



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Feb 10, 2018 – 08:20 PM EST

PDB ID : 6EPF
EMDB ID: : EMD-3916
Title : Ground state 26S proteasome (GS1)
Authors : Guo, Q.; Lehmer, C.; Martinez-Sanchez, A.; Rudack, T.; Beck, F.; Hartmann, H.; Hipp, M.S.; Hartl, F.U.; Edbauer, D.; Baumeister, W.; Fernandez-Busnadiego, R.
Deposited on : 2017-10-11
Resolution : 11.80 Å(reported)

This is a Full wwPDB/EMDatabank EM Map/Model Validation Report
for a publicly released PDB/EMDB entry.

We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

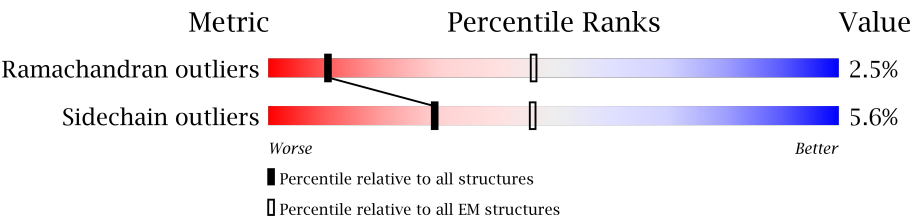
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : rb-20030736

1 Overall quality at a glance i

The following experimental techniques were used to determine the structure:
ELECTRON MICROSCOPY

The reported resolution of this entry is 11.80 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.











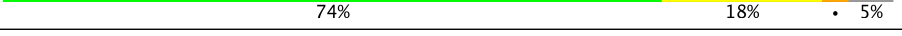
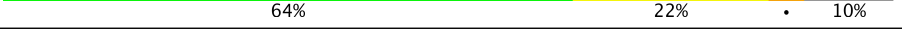
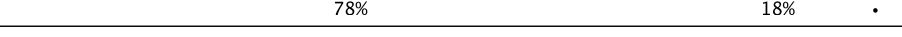

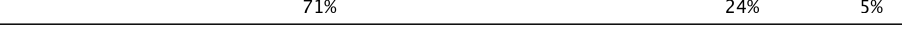
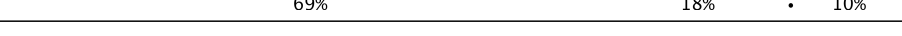
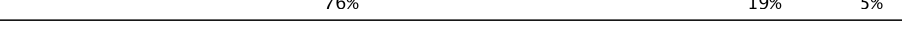


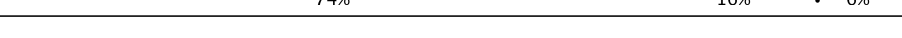
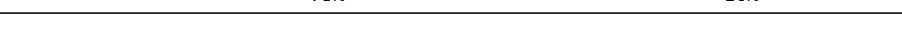


Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

The table below summarises the geometric issues observed across the polymeric chains. The red, orange, yellow and green segments on the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$

Mol	Chain	Length	Quality of chain
1	A	246	<div><div>76%</div><div>20%</div><div>• •</div></div>
2	B	234	<div><div>77%</div><div>18%</div><div>•</div></div>
3	C	261	<div><div>67%</div><div>24%</div><div>• 5%</div></div>
4	D	254	<div><div>73%</div><div>21%</div><div>• •</div></div>
5	E	241	<div><div>76%</div><div>19%</div><div>• •</div></div>
6	F	263	<div><div>69%</div><div>17%</div><div>• 10%</div></div>
7	G	255	<div><div>74%</div><div>20%</div><div>• •</div></div>
8	1	238	<div><div>61%</div><div>19%</div><div>• • 15%</div></div>
9	2	277	<div><div>55%</div><div>18%</div><div>6% 21%</div></div>
10	3	205	<div><div>68%</div><div>25%</div><div>6%</div></div>
11	4	201	<div><div>65%</div><div>27%</div><div>5% •</div></div>

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Mol	Chain	Length	Quality of chain
12	5	263	
13	6	240	
14	7	263	
15	W	377	
16	V	310	
17	T	353	
18	Y	70	
19	Z	908	
20	N	953	
21	S	530	
22	P	456	
23	Q	422	
24	R	389	
25	U	320	
26	O	376	
27	H	433	
28	I	440	
29	K	418	
30	L	403	
31	M	442	
32	J	406	

2 Entry composition

There are 32 unique types of molecules in this entry. The entry contains 82757 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	246	Total	C	N	O	S	0	0
			1920	1215	322	369	14		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	234	Total	C	N	O	S	0	0
			1828	1166	311	344	7		

- Molecule 3 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	C	249	Total	C	N	O	S	0	0
			1960	1238	337	374	11		

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	D	246	Total	C	N	O	S	0	0
			1926	1209	340	371	6		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	E	233	Total	C	N	O	S	0	0
			1778	1114	296	358	10		

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	F	238	Total	C	N	O	S	0	0
			1871	1170	337	353	11		

- Molecule 7 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	245	Total	C	N	O	S	0	0
			1912	1212	326	362	12		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	202	Total	C	N	O	S	0	0
			1516	948	259	297	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	219	Total	C	N	O	S	0	0
			1651	1042	281	316	12		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	205	Total	C	N	O	S	0	0
			1600	1018	266	296	20		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	4	196	Total	C	N	O	S	0	0
			1572	1007	267	289	9		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	5	201	Total	C	N	O	S	0	0
			1560	984	272	295	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	6	213	Total	C	N	O	S	0	0
			1659	1050	284	315	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	216	Total	C	N	O	S	0	0
			1686	1065	292	317	12		

- Molecule 15 is a protein called 26S proteasome subunit S5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	195	Total	C	N	O	S	0	0
			1480	922	265	285	8		

- Molecule 16 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	289	Total	C	N	O	S	0	0
			2272	1438	391	424	19		

- Molecule 17 is a protein called Proteasome 26S subunit, non-ATPase 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	263	Total	C	N	O	S	0	0
			2149	1390	351	398	10		

- Molecule 18 is a protein called RCG28037.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	24	Total	C	N	O	S	0	0
			199	120	34	44	1		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	896	Total	C	N	O	S	0	0
			6913	4342	1178	1346	47		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	905	Total	C	N	O	S	0	0
			7082	4487	1193	1356	46		

- Molecule 21 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	476	Total	C	N	O	S	0	0
			3844	2438	685	707	14		

- Molecule 22 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	456	Total	C	N	O	S	0	0
			3706	2338	635	709	24		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Q	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		

- Molecule 24 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	389	Total	C	N	O	S	0	0
			3204	2042	542	600	20		

- Molecule 25 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 7 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	288	Total	C	N	O	S	0	0
			2299	1470	395	428	6		

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	376	Total	C	N	O	S	0	0
			3011	1918	514	564	15		

- Molecule 27 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	396	Total	C	N	O	S	0	0
			3113	1960	546	589	18		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	I	385	Total	C	N	O	S	0	0
			3042	1913	516	598	15		

- Molecule 29 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	K	391	Total	C	N	O	S	0	0
			3125	1978	535	599	13		

- Molecule 30 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L	389	Total	C	N	O	S	0	0
			3098	1947	552	582	17		

- Molecule 31 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	M	415	Total	C	N	O	S	0	0
			3252	2038	561	635	18		

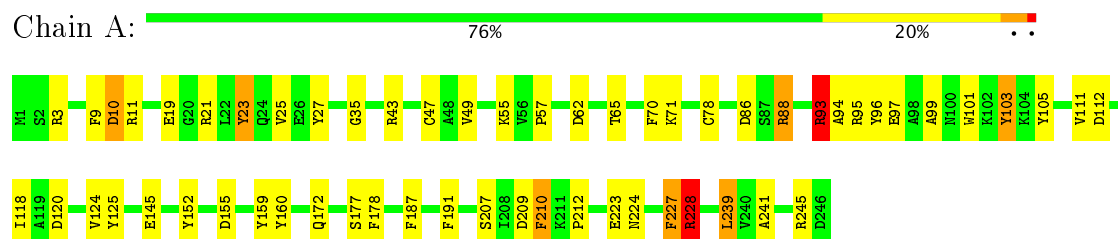
- Molecule 32 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	J	406	Total	C	N	O	S	0	0
			3194	2006	569	599	20		

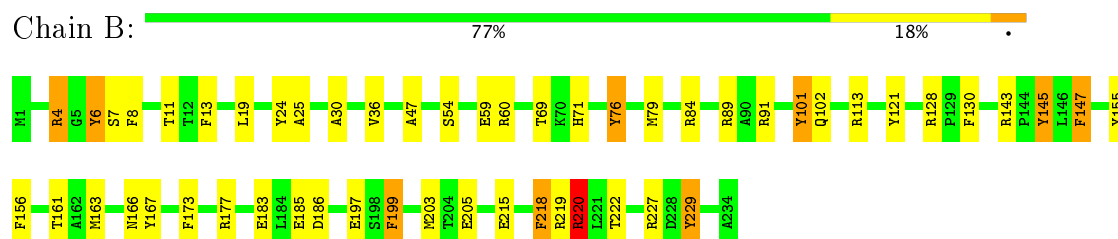
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

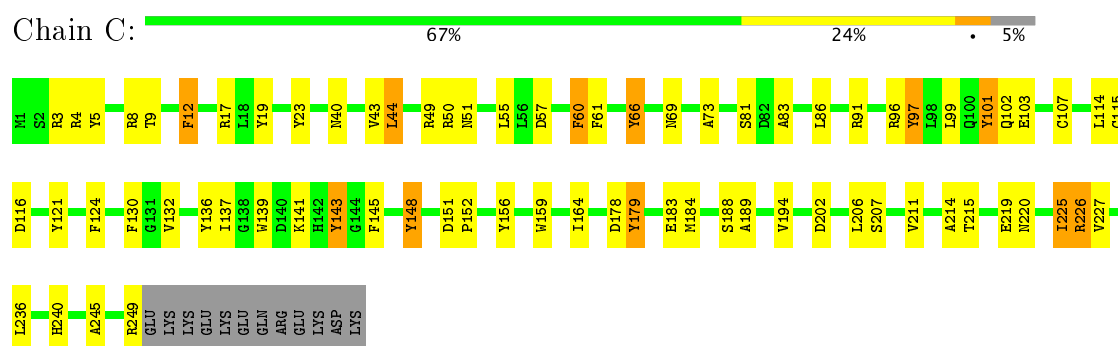
- Molecule 1: Proteasome subunit alpha type-6



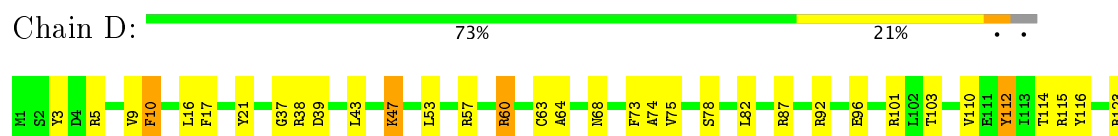
- Molecule 2: Proteasome subunit alpha type-2



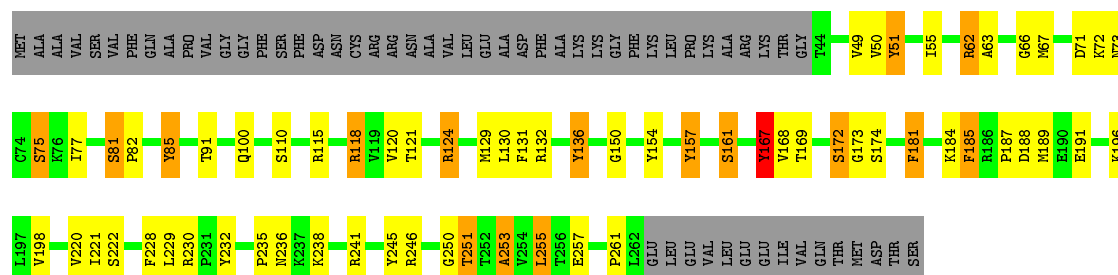
- Molecule 3: Proteasome subunit alpha type-4



- Molecule 4: Proteasome subunit alpha type-7

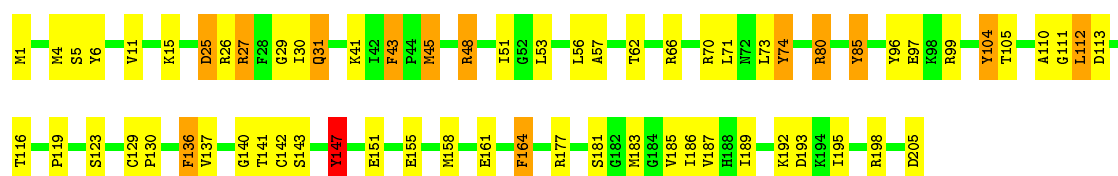


Chain 2:  55% 18% 6% 21%



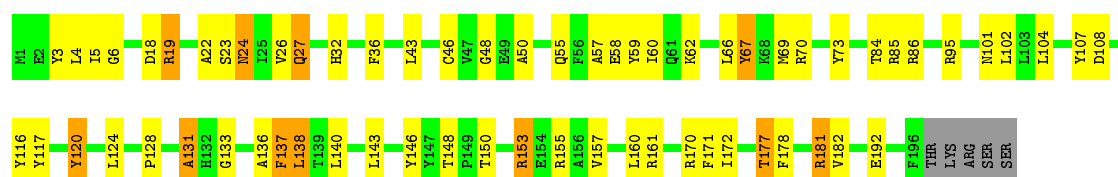
• Molecule 10: Proteasome subunit beta type-3

Chain 3:  68% 25% 6%



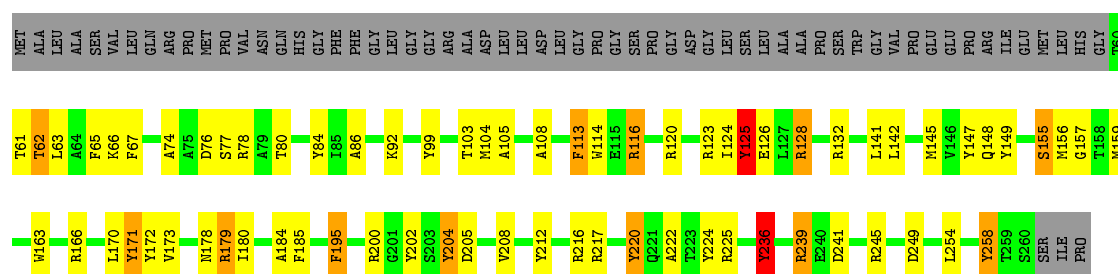
• Molecule 11: Proteasome subunit beta type-2

Chain 4:  65% 27% 5% •



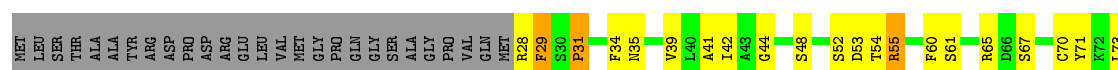
• Molecule 12: Proteasome subunit beta type-5

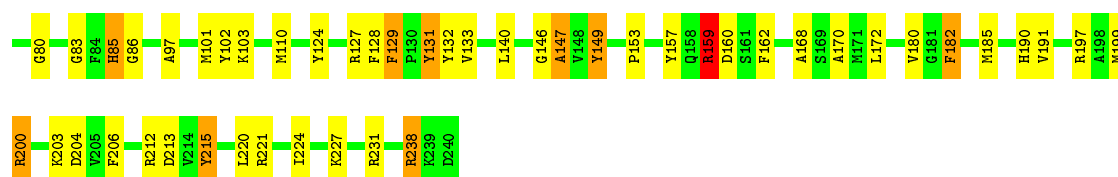
Chain 5:  50% 21% 5% • 24%



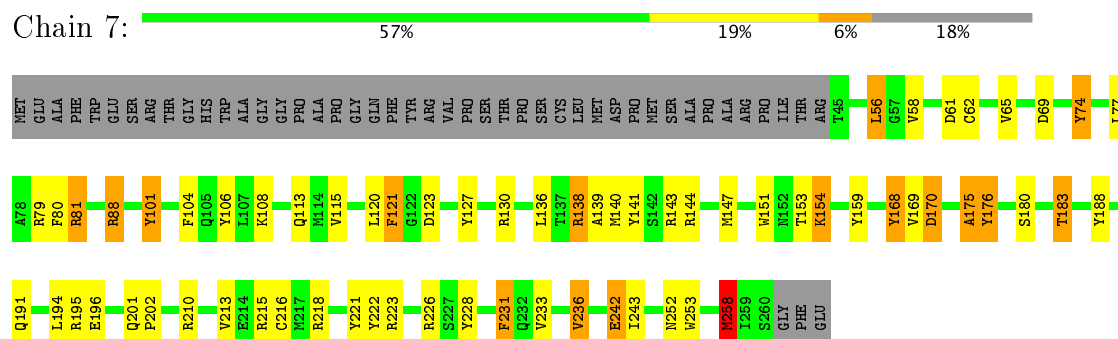
• Molecule 13: Proteasome subunit beta type-1

Chain 6:  60% 23% 5% 11%

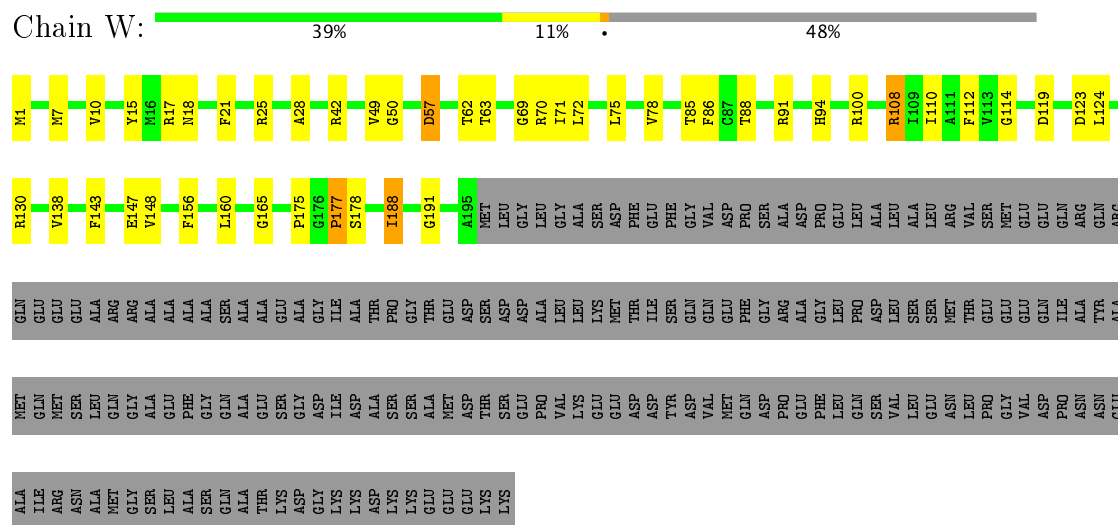




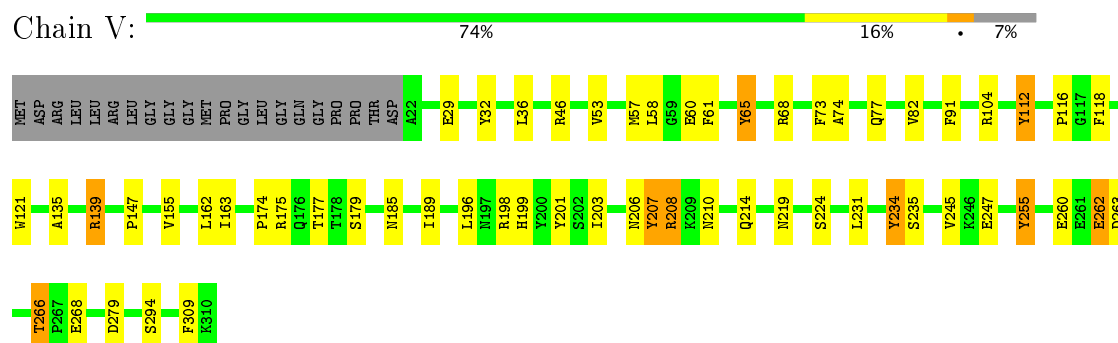
- Molecule 14: Proteasome subunit beta-4



- Molecule 15: 26S proteasome subunit S5a



- Molecule 16: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 14



- Molecule 17: Proteasome 26S subunit, non-ATPase 8

- Molecule 18: RCG28037

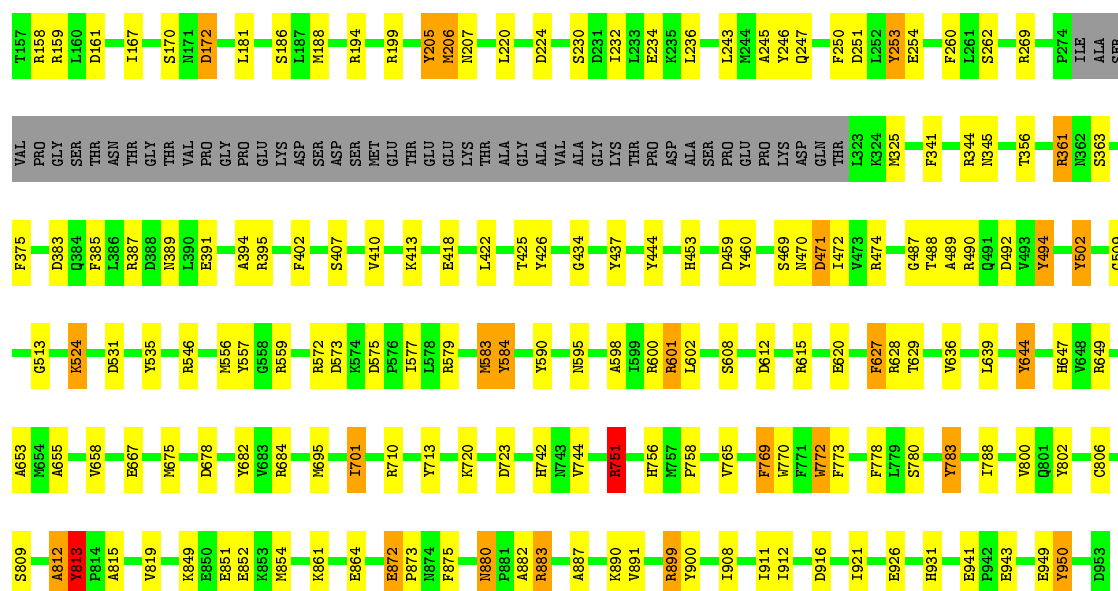
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- Molecule 19: 26S proteasome non-ATPase regulatory subunit 2

LEU	F590	R431	R300	D175	M1
ARG	R763	Y432	F304	K178	E2
LNS	C598	L433	F304		B6
ASN	A599	Y434	E209	R181	P16
PRD	Y600	S435	E313	E182	
ASN	A601	Y439	E313	K189	A24
TYR	G604	L445	Y314	E190	S28
LEU	L787	S617	N323	I191	
				Y192	
L300	F620	Y455	L326	P193	K31
B601	D621	R456	N327		E32
S802	F803	Y457	S328	M196	R33
R803	K632	Y469	N329	H202	R34
L204			F330		
R805	A644	R478	L331		E42
B806	D645		A332	M209	
R807	M646	T482	L333	E210	L45
B808	F483				
I809			L337	D222	R62
I810	V652	Y489	M340	A225	R72
			E341	Z226	
Y819	R673	S492		S227	R79
R828	T674	Y493	V344		
	F675	R494		Y232	R83
E336	R630	E495			
L837		D496	Y349		
R338	P634			H238	T86
		M505	R357	Y239	
P841	R637	G506	F358	T240	T90
V842	R638	D507		P241	
		S508	S363		P95
R845	L636	A515	Q364	R250	R100
			V365	C251	
K858	R703	A519	D366		Y103
	L704		S367	R257	
T861		D633	A368	R258	Y110
F365	K712	V534	F376	F259	
R666	H715	T535		S260	M113
T867	D716	L539	F380	R261	A114
B868	A717			F262	
	R718		A384		K119
V872		T553	F385	A265	
		Y554	G386	L266	A130
A875	S722			R267	
	Y723	M557	T392	D274	R137
E878		L564	W398	S284	Y142
R879	M738		L399	R143	
A880	A739	L567	Y400	Q291	L151
E881	R740			K292	
		B574	G406	Q293	
P892	R746			M294	Y158
		S584	M416	A295	V159
E895	Y751			F296	R160
G896		F587	W420	K397	H161
PHE	M757	R588		L298	L162
VAL	T760				

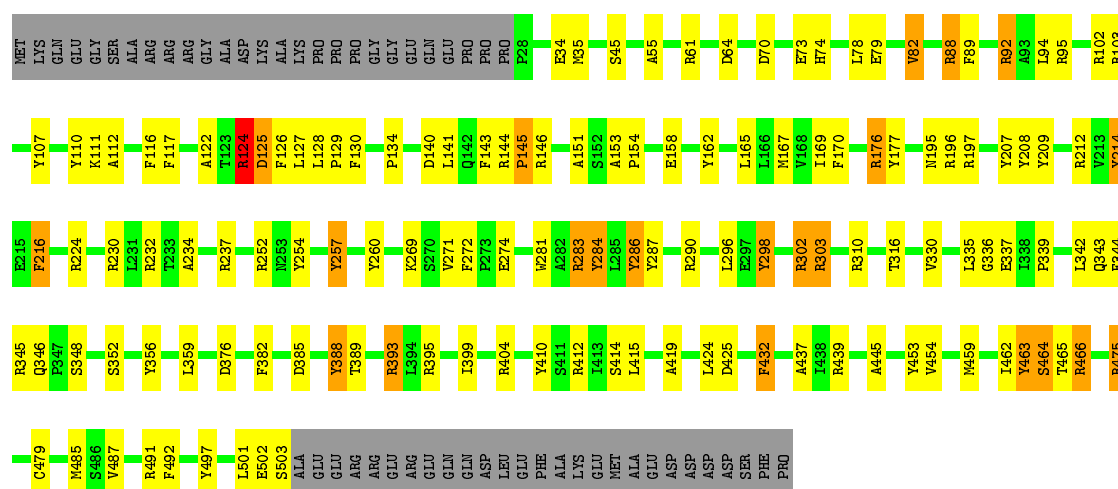
- Molecule 20: 26S proteasome non-ATPase regulatory subunit 1

M1	E21	F22	A23	L24	H25	A29	W35	D43	D51	F54	A55	S56	S57	F68	L71	G72	A73	F74	Y80	A81	L82	F88	D92	Y96	T109	V113	L118	G121	T126	D127	Q128	R129	F138	Q139	R140	C141	L142	D143	D144	T145
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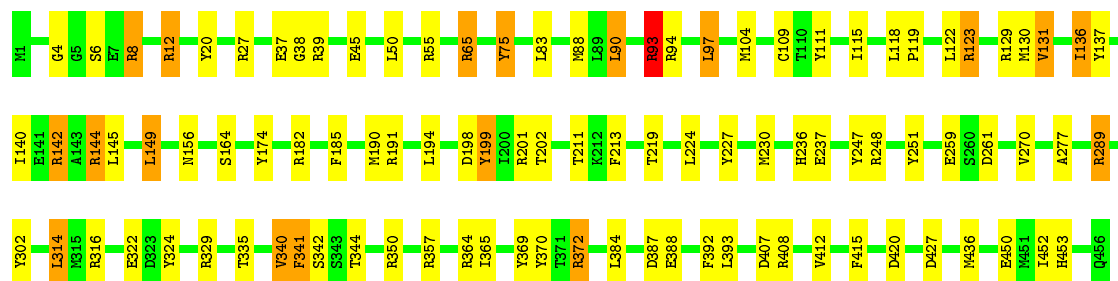
- Molecule 21: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 3

Chain S: 64% 22% 10%

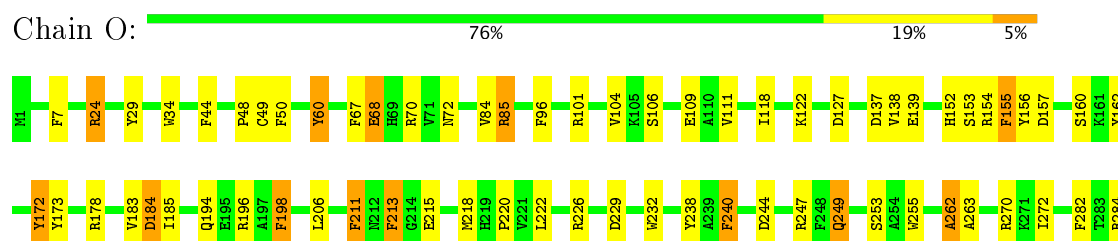
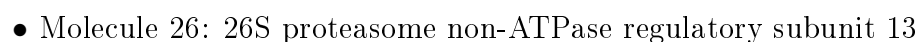
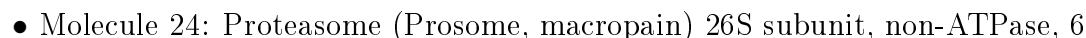


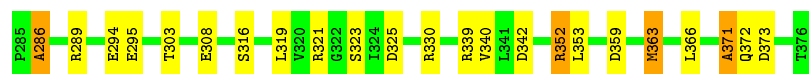
- Molecule 22: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 12

Chain P: 78% 18%



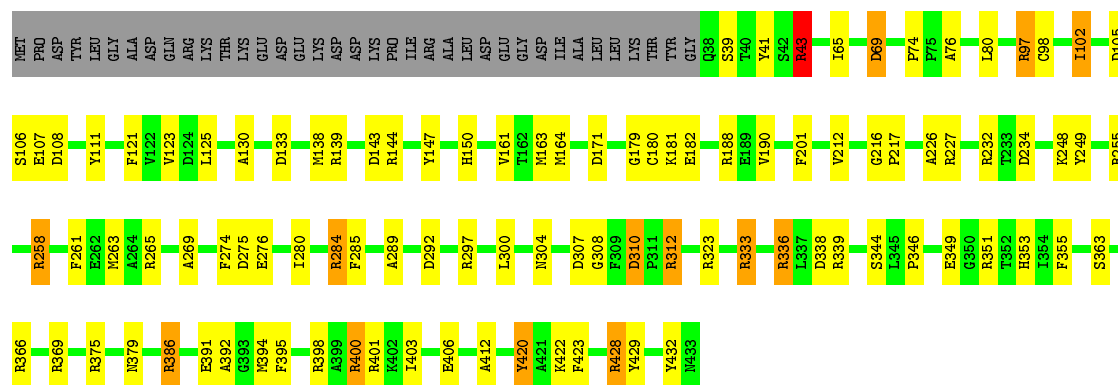
- Molecule 23: 26S proteasome non-ATPase regulatory subunit 11





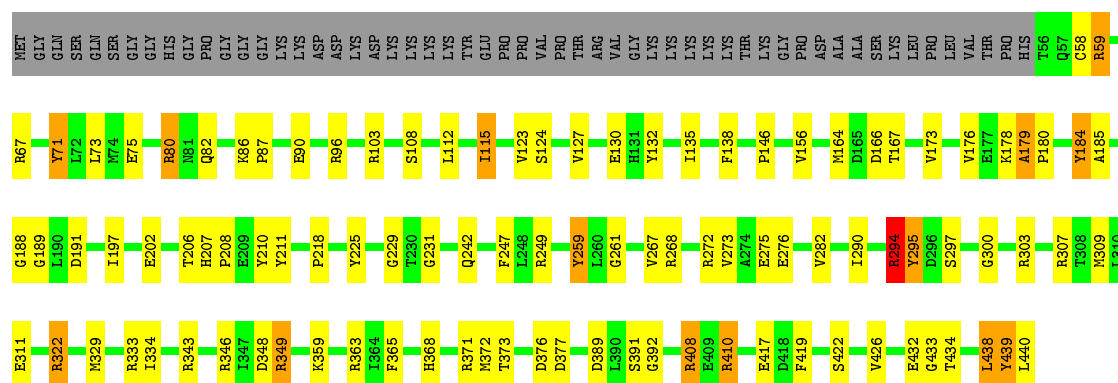
• Molecule 27: 26S proteasome regulatory subunit 7

Chain H: 68% 20% 9%



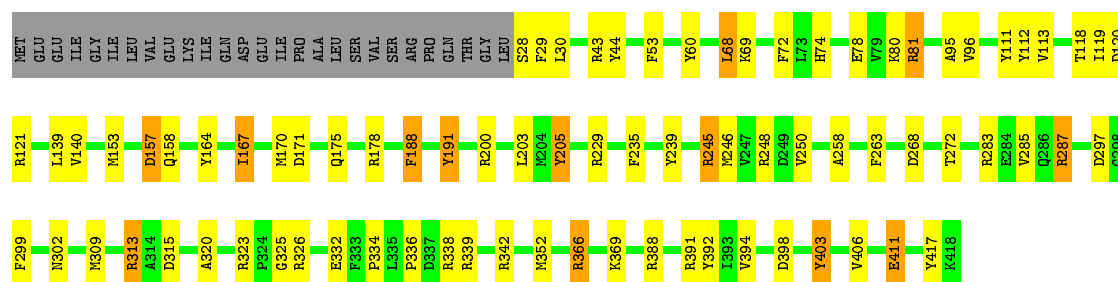
• Molecule 28: 26S proteasome regulatory subunit 4

Chain I: 64% 20% 13%



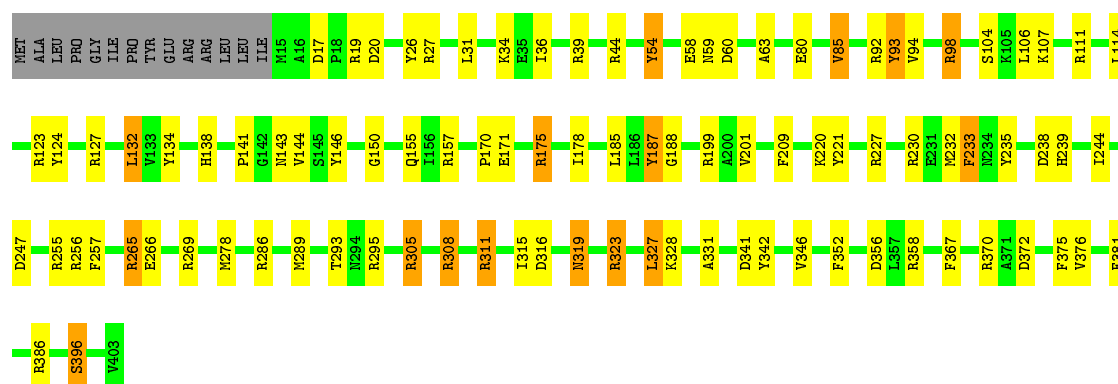
• Molecule 29: 26S proteasome regulatory subunit 6B

Chain K: 74% 16% 6%



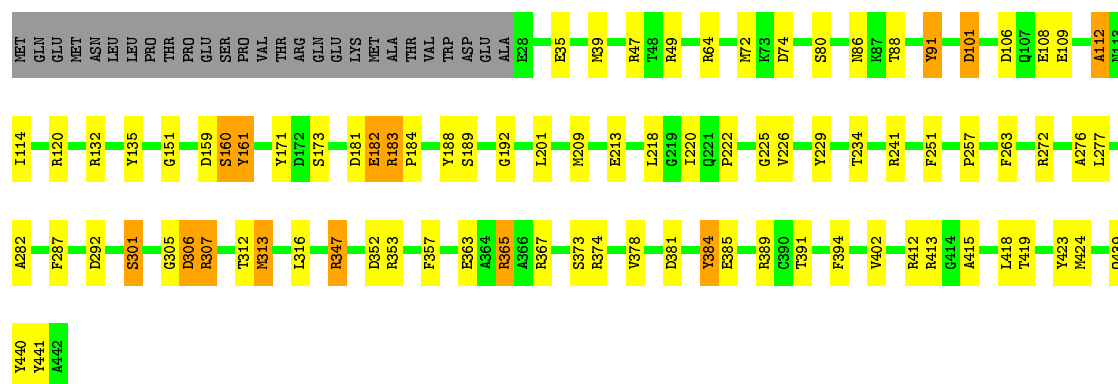
• Molecule 30: Proteasome 26S subunit, ATPase 6

Chain L: 73% 20% 7%



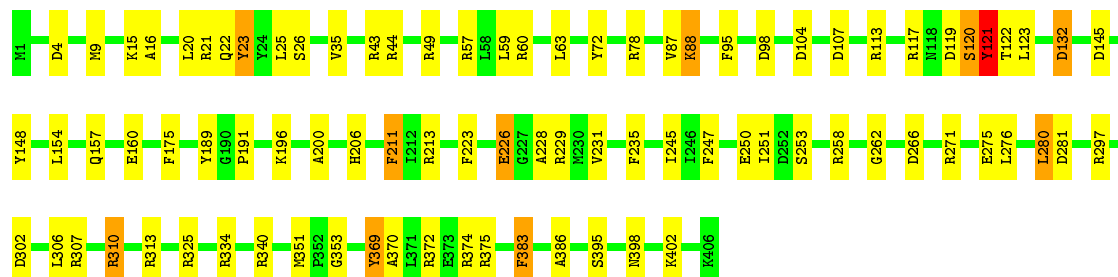
- Molecule 31: 26S proteasome regulatory subunit 6A

Chain M: 74% 17% 6%



- Molecule 32: 26S proteasome regulatory subunit 8

Chain J: 79% 19%



4 Experimental information

Property	Value	Source
Reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	7393	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.8	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	7000	Depositor
Magnification	42000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

The Z score for a bond length (or angle) is the number of standard deviations the observed value is removed from the expected value. A bond length (or angle) with $|Z| > 5$ is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z > 2$	RMSZ	$\# Z > 2$
1	A	1.74	16/1954 (0.8%)	2.01	43/2638 (1.6%)
10	3	1.63	15/1629 (0.9%)	2.06	44/2195 (2.0%)
11	4	1.76	17/1604 (1.1%)	2.00	48/2170 (2.2%)
12	5	2.53	19/1592 (1.2%)	2.17	63/2152 (2.9%)
13	6	1.77	17/1690 (1.0%)	2.03	54/2278 (2.4%)
14	7	1.78	19/1720 (1.1%)	2.05	58/2327 (2.5%)
15	W	1.68	11/1500 (0.7%)	1.87	24/2030 (1.2%)
16	V	1.68	13/2315 (0.6%)	1.85	37/3129 (1.2%)
17	T	1.71	17/2195 (0.8%)	1.94	58/2964 (2.0%)
18	Y	1.90	3/201 (1.5%)	1.89	9/266 (3.4%)
19	Z	1.72	61/7026 (0.9%)	1.94	164/9495 (1.7%)
2	B	1.73	13/1867 (0.7%)	2.10	54/2527 (2.1%)
20	N	1.73	68/7206 (0.9%)	1.87	164/9738 (1.7%)
21	S	1.75	34/3918 (0.9%)	2.01	110/5287 (2.1%)
22	P	1.70	32/3754 (0.9%)	1.91	86/5049 (1.7%)
23	Q	1.69	25/3381 (0.7%)	1.89	74/4558 (1.6%)
24	R	1.78	45/3263 (1.4%)	2.04	106/4393 (2.4%)
25	U	1.67	17/2344 (0.7%)	1.98	51/3178 (1.6%)
26	O	1.69	27/3066 (0.9%)	1.94	74/4148 (1.8%)
27	H	1.69	26/3166 (0.8%)	1.97	90/4275 (2.1%)
28	I	1.74	37/3085 (1.2%)	1.98	72/4158 (1.7%)
29	K	1.69	20/3178 (0.6%)	1.95	70/4290 (1.6%)
3	C	1.75	18/1990 (0.9%)	2.06	71/2680 (2.6%)
30	L	1.73	28/3146 (0.9%)	1.94	72/4233 (1.7%)
31	M	1.69	28/3293 (0.9%)	1.92	80/4436 (1.8%)
32	J	1.72	22/3236 (0.7%)	1.95	68/4347 (1.6%)
4	D	1.78	16/1953 (0.8%)	1.97	49/2637 (1.9%)
5	E	2.35	12/1806 (0.7%)	1.85	38/2439 (1.6%)
6	F	1.75	21/1906 (1.1%)	1.96	46/2577 (1.8%)
7	G	1.72	19/1947 (1.0%)	1.96	47/2620 (1.8%)
8	1	1.72	17/1542 (1.1%)	2.09	42/2089 (2.0%)
9	2	1.71	17/1679 (1.0%)	2.03	49/2271 (2.2%)
All	All	1.76	750/84152 (0.9%)	1.96	2115/113574 (1.9%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand. A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
10	3	0	9
11	4	0	4
12	5	0	11
13	6	0	9
14	7	0	4
15	W	0	3
16	V	0	5
17	T	0	11
18	Y	0	1
19	Z	0	19
2	B	0	11
20	N	0	17
21	S	0	22
22	P	0	12
23	Q	0	10
24	R	0	12
25	U	0	6
26	O	0	9
27	H	0	11
28	I	0	12
29	K	0	11
3	C	0	6
30	L	0	11
31	M	0	8
32	J	0	11
4	D	0	8
5	E	0	2
6	F	0	8
7	G	0	8
8	1	0	6
9	2	0	6
All	All	0	291

All (750) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	97	GLN	CG-CD	71.39	3.15	1.51
12	5	125	TYR	CE2-CZ	32.57	1.80	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	125	TYR	CG-CD1	30.78	1.79	1.39
12	5	125	TYR	CD1-CE1	29.68	1.83	1.39
12	5	125	TYR	CG-CD2	28.75	1.76	1.39
12	5	125	TYR	CD2-CE2	27.92	1.81	1.39
12	5	125	TYR	CE1-CZ	26.66	1.73	1.38
11	4	155	ARG	CZ-NH2	9.62	1.45	1.33
21	S	393	ARG	CD-NE	9.25	1.62	1.46
32	J	310	ARG	NE-CZ	9.03	1.44	1.33
17	T	340	ARG	CD-NE	8.96	1.61	1.46
23	Q	231	TYR	CE2-CZ	8.85	1.50	1.38
28	I	417	GLU	CG-CD	8.49	1.64	1.51
29	K	28	SER	CA-CB	8.47	1.65	1.52
19	Z	763	ARG	CD-NE	8.41	1.60	1.46
23	Q	72	TYR	CD1-CE1	8.21	1.51	1.39
28	I	108	SER	CA-CB	8.20	1.65	1.52
19	Z	807	ARG	CZ-NH2	8.10	1.43	1.33
22	P	129	ARG	CD-NE	8.09	1.60	1.46
12	5	123	ARG	CD-NE	8.01	1.60	1.46
24	R	293	ARG	CZ-NH1	7.95	1.43	1.33
27	H	333	ARG	CZ-NH1	7.84	1.43	1.33
28	I	322	ARG	CZ-NH2	7.83	1.43	1.33
20	N	502	TYR	CD2-CE2	7.81	1.51	1.39
31	M	160	SER	CA-CB	7.79	1.64	1.52
20	N	600	ARG	CZ-NH1	7.77	1.43	1.33
16	V	29	GLU	CG-CD	7.76	1.63	1.51
18	Y	57	ARG	CZ-NH1	7.68	1.43	1.33
21	S	146	ARG	NE-CZ	7.68	1.43	1.33
30	L	104	SER	CA-CB	7.67	1.64	1.52
32	J	120	SER	CA-CB	7.66	1.64	1.52
15	W	100	ARG	NE-CZ	7.60	1.43	1.33
30	L	27	ARG	CD-NE	7.59	1.59	1.46
13	6	65	ARG	CD-NE	7.55	1.59	1.46
15	W	15	TYR	CE2-CZ	7.55	1.48	1.38
29	K	178	ARG	NE-CZ	7.49	1.42	1.33
11	4	107	TYR	CG-CD2	7.49	1.48	1.39
4	D	124	TYR	CE1-CZ	7.46	1.48	1.38
31	M	135	TYR	CE2-CZ	7.46	1.48	1.38
22	P	129	ARG	CZ-NH2	7.44	1.42	1.33
11	4	95	ARG	NE-CZ	7.43	1.42	1.33
27	H	420	TYR	CZ-OH	7.43	1.50	1.37
1	A	47	CYS	CB-SG	7.40	1.94	1.82
7	G	119	TYR	CZ-OH	7.38	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	802	TYR	CE2-CZ	7.38	1.48	1.38
28	I	349	ARG	CZ-NH2	7.38	1.42	1.33
31	M	49	ARG	NE-CZ	7.37	1.42	1.33
6	F	126	ARG	CZ-NH1	7.34	1.42	1.33
31	M	241	ARG	NE-CZ	7.33	1.42	1.33
20	N	96	TYR	CD2-CE2	7.31	1.50	1.39
28	I	343	ARG	NE-CZ	7.27	1.42	1.33
24	R	324	GLY	CA-C	-7.27	1.40	1.51
17	T	109	SER	CA-CB	7.25	1.63	1.52
1	A	95	ARG	NE-CZ	7.24	1.42	1.33
12	5	239	ARG	NE-CZ	7.21	1.42	1.33
20	N	494	TYR	CG-CD1	7.21	1.48	1.39
14	7	180	SER	CA-CB	7.20	1.63	1.52
27	H	386	ARG	CZ-NH1	7.20	1.42	1.33
19	Z	406	GLY	N-CA	-7.18	1.35	1.46
26	O	330	ARG	CZ-NH1	7.17	1.42	1.33
6	F	123	TYR	CG-CD2	7.17	1.48	1.39
24	R	233	ARG	CZ-NH1	7.16	1.42	1.33
26	O	156	TYR	CE1-CZ	7.15	1.47	1.38
13	6	149	TYR	CG-CD2	7.14	1.48	1.39
28	I	363	ARG	NE-CZ	7.10	1.42	1.33
32	J	258	ARG	CZ-NH2	7.08	1.42	1.33
2	B	69	THR	N-CA	-7.07	1.32	1.46
26	O	340	VAL	CB-CG2	7.07	1.67	1.52
14	7	88	ARG	CD-NE	7.05	1.58	1.46
8	1	123	TYR	CG-CD2	7.05	1.48	1.39
21	S	257	TYR	CB-CG	7.04	1.62	1.51
8	1	219	ARG	NE-CZ	7.03	1.42	1.33
22	P	111	TYR	CG-CD2	7.03	1.48	1.39
30	L	175	ARG	CZ-NH1	7.02	1.42	1.33
3	C	226	ARG	CZ-NH2	6.99	1.42	1.33
20	N	872	GLU	CA-C	6.99	1.71	1.52
23	Q	214	SER	CA-CB	6.97	1.63	1.52
10	3	198	ARG	CD-NE	6.95	1.58	1.46
24	R	268	TYR	CE2-CZ	6.94	1.47	1.38
31	M	49	ARG	CD-NE	6.94	1.58	1.46
29	K	325	GLY	N-CA	-6.93	1.35	1.46
25	U	25	ARG	NE-CZ	6.92	1.42	1.33
28	I	210	TYR	CE1-CZ	6.92	1.47	1.38
4	D	133	PHE	CG-CD2	6.87	1.49	1.38
23	Q	52	GLU	CG-CD	6.86	1.62	1.51
20	N	80	TYR	CG-CD1	6.85	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	U	283	ARG	CZ-NH1	6.85	1.42	1.33
32	J	223	PHE	CG-CD2	6.84	1.49	1.38
2	B	60	ARG	NE-CZ	6.83	1.42	1.33
14	7	168	TYR	CG-CD1	6.83	1.48	1.39
24	R	125	ARG	NE-CZ	6.83	1.42	1.33
30	L	221	TYR	CG-CD2	6.83	1.48	1.39
23	Q	342	PHE	CG-CD1	6.83	1.49	1.38
7	G	72	ARG	CZ-NH2	6.82	1.42	1.33
14	7	101	TYR	CG-CD2	6.81	1.48	1.39
21	S	335	LEU	C-N	6.81	1.45	1.33
23	Q	87	ARG	CD-NE	6.81	1.58	1.46
12	5	78	ARG	CD-NE	6.79	1.57	1.46
26	O	321	ARG	NE-CZ	6.79	1.41	1.33
24	R	176	ARG	CD-NE	6.78	1.57	1.46
20	N	474	ARG	NE-CZ	6.77	1.41	1.33
9	2	250	GLY	CA-C	-6.76	1.41	1.51
28	I	307	ARG	CZ-NH1	6.76	1.41	1.33
20	N	682	TYR	CB-CG	-6.73	1.41	1.51
13	6	127	ARG	NE-CZ	6.72	1.41	1.33
19	Z	703	ARG	NE-CZ	6.72	1.41	1.33
20	N	780	SER	CA-CB	6.71	1.63	1.52
14	7	215	ARG	CD-NE	6.69	1.57	1.46
23	Q	281	GLY	CA-C	-6.69	1.41	1.51
8	1	177	ARG	CZ-NH2	6.69	1.41	1.33
17	T	181	TYR	CG-CD1	6.67	1.47	1.39
24	R	336	ARG	CD-NE	6.66	1.57	1.46
28	I	259	TYR	CG-CD2	6.64	1.47	1.39
19	Z	435	SER	CA-CB	6.64	1.62	1.52
14	7	242	GLU	CD-OE1	6.64	1.32	1.25
1	A	25	VAL	CA-CB	-6.64	1.40	1.54
14	7	176	TYR	CG-CD1	6.63	1.47	1.39
12	5	78	ARG	CZ-NH2	6.63	1.41	1.33
16	V	175	ARG	NE-CZ	6.63	1.41	1.33
32	J	297	ARG	NE-CZ	6.62	1.41	1.33
10	3	85	TYR	CZ-OH	6.62	1.49	1.37
22	P	213	PHE	CG-CD1	6.61	1.48	1.38
24	R	298	GLU	CG-CD	6.61	1.61	1.51
11	4	178	PHE	CG-CD2	6.60	1.48	1.38
20	N	572	ARG	CZ-NH1	6.58	1.41	1.33
32	J	72	TYR	CE2-CZ	6.58	1.47	1.38
21	S	110	TYR	CZ-OH	6.58	1.49	1.37
19	Z	239	TYR	CD1-CE1	6.57	1.49	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	255	ARG	CZ-NH1	6.57	1.41	1.33
24	R	166	SER	CA-CB	6.56	1.62	1.52
30	L	26	TYR	CG-CD2	6.56	1.47	1.39
17	T	238	TYR	CG-CD1	6.55	1.47	1.39
19	Z	137	ARG	CZ-NH1	6.55	1.41	1.33
21	S	466	ARG	NE-CZ	6.55	1.41	1.33
25	U	25	ARG	CD-NE	6.55	1.57	1.46
4	D	21	TYR	CG-CD2	6.54	1.47	1.39
21	S	345	ARG	CZ-NH1	6.54	1.41	1.33
28	I	261	GLY	N-CA	-6.54	1.36	1.46
24	R	24	PHE	CG-CD1	6.53	1.48	1.38
22	P	39	ARG	CZ-NH2	6.51	1.41	1.33
20	N	387	ARG	CZ-NH1	6.51	1.41	1.33
20	N	186	SER	CA-CB	6.50	1.62	1.52
8	1	199	ARG	CZ-NH2	6.49	1.41	1.33
19	Z	261	ARG	CZ-NH2	6.48	1.41	1.33
4	D	87	ARG	CZ-NH1	6.48	1.41	1.33
27	H	369	ARG	NE-CZ	6.48	1.41	1.33
6	F	4	ASN	N-CA	6.48	1.59	1.46
24	R	381	GLN	CG-CD	6.48	1.66	1.51
21	S	212	ARG	CZ-NH2	6.47	1.41	1.33
4	D	141	GLY	CA-C	6.46	1.62	1.51
4	D	176	GLU	CB-CG	6.46	1.64	1.52
8	1	121	TYR	CB-CG	-6.46	1.42	1.51
23	Q	142	ARG	CD-NE	6.46	1.57	1.46
15	W	15	TYR	CG-CD1	6.46	1.47	1.39
24	R	54	TYR	CE1-CZ	6.46	1.47	1.38
27	H	107	GLU	CD-OE2	6.44	1.32	1.25
3	C	5	TYR	CZ-OH	6.43	1.48	1.37
32	J	206	HIS	CG-CD2	6.42	1.46	1.35
19	Z	328	SER	CA-CB	6.42	1.62	1.52
30	L	27	ARG	NE-CZ	6.42	1.41	1.33
9	2	115	ARG	CZ-NH1	6.42	1.41	1.33
6	F	157	ARG	NE-CZ	6.40	1.41	1.33
6	F	193	ARG	CZ-NH1	6.40	1.41	1.33
11	4	117	TYR	CE2-CZ	6.40	1.46	1.38
29	K	78	GLU	CG-CD	6.40	1.61	1.51
19	Z	259	PHE	CG-CD1	6.40	1.48	1.38
20	N	35	TRP	CB-CG	6.39	1.61	1.50
28	I	225	TYR	CZ-OH	6.39	1.48	1.37
20	N	234	GLU	CD-OE2	6.38	1.32	1.25
13	6	86	GLY	N-CA	-6.36	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	88	PHE	CG-CD1	6.35	1.48	1.38
16	V	247	GLU	CD-OE2	6.34	1.32	1.25
26	O	173	TYR	CB-CG	-6.33	1.42	1.51
31	M	307	ARG	CZ-NH2	6.33	1.41	1.33
3	C	50	ARG	CZ-NH2	6.33	1.41	1.33
10	3	43	PHE	CB-CG	-6.32	1.40	1.51
5	E	168	ARG	CZ-NH1	6.30	1.41	1.33
21	S	352	SER	CA-CB	6.30	1.62	1.52
1	A	88	ARG	NE-CZ	6.30	1.41	1.33
32	J	175	PHE	N-CA	-6.30	1.33	1.46
26	O	316	SER	CA-CB	6.29	1.62	1.52
11	4	85	ARG	CD-NE	6.28	1.57	1.46
17	T	297	SER	CB-OG	6.27	1.50	1.42
20	N	57	ARG	NE-CZ	6.27	1.41	1.33
24	R	257	ARG	CZ-NH1	6.27	1.41	1.33
25	U	138	TYR	CE1-CZ	6.27	1.46	1.38
2	B	227	ARG	CZ-NH2	6.27	1.41	1.33
2	B	218	PHE	CG-CD2	6.26	1.48	1.38
19	Z	881	GLU	CD-OE2	6.26	1.32	1.25
20	N	535	TYR	CG-CD2	6.26	1.47	1.39
20	N	269	ARG	CZ-NH2	6.25	1.41	1.33
5	E	193	GLU	CG-CD	6.25	1.61	1.51
16	V	68	ARG	NE-CZ	6.25	1.41	1.33
27	H	179	GLY	CA-C	-6.25	1.41	1.51
7	G	215	SER	CA-CB	6.24	1.62	1.52
13	6	200	ARG	CZ-NH2	6.22	1.41	1.33
31	M	347	ARG	CD-NE	6.22	1.57	1.46
2	B	183	GLU	CD-OE1	6.22	1.32	1.25
10	3	198	ARG	CZ-NH2	6.22	1.41	1.33
19	Z	895	GLU	CD-OE2	6.21	1.32	1.25
19	Z	456	ARG	CZ-NH2	6.21	1.41	1.33
29	K	43	ARG	CZ-NH2	6.20	1.41	1.33
28	I	333	ARG	NE-CZ	6.20	1.41	1.33
3	C	97	TYR	CB-CG	6.19	1.60	1.51
17	T	347	ARG	CD-NE	6.19	1.56	1.46
9	2	124	ARG	CZ-NH2	6.19	1.41	1.33
11	4	6	GLY	N-CA	-6.18	1.36	1.46
3	C	245	ALA	CA-CB	6.18	1.65	1.52
20	N	426	TYR	CE1-CZ	6.18	1.46	1.38
8	1	41	PHE	CG-CD1	6.18	1.48	1.38
20	N	513	GLY	CA-C	-6.18	1.42	1.51
20	N	941	GLU	CD-OE2	6.17	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	228	ARG	NE-CZ	6.17	1.41	1.33
30	L	230	ARG	NE-CZ	6.17	1.41	1.33
24	R	183	TYR	CE2-CZ	6.16	1.46	1.38
25	U	90	ARG	CZ-NH2	6.16	1.41	1.33
16	V	104	ARG	CD-NE	6.16	1.56	1.46
9	2	110	SER	CA-CB	6.15	1.62	1.52
32	J	72	TYR	CG-CD2	6.14	1.47	1.39
19	Z	508	SER	CA-CB	6.14	1.62	1.52
19	Z	688	ARG	CZ-NH2	6.14	1.41	1.33
17	T	115	CYS	CB-SG	6.13	1.92	1.82
15	W	86	PHE	CG-CD1	6.13	1.48	1.38
19	Z	160	ARG	CD-NE	6.13	1.56	1.46
25	U	88	ARG	NE-CZ	6.12	1.41	1.33
31	M	440	TYR	CZ-OH	6.12	1.48	1.37
20	N	129	ARG	CZ-NH2	6.11	1.41	1.33
30	L	269	ARG	CD-NE	6.10	1.56	1.46
26	O	178	ARG	CZ-NH2	6.10	1.41	1.33
10	3	181	SER	C-N	6.09	1.44	1.33
21	S	502	GLU	CD-OE2	6.09	1.32	1.25
32	J	247	PHE	CG-CD2	6.09	1.47	1.38
19	Z	836	GLU	CB-CG	6.08	1.63	1.52
20	N	600	ARG	NE-CZ	6.08	1.41	1.33
31	M	161	TYR	CB-CG	-6.07	1.42	1.51
24	R	336	ARG	CZ-NH2	6.07	1.41	1.33
4	D	63	CYS	CB-SG	-6.06	1.72	1.82
1	A	78	CYS	CB-SG	6.06	1.92	1.82
2	B	30	ALA	CA-CB	6.06	1.65	1.52
20	N	389	ASN	CB-CG	6.05	1.65	1.51
23	Q	104	GLY	CA-C	-6.04	1.42	1.51
19	Z	505	MET	N-CA	-6.04	1.34	1.46
9	2	75	SER	CA-CB	6.04	1.62	1.52
20	N	57	ARG	CZ-NH2	6.03	1.40	1.33
28	I	410	ARG	CD-NE	6.03	1.56	1.46
27	H	428	ARG	CZ-NH2	6.03	1.40	1.33
27	H	406	GLU	CD-OE2	6.02	1.32	1.25
24	R	297	ARG	CD-NE	6.01	1.56	1.46
21	S	388	TYR	CG-CD2	6.01	1.47	1.39
22	P	322	GLU	CD-OE2	6.01	1.32	1.25
12	5	216	ARG	NE-CZ	6.00	1.40	1.33
20	N	56	SER	CA-CB	6.00	1.61	1.52
6	F	157	ARG	CZ-NH1	5.99	1.40	1.33
13	6	28	ARG	NE-CZ	5.99	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	321	PHE	CG-CD1	5.99	1.47	1.38
7	G	103	PHE	CG-CD2	5.99	1.47	1.38
4	D	92	ARG	CZ-NH2	5.99	1.40	1.33
29	K	323	ARG	CZ-NH1	5.98	1.40	1.33
11	4	67	TYR	CE2-CZ	5.96	1.46	1.38
29	K	326	ARG	CZ-NH2	5.96	1.40	1.33
30	L	123	ARG	NE-CZ	5.96	1.40	1.33
14	7	144	ARG	CZ-NH2	5.96	1.40	1.33
16	V	235	SER	CA-CB	5.95	1.61	1.52
8	1	116	PHE	CG-CD1	5.95	1.47	1.38
13	6	128	PHE	CG-CD1	5.95	1.47	1.38
27	H	130	ALA	C-N	5.95	1.45	1.34
20	N	55	ARG	NE-CZ	5.95	1.40	1.33
26	O	247	ARG	NE-CZ	5.95	1.40	1.33
20	N	159	ARG	CZ-NH1	5.95	1.40	1.33
27	H	147	TYR	CG-CD2	5.94	1.46	1.39
30	L	171	GLU	CG-CD	5.94	1.60	1.51
7	G	161	TYR	CG-CD1	5.93	1.46	1.39
28	I	333	ARG	CZ-NH2	5.93	1.40	1.33
8	1	124	ARG	CZ-NH1	5.92	1.40	1.33
15	W	91	ARG	CZ-NH2	5.92	1.40	1.33
18	Y	52	PHE	CE2-CZ	5.92	1.48	1.37
31	M	91	TYR	CG-CD1	5.91	1.46	1.39
21	S	110	TYR	CG-CD2	5.91	1.46	1.39
8	1	122	ARG	NE-CZ	5.91	1.40	1.33
5	E	220	VAL	CB-CG1	5.90	1.65	1.52
31	M	374	ARG	NE-CZ	5.90	1.40	1.33
8	1	182	LYS	CD-CE	5.90	1.66	1.51
21	S	283	ARG	CZ-NH1	5.89	1.40	1.33
27	H	258	ARG	CZ-NH1	5.88	1.40	1.33
31	M	64	ARG	CZ-NH2	5.88	1.40	1.33
30	L	111	ARG	NE-CZ	5.88	1.40	1.33
7	G	13	SER	CA-CB	-5.88	1.44	1.52
10	3	26	ARG	CZ-NH1	5.88	1.40	1.33
11	4	161	ARG	CD-NE	5.87	1.56	1.46
31	M	183	ARG	CZ-NH2	5.87	1.40	1.33
20	N	628	ARG	NE-CZ	5.87	1.40	1.33
23	Q	181	SER	CA-CB	5.85	1.61	1.52
12	5	212	TYR	CG-CD1	5.85	1.46	1.39
22	P	227	TYR	CA-CB	5.85	1.66	1.53
12	5	77	SER	CA-CB	5.84	1.61	1.52
19	Z	574	GLU	CD-OE2	5.84	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	899	ARG	CD-NE	5.84	1.56	1.46
20	N	460	TYR	CG-CD1	5.83	1.46	1.39
28	I	272	ARG	NE-CZ	5.83	1.40	1.33
3	C	55	LEU	N-CA	-5.83	1.34	1.46
27	H	349	GLU	CB-CG	5.83	1.63	1.52
12	5	212	TYR	CG-CD2	5.82	1.46	1.39
13	6	221	ARG	CZ-NH2	5.82	1.40	1.33
7	G	41	ARG	CD-NE	5.81	1.56	1.46
10	3	80	ARG	CZ-NH2	5.81	1.40	1.33
13	6	55	ARG	CZ-NH1	5.81	1.40	1.33
23	Q	122	ARG	CD-NE	5.81	1.56	1.46
24	R	379	ARG	CD-NE	5.81	1.56	1.46
6	F	136	GLY	N-CA	-5.80	1.37	1.46
23	Q	348	GLU	CG-CD	5.80	1.60	1.51
1	A	11	ARG	NE-CZ	5.80	1.40	1.33
20	N	572	ARG	CZ-NH2	5.80	1.40	1.33
22	P	329	ARG	CZ-NH1	5.80	1.40	1.33
26	O	282	PHE	CB-CG	-5.80	1.41	1.51
9	2	235	PRO	CA-CB	5.80	1.65	1.53
1	A	145	GLU	CD-OE1	5.80	1.32	1.25
20	N	490	ARG	NE-CZ	5.79	1.40	1.33
28	I	349	ARG	CZ-NH1	5.79	1.40	1.33
24	R	366	TYR	CD1-CE1	5.79	1.48	1.39
24	R	40	GLU	CD-OE1	5.79	1.32	1.25
21	S	102	ARG	CZ-NH2	5.78	1.40	1.33
26	O	352	ARG	CZ-NH2	5.78	1.40	1.33
13	6	102	TYR	CE2-CZ	5.78	1.46	1.38
20	N	407	SER	CB-OG	5.78	1.49	1.42
10	3	66	ARG	NE-CZ	5.77	1.40	1.33
26	O	109	GLU	CG-CD	-5.77	1.43	1.51
20	N	434	GLY	CA-C	5.76	1.61	1.51
22	P	27	ARG	NE-CZ	5.76	1.40	1.33
28	I	268	ARG	CD-NE	5.76	1.56	1.46
23	Q	244	SER	CA-CB	5.76	1.61	1.52
21	S	337	GLU	N-CA	-5.75	1.34	1.46
12	5	220	TYR	CG-CD1	5.75	1.46	1.39
11	4	86	ARG	CZ-NH1	5.74	1.40	1.33
24	R	177	ARG	CZ-NH1	5.74	1.40	1.33
6	F	221	PHE	CE2-CZ	5.73	1.48	1.37
26	O	196	ARG	NE-CZ	5.73	1.40	1.33
3	C	81	SER	CA-CB	5.72	1.61	1.52
22	P	123	ARG	CZ-NH1	5.72	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	129	PHE	CG-CD2	5.72	1.47	1.38
16	V	224	SER	CA-CB	5.72	1.61	1.52
31	M	220	ILE	CA-CB	-5.72	1.41	1.54
7	G	224	ARG	CZ-NH1	5.71	1.40	1.33
32	J	113	ARG	CZ-NH2	5.71	1.40	1.33
20	N	413	LYS	C-N	5.70	1.43	1.33
27	H	401	ARG	CZ-NH1	5.70	1.40	1.33
7	G	48	PHE	N-CA	-5.70	1.34	1.46
7	G	8	TYR	CE2-CZ	5.70	1.46	1.38
20	N	943	GLU	CD-OE2	5.70	1.31	1.25
25	U	249	PHE	CG-CD1	5.70	1.47	1.38
24	R	30	GLU	CD-OE2	5.69	1.31	1.25
32	J	189	TYR	CZ-OH	5.69	1.47	1.37
3	C	152	PRO	N-CD	5.68	1.55	1.47
21	S	74	HIS	CG-CD2	5.68	1.45	1.35
14	7	151	TRP	CG-CD1	5.67	1.44	1.36
24	R	294	TYR	CZ-OH	5.67	1.47	1.37
24	R	83	ARG	NE-CZ	5.67	1.40	1.33
20	N	469	SER	CB-OG	5.67	1.49	1.42
2	B	229	TYR	CZ-OH	5.66	1.47	1.37
26	O	153	SER	CA-CB	5.66	1.61	1.52
16	V	206	ASN	N-CA	-5.65	1.35	1.46
6	F	89	ARG	NE-CZ	5.65	1.40	1.33
13	6	159	ARG	CD-NE	5.65	1.56	1.46
28	I	180	PRO	N-CD	-5.65	1.40	1.47
22	P	364	ARG	CZ-NH1	5.64	1.40	1.33
4	D	115	ARG	CZ-NH1	5.64	1.40	1.33
6	F	171	TYR	CE2-CZ	5.64	1.45	1.38
8	1	57	SER	CA-CB	5.64	1.61	1.52
21	S	290	ARG	CD-NE	5.64	1.56	1.46
25	U	41	GLY	CA-C	-5.64	1.42	1.51
19	Z	257	ARG	NE-CZ	5.63	1.40	1.33
19	Z	557	TRP	CZ2-CH2	5.63	1.48	1.37
19	Z	584	SER	CA-CB	5.63	1.61	1.52
20	N	121	GLY	CA-C	-5.63	1.42	1.51
28	I	363	ARG	CZ-NH1	5.63	1.40	1.33
19	Z	341	GLU	C-N	5.63	1.45	1.34
20	N	601	ARG	CZ-NH2	5.63	1.40	1.33
6	F	173	GLU	CD-OE1	-5.62	1.19	1.25
13	6	70	CYS	CB-SG	5.62	1.91	1.82
21	S	503	SER	CB-OG	5.62	1.49	1.42
27	H	375	ARG	NE-CZ	5.62	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	I	300	GLY	N-CA	-5.62	1.37	1.46
10	3	193	ASP	N-CA	-5.61	1.35	1.46
21	S	252	ARG	CZ-NH2	5.61	1.40	1.33
24	R	379	ARG	CZ-NH1	5.61	1.40	1.33
31	M	192	GLY	C-N	5.61	1.43	1.33
24	R	292	TYR	CZ-OH	5.61	1.47	1.37
19	Z	588	ARG	CD-NE	5.60	1.55	1.46
9	2	191	GLU	CD-OE1	5.60	1.31	1.25
8	1	52	ARG	CD-NE	5.60	1.55	1.46
28	I	231	GLY	CA-C	-5.59	1.43	1.51
14	7	79	ARG	CZ-NH1	5.59	1.40	1.33
26	O	284	ARG	NE-CZ	5.59	1.40	1.33
28	I	207	HIS	CB-CG	5.58	1.60	1.50
5	E	150	GLY	N-CA	-5.58	1.37	1.46
31	M	47	ARG	NE-CZ	5.58	1.40	1.33
6	F	237	GLU	CD-OE2	5.57	1.31	1.25
16	V	104	ARG	CZ-NH1	5.57	1.40	1.33
21	S	237	ARG	CZ-NH1	5.57	1.40	1.33
22	P	164	SER	CA-CB	5.57	1.61	1.52
8	1	138	PRO	N-CA	-5.57	1.37	1.47
21	S	224	ARG	CD-NE	5.57	1.55	1.46
11	4	120	TYR	CE1-CZ	5.57	1.45	1.38
19	Z	363	SER	CA-CB	5.56	1.61	1.52
13	6	231	ARG	CZ-NH1	5.56	1.40	1.33
6	F	239	ARG	NE-CZ	5.55	1.40	1.33
3	C	148	TYR	CE2-CZ	5.55	1.45	1.38
27	H	97	ARG	CZ-NH1	5.54	1.40	1.33
30	L	370	ARG	CZ-NH2	5.54	1.40	1.33
5	E	222	PRO	N-CD	-5.54	1.40	1.47
20	N	575	ASP	C-N	5.54	1.44	1.34
24	R	295	TYR	CZ-OH	5.54	1.47	1.37
20	N	649	ARG	CZ-NH1	5.54	1.40	1.33
30	L	386	ARG	NE-CZ	5.54	1.40	1.33
28	I	392	GLY	N-CA	-5.54	1.37	1.46
14	7	196	GLU	CD-OE2	5.53	1.31	1.25
16	V	139	ARG	CZ-NH2	5.53	1.40	1.33
19	Z	33	ARG	CZ-NH2	5.53	1.40	1.33
27	H	274	PHE	CG-CD1	5.53	1.47	1.38
1	A	94	ALA	CA-CB	5.53	1.64	1.52
26	O	194	GLN	CG-CD	5.52	1.63	1.51
27	H	429	TYR	CZ-OH	5.52	1.47	1.37
19	Z	478	ARG	CZ-NH1	5.52	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K	248	ARG	CD-NE	5.52	1.55	1.46
22	P	316	ARG	CZ-NH2	5.52	1.40	1.33
20	N	615	ARG	CZ-NH2	5.51	1.40	1.33
21	S	237	ARG	NE-CZ	5.51	1.40	1.33
26	O	294	GLU	CG-CD	5.51	1.60	1.51
19	Z	598	CYS	CB-SG	-5.51	1.72	1.81
27	H	363	SER	CA-CB	5.51	1.61	1.52
31	M	151	GLY	N-CA	-5.51	1.37	1.46
22	P	302	TYR	CZ-OH	5.50	1.47	1.37
21	S	197	ARG	CA-CB	5.50	1.66	1.53
24	R	174	TRP	CB-CG	5.50	1.60	1.50
2	B	173	PHE	CE1-CZ	5.50	1.47	1.37
25	U	190	ARG	CZ-NH2	5.50	1.40	1.33
28	I	322	ARG	CZ-NH1	5.50	1.40	1.33
23	Q	363	ARG	CZ-NH1	5.49	1.40	1.33
27	H	398	ARG	CZ-NH1	5.49	1.40	1.33
32	J	313	ARG	NE-CZ	5.49	1.40	1.33
10	3	104	TYR	CB-CG	-5.49	1.43	1.51
3	C	96	ARG	CZ-NH1	5.48	1.40	1.33
12	5	225	ARG	CZ-NH1	5.48	1.40	1.33
15	W	191	GLY	N-CA	-5.48	1.37	1.46
11	4	120	TYR	CG-CD1	5.48	1.46	1.39
1	A	177	SER	CA-CB	5.48	1.61	1.52
19	Z	95	PRO	N-CD	-5.48	1.40	1.47
27	H	344	SER	CA-CB	5.48	1.61	1.52
29	K	158	GLN	N-CA	-5.48	1.35	1.46
19	Z	482	ILE	CA-CB	-5.48	1.42	1.54
28	I	268	ARG	CZ-NH2	5.46	1.40	1.33
19	Z	478	ARG	CD-NE	5.46	1.55	1.46
19	Z	506	GLY	CA-C	-5.46	1.43	1.51
7	G	100	ARG	NE-CZ	5.45	1.40	1.33
28	I	439	TYR	CG-CD1	5.45	1.46	1.39
20	N	71	LEU	C-N	5.45	1.42	1.33
20	N	883	ARG	NE-CZ	5.45	1.40	1.33
21	S	92	ARG	CZ-NH2	5.45	1.40	1.33
32	J	395	SER	CA-CB	5.44	1.61	1.52
17	T	190	TYR	CG-CD2	5.44	1.46	1.39
19	Z	357	ARG	NE-CZ	5.44	1.40	1.33
19	Z	703	ARG	CZ-NH2	5.44	1.40	1.33
2	B	4	ARG	CZ-NH2	5.44	1.40	1.33
1	A	19	GLU	CG-CD	5.43	1.60	1.51
32	J	372	ARG	NE-CZ	5.43	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	142	PHE	CG-CD2	5.43	1.46	1.38
1	A	35	GLY	C-N	5.43	1.42	1.33
19	Z	723	TYR	CG-CD2	5.42	1.46	1.39
22	P	4	GLY	C-N	5.42	1.42	1.33
30	L	286	ARG	CZ-NH1	5.42	1.40	1.33
23	Q	142	ARG	CZ-NH1	5.42	1.40	1.33
25	U	267	ARG	CZ-NH1	5.42	1.40	1.33
24	R	201	PHE	CG-CD1	5.41	1.46	1.38
23	Q	132	ARG	CD-NE	5.41	1.55	1.46
25	U	255	ASP	CB-CG	5.41	1.63	1.51
6	F	196	ARG	CZ-NH1	5.41	1.40	1.33
9	2	51	TYR	CB-CG	-5.40	1.43	1.51
30	L	235	TYR	CD2-CE2	5.40	1.47	1.39
21	S	404	ARG	NE-CZ	5.40	1.40	1.33
24	R	219	PHE	CG-CD1	5.40	1.46	1.38
26	O	270	ARG	CD-NE	5.40	1.55	1.46
7	G	235	GLU	CD-OE1	5.40	1.31	1.25
26	O	139	GLU	CD-OE1	5.39	1.31	1.25
19	Z	182	GLU	CB-CG	5.39	1.62	1.52
12	5	128	ARG	NE-CZ	5.39	1.40	1.33
11	4	36	PHE	CG-CD1	5.38	1.46	1.38
10	3	143	SER	CA-CB	5.38	1.61	1.52
23	Q	11	ARG	NE-CZ	5.38	1.40	1.33
32	J	313	ARG	CD-NE	5.38	1.55	1.46
9	2	257	GLU	CA-CB	5.38	1.65	1.53
20	N	407	SER	CA-CB	5.38	1.61	1.52
26	O	289	ARG	CZ-NH1	5.38	1.40	1.33
6	F	193	ARG	CZ-NH2	5.38	1.40	1.33
30	L	311	ARG	CZ-NH1	5.37	1.40	1.33
7	G	15	PHE	CG-CD2	5.37	1.46	1.38
20	N	509	GLY	N-CA	-5.37	1.38	1.46
32	J	253	SER	CA-CB	5.37	1.61	1.52
8	1	95	GLN	CG-CD	5.37	1.63	1.51
29	K	258	ALA	CA-CB	5.37	1.63	1.52
23	Q	397	TYR	CE1-CZ	5.36	1.45	1.38
11	4	137	PHE	CG-CD1	5.36	1.46	1.38
15	W	69	GLY	CA-C	-5.36	1.43	1.51
19	Z	284	SER	CA-CB	5.36	1.60	1.52
21	S	214	TYR	CG-CD2	5.36	1.46	1.39
22	P	251	TYR	CG-CD1	5.36	1.46	1.39
5	E	20	ARG	NE-CZ	5.35	1.40	1.33
10	3	48	ARG	CD-NE	5.35	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	841	PRO	N-CD	-5.35	1.40	1.47
21	S	336	GLY	CA-C	-5.35	1.43	1.51
5	E	62	SER	CA-CB	5.35	1.60	1.52
22	P	142	ARG	CZ-NH2	5.35	1.40	1.33
26	O	29	TYR	CE1-CZ	-5.34	1.31	1.38
19	Z	712	LYS	CD-CE	5.34	1.64	1.51
29	K	366	ARG	CZ-NH1	5.34	1.40	1.33
14	7	138	ARG	CZ-NH2	5.34	1.40	1.33
23	Q	155	ARG	CZ-NH2	5.33	1.40	1.33
3	C	219	GLU	CD-OE2	-5.33	1.19	1.25
19	Z	456	ARG	CZ-NH1	5.33	1.40	1.33
24	R	293	ARG	CZ-NH2	5.33	1.40	1.33
4	D	78	SER	CB-OG	5.33	1.49	1.42
16	V	260	GLU	CG-CD	5.33	1.59	1.51
6	F	18	ARG	CD-NE	5.32	1.55	1.46
13	6	67	SER	CA-CB	5.31	1.60	1.52
22	P	316	ARG	CD-NE	5.31	1.55	1.46
29	K	72	PHE	CG-CD1	5.31	1.46	1.38
30	L	157	ARG	CD-NE	5.31	1.55	1.46
30	L	17	ASP	C-N	5.31	1.44	1.34
17	T	232	PRO	N-CD	-5.31	1.40	1.47
31	M	439	GLN	CA-CB	5.30	1.65	1.53
1	A	27	TYR	CZ-OH	5.30	1.46	1.37
21	S	79	GLU	CG-CD	5.30	1.59	1.51
20	N	156	GLU	CD-OE1	5.30	1.31	1.25
3	C	12	PHE	CG-CD1	5.30	1.46	1.38
26	O	101	ARG	CZ-NH2	5.30	1.40	1.33
29	K	332	GLU	CD-OE1	-5.30	1.19	1.25
4	D	92	ARG	CD-NE	5.29	1.55	1.46
10	3	105	THR	N-CA	-5.29	1.35	1.46
19	Z	257	ARG	CZ-NH1	5.29	1.40	1.33
20	N	230	SER	CA-CB	5.29	1.60	1.52
31	M	305	GLY	N-CA	-5.29	1.38	1.46
24	R	143	TYR	CG-CD2	5.29	1.46	1.39
29	K	263	PHE	CG-CD2	5.28	1.46	1.38
14	7	81	ARG	CZ-NH2	5.28	1.40	1.33
19	Z	617	SER	CA-CB	5.28	1.60	1.52
20	N	254	GLU	CD-OE1	5.28	1.31	1.25
15	W	88	THR	N-CA	-5.28	1.35	1.46
22	P	237	GLU	CD-OE2	5.27	1.31	1.25
30	L	157	ARG	NE-CZ	5.27	1.40	1.33
31	M	189	SER	CA-CB	5.27	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	215	GLU	CD-OE2	5.27	1.31	1.25
17	T	232	PRO	CA-C	-5.27	1.42	1.52
19	Z	227	SER	CA-CB	-5.27	1.45	1.52
21	S	453	TYR	CG-CD2	5.27	1.46	1.39
25	U	3	GLU	CD-OE2	-5.26	1.19	1.25
7	G	93	ARG	NE-CZ	5.26	1.39	1.33
24	R	4	GLU	CG-CD	5.26	1.59	1.51
30	L	58	GLU	CG-CD	5.26	1.59	1.51
30	L	358	ARG	CZ-NH1	5.26	1.39	1.33
19	Z	239	TYR	CG-CD1	5.26	1.46	1.39
19	Z	337	LEU	N-CA	-5.26	1.35	1.46
26	O	70	ARG	NE-CZ	5.26	1.39	1.33
14	7	252	ASN	CB-CG	5.25	1.63	1.51
4	D	101	ARG	CD-NE	5.25	1.55	1.46
5	E	100	TRP	CZ2-CH2	5.25	1.47	1.37
29	K	398	ASP	CA-CB	5.25	1.65	1.53
12	5	171	TYR	CG-CD1	5.25	1.46	1.39
19	Z	644	ALA	N-CA	-5.25	1.35	1.46
20	N	579	ARG	NE-CZ	5.25	1.39	1.33
32	J	275	GLU	CD-OE1	-5.25	1.19	1.25
22	P	213	PHE	CG-CD2	5.24	1.46	1.38
20	N	899	ARG	CZ-NH2	5.24	1.39	1.33
20	N	667	GLU	CB-CG	5.23	1.62	1.52
24	R	38	ARG	CZ-NH1	5.23	1.39	1.33
11	4	70	ARG	CD-NE	5.23	1.55	1.46
10	3	73	LEU	CA-CB	5.23	1.65	1.53
24	R	379	ARG	CB-CG	5.23	1.66	1.52
31	M	120	ARG	NE-CZ	5.23	1.39	1.33
8	1	50	ASP	CA-CB	5.22	1.65	1.53
28	I	272	ARG	CD-NE	5.22	1.55	1.46
11	4	117	TYR	CZ-OH	5.22	1.46	1.37
21	S	388	TYR	CG-CD1	-5.22	1.32	1.39
23	Q	55	SER	CA-CB	5.22	1.60	1.52
30	L	233	PHE	CB-CG	-5.22	1.42	1.51
17	T	252	GLY	CA-C	-5.21	1.43	1.51
18	Y	63	HIS	CB-CG	5.21	1.59	1.50
23	Q	282	ARG	CZ-NH1	5.21	1.39	1.33
30	L	311	ARG	NE-CZ	5.21	1.39	1.33
19	Z	274	ASP	N-CA	5.21	1.56	1.46
23	Q	74	ARG	NE-CZ	5.21	1.39	1.33
24	R	385	ARG	CD-NE	5.21	1.55	1.46
17	T	107	ARG	CZ-NH1	5.21	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	37	GLU	C-N	5.21	1.42	1.33
24	R	314	LEU	N-CA	-5.21	1.35	1.46
20	N	864	GLU	CG-CD	5.21	1.59	1.51
25	U	209	ARG	CZ-NH2	5.20	1.39	1.33
31	M	35	GLU	CG-CD	5.20	1.59	1.51
1	A	97	GLU	C-N	5.20	1.46	1.34
15	W	112	PHE	CG-CD1	5.20	1.46	1.38
21	S	116	PHE	CG-CD1	5.20	1.46	1.38
20	N	170	SER	CB-OG	5.19	1.49	1.42
3	C	17	ARG	NE-CZ	5.19	1.39	1.33
28	I	275	GLU	CG-CD	5.19	1.59	1.51
3	C	107	CYS	CB-SG	-5.19	1.73	1.81
29	K	96	VAL	CB-CG2	5.19	1.63	1.52
2	B	24	TYR	CZ-OH	5.19	1.46	1.37
7	G	188	ARG	CZ-NH1	5.19	1.39	1.33
20	N	620	GLU	CA-C	-5.19	1.39	1.52
19	Z	433	LEU	CA-CB	5.19	1.65	1.53
28	I	422	SER	CA-CB	5.18	1.60	1.52
15	W	147	GLU	CD-OE2	5.18	1.31	1.25
22	P	55	ARG	CZ-NH2	5.18	1.39	1.33
6	F	44	ALA	N-CA	-5.18	1.35	1.46
9	2	161	SER	CA-CB	5.18	1.60	1.52
11	4	58	GLU	CG-CD	5.18	1.59	1.51
1	A	105	TYR	CE2-CZ	5.17	1.45	1.38
6	F	68	ASN	CB-CG	5.17	1.62	1.51
20	N	437	TYR	CZ-OH	5.17	1.46	1.37
32	J	88	LYS	N-CA	-5.17	1.36	1.46
4	D	221	GLN	CA-CB	5.17	1.65	1.53
19	Z	190	GLU	CB-CG	5.17	1.61	1.52
6	F	97	PHE	CG-CD1	5.17	1.46	1.38
25	U	217	SER	CA-CB	5.17	1.60	1.52
8	1	208	ARG	N-CA	-5.17	1.36	1.46
32	J	235	PHE	CE1-CZ	5.17	1.47	1.37
9	2	62	ARG	CZ-NH1	5.16	1.39	1.33
19	Z	209	MET	CA-C	-5.16	1.39	1.52
19	Z	807	ARG	CD-NE	5.16	1.55	1.46
22	P	182	ARG	NE-CZ	5.16	1.39	1.33
25	U	224	HIS	CB-CG	5.16	1.59	1.50
7	G	141	TYR	CD2-CE2	5.16	1.47	1.39
31	M	384	TYR	CD2-CE2	5.16	1.47	1.39
32	J	16	ALA	C-N	5.16	1.42	1.33
28	I	311	GLU	CB-CG	5.16	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	P	109	CYS	CB-SG	5.15	1.91	1.82
16	V	309	PHE	CG-CD1	5.15	1.46	1.38
19	Z	588	ARG	CZ-NH1	5.15	1.39	1.33
20	N	391	GLU	CD-OE1	5.15	1.31	1.25
2	B	185	GLU	CD-OE1	-5.15	1.20	1.25
23	Q	236	PHE	CA-CB	5.15	1.65	1.53
21	S	272	PHE	CG-CD2	5.15	1.46	1.38
27	H	432	TYR	CA-CB	5.14	1.65	1.53
5	E	168	ARG	CD-NE	5.14	1.55	1.46
17	T	98	TYR	CG-CD1	5.14	1.45	1.39
22	P	38	GLY	CA-C	-5.14	1.43	1.51
9	2	157	TYR	CE2-CZ	5.14	1.45	1.38
26	O	196	ARG	CZ-NH2	5.14	1.39	1.33
7	G	48	PHE	CD2-CE2	5.14	1.49	1.39
13	6	102	TYR	CG-CD1	5.14	1.45	1.39
23	Q	312	GLU	CG-CD	5.14	1.59	1.51
24	R	310	SER	CA-CB	5.13	1.60	1.52
20	N	80	TYR	CB-CG	5.13	1.59	1.51
19	Z	6	ARG	NE-CZ	5.13	1.39	1.33
20	N	35	TRP	CE3-CZ3	5.13	1.47	1.38
27	H	144	ARG	CZ-NH2	5.12	1.39	1.33
7	G	100	ARG	CZ-NH1	5.12	1.39	1.33
3	C	179	TYR	CE2-CZ	5.11	1.45	1.38
20	N	345	ASN	CA-CB	5.11	1.66	1.53
8	1	177	ARG	NE-CZ	5.11	1.39	1.33
14	7	88	ARG	CZ-NH2	5.11	1.39	1.33
29	K	297	ASP	N-CA	-5.10	1.36	1.46
9	2	118	ARG	CZ-NH2	5.10	1.39	1.33
25	U	184	VAL	C-N	5.10	1.42	1.33
28	I	294	ARG	CD-NE	5.10	1.55	1.46
15	W	50	GLY	N-CA	-5.10	1.38	1.46
3	C	23	TYR	CZ-OH	5.10	1.46	1.37
4	D	37	GLY	CA-C	-5.10	1.43	1.51
17	T	179	PHE	CG-CD1	5.10	1.46	1.38
29	K	283	ARG	CD-NE	5.10	1.55	1.46
19	Z	181	ARG	CZ-NH1	5.10	1.39	1.33
27	H	412	ALA	N-CA	-5.10	1.36	1.46
28	I	202	GLU	CG-CD	5.10	1.59	1.51
28	I	282	VAL	CB-CG2	5.10	1.63	1.52
31	M	301	SER	CA-CB	5.10	1.60	1.52
9	2	131	PHE	CG-CD2	5.09	1.46	1.38
24	R	300	ARG	CD-NE	5.09	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	183	GLU	CB-CG	5.09	1.61	1.52
30	L	188	GLY	CA-C	-5.09	1.43	1.51
28	I	346	ARG	CZ-NH2	5.09	1.39	1.33
9	2	73	ASN	N-CA	-5.09	1.36	1.46
19	Z	879	ARG	CZ-NH1	5.09	1.39	1.33
31	M	173	SER	CA-CB	5.09	1.60	1.52
26	O	215	GLU	CB-CG	5.09	1.61	1.52
19	Z	838	ARG	CZ-NH1	5.08	1.39	1.33
9	2	236	ASN	CB-CG	5.08	1.62	1.51
20	N	819	VAL	C-N	-5.08	1.24	1.34
25	U	82	PHE	CB-CG	5.08	1.59	1.51
2	B	4	ARG	CZ-NH1	5.08	1.39	1.33
4	D	64	ALA	CA-C	-5.08	1.39	1.52
27	H	111	TYR	CZ-OH	5.07	1.46	1.37
32	J	26	SER	CA-CB	5.07	1.60	1.52
22	P	65	ARG	CZ-NH1	5.07	1.39	1.33
31	M	385	GLU	CG-CD	5.07	1.59	1.51
14	7	159	TYR	CE2-CZ	5.07	1.45	1.38
17	T	121	ARG	NE-CZ	5.07	1.39	1.33
14	7	233	VAL	CB-CG1	5.07	1.63	1.52
5	E	175	GLU	CD-OE1	5.06	1.31	1.25
24	R	337	PHE	CG-CD2	5.06	1.46	1.38
3	C	179	TYR	CZ-OH	5.06	1.46	1.37
19	Z	72	ARG	NE-CZ	5.06	1.39	1.33
19	Z	267	ARG	CZ-NH1	5.06	1.39	1.33
21	S	110	TYR	CD2-CE2	5.06	1.47	1.39
28	I	75	GLU	N-CA	-5.06	1.36	1.46
22	P	289	ARG	NE-CZ	5.06	1.39	1.33
24	R	118	GLU	CB-CG	5.06	1.61	1.52
29	K	95	ALA	CA-CB	5.06	1.63	1.52
14	7	222	TYR	CG-CD2	-5.06	1.32	1.39
31	M	353	ARG	CZ-NH1	5.06	1.39	1.33
20	N	207	ASN	CB-CG	5.05	1.62	1.51
31	M	80	SER	CB-OG	5.05	1.48	1.42
6	F	230	SER	CA-CB	5.05	1.60	1.52
26	O	68	GLU	CD-OE1	5.05	1.31	1.25
30	L	221	TYR	CG-CD1	5.05	1.45	1.39
20	N	23	ALA	CA-CB	5.04	1.63	1.52
20	N	72	GLY	CA-C	-5.04	1.43	1.51
22	P	387	ASP	CA-CB	5.04	1.65	1.53
26	O	60	TYR	CE1-CZ	5.04	1.45	1.38
29	K	245	ARG	NE-CZ	5.04	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	595	ASN	CA-C	-5.04	1.39	1.52
24	R	297	ARG	CZ-NH1	5.04	1.39	1.33
22	P	259	GLU	CG-CD	5.04	1.59	1.51
22	P	388	GLU	CG-CD	5.03	1.59	1.51
24	R	216	TYR	CE1-CZ	5.03	1.45	1.38
23	Q	314	ARG	CD-NE	5.03	1.55	1.46
6	F	153	TYR	CB-CG	5.03	1.59	1.51
13	6	44	GLY	CA-C	-5.03	1.43	1.51
22	P	8	ARG	CD-NE	5.03	1.54	1.46
26	O	44	PHE	CG-CD1	5.03	1.46	1.38
5	E	179	SER	CA-CB	5.03	1.60	1.52
14	7	61	ASP	CA-CB	5.03	1.65	1.53
19	Z	838	ARG	CD-NE	5.03	1.54	1.46
20	N	489	ALA	N-CA	-5.03	1.36	1.46
24	R	323	PHE	CE1-CZ	5.02	1.46	1.37
27	H	190	VAL	N-CA	-5.02	1.36	1.46
28	I	276	GLU	CG-CD	5.02	1.59	1.51
28	I	80	ARG	CZ-NH2	5.02	1.39	1.33
30	L	98	ARG	CZ-NH2	5.02	1.39	1.33
17	T	244	TYR	CG-CD1	5.02	1.45	1.39
24	R	87	GLU	CG-CD	5.02	1.59	1.51
21	S	432	PHE	CE2-CZ	5.01	1.46	1.37
7	G	19	GLY	N-CA	-5.01	1.38	1.46
22	P	94	ARG	NE-CZ	5.01	1.39	1.33
9	2	118	ARG	NE-CZ	5.01	1.39	1.33
10	3	161	GLU	CD-OE2	5.01	1.31	1.25
16	V	294	SER	CB-OG	-5.01	1.35	1.42
1	A	70	PHE	CG-CD1	5.01	1.46	1.38
30	L	146	TYR	CZ-OH	5.01	1.46	1.37
12	5	156	MET	C-N	5.00	1.42	1.33
19	Z	6	ARG	CZ-NH2	5.00	1.39	1.33
19	Z	250	ARG	NE-CZ	5.00	1.39	1.33
24	R	80	GLU	CD-OE2	5.00	1.31	1.25
27	H	255	ARG	CD-NE	5.00	1.54	1.46

All (2115) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	L	308	ARG	NE-CZ-NH2	-19.32	110.64	120.30
2	B	130	PHE	CB-CG-CD2	-19.11	107.42	120.80
21	S	146	ARG	NE-CZ-NH2	-18.99	110.81	120.30
28	I	303	ARG	NE-CZ-NH2	-18.67	110.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	170	ARG	NE-CZ-NH2	-18.38	111.11	120.30
1	A	27	TYR	CB-CG-CD2	-17.70	110.38	121.00
4	D	92	ARG	NE-CZ-NH1	17.66	129.13	120.30
19	Z	554	TYR	CB-CG-CD1	-17.47	110.52	121.00
7	G	170	ARG	NE-CZ-NH1	17.40	129.00	120.30
8	1	219	ARG	NE-CZ-NH2	-16.99	111.80	120.30
19	Z	763	ARG	NE-CZ-NH1	16.23	128.42	120.30
23	Q	72	TYR	CB-CG-CD2	-16.18	111.29	121.00
21	S	146	ARG	NE-CZ-NH1	16.06	128.33	120.30
8	1	208	ARG	NE-CZ-NH2	-15.94	112.33	120.30
8	1	62	ARG	NE-CZ-NH1	15.53	128.07	120.30
19	Z	688	ARG	NE-CZ-NH1	15.48	128.04	120.30
23	Q	342	PHE	CB-CG-CD1	15.41	131.59	120.80
19	Z	469	TYR	CB-CG-CD1	15.38	130.22	121.00
26	O	289	ARG	NE-CZ-NH1	15.35	127.97	120.30
13	6	221	ARG	NE-CZ-NH2	-15.34	112.63	120.30
28	I	103	ARG	NE-CZ-NH2	-15.34	112.63	120.30
26	O	178	ARG	NE-CZ-NH1	15.32	127.96	120.30
25	U	283	ARG	NE-CZ-NH2	-15.28	112.66	120.30
25	U	114	ARG	NE-CZ-NH1	15.23	127.92	120.30
29	K	43	ARG	NE-CZ-NH1	15.22	127.91	120.30
3	C	23	TYR	CB-CG-CD2	-15.20	111.88	121.00
25	U	25	ARG	NE-CZ-NH2	-15.16	112.72	120.30
32	J	44	ARG	NE-CZ-NH1	15.09	127.84	120.30
28	I	103	ARG	NE-CZ-NH1	15.05	127.83	120.30
24	R	179	ARG	NE-CZ-NH2	-15.03	112.78	120.30
22	P	65	ARG	NE-CZ-NH1	14.22	127.41	120.30
24	R	292	TYR	CB-CG-CD2	-14.15	112.51	121.00
16	V	32	TYR	CB-CG-CD1	-14.13	112.52	121.00
1	A	178	PHE	CB-CG-CD1	14.11	130.68	120.80
29	K	366	ARG	NE-CZ-NH1	14.11	127.35	120.30
2	B	24	TYR	CB-CG-CD1	13.95	129.37	121.00
29	K	164	TYR	CB-CG-CD1	-13.91	112.65	121.00
25	U	79	TYR	CB-CG-CD2	-13.88	112.67	121.00
22	P	185	PHE	CB-CG-CD2	-13.84	111.11	120.80
29	K	283	ARG	NE-CZ-NH2	-13.58	113.51	120.30
26	O	247	ARG	NE-CZ-NH2	-13.53	113.53	120.30
27	H	249	TYR	CB-CG-CD1	13.44	129.06	121.00
4	D	73	PHE	CB-CG-CD1	-13.37	111.44	120.80
21	S	298	TYR	CB-CG-CD2	13.35	129.01	121.00
7	G	126	TYR	CB-CG-CD1	13.34	129.00	121.00
24	R	358	ARG	NE-CZ-NH2	-13.26	113.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	K	326	ARG	NE-CZ-NH1	13.26	126.93	120.30
28	I	247	PHE	CB-CG-CD2	13.07	129.95	120.80
28	I	247	PHE	CB-CG-CD1	-13.01	111.69	120.80
29	K	112	TYR	CB-CG-CD1	-12.98	113.21	121.00
3	C	8	ARG	NE-CZ-NH2	-12.96	113.82	120.30
19	Z	160	ARG	NE-CZ-NH2	12.95	126.77	120.30
27	H	249	TYR	CB-CG-CD2	-12.87	113.28	121.00
32	J	369	TYR	CB-CG-CD1	-12.87	113.28	121.00
27	H	285	PHE	CB-CG-CD1	-12.84	111.81	120.80
8	1	52	ARG	NE-CZ-NH2	-12.81	113.89	120.30
2	B	130	PHE	CB-CG-CD1	12.81	129.76	120.80
24	R	176	ARG	NE-CZ-NH2	-12.80	113.90	120.30
2	B	121	TYR	CB-CG-CD2	12.76	128.66	121.00
3	C	23	TYR	CB-CG-CD1	12.59	128.55	121.00
32	J	43	ARG	NE-CZ-NH2	-12.54	114.03	120.30
20	N	546	ARG	NE-CZ-NH2	-12.50	114.05	120.30
13	6	215	TYR	CB-CG-CD2	-12.49	113.51	121.00
2	B	143	ARG	NE-CZ-NH1	12.48	126.54	120.30
29	K	81	ARG	NE-CZ-NH1	12.48	126.54	120.30
1	A	27	TYR	CB-CG-CD1	12.45	128.47	121.00
24	R	146	ARG	NE-CZ-NH2	-12.44	114.08	120.30
6	F	164	ARG	NE-CZ-NH1	12.43	126.52	120.30
26	O	178	ARG	NE-CZ-NH2	-12.42	114.09	120.30
12	5	147	TYR	CB-CG-CD2	12.42	128.45	121.00
22	P	129	ARG	NE-CZ-NH2	-12.31	114.14	120.30
21	S	439	ARG	NE-CZ-NH2	-12.29	114.16	120.30
9	2	167	TYR	CB-CG-CD1	-12.27	113.64	121.00
14	7	221	TYR	CB-CG-CD1	12.25	128.35	121.00
23	Q	342	PHE	CB-CG-CD2	-12.23	112.24	120.80
28	I	259	TYR	CB-CG-CD1	12.19	128.31	121.00
32	J	325	ARG	NE-CZ-NH1	12.17	126.38	120.30
26	O	284	ARG	NE-CZ-NH1	12.13	126.37	120.30
31	M	47	ARG	NE-CZ-NH2	-12.12	114.24	120.30
27	H	366	ARG	NE-CZ-NH1	12.08	126.34	120.30
2	B	121	TYR	CB-CG-CD1	-12.05	113.77	121.00
25	U	114	ARG	NE-CZ-NH2	-12.03	114.28	120.30
17	T	178	TYR	CB-CG-CD1	12.03	128.22	121.00
1	A	152	TYR	CB-CG-CD2	-12.02	113.79	121.00
17	T	178	TYR	CB-CG-CD2	-12.02	113.78	121.00
26	O	352	ARG	NE-CZ-NH1	11.98	126.29	120.30
1	A	152	TYR	CB-CG-CD1	11.86	128.12	121.00
2	B	24	TYR	CB-CG-CD2	-11.85	113.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	L	227	ARG	NE-CZ-NH1	11.82	126.21	120.30
19	Z	137	ARG	NE-CZ-NH2	-11.82	114.39	120.30
9	2	124	ARG	NE-CZ-NH2	-11.82	114.39	120.30
12	5	179	ARG	NE-CZ-NH2	-11.81	114.40	120.30
26	O	284	ARG	NE-CZ-NH2	-11.79	114.40	120.30
24	R	295	TYR	CB-CG-CD1	11.77	128.06	121.00
15	W	108	ARG	NE-CZ-NH2	-11.76	114.42	120.30
31	M	413	ARG	NE-CZ-NH1	11.75	126.17	120.30
19	Z	239	TYR	CB-CG-CD2	-11.75	113.95	121.00
25	U	79	TYR	CB-CG-CD1	11.72	128.03	121.00
17	T	181	TYR	CB-CG-CD1	11.65	127.99	121.00
22	P	357	ARG	NE-CZ-NH2	11.63	126.11	120.30
6	F	107	ARG	NE-CZ-NH1	11.63	126.11	120.30
27	H	111	TYR	CB-CG-CD2	-11.62	114.03	121.00
2	B	8	PHE	CB-CG-CD2	-11.59	112.69	120.80
21	S	126	PHE	CB-CG-CD2	-11.56	112.70	120.80
31	M	307	ARG	NE-CZ-NH2	-11.56	114.52	120.30
22	P	427	ASP	CB-CG-OD2	11.53	128.68	118.30
30	L	54	TYR	CB-CG-CD2	-11.53	114.08	121.00
25	U	90	ARG	NE-CZ-NH1	-11.52	114.54	120.30
6	F	24	TYR	CB-CG-CD1	11.44	127.86	121.00
12	5	84	TYR	CG-CD2-CE2	-11.43	112.16	121.30
19	Z	763	ARG	NE-CZ-NH2	-11.41	114.59	120.30
23	Q	310	ARG	NE-CZ-NH2	-11.39	114.61	120.30
19	Z	675	PHE	CB-CG-CD2	-11.36	112.85	120.80
32	J	310	ARG	NE-CZ-NH2	-11.36	114.62	120.30
12	5	78	ARG	NE-CZ-NH1	11.29	125.95	120.30
30	L	26	TYR	CB-CG-CD1	11.28	127.77	121.00
27	H	274	PHE	CB-CG-CD2	11.27	128.69	120.80
20	N	199	ARG	NE-CZ-NH2	-11.25	114.67	120.30
24	R	159	ARG	NE-CZ-NH2	-11.18	114.71	120.30
31	M	120	ARG	NE-CZ-NH2	-11.18	114.71	120.30
28	I	272	ARG	NE-CZ-NH2	-11.16	114.72	120.30
10	3	96	TYR	CB-CG-CD2	-11.16	114.30	121.00
9	2	136	TYR	CB-CG-CD2	-11.15	114.31	121.00
29	K	164	TYR	CB-CG-CD2	11.13	127.68	121.00
20	N	490	ARG	NE-CZ-NH2	-11.10	114.75	120.30
3	C	60	PHE	CB-CG-CD1	-11.08	113.04	120.80
21	S	237	ARG	NE-CZ-NH2	-11.00	114.80	120.30
25	U	267	ARG	NE-CZ-NH2	-10.98	114.81	120.30
12	5	116	ARG	NE-CZ-NH2	-10.97	114.81	120.30
21	S	439	ARG	NE-CZ-NH1	10.97	125.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	S	382	PHE	CB-CG-CD2	10.96	128.47	120.80
19	Z	673	ARG	NE-CZ-NH2	-10.92	114.84	120.30
17	T	121	ARG	NE-CZ-NH2	-10.91	114.84	120.30
17	T	319	TYR	CB-CG-CD1	-10.91	114.45	121.00
32	J	340	ARG	NE-CZ-NH2	-10.89	114.86	120.30
20	N	474	ARG	NE-CZ-NH2	-10.88	114.86	120.30
23	Q	177	TYR	CB-CG-CD2	-10.84	114.50	121.00
22	P	341	PHE	CB-CG-CD2	-10.78	113.25	120.80
3	C	249	ARG	NE-CZ-NH1	10.77	125.68	120.30
29	K	235	PHE	CB-CG-CD1	10.76	128.34	120.80
16	V	208	ARG	NE-CZ-NH1	10.75	125.67	120.30
28	I	346	ARG	NE-CZ-NH2	-10.75	114.93	120.30
31	M	287	PHE	CB-CG-CD2	-10.75	113.28	120.80
21	S	395	ARG	NE-CZ-NH1	10.74	125.67	120.30
9	2	62	ARG	NE-CZ-NH1	10.73	125.66	120.30
32	J	375	ARG	NE-CZ-NH1	-10.71	114.94	120.30
24	R	192	ARG	NE-CZ-NH1	-10.69	114.95	120.30
32	J	375	ARG	NE-CZ-NH2	10.69	125.64	120.30
21	S	453	TYR	CB-CG-CD1	10.69	127.41	121.00
20	N	559	ARG	NE-CZ-NH1	10.67	125.63	120.30
21	S	232	ARG	NE-CZ-NH1	10.66	125.63	120.30
21	S	284	TYR	CB-CG-CD2	-10.66	114.60	121.00
17	T	318	TYR	CB-CG-CD2	-10.65	114.61	121.00
23	Q	337	ARG	NE-CZ-NH2	-10.63	114.98	120.30
24	R	267	ARG	NE-CZ-NH1	10.63	125.62	120.30
24	R	336	ARG	NE-CZ-NH1	10.63	125.61	120.30
21	S	345	ARG	NE-CZ-NH1	10.62	125.61	120.30
10	3	99	ARG	NE-CZ-NH2	-10.61	114.99	120.30
1	A	3	ARG	NE-CZ-NH2	10.55	125.58	120.30
27	H	375	ARG	NE-CZ-NH2	-10.54	115.03	120.30
20	N	194	ARG	NE-CZ-NH2	10.53	125.56	120.30
20	N	572	ARG	NE-CZ-NH1	10.52	125.56	120.30
20	N	590	TYR	CG-CD1-CE1	-10.52	112.88	121.30
29	K	313	ARG	NE-CZ-NH2	-10.52	115.04	120.30
12	5	125	TYR	CB-CG-CD2	-10.46	114.72	121.00
15	W	156	PHE	CB-CG-CD1	-10.45	113.49	120.80
23	Q	229	TYR	CB-CG-CD1	10.44	127.26	121.00
20	N	678	ASP	CB-CG-OD1	-10.43	108.91	118.30
7	G	145	ASP	CB-CG-OD1	-10.41	108.93	118.30
3	C	8	ARG	NE-CZ-NH1	10.40	125.50	120.30
17	T	107	ARG	NE-CZ-NH1	10.40	125.50	120.30
7	G	100	ARG	NE-CZ-NH1	-10.39	115.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	157	ASP	CB-CG-OD2	10.38	127.64	118.30
20	N	140	ARG	NE-CZ-NH1	10.35	125.48	120.30
21	S	208	TYR	CB-CG-CD2	10.35	127.21	121.00
27	H	232	ARG	NE-CZ-NH2	-10.33	115.13	120.30
32	J	21	ARG	NE-CZ-NH2	-10.29	115.16	120.30
3	C	61	PHE	CB-CG-CD1	-10.28	113.60	120.80
31	M	132	ARG	NE-CZ-NH2	-10.24	115.18	120.30
12	5	212	TYR	CB-CG-CD1	10.23	127.14	121.00
17	T	144	LEU	CB-CG-CD1	10.20	128.34	111.00
14	7	223	ARG	NE-CZ-NH1	10.16	125.38	120.30
32	J	369	TYR	CB-CG-CD2	10.15	127.09	121.00
19	Z	588	ARG	NE-CZ-NH1	10.14	125.37	120.30
20	N	751	ARG	NE-CZ-NH2	-10.13	115.23	120.30
8	1	176	TYR	CB-CG-CD2	10.13	127.08	121.00
24	R	360	ASP	CB-CG-OD2	-10.12	109.19	118.30
24	R	323	PHE	CB-CG-CD2	-10.11	113.72	120.80
29	K	342	ARG	NE-CZ-NH2	-10.07	115.26	120.30
24	R	312	ARG	NE-CZ-NH2	10.07	125.33	120.30
12	5	84	TYR	CB-CG-CD2	-10.06	114.96	121.00
21	S	230	ARG	NE-CZ-NH1	10.04	125.32	120.30
28	I	211	TYR	CB-CG-CD2	-10.04	114.98	121.00
3	C	121	TYR	CB-CG-CD2	-10.02	114.99	121.00
22	P	408	ARG	NE-CZ-NH2	-10.02	115.29	120.30
22	P	251	TYR	CB-CG-CD1	10.01	127.01	121.00
6	F	82	ARG	NE-CZ-NH2	-9.98	115.31	120.30
24	R	222	TYR	CB-CG-CD2	-9.95	115.03	121.00
3	C	91	ARG	NE-CZ-NH1	9.94	125.27	120.30
19	Z	554	TYR	CB-CG-CD2	9.92	126.95	121.00
20	N	54	PHE	CB-CG-CD2	-9.91	113.86	120.80
1	A	43	ARG	NE-CZ-NH2	-9.91	115.35	120.30
12	5	200	ARG	NE-CZ-NH1	9.90	125.25	120.30
19	Z	845	ARG	NE-CZ-NH1	9.88	125.24	120.30
26	O	70	ARG	NE-CZ-NH1	-9.88	115.36	120.30
19	Z	533	ASP	CB-CG-OD1	9.88	127.19	118.30
4	D	175	ARG	NE-CZ-NH1	-9.87	115.36	120.30
10	3	177	ARG	NE-CZ-NH1	9.87	125.23	120.30
14	7	170	ASP	CB-CG-OD1	-9.85	109.44	118.30
15	W	156	PHE	CB-CG-CD2	9.85	127.69	120.80
24	R	143	TYR	CB-CG-CD1	-9.85	115.09	121.00
32	J	374	ARG	NE-CZ-NH1	-9.84	115.38	120.30
24	R	295	TYR	CB-CG-CD2	-9.80	115.12	121.00
14	7	101	TYR	CB-CG-CD2	9.79	126.88	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	18	ARG	NE-CZ-NH1	-9.78	115.41	120.30
27	H	420	TYR	CB-CG-CD2	-9.77	115.14	121.00
30	L	209	PHE	CB-CG-CD2	-9.76	113.97	120.80
19	Z	175	ASP	CB-CG-OD2	9.73	127.06	118.30
32	J	23	TYR	CB-CG-CD1	9.71	126.83	121.00
11	4	59	TYR	CB-CG-CD1	-9.70	115.18	121.00
2	B	177	ARG	NE-CZ-NH1	-9.70	115.45	120.30
6	F	24	TYR	CB-CG-CD2	-9.69	115.18	121.00
31	M	367	ARG	NE-CZ-NH2	-9.68	115.46	120.30
9	2	167	TYR	CB-CG-CD2	9.68	126.81	121.00
10	3	80	ARG	NE-CZ-NH1	9.67	125.13	120.30
9	2	230	ARG	NE-CZ-NH2	9.66	125.13	120.30
30	L	124	TYR	CB-CG-CD2	9.66	126.80	121.00
32	J	340	ARG	NE-CZ-NH1	9.64	125.12	120.30
21	S	224	ARG	NE-CZ-NH1	9.63	125.12	120.30
28	I	96	ARG	NE-CZ-NH2	9.61	125.11	120.30
4	D	92	ARG	NE-CZ-NH2	-9.59	115.50	120.30
32	J	117	ARG	NE-CZ-NH2	-9.55	115.52	120.30
19	Z	400	TYR	CB-CG-CD2	-9.55	115.27	121.00
25	U	245	PHE	CB-CG-CD1	-9.55	114.12	120.80
27	H	400	ARG	NE-CZ-NH1	9.54	125.07	120.30
19	Z	496	ASP	CB-CG-OD1	-9.53	109.72	118.30
32	J	383	PHE	CB-CG-CD1	-9.46	114.18	120.80
1	A	178	PHE	CB-CG-CD2	-9.46	114.18	120.80
6	F	145	PHE	CB-CG-CD2	-9.46	114.18	120.80
14	7	228	TYR	CG-CD1-CE1	-9.45	113.74	121.30
27	H	105	ASP	CB-CG-OD2	-9.46	109.79	118.30
30	L	93	TYR	CB-CG-CD1	-9.44	115.34	121.00
20	N	492	ASP	CB-CG-OD1	-9.43	109.82	118.30
10	3	85	TYR	CB-CG-CD1	9.42	126.65	121.00
21	S	170	PHE	CB-CG-CD1	-9.42	114.20	120.80
20	N	590	TYR	CD1-CE1-CZ	9.42	128.28	119.80
21	S	492	PHE	CB-CG-CD1	-9.41	114.21	120.80
14	7	222	TYR	CB-CG-CD2	-9.40	115.36	121.00
19	Z	469	TYR	CB-CG-CD2	-9.35	115.39	121.00
2	B	60	ARG	NE-CZ-NH1	-9.34	115.63	120.30
29	K	81	ARG	NE-CZ-NH2	-9.34	115.63	120.30
17	T	340	ARG	NE-CZ-NH1	9.33	124.97	120.30
1	A	93	ARG	NE-CZ-NH1	-9.32	115.64	120.30
24	R	225	TYR	CB-CG-CD1	9.32	126.59	121.00
32	J	121	TYR	N-CA-CB	9.32	127.38	110.60
3	C	179	TYR	CB-CG-CD2	-9.31	115.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	200	ASP	CB-CG-OD1	-9.31	109.92	118.30
21	S	252	ARG	NE-CZ-NH1	9.28	124.94	120.30
6	F	97	PHE	CB-CG-CD1	9.27	127.29	120.80
32	J	49	ARG	NE-CZ-NH2	-9.27	115.66	120.30
30	L	311	ARG	NE-CZ-NH1	9.26	124.93	120.30
31	M	357	PHE	CB-CG-CD2	-9.26	114.32	120.80
14	7	223	ARG	NE-CZ-NH2	-9.26	115.67	120.30
29	K	188	PHE	CB-CG-CD2	-9.25	114.32	120.80
20	N	601	ARG	NE-CZ-NH2	-9.22	115.69	120.30
21	S	162	TYR	CB-CG-CD1	-9.22	115.47	121.00
17	T	319	TYR	CB-CG-CD2	9.21	126.53	121.00
5	E	97	GLN	CB-CG-CD	9.21	135.55	111.60
30	L	342	TYR	CB-CG-CD2	-9.21	115.47	121.00
21	S	303	ARG	NE-CZ-NH1	-9.20	115.70	120.30
20	N	950	TYR	CB-CG-CD2	9.18	126.51	121.00
24	R	292	TYR	CB-CG-CD1	9.17	126.50	121.00
1	A	43	ARG	NE-CZ-NH1	9.16	124.88	120.30
12	5	116	ARG	NE-CZ-NH1	9.16	124.88	120.30
27	H	355	PHE	CB-CG-CD1	-9.16	114.39	120.80
5	E	93	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	A	227	PHE	CB-CG-CD2	-9.14	114.40	120.80
19	Z	304	PHE	CB-CG-CD1	9.14	127.20	120.80
29	K	188	PHE	CB-CG-CD1	9.11	127.18	120.80
17	T	262	PHE	CB-CG-CD2	-9.09	114.44	120.80
19	Z	620	PHE	CB-CG-CD2	9.09	127.16	120.80
20	N	444	TYR	CB-CG-CD1	9.09	126.45	121.00
21	S	88	ARG	NE-CZ-NH1	-9.09	115.76	120.30
24	R	179	ARG	NE-CZ-NH1	9.08	124.84	120.30
26	O	184	ASP	CB-CG-OD2	-9.08	110.13	118.30
10	3	104	TYR	CB-CG-CD2	-9.07	115.56	121.00
31	M	357	PHE	CB-CG-CD1	9.05	127.14	120.80
20	N	556	MET	CG-SD-CE	-9.05	85.72	100.20
9	2	157	TYR	CG-CD1-CE1	-9.04	114.06	121.30
14	7	226	ARG	CD-NE-CZ	9.04	136.25	123.60
20	N	502	TYR	CB-CG-CD2	-9.04	115.58	121.00
23	Q	232	PHE	CB-CG-CD2	-9.03	114.48	120.80
26	O	154	ARG	NE-CZ-NH1	9.02	124.81	120.30
8	1	176	TYR	CB-CG-CD1	-9.02	115.59	121.00
19	Z	358	PHE	CB-CG-CD1	-8.95	114.53	120.80
11	4	155	ARG	NE-CZ-NH1	8.95	124.77	120.30
21	S	208	TYR	CB-CG-CD1	-8.94	115.63	121.00
15	W	91	ARG	NE-CZ-NH2	8.94	124.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	143	TYR	CB-CG-CD2	8.93	126.36	121.00
10	3	123	SER	N-CA-CB	8.91	123.87	110.50
22	P	370	TYR	CB-CG-CD1	-8.91	115.65	121.00
2	B	60	ARG	NE-CZ-NH2	-8.90	115.85	120.30
19	Z	746	ARG	NE-CZ-NH1	-8.90	115.85	120.30
12	5	202	TYR	CB-CG-CD1	8.89	126.33	121.00
32	J	21	ARG	NE-CZ-NH1	8.87	124.73	120.30
21	S	344	PHE	CB-CG-CD2	8.86	127.00	120.80
15	W	100	ARG	NE-CZ-NH1	-8.85	115.87	120.30
18	Y	57	ARG	NE-CZ-NH1	8.85	124.72	120.30
20	N	559	ARG	NE-CZ-NH2	-8.84	115.88	120.30
32	J	57	ARG	NE-CZ-NH1	8.84	124.72	120.30
19	Z	376	PHE	CB-CG-CD1	8.83	126.98	120.80
32	J	72	TYR	CB-CG-CD1	-8.82	115.71	121.00
9	2	181	PHE	CB-CG-CD2	8.81	126.97	120.80
21	S	298	TYR	CB-CG-CD1	-8.80	115.72	121.00
11	4	73	TYR	CB-CG-CD1	-8.79	115.72	121.00
27	H	97	ARG	NE-CZ-NH2	8.79	124.70	120.30
3	C	101	TYR	CB-CG-CD1	8.79	126.28	121.00
10	3	27	ARG	NE-CZ-NH2	-8.78	115.91	120.30
22	P	144	ARG	NE-CZ-NH1	-8.77	115.92	120.30
9	2	62	ARG	NE-CZ-NH2	-8.77	115.92	120.30
26	O	111	VAL	CA-CB-CG1	8.77	124.05	110.90
2	B	6	TYR	CG-CD2-CE2	-8.76	114.30	121.30
12	5	128	ARG	NE-CZ-NH1	8.75	124.67	120.30
20	N	678	ASP	CB-CG-OD2	8.75	126.17	118.30
9	2	241	ARG	NE-CZ-NH2	-8.74	115.93	120.30
14	7	79	ARG	NE-CZ-NH1	8.73	124.67	120.30
19	Z	456	ARG	NE-CZ-NH1	-8.73	115.93	120.30
25	U	250	TYR	CB-CG-CD1	8.73	126.24	121.00
28	I	268	ARG	NE-CZ-NH1	8.71	124.66	120.30
28	I	71	TYR	CB-CG-CD1	-8.71	115.78	121.00
31	M	171	TYR	CB-CG-CD2	8.70	126.22	121.00
31	M	64	ARG	NE-CZ-NH2	-8.70	115.95	120.30
9	2	136	TYR	CB-CG-CD1	8.69	126.22	121.00
28	I	371	ARG	NE-CZ-NH1	8.69	124.64	120.30
14	7	143	ARG	NE-CZ-NH2	8.67	124.63	120.30
23	Q	76	PHE	CB-CG-CD1	8.67	126.87	120.80
21	S	412	ARG	NE-CZ-NH2	-8.66	115.97	120.30
29	K	178	ARG	NE-CZ-NH2	-8.66	115.97	120.30
19	Z	300	ARG	NE-CZ-NH1	8.65	124.63	120.30
19	Z	296	PHE	CB-CG-CD2	-8.64	114.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	I	67	ARG	NE-CZ-NH1	8.60	124.60	120.30
29	K	53	PHE	CB-CG-CD2	-8.60	114.78	120.80
30	L	111	ARG	NE-CZ-NH2	-8.60	116.00	120.30
3	C	179	TYR	CB-CG-CD1	8.57	126.14	121.00
19	Z	314	TYR	CB-CG-CD1	8.57	126.14	121.00
21	S	116	PHE	CB-CG-CD2	8.57	126.80	120.80
7	G	8	TYR	CB-CG-CD2	8.53	126.12	121.00
24	R	18	ARG	NE-CZ-NH2	8.53	124.57	120.30
8	1	149	MET	CG-SD-CE	-8.53	86.56	100.20
9	2	132	ARG	NE-CZ-NH1	8.52	124.56	120.30
22	P	350	ARG	NE-CZ-NH2	-8.52	116.04	120.30
24	R	257	ARG	NE-CZ-NH2	-8.52	116.04	120.30
16	V	68	ARG	NE-CZ-NH1	8.51	124.56	120.30
2	B	76	TYR	CB-CG-CD2	-8.51	115.90	121.00
14	7	121	PHE	CB-CG-CD1	8.51	126.75	120.80
13	6	162	PHE	CB-CG-CD2	8.50	126.75	120.80
9	2	71	ASP	CB-CG-OD2	-8.49	110.66	118.30
28	I	59	ARG	NE-CZ-NH2	-8.49	116.06	120.30
30	L	367	PHE	CB-CG-CD1	8.45	126.72	120.80
17	T	318	TYR	CB-CG-CD1	8.45	126.07	121.00
27	H	234	ASP	CB-CG-OD2	-8.44	110.70	118.30
12	5	205	ASP	CB-CG-OD2	-8.44	110.70	118.30
10	3	96	TYR	CB-CG-CD1	8.43	126.06	121.00
19	Z	226	TYR	CB-CG-CD2	8.43	126.06	121.00
22	P	302	TYR	CB-CG-CD1	8.43	126.06	121.00
2	B	91	ARG	NE-CZ-NH1	8.42	124.51	120.30
26	O	240	PHE	CB-CG-CD2	-8.42	114.91	120.80
19	Z	103	TYR	CB-CG-CD1	8.40	126.04	121.00
24	R	366	TYR	CB-CG-CD1	8.39	126.04	121.00
6	F	97	PHE	CB-CG-CD2	-8.39	114.93	120.80
13	6	71	TYR	CG-CD2-CE2	8.39	128.01	121.30
2	B	173	PHE	CB-CG-CD1	8.38	126.67	120.80
19	Z	376	PHE	CB-CG-CD2	-8.38	114.93	120.80
24	R	204	THR	CA-CB-CG2	-8.38	100.67	112.40
17	T	217	ARG	NE-CZ-NH2	-8.37	116.12	120.30
20	N	426	TYR	CB-CG-CD2	8.37	126.02	121.00
13	6	60	PHE	CB-CG-CD2	-8.37	114.94	120.80
9	2	232	TYR	CB-CG-CD1	8.36	126.01	121.00
10	3	198	ARG	NE-CZ-NH1	8.35	124.47	120.30
2	B	173	PHE	CB-CG-CD2	-8.34	114.96	120.80
22	P	364	ARG	NE-CZ-NH1	8.33	124.47	120.30
13	6	127	ARG	NE-CZ-NH2	-8.31	116.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	314	ARG	NE-CZ-NH2	8.30	124.45	120.30
14	7	58	VAL	CG1-CB-CG2	8.29	124.17	110.90
2	B	60	ARG	NH1-CZ-NH2	8.29	128.52	119.40
24	R	366	TYR	CB-CG-CD2	-8.29	116.03	121.00
11	4	171	PHE	CB-CG-CD2	-8.29	115.00	120.80
21	S	283	ARG	NE-CZ-NH1	8.28	124.44	120.30
1	A	105	TYR	CB-CG-CD1	-8.27	116.04	121.00
20	N	253	TYR	CB-CG-CD2	-8.27	116.04	121.00
23	Q	397	TYR	CG-CD2-CE2	-8.27	114.69	121.30
9	2	172	SER	N-CA-CB	8.27	122.90	110.50
1	A	187	PHE	CB-CG-CD2	-8.25	115.02	120.80
27	H	274	PHE	CB-CG-CD1	-8.25	115.02	120.80
20	N	206	MET	CG-SD-CE	8.25	113.40	100.20
26	O	371	ALA	N-CA-CB	8.25	121.65	110.10
24	R	67	MET	CG-SD-CE	-8.24	87.01	100.20
26	O	262	ALA	CB-CA-C	-8.24	97.74	110.10
6	F	193	ARG	NE-CZ-NH2	8.24	124.42	120.30
22	P	129	ARG	NE-CZ-NH1	8.23	124.42	120.30
30	L	295	ARG	NE-CZ-NH2	-8.22	116.19	120.30
32	J	148	TYR	CB-CG-CD1	8.22	125.93	121.00
14	7	221	TYR	CB-CG-CD2	-8.18	116.09	121.00
12	5	132	ARG	NE-CZ-NH2	-8.18	116.21	120.30
2	B	84	ARG	NE-CZ-NH2	-8.17	116.21	120.30
22	P	123	ARG	NE-CZ-NH2	8.17	124.39	120.30
7	G	126	TYR	CB-CG-CD2	-8.17	116.10	121.00
23	Q	143	TYR	CB-CG-CD2	-8.17	116.10	121.00
26	O	127	ASP	CB-CG-OD1	-8.17	110.95	118.30
19	Z	296	PHE	CB-CG-CD1	8.16	126.51	120.80
21	S	126	PHE	CB-CG-CD1	8.16	126.51	120.80
21	S	344	PHE	CB-CG-CD1	-8.15	115.09	120.80
11	4	73	TYR	CB-CG-CD2	8.15	125.89	121.00
21	S	492	PHE	CB-CG-CD2	8.15	126.50	120.80
4	D	159	TYR	CB-CG-CD2	-8.14	116.12	121.00
11	4	137	PHE	CB-CG-CD1	8.14	126.50	120.80
24	R	177	ARG	NE-CZ-NH1	8.12	124.36	120.30
23	Q	229	TYR	CB-CG-CD2	-8.12	116.13	121.00
6	F	145	PHE	CB-CG-CD1	8.12	126.48	120.80
9	2	115	ARG	NE-CZ-NH1	8.12	124.36	120.30
30	L	209	PHE	CB-CG-CD1	8.12	126.48	120.80
20	N	769	PHE	CB-CG-CD1	-8.11	115.12	120.80
24	R	300	ARG	NE-CZ-NH1	8.11	124.36	120.30
31	M	106	ASP	CB-CG-OD2	8.10	125.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	828	ARG	NE-CZ-NH1	8.10	124.35	120.30
28	I	303	ARG	NE-CZ-NH1	8.10	124.35	120.30
12	5	78	ARG	NE-CZ-NH2	-8.09	116.25	120.30
29	K	120	ASP	CB-CG-OD1	-8.08	111.03	118.30
30	L	367	PHE	CB-CG-CD2	-8.08	115.14	120.80
22	P	190	MET	CG-SD-CE	-8.07	87.28	100.20
30	L	255	ARG	NE-CZ-NH1	8.06	124.33	120.30
24	R	323	PHE	CB-CG-CD1	8.05	126.44	120.80
29	K	43	ARG	NE-CZ-NH2	-8.05	116.27	120.30
19	Z	332	ALA	N-CA-CB	8.05	121.37	110.10
9	2	157	TYR	CB-CG-CD1	-8.04	116.18	121.00
20	N	55	ARG	NE-CZ-NH2	-8.04	116.28	120.30
30	L	265	ARG	NE-CZ-NH2	8.03	124.32	120.30
32	J	72	TYR	CB-CG-CD2	8.03	125.82	121.00
24	R	142	PHE	CB-CG-CD2	-8.03	115.18	120.80
4	D	110	VAL	CG1-CB-CG2	-8.02	98.06	110.90
21	S	197	ARG	NE-CZ-NH2	8.02	124.31	120.30
26	O	339	ARG	NE-CZ-NH2	-8.02	116.29	120.30
31	M	159	ASP	CB-CG-OD1	-8.02	111.08	118.30
32	J	122	THR	CA-CB-CG2	-8.02	101.17	112.40
13	6	206	PHE	CB-CG-CD2	-8.01	115.19	120.80
26	O	24	ARG	NE-CZ-NH2	-8.01	116.30	120.30
20	N	144	ASP	CB-CG-OD1	-7.99	111.11	118.30
30	L	376	VAL	CA-CB-CG1	7.99	122.89	110.90
21	S	356	TYR	CB-CG-CD2	7.99	125.79	121.00
31	M	389	ARG	NE-CZ-NH2	-7.99	116.31	120.30
22	P	75	TYR	CB-CG-CD2	-7.99	116.21	121.00
14	7	141	TYR	CB-CG-CD1	-7.98	116.21	121.00
3	C	19	TYR	CG-CD1-CE1	-7.98	114.92	121.30
11	4	116	TYR	CB-CG-CD2	-7.97	116.22	121.00
19	Z	620	PHE	CB-CG-CD1	-7.96	115.23	120.80
30	L	26	TYR	CB-CG-CD2	-7.96	116.22	121.00
19	Z	400	TYR	CB-CG-CD1	7.96	125.78	121.00
4	D	10	PHE	CB-CG-CD1	7.96	126.37	120.80
27	H	307	ASP	CB-CG-OD2	-7.96	111.14	118.30
23	Q	397	TYR	CB-CG-CD1	-7.96	116.23	121.00
23	Q	72	TYR	CG-CD1-CE1	-7.95	114.94	121.30
3	C	49	ARG	NE-CZ-NH1	7.95	124.27	120.30
31	M	72	MET	CG-SD-CE	-7.95	87.49	100.20
24	R	222	TYR	CB-CG-CD1	7.94	125.76	121.00
3	C	101	TYR	CB-CG-CD2	-7.93	116.25	121.00
25	U	64	ASP	CB-CG-OD2	7.93	125.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	H	369	ARG	NE-CZ-NH1	-7.93	116.34	120.30
28	I	410	ARG	NE-CZ-NH2	-7.93	116.34	120.30
27	H	284	ARG	NE-CZ-NH2	-7.92	116.34	120.30
27	H	338	ASP	CB-CG-OD2	-7.91	111.18	118.30
27	H	41	TYR	CB-CG-CD1	-7.90	116.26	121.00
30	L	269	ARG	NE-CZ-NH2	7.89	124.24	120.30
32	J	72	TYR	CD1-CE1-CZ	7.88	126.89	119.80
22	P	302	TYR	CB-CG-CD2	-7.87	116.28	121.00
19	Z	158	TYR	CB-CG-CD2	-7.87	116.28	121.00
7	G	14	THR	CA-CB-CG2	-7.87	101.39	112.40
12	5	224	TYR	CB-CG-CD1	-7.87	116.28	121.00
13	6	221	ARG	NE-CZ-NH1	7.86	124.23	120.30
26	O	155	PHE	CB-CG-CD1	-7.86	115.30	120.80
29	K	285	VAL	CA-CB-CG2	-7.86	99.12	110.90
8	1	173	ASP	CB-CG-OD1	-7.85	111.24	118.30
20	N	875	PHE	CB-CG-CD1	7.84	126.29	120.80
21	S	103	ARG	NE-CZ-NH2	7.84	124.22	120.30
22	P	344	THR	CA-CB-CG2	-7.84	101.43	112.40
20	N	395	ARG	NE-CZ-NH2	-7.83	116.39	120.30
13	6	34	PHE	CB-CG-CD2	7.82	126.27	120.80
14	7	258	MET	CA-CB-CG	7.80	126.57	113.30
23	Q	298	SER	N-CA-CB	7.80	122.20	110.50
12	5	236	TYR	CB-CG-CD2	-7.80	116.32	121.00
30	L	375	PHE	CB-CG-CD1	-7.80	115.34	120.80
24	R	360	ASP	CB-CG-OD1	7.79	125.31	118.30
13	6	215	TYR	CB-CG-CD1	7.79	125.67	121.00
28	I	259	TYR	CB-CG-CD2	-7.78	116.33	121.00
27	H	171	ASP	CB-CG-OD1	7.77	125.30	118.30
1	A	210	PHE	CB-CG-CD1	-7.77	115.36	120.80
16	V	118	PHE	CB-CG-CD2	-7.76	115.37	120.80
20	N	950	TYR	CB-CG-CD1	-7.76	116.34	121.00
22	P	93	ARG	NE-CZ-NH1	7.74	124.17	120.30
21	S	475	ARG	NE-CZ-NH2	-7.73	116.43	120.30
22	P	219	THR	CA-CB-CG2	-7.73	101.58	112.40
25	U	62	ASP	CB-CG-OD1	7.72	125.25	118.30
22	P	191	ARG	NE-CZ-NH1	7.72	124.16	120.30
28	I	71	TYR	CG-CD2-CE2	-7.72	115.13	121.30
16	V	201	TYR	CB-CG-CD1	7.72	125.63	121.00
14	7	101	TYR	CB-CG-CD1	-7.71	116.38	121.00
29	K	235	PHE	CB-CG-CD2	-7.70	115.41	120.80
25	U	245	PHE	CG-CD2-CE2	-7.69	112.34	120.80
20	N	615	ARG	NE-CZ-NH1	7.69	124.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	68	PHE	CB-CG-CD1	7.68	126.17	120.80
20	N	426	TYR	CB-CG-CD1	-7.68	116.39	121.00
22	P	185	PHE	CG-CD2-CE2	-7.68	112.36	120.80
8	1	177	ARG	NE-CZ-NH1	7.68	124.14	120.30
19	Z	439	TYR	CB-CG-CD1	-7.67	116.40	121.00
19	Z	645	ASP	CB-CG-OD1	-7.67	111.40	118.30
25	U	211	TYR	CB-CG-CD1	-7.67	116.40	121.00
4	D	131	ARG	NE-CZ-NH1	7.67	124.13	120.30
20	N	199	ARG	NE-CZ-NH1	7.67	124.13	120.30
17	T	264	ASP	CB-CG-OD2	-7.66	111.41	118.30
32	J	229	ARG	NE-CZ-NH1	7.64	124.12	120.30
19	Z	222	ASP	CB-CG-OD1	7.64	125.17	118.30
11	4	137	PHE	CB-CG-CD2	-7.63	115.46	120.80
24	R	267	ARG	NE-CZ-NH2	-7.63	116.48	120.30
25	U	95	TYR	CB-CG-CD1	-7.63	116.42	121.00
28	I	419	PHE	CB-CG-CD1	7.62	126.14	120.80
16	V	262	GLU	N-CA-CB	7.62	124.31	110.60
17	T	181	TYR	CB-CG-CD2	-7.59	116.44	121.00
22	P	427	ASP	CB-CG-OD1	-7.58	111.48	118.30
12	5	149	TYR	CB-CG-CD1	-7.58	116.45	121.00
14	7	147	MET	CG-SD-CE	-7.57	88.08	100.20
26	O	7	PHE	CB-CG-CD1	7.57	126.10	120.80
1	A	210	PHE	CB-CG-CD2	7.56	126.09	120.80
3	C	4	ARG	NE-CZ-NH1	7.56	124.08	120.30
7	G	89	ALA	N-CA-CB	7.56	120.68	110.10
17	T	107	ARG	NE-CZ-NH2	-7.55	116.52	120.30
20	N	583	MET	CG-SD-CE	-7.55	88.13	100.20
1	A	125	TYR	CB-CG-CD2	7.54	125.53	121.00
12	5	245	ARG	NE-CZ-NH2	-7.54	116.53	120.30
20	N	51	ASP	CB-CG-OD2	-7.53	111.52	118.30
22	P	370	TYR	CB-CG-CD2	7.53	125.52	121.00
25	U	81	MET	CA-CB-CG	7.53	126.10	113.30
31	M	182	GLU	N-CA-CB	7.53	124.16	110.60
3	C	139	TRP	CH2-CZ2-CE2	7.52	124.92	117.40
19	Z	175	ASP	N-CA-CB	7.52	124.14	110.60
12	5	149	TYR	CB-CG-CD2	7.52	125.51	121.00
2	B	156	PHE	CB-CG-CD2	-7.52	115.54	120.80
30	L	311	ARG	NE-CZ-NH2	-7.52	116.54	120.30
16	V	32	TYR	CB-CG-CD2	7.51	125.51	121.00
31	M	352	ASP	CB-CG-OD2	-7.51	111.54	118.30
26	O	24	ARG	NE-CZ-NH1	7.51	124.06	120.30
26	O	85	ARG	NE-CZ-NH1	7.51	124.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	O	373	ASP	CB-CG-OD2	-7.50	111.55	118.30
17	T	190	TYR	CG-CD2-CE2	-7.50	115.30	121.30
19	Z	142	TYR	CG-CD1-CE1	-7.49	115.31	121.30
11	4	171	PHE	CB-CG-CD1	7.49	126.04	120.80
20	N	615	ARG	NE-CZ-NH2	-7.49	116.56	120.30
7	G	141	TYR	CZ-CE2-CD2	-7.49	113.06	119.80
29	K	283	ARG	NE-CZ-NH1	7.49	124.04	120.30
27	H	339	ARG	NE-CZ-NH1	7.48	124.04	120.30
15	W	25	ARG	NE-CZ-NH2	-7.48	116.56	120.30
6	F	126	ARG	NE-CZ-NH2	7.47	124.03	120.30
11	4	131	ALA	N-CA-CB	7.47	120.56	110.10
2	B	163	MET	CG-SD-CE	-7.46	88.27	100.20
19	Z	533	ASP	CB-CG-OD2	-7.45	111.59	118.30
31	M	353	ARG	NE-CZ-NH2	7.45	124.03	120.30
28	I	307	ARG	NE-CZ-NH1	-7.45	116.58	120.30
22	P	174	TYR	CG-CD2-CE2	-7.45	115.34	121.30
3	C	17	ARG	NE-CZ-NH1	-7.44	116.58	120.30
28	I	272	ARG	NE-CZ-NH1	7.44	124.02	120.30
27	H	138	MET	CG-SD-CE	-7.44	88.30	100.20
28	I	267	VAL	CA-CB-CG2	-7.43	99.75	110.90
14	7	226	ARG	NE-CZ-NH1	7.43	124.01	120.30
4	D	3	TYR	CB-CG-CD2	-7.42	116.55	121.00
9	2	230	ARG	NE-CZ-NH1	-7.42	116.59	120.30
4	D	39	ASP	CB-CG-OD2	7.42	124.97	118.30
6	F	137	TYR	CB-CG-CD2	7.41	125.44	121.00
12	5	171	TYR	CG-CD1-CE1	-7.40	115.38	121.30
32	J	189	TYR	CB-CG-CD2	-7.40	116.56	121.00
20	N	644	TYR	CB-CG-CD1	-7.40	116.56	121.00
24	R	225	TYR	CB-CG-CD2	-7.40	116.56	121.00
26	O	162	TYR	CB-CG-CD2	-7.39	116.56	121.00
27	H	147	TYR	CG-CD2-CE2	-7.38	115.39	121.30
25	U	250	TYR	CB-CG-CD2	-7.38	116.57	121.00
24	R	289	ALA	CB-CA-C	-7.37	99.04	110.10
4	D	38	ARG	NE-CZ-NH1	-7.37	116.62	120.30
29	K	200	ARG	NE-CZ-NH2	-7.36	116.62	120.30
4	D	47	LYS	N-CA-CB	7.36	123.84	110.60
29	K	60	TYR	CG-CD1-CE1	-7.36	115.42	121.30
5	E	143	PHE	CB-CG-CD2	-7.35	115.66	120.80
27	H	139	ARG	NE-CZ-NH2	-7.35	116.63	120.30
31	M	312	THR	CA-CB-OG1	7.35	124.44	109.00
3	C	50	ARG	NE-CZ-NH2	-7.35	116.63	120.30
19	Z	304	PHE	CB-CG-CD2	-7.34	115.66	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	187	ARG	CD-NE-CZ	7.34	133.88	123.60
3	C	61	PHE	CB-CG-CD2	7.32	125.93	120.80
3	C	96	ARG	NE-CZ-NH1	7.32	123.96	120.30
15	W	108	ARG	NE-CZ-NH1	7.32	123.96	120.30
20	N	383	ASP	CB-CG-OD1	7.32	124.89	118.30
4	D	73	PHE	CB-CG-CD2	7.32	125.92	120.80
20	N	494	TYR	CB-CG-CD2	7.31	125.39	121.00
19	Z	295	ALA	CB-CA-C	-7.31	99.13	110.10
20	N	383	ASP	CB-CG-OD2	-7.30	111.73	118.30
24	R	259	TYR	CB-CG-CD1	-7.30	116.62	121.00
25	U	155	PHE	CB-CG-CD1	7.30	125.91	120.80
13	6	147	ALA	N-CA-CB	7.30	120.31	110.10
24	R	264	TYR	CB-CG-CD2	-7.29	116.62	121.00
23	Q	337	ARG	NE-CZ-NH1	7.28	123.94	120.30
26	O	84	VAL	CA-CB-CG2	-7.28	99.98	110.90
29	K	391	ARG	NE-CZ-NH1	7.28	123.94	120.30
3	C	116	ASP	CB-CG-OD1	-7.28	111.75	118.30
15	W	17	ARG	NE-CZ-NH2	-7.28	116.66	120.30
13	6	191	VAL	CG1-CB-CG2	7.26	122.52	110.90
31	M	415	ALA	N-CA-CB	7.26	120.27	110.10
32	J	313	ARG	NE-CZ-NH2	-7.26	116.67	120.30
28	I	408	ARG	NE-CZ-NH2	-7.26	116.67	120.30
30	L	201	VAL	CA-CB-CG1	7.26	121.79	110.90
8	1	155	ARG	NE-CZ-NH1	7.26	123.93	120.30
11	4	70	ARG	NE-CZ-NH2	-7.25	116.67	120.30
24	R	23	ARG	NE-CZ-NH1	7.25	123.92	120.30
12	5	105	ALA	N-CA-CB	7.25	120.24	110.10
31	M	188	TYR	CB-CG-CD1	-7.25	116.65	121.00
10	3	177	ARG	NE-CZ-NH2	-7.24	116.68	120.30
29	K	391	ARG	NE-CZ-NH2	-7.24	116.68	120.30
11	4	116	TYR	CB-CG-CD1	7.23	125.34	121.00
30	L	54	TYR	CB-CG-CD1	7.23	125.34	121.00
10	3	4	MET	CG-SD-CE	-7.22	88.65	100.20
24	R	183	TYR	CB-CG-CD2	-7.22	116.67	121.00
24	R	219	PHE	CB-CG-CD2	-7.22	115.75	120.80
30	L	327	LEU	CB-CG-CD1	7.22	123.27	111.00
32	J	107	ASP	CB-CG-OD1	-7.22	111.80	118.30
20	N	655	ALA	CB-CA-C	-7.21	99.28	110.10
30	L	257	PHE	CB-CG-CD2	-7.21	115.75	120.80
29	K	268	ASP	CB-CG-OD1	-7.20	111.82	118.30
13	6	133	VAL	CG1-CB-CG2	7.20	122.42	110.90
6	F	140	MET	CG-SD-CE	7.19	111.71	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	20	TYR	CB-CG-CD2	-7.19	116.69	121.00
20	N	531	ASP	N-CA-CB	7.19	123.53	110.60
12	5	65	PHE	CB-CG-CD1	7.18	125.83	120.80
19	Z	262	PHE	CB-CG-CD2	-7.18	115.77	120.80
30	L	323	ARG	NE-CZ-NH2	7.18	123.89	120.30
31	M	101	ASP	CB-CG-OD1	-7.18	111.84	118.30
20	N	900	TYR	CB-CG-CD2	-7.17	116.70	121.00
27	H	171	ASP	CB-CG-OD2	-7.17	111.84	118.30
32	J	325	ARG	NE-CZ-NH2	-7.17	116.71	120.30
12	5	202	TYR	CB-CG-CD2	-7.17	116.70	121.00
21	S	209	TYR	CB-CG-CD1	-7.17	116.70	121.00
17	T	148	ARG	NE-CZ-NH1	7.17	123.88	120.30
19	Z	100	ARG	NE-CZ-NH2	-7.17	116.72	120.30
20	N	402	PHE	CZ-CE2-CD2	-7.17	111.50	120.10
7	G	206	LYS	CB-CA-C	-7.17	96.07	110.40
16	V	198	ARG	NE-CZ-NH2	7.16	123.88	120.30
1	A	155	ASP	CB-CG-OD2	7.16	124.74	118.30
19	Z	83	ARG	NE-CZ-NH2	7.16	123.88	120.30
31	M	307	ARG	NE-CZ-NH1	7.16	123.88	120.30
26	O	70	ARG	NE-CZ-NH2	-7.16	116.72	120.30
23	Q	282	ARG	NE-CZ-NH1	-7.16	116.72	120.30
21	S	345	ARG	NH1-CZ-NH2	-7.15	111.54	119.40
20	N	68	PHE	CB-CG-CD2	-7.14	115.80	120.80
5	E	71	ASP	CB-CG-OD2	7.14	124.72	118.30
11	4	133	GLY	N-CA-C	-7.14	95.26	113.10
21	S	151	ALA	N-CA-CB	7.13	120.08	110.10
15	W	119	ASP	CB-CG-OD2	-7.12	111.89	118.30
32	J	200	ALA	N-CA-CB	7.12	120.07	110.10
20	N	900	TYR	CG-CD1-CE1	-7.12	115.60	121.30
11	4	67	TYR	CB-CG-CD2	-7.11	116.73	121.00
3	C	19	TYR	CB-CG-CD1	-7.11	116.74	121.00
20	N	460	TYR	CB-CG-CD2	-7.09	116.75	121.00
19	Z	368	ALA	N-CA-CB	7.08	120.02	110.10
6	F	137	TYR	CB-CG-CD1	-7.08	116.75	121.00
24	R	194	PHE	CB-CG-CD2	-7.07	115.85	120.80
31	M	394	PHE	CZ-CE2-CD2	-7.07	111.62	120.10
1	A	245	ARG	NE-CZ-NH1	-7.06	116.77	120.30
21	S	141	LEU	CB-CG-CD1	7.06	123.01	111.00
9	2	157	TYR	CD1-CG-CD2	7.06	125.66	117.90
1	A	105	TYR	CB-CG-CD2	7.05	125.23	121.00
29	K	44	TYR	CB-CG-CD2	-7.05	116.77	121.00
21	S	209	TYR	CD1-CE1-CZ	7.05	126.14	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	13	PHE	CB-CG-CD1	7.04	125.73	120.80
19	Z	535	THR	CA-CB-CG2	-7.04	102.54	112.40
26	O	70	ARG	NH1-CZ-NH2	7.04	127.14	119.40
16	V	214	GLN	CA-CB-CG	-7.04	97.91	113.40
8	1	37	MET	N-CA-CB	7.04	123.27	110.60
11	4	23	SER	N-CA-CB	7.04	121.06	110.50
5	E	116	VAL	CA-CB-CG2	-7.04	100.34	110.90
9	2	185	PHE	CB-CG-CD1	-7.03	115.88	120.80
23	Q	308	ASP	CB-CG-OD1	7.03	124.63	118.30
17	T	170	TYR	CB-CG-CD1	-7.03	116.78	121.00
20	N	546	ARG	NE-CZ-NH1	7.02	123.81	120.30
10	3	53	LEU	N-CA-CB	7.02	124.45	110.40
17	T	238	TYR	CB-CG-CD2	7.02	125.21	121.00
19	Z	113	MET	CG-SD-CE	-7.01	88.99	100.20
29	K	417	TYR	CB-CG-CD2	-7.01	116.80	121.00
25	U	155	PHE	CB-CG-CD2	-7.00	115.90	120.80
32	J	43	ARG	NE-CZ-NH1	7.00	123.80	120.30
27	H	366	ARG	NE-CZ-NH2	-7.00	116.80	120.30
10	3	51	ILE	CA-CB-CG1	7.00	124.29	111.00
13	6	160	ASP	CB-CG-OD1	6.99	124.59	118.30
24	R	379	ARG	NE-CZ-NH1	6.98	123.79	120.30
31	M	86	ASN	CB-CG-OD1	-6.97	107.65	121.60
13	6	29	PHE	N-CA-CB	6.97	123.15	110.60
3	C	66	TYR	CB-CG-CD2	-6.97	116.82	121.00
24	R	342	ARG	NE-CZ-NH2	-6.97	116.81	120.30
27	H	108	ASP	CB-CG-OD2	-6.96	112.03	118.30
26	O	157	ASP	CB-CG-OD2	6.96	124.56	118.30
13	6	132	TYR	CB-CG-CD1	-6.96	116.83	121.00
4	D	142	PHE	CB-CG-CD1	6.96	125.67	120.80
28	I	365	PHE	CB-CG-CD1	6.96	125.67	120.80
19	Z	294	MET	CG-SD-CE	-6.95	89.08	100.20
30	L	289	MET	CG-SD-CE	-6.95	89.08	100.20
32	J	132	ASP	CB-CG-OD2	6.95	124.55	118.30
30	L	127	ARG	NE-CZ-NH2	6.95	123.77	120.30
22	P	289	ARG	NE-CZ-NH1	-6.94	116.83	120.30
27	H	423	PHE	CB-CG-CD1	-6.94	115.94	120.80
26	O	238	TYR	CZ-CE2-CD2	-6.94	113.55	119.80
15	W	177	PRO	N-CA-CB	6.94	111.63	103.30
22	P	119	PRO	N-CD-CG	6.93	113.60	103.20
13	6	197	ARG	NE-CZ-NH2	-6.92	116.84	120.30
20	N	783	TYR	CB-CG-CD1	6.92	125.15	121.00
10	3	99	ARG	NE-CZ-NH1	6.92	123.76	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	232	TYR	CD1-CE1-CZ	6.91	126.02	119.80
21	S	162	TYR	CB-CG-CD2	6.90	125.14	121.00
25	U	49	ASP	CB-CG-OD2	-6.90	112.09	118.30
11	4	46	CYS	N-CA-CB	6.89	123.00	110.60
24	R	358	ARG	NE-CZ-NH1	6.88	123.74	120.30
3	C	97	TYR	CG-CD1-CE1	-6.87	115.80	121.30
6	F	185	ASP	CB-CG-OD2	-6.87	112.12	118.30
20	N	601	ARG	NE-CZ-NH1	6.87	123.74	120.30
27	H	275	ASP	CB-CG-OD1	6.86	124.47	118.30
14	7	231	PHE	CB-CG-CD2	6.86	125.60	120.80
32	J	395	SER	N-CA-CB	6.85	120.78	110.50
29	K	118	THR	CA-CB-CG2	6.85	121.99	112.40
25	U	97	THR	CA-CB-CG2	-6.84	102.82	112.40
29	K	60	TYR	CB-CG-CD2	-6.84	116.90	121.00
30	L	146	TYR	CB-CG-CD1	6.83	125.10	121.00
23	Q	309	TYR	CG-CD2-CE2	-6.83	115.84	121.30
32	J	310	ARG	NH1-CZ-NH2	6.83	126.91	119.40
21	S	284	TYR	CB-CG-CD1	6.82	125.09	121.00
28	I	184	TYR	CB-CG-CD2	6.82	125.09	121.00
31	M	272	ARG	NE-CZ-NH1	6.80	123.70	120.30
5	E	100	TRP	CZ3-CH2-CZ2	-6.80	113.44	121.60
7	G	8	TYR	CB-CG-CD1	-6.79	116.92	121.00
1	A	96	TYR	CB-CG-CD1	-6.79	116.92	121.00
19	Z	687	ARG	NE-CZ-NH2	-6.79	116.90	120.30
2	B	156	PHE	CB-CG-CD1	6.78	125.55	120.80
21	S	310	ARG	NE-CZ-NH1	6.78	123.69	120.30
24	R	237	ARG	NE-CZ-NH2	6.77	123.69	120.30
3	C	12	PHE	CB-CG-CD1	6.77	125.54	120.80
19	Z	262	PHE	CB-CG-CD1	6.76	125.53	120.80
10	3	140	GLY	N-CA-C	-6.76	96.21	113.10
11	4	120	TYR	CZ-CE2-CD2	-6.76	113.72	119.80
20	N	269	ARG	NE-CZ-NH2	-6.76	116.92	120.30
20	N	778	PHE	CB-CG-CD2	6.75	125.53	120.80
27	H	97	ARG	NH1-CZ-NH2	-6.75	111.97	119.40
8	1	50	ASP	CB-CG-OD1	-6.75	112.23	118.30
25	U	237	LEU	CB-CG-CD1	6.75	122.47	111.00
12	5	155	SER	N-CA-CB	6.74	120.61	110.50
13	6	41	ALA	CB-CA-C	-6.74	99.99	110.10
19	Z	226	TYR	CB-CG-CD1	-6.74	116.95	121.00
10	3	110	ALA	N-CA-CB	6.74	119.53	110.10
4	D	234	TYR	CB-CG-CD1	-6.73	116.96	121.00
23	Q	76	PHE	CB-CG-CD2	-6.73	116.09	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	201	PHE	CB-CG-CD2	6.72	125.51	120.80
20	N	813	TYR	CB-CG-CD2	-6.72	116.97	121.00
3	C	83	ALA	CB-CA-C	-6.71	100.04	110.10
22	P	387	ASP	CB-CG-OD1	6.70	124.33	118.30
23	Q	142	ARG	NE-CZ-NH2	-6.70	116.95	120.30
28	I	225	TYR	CB-CG-CD1	6.70	125.02	121.00
29	K	313	ARG	NE-CZ-NH1	6.70	123.65	120.30
3	C	19	TYR	CD1-CE1-CZ	6.68	125.82	119.80
5	E	39	GLY	N-CA-C	-6.68	96.39	113.10
17	T	296	PHE	CB-CG-CD1	-6.68	116.12	120.80
19	Z	621	ASP	CB-CG-OD2	6.68	124.31	118.30
12	5	239	ARG	NE-CZ-NH1	6.68	123.64	120.30
20	N	251	ASP	CB-CG-OD1	-6.68	112.29	118.30
4	D	39	ASP	CB-CG-OD1	-6.68	112.29	118.30
3	C	121	TYR	CB-CG-CD1	6.67	125.00	121.00
31	M	441	TYR	CG-CD2-CE2	-6.67	115.96	121.30
11	4	146	TYR	CB-CG-CD2	6.67	125.00	121.00
6	F	122	ARG	NE-CZ-NH1	-6.66	116.97	120.30
10	3	136	PHE	CB-CG-CD1	-6.66	116.14	120.80
14	7	127	TYR	CB-CG-CD1	6.66	125.00	121.00
26	O	240	PHE	CB-CG-CD1	6.66	125.47	120.80
22	P	130	MET	CG-SD-CE	6.66	110.86	100.20
20	N	375	PHE	CB-CG-CD2	-6.66	116.14	120.80
21	S	35	MET	CG-SD-CE	-6.66	89.55	100.20
19	Z	600	TYR	CG-CD2-CE2	-6.65	115.98	121.30
20	N	113	VAL	CA-CB-CG1	6.65	120.87	110.90
21	S	382	PHE	CB-CG-CD1	-6.65	116.15	120.80
21	S	497	TYR	CB-CG-CD2	-6.64	117.01	121.00
22	P	149	LEU	CB-CG-CD1	6.64	122.29	111.00
29	K	403	TYR	CG-CD1-CE1	-6.64	115.99	121.30
7	G	141	TYR	CB-CG-CD1	6.64	124.98	121.00
20	N	684	ARG	NE-CZ-NH1	6.64	123.62	120.30
3	C	202	ASP	CB-CG-OD2	-6.64	112.33	118.30
28	I	372	MET	C-N-CA	6.64	138.29	121.70
29	K	394	VAL	CA-CB-CG1	6.64	120.86	110.90
17	T	149	ASP	CB-CG-OD1	6.63	124.27	118.30
29	K	157	ASP	CB-CG-OD1	6.63	124.27	118.30
2	B	227	ARG	NE-CZ-NH1	6.63	123.62	120.30
14	7	183	THR	N-CA-CB	6.63	122.90	110.30
27	H	369	ARG	NE-CZ-NH2	-6.63	116.98	120.30
28	I	343	ARG	NE-CZ-NH1	6.63	123.61	120.30
3	C	220	ASN	CB-CG-OD1	-6.63	108.35	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	131	PHE	CB-CG-CD1	-6.62	116.17	120.80
21	S	388	TYR	CG-CD1-CE1	6.62	126.59	121.30
23	Q	17	SER	N-CA-CB	6.62	120.42	110.50
12	5	217	ARG	NE-CZ-NH2	-6.61	116.99	120.30
29	K	170	MET	CA-CB-CG	6.61	124.54	113.30
19	Z	392	THR	CA-CB-CG2	-6.61	103.15	112.40
22	P	420	ASP	CB-CG-OD1	6.61	124.25	118.30
20	N	584	TYR	CB-CG-CD2	-6.60	117.04	121.00
20	N	783	TYR	CB-CG-CD2	-6.60	117.04	121.00
4	D	103	THR	CA-CB-CG2	-6.60	103.16	112.40
3	C	12	PHE	CB-CG-CD2	-6.60	116.18	120.80
24	R	385	ARG	NE-CZ-NH2	-6.60	117.00	120.30
27	H	386	ARG	NE-CZ-NH1	-6.60	117.00	120.30
13	6	73	LEU	C-N-CA	6.59	138.19	121.70
27	H	420	TYR	CB-CG-CD1	6.59	124.96	121.00
8	1	152	MET	CA-CB-CG	6.59	124.50	113.30
5	E	215	ILE	CA-CB-CG1	6.59	123.52	111.00
29	K	229	ARG	NE-CZ-NH2	6.59	123.59	120.30
10	3	80	ARG	CD-NE-CZ	-6.58	114.39	123.60
26	O	286	ALA	N-CA-CB	6.58	119.31	110.10
21	S	487	VAL	CG1-CB-CG2	-6.58	100.38	110.90
28	I	329	MET	CG-SD-CE	6.58	110.72	100.20
27	H	401	ARG	NE-CZ-NH2	-6.57	117.01	120.30
32	J	229	ARG	NE-CZ-NH2	-6.57	117.02	120.30
19	Z	314	TYR	CB-CG-CD2	-6.57	117.06	121.00
2	B	186	ASP	CB-CG-OD2	6.56	124.20	118.30
19	Z	456	ARG	C-N-CA	6.56	138.09	121.70
19	Z	519	ALA	CB-CA-C	-6.55	100.27	110.10
21	S	491	ARG	NE-CZ-NH2	6.55	123.58	120.30
22	P	90	LEU	CB-CG-CD1	6.55	122.13	111.00
16	V	135	ALA	CB-CA-C	-6.55	100.28	110.10
19	Z	740	ARG	NE-CZ-NH2	6.55	123.57	120.30
29	K	178	ARG	NE-CZ-NH1	-6.55	117.03	120.30
20	N	205	TYR	CG-CD2-CE2	-6.54	116.06	121.30
4	D	169	ARG	NE-CZ-NH1	6.54	123.57	120.30
13	6	159	ARG	NE-CZ-NH2	-6.54	117.03	120.30
20	N	194	ARG	NE-CZ-NH1	-6.54	117.03	120.30
5	E	226	PHE	CB-CG-CD2	-6.54	116.22	120.80
20	N	770	TRP	CB-CG-CD1	6.54	135.50	127.00
29	K	68	LEU	CB-CG-CD1	6.53	122.10	111.00
14	7	195	ARG	NE-CZ-NH1	-6.52	117.04	120.30
20	N	172	ASP	N-CA-C	-6.52	93.39	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	385	PHE	CB-CG-CD1	-6.52	116.23	120.80
20	N	682	TYR	CB-CG-CD1	-6.52	117.09	121.00
21	S	302	ARG	NE-CZ-NH2	-6.52	117.04	120.30
27	H	265	ARG	NE-CZ-NH1	6.52	123.56	120.30
12	5	200	ARG	NE-CZ-NH2	-6.52	117.04	120.30
16	V	112	TYR	CB-CG-CD2	-6.52	117.09	121.00
12	5	166	ARG	NE-CZ-NH1	-6.51	117.04	120.30
20	N	425	THR	CA-CB-CG2	-6.51	103.28	112.40
27	H	351	ARG	NE-CZ-NH1	6.51	123.56	120.30
4	D	125	THR	CA-CB-CG2	-6.50	103.29	112.40
19	Z	142	TYR	CB-CG-CD1	-6.50	117.10	121.00
11	4	104	LEU	N-CA-CB	6.50	123.40	110.40
22	P	12	ARG	NE-CZ-NH1	6.50	123.55	120.30
23	Q	137	TYR	CG-CD2-CE2	6.50	126.50	121.30
8	1	199	ARG	NE-CZ-NH1	6.50	123.55	120.30
10	3	164	PHE	CB-CG-CD2	-6.50	116.25	120.80
2	B	8	PHE	CB-CG-CD1	6.50	125.35	120.80
29	K	320	ALA	C-N-CA	6.50	137.94	121.70
21	S	143	PHE	CB-CG-CD2	6.50	125.35	120.80
24	R	26	LEU	CB-CG-CD2	-6.50	99.96	111.00
20	N	260	PHE	CB-CG-CD2	-6.49	116.25	120.80
32	J	154	LEU	N-CA-C	-6.49	93.47	111.00
10	3	56	LEU	CB-CG-CD2	6.49	122.03	111.00
19	Z	800	LEU	CB-CG-CD2	6.48	122.02	111.00
28	I	138	PHE	CB-CG-CD2	-6.48	116.26	120.80
22	P	387	ASP	CB-CG-OD2	-6.48	112.47	118.30
23	Q	297	ARG	NE-CZ-NH1	-6.48	117.06	120.30
28	I	188	GLY	C-N-CA	6.48	135.90	122.30
21	S	459	MET	N-CA-CB	6.47	122.24	110.60
8	1	167	TYR	CB-CG-CD2	6.46	124.87	121.00
24	R	142	PHE	CB-CG-CD1	6.45	125.32	120.80
32	J	59	LEU	CB-CG-CD1	6.45	121.97	111.00
3	C	99	LEU	CB-CG-CD2	6.45	121.96	111.00
19	Z	456	ARG	NE-CZ-NH2	6.45	123.52	120.30
21	S	453	TYR	CB-CG-CD2	-6.45	117.13	121.00
20	N	490	ARG	NE-CZ-NH1	6.45	123.52	120.30
27	H	355	PHE	CB-CG-CD2	6.44	125.31	120.80
7	G	153	ASP	CB-CG-OD2	6.44	124.10	118.30
6	F	179	PHE	CB-CG-CD2	-6.44	116.29	120.80
8	1	123	TYR	CB-CG-CD2	-6.44	117.14	121.00
15	W	123	ASP	N-CA-CB	6.43	122.18	110.60
11	4	24	ASN	CB-CG-OD1	-6.43	108.74	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	S	209	TYR	CG-CD1-CE1	-6.43	116.16	121.30
11	4	138	LEU	CA-CB-CG	6.43	130.08	115.30
23	Q	166	LEU	CB-CG-CD1	6.43	121.92	111.00
13	6	185	MET	CG-SD-CE	-6.42	89.92	100.20
28	I	179	ALA	N-CA-CB	6.42	119.09	110.10
32	J	280	LEU	N-CA-CB	6.42	123.24	110.40
2	B	11	THR	CA-CB-CG2	-6.42	103.42	112.40
28	I	268	ARG	NE-CZ-NH2	-6.42	117.09	120.30
29	K	74	HIS	O-C-N	-6.42	112.44	122.70
21	S	388	TYR	CG-CD2-CE2	-6.41	116.17	121.30
21	S	158	GLU	OE1-CD-OE2	-6.41	115.61	123.30
16	V	53	VAL	CA-CB-CG2	-6.40	101.30	110.90
16	V	201	TYR	CB-CG-CD2	-6.40	117.16	121.00
20	N	253	TYR	CB-CG-CD1	6.40	124.84	121.00
3	C	124	PHE	N-CA-CB	6.39	122.11	110.60
19	Z	62	ARG	NE-CZ-NH2	6.39	123.50	120.30
27	H	163	MET	CG-SD-CE	-6.39	89.97	100.20
6	F	125	ARG	NE-CZ-NH1	-6.39	117.11	120.30
9	2	124	ARG	NE-CZ-NH1	6.39	123.49	120.30
7	G	221	THR	CA-CB-CG2	-6.38	103.47	112.40
26	O	232	TRP	CB-CG-CD2	-6.38	118.30	126.60
26	O	34	TRP	CG-CD2-CE3	-6.38	128.16	133.90
32	J	191	PRO	N-CA-CB	6.38	110.96	103.30
7	G	59	TYR	CB-CG-CD1	6.38	124.83	121.00
29	K	167	ILE	CA-CB-CG2	-6.38	98.14	110.90
7	G	224	ARG	NE-CZ-NH2	-6.38	117.11	120.30
3	C	44	LEU	CB-CG-CD2	6.37	121.83	111.00
4	D	96	GLU	OE1-CD-OE2	6.37	130.94	123.30
17	T	149	ASP	CB-CG-OD2	-6.37	112.57	118.30
3	C	189	ALA	N-CA-CB	6.37	119.01	110.10
2	B	145	TYR	CB-CG-CD2	-6.36	117.18	121.00
19	Z	819	TYR	CG-CD2-CE2	-6.36	116.21	121.30
20	N	161	ASP	CB-CG-OD1	6.36	124.03	118.30
25	U	68	TRP	CG-CD2-CE3	-6.36	128.18	133.90
3	C	156	TYR	CD1-CE1-CZ	-6.36	114.08	119.80
19	Z	587	PHE	CB-CG-CD1	-6.36	116.35	120.80
21	S	260	TYR	CB-CG-CD2	-6.36	117.19	121.00
29	K	178	ARG	NH1-CZ-NH2	6.35	126.39	119.40
2	B	113	ARG	NE-CZ-NH1	-6.35	117.12	120.30
24	R	85	ASP	CB-CG-OD2	6.35	124.02	118.30
20	N	502	TYR	CB-CG-CD1	6.35	124.81	121.00
16	V	279	ASP	CB-CG-OD2	6.35	124.01	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	S	34	GLU	OE1-CD-OE2	6.33	130.90	123.30
26	O	162	TYR	CB-CG-CD1	6.33	124.80	121.00
27	H	201	PHE	CB-CG-CD2	6.33	125.23	120.80
30	L	316	ASP	C-N-CA	6.33	137.53	121.70
10	3	85	TYR	CB-CG-CD2	-6.32	117.21	121.00
24	R	293	ARG	NE-CZ-NH2	6.32	123.46	120.30
19	Z	483	PHE	CB-CG-CD1	6.32	125.22	120.80
1	A	209	ASP	CB-CG-OD2	-6.32	112.62	118.30
24	R	176	ARG	NE-CZ-NH1	6.32	123.46	120.30
28	I	130	GLU	OE1-CD-OE2	6.31	130.87	123.30
2	B	36	VAL	CG1-CB-CG2	6.31	120.99	110.90
19	Z	261	ARG	NE-CZ-NH2	-6.30	117.15	120.30
15	W	143	PHE	CB-CG-CD2	6.30	125.21	120.80
19	Z	688	ARG	NE-CZ-NH2	-6.30	117.15	120.30
17	T	131	PHE	CB-CG-CD2	6.30	125.21	120.80
16	V	255	TYR	CG-CD1-CE1	-6.29	116.26	121.30
21	S	154	PRO	N-CD-CG	6.29	112.64	103.20
23	Q	415	TYR	CB-CG-CD1	-6.29	117.22	121.00
28	I	225	TYR	CB-CG-CD2	-6.29	117.22	121.00
4	D	74	ALA	CB-CA-C	-6.29	100.67	110.10
8	1	225	ASP	CB-CG-OD2	6.29	123.96	118.30
9	2	253	ALA	N-CA-CB	6.29	118.90	110.10
23	Q	87	ARG	NE-CZ-NH2	-6.29	117.16	120.30
24	R	288	PHE	CB-CG-CD1	6.29	125.20	120.80
1	A	209	ASP	CB-CG-OD1	6.28	123.95	118.30
19	Z	588	ARG	NE-CZ-NH2	-6.28	117.16	120.30
10	3	4	MET	N-CA-CB	6.28	121.91	110.60
9	2	174	SER	N-CA-CB	6.28	119.92	110.50
29	K	315	ASP	CB-CG-OD2	-6.28	112.65	118.30
13	6	182	PHE	CB-CG-CD1	-6.28	116.41	120.80
24	R	20	ALA	O-C-N	6.28	132.74	122.70
30	L	111	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	B	218	PHE	CB-CG-CD1	-6.27	116.41	120.80
3	C	151	ASP	CB-CG-OD1	-6.27	112.66	118.30
16	V	57	MET	CG-SD-CE	6.27	110.23	100.20
28	I	218	PRO	N-CA-CB	6.27	110.82	103.30
19	Z	79	ARG	NE-CZ-NH2	6.27	123.43	120.30
12	5	86	ALA	CB-CA-C	-6.26	100.70	110.10
17	T	305	TYR	CG-CD1-CE1	-6.26	116.29	121.30
24	R	24	PHE	CB-CG-CD1	-6.26	116.42	120.80
31	M	64	ARG	NE-CZ-NH1	6.26	123.43	120.30
17	T	304	ASP	CB-CG-OD2	6.26	123.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	802	TYR	CZ-CE2-CD2	-6.26	114.17	119.80
6	F	204	ASP	CB-CG-OD2	-6.25	112.67	118.30
9	2	130	LEU	CB-CG-CD2	6.25	121.63	111.00
19	Z	103	TYR	CB-CG-CD2	-6.25	117.25	121.00
14	7	62	CYS	CA-CB-SG	-6.25	102.75	114.00
20	N	494	TYR	CB-CG-CD1	-6.25	117.25	121.00
14	7	69	ASP	N-CA-C	-6.25	94.14	111.00
20	N	773	PHE	CG-CD1-CE1	-6.25	113.93	120.80
4	D	115	ARG	NE-CZ-NH1	-6.24	117.18	120.30
4	D	10	PHE	CB-CG-CD2	-6.24	116.43	120.80
27	H	369	ARG	NH1-CZ-NH2	6.23	126.25	119.40
7	G	20	ARG	NE-CZ-NH2	-6.22	117.19	120.30
31	M	287	PHE	CG-CD1-CE1	-6.22	113.96	120.80
13	6	204	ASP	CB-CG-OD2	-6.22	112.70	118.30
19	Z	838	ARG	NE-CZ-NH1	-6.22	117.19	120.30
3	C	236	LEU	CB-CG-CD1	6.21	121.56	111.00
19	Z	239	TYR	CB-CG-CD1	6.21	124.73	121.00
14	7	144	ARG	NE-CZ-NH2	-6.21	117.19	120.30
22	P	251	TYR	CB-CG-CD2	-6.21	117.27	121.00
10	3	27	ARG	N-CA-CB	6.20	121.77	110.60
19	Z	567	LEU	CB-CG-CD2	-6.20	100.45	111.00
30	L	256	ARG	NE-CZ-NH2	6.20	123.40	120.30
24	R	228	MET	CG-SD-CE	-6.20	90.28	100.20
26	O	229	ASP	CB-CG-OD2	-6.20	112.72	118.30
20	N	773	PHE	CB-CG-CD2	-6.20	116.46	120.80
28	I	307	ARG	NE-CZ-NH2	6.19	123.39	120.30
6	F	229	VAL	CA-CB-CG2	-6.19	101.62	110.90
7	G	233	ARG	NE-CZ-NH1	-6.18	117.21	120.30
20	N	472	ILE	CA-CB-CG1	6.18	122.75	111.00
22	P	39	ARG	NE-CZ-NH1	6.18	123.39	120.30
8	1	98	PHE	N-CA-CB	6.18	121.73	110.60
14	7	106	TYR	CB-CG-CD2	6.18	124.71	121.00
31	M	389	ARG	NE-CZ-NH1	6.18	123.39	120.30
17	T	185	LEU	CB-CG-CD1	6.18	121.51	111.00
29	K	268	ASP	CB-CG-OD2	6.18	123.86	118.30
32	J	383	PHE	CG-CD1-CE1	-6.18	114.01	120.80
17	T	98	TYR	CB-CG-CD2	-6.17	117.30	121.00
27	H	216	GLY	N-CA-C	-6.17	97.68	113.10
11	4	101	ASN	N-CA-C	-6.17	94.35	111.00
23	Q	177	TYR	CG-CD2-CE2	-6.17	116.37	121.30
1	A	101	TRP	CD1-CG-CD2	-6.16	101.37	106.30
19	Z	837	LEU	N-CA-CB	6.16	122.73	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	412	VAL	CG1-CB-CG2	-6.16	101.04	110.90
24	R	222	TYR	CG-CD1-CE1	-6.16	116.37	121.30
32	J	60	ARG	NE-CZ-NH2	-6.16	117.22	120.30
8	1	163	SER	N-CA-CB	6.16	119.73	110.50
20	N	96	TYR	CB-CG-CD1	-6.16	117.31	121.00
21	S	339	PRO	N-CD-CG	6.15	112.43	103.20
21	S	95	ARG	NE-CZ-NH2	6.15	123.38	120.30
2	B	25	ALA	N-CA-CB	6.15	118.71	110.10
1	A	159	TYR	CB-CG-CD2	-6.14	117.31	121.00
19	Z	600	TYR	CB-CG-CD2	-6.14	117.31	121.00
19	Z	696	LEU	CB-CG-CD2	6.14	121.44	111.00
24	R	329	PHE	CB-CG-CD2	-6.14	116.50	120.80
29	K	403	TYR	CB-CG-CD1	-6.14	117.31	121.00
31	M	181	ASP	CB-CG-OD1	-6.14	112.77	118.30
10	3	111	GLY	N-CA-C	-6.14	97.75	113.10
27	H	261	PHE	CB-CG-CD2	-6.14	116.50	120.80
2	B	219	ARG	NE-CZ-NH2	6.14	123.37	120.30
1	A	23	TYR	CB-CG-CD1	-6.13	117.32	121.00
12	5	171	TYR	CG-CD2-CE2	-6.13	116.39	121.30
5	E	240	ASP	CB-CG-OD1	6.13	123.81	118.30
9	2	51	TYR	N-CA-C	-6.13	94.45	111.00
21	S	78	LEU	CB-CG-CD2	6.13	121.42	111.00
20	N	181	LEU	CB-CG-CD2	6.13	121.41	111.00
22	P	372	ARG	NE-CZ-NH2	-6.12	117.24	120.30
11	4	138	LEU	CB-CG-CD2	6.12	121.41	111.00
30	L	39	ARG	NE-CZ-NH2	-6.12	117.24	120.30
11	4	170	ARG	NE-CZ-NH2	6.12	123.36	120.30
19	Z	24	ALA	N-CA-CB	6.12	118.66	110.10
32	J	374	ARG	NH1-CZ-NH2	6.11	126.12	119.40
22	P	365	ILE	CA-CB-CG1	6.11	122.61	111.00
23	Q	239	TYR	CD1-CE1-CZ	-6.11	114.30	119.80
14	7	159	TYR	CB-CG-CD2	-6.11	117.33	121.00
9	2	174	SER	N-CA-C	-6.11	94.51	111.00
21	S	153	ALA	N-CA-CB	6.11	118.65	110.10
8	1	152	MET	CB-CA-C	-6.11	98.19	110.40
9	2	198	VAL	CA-CB-CG2	-6.11	101.74	110.90
20	N	655	ALA	N-CA-CB	6.11	118.65	110.10
22	P	65	ARG	NE-CZ-NH2	-6.11	117.25	120.30
18	Y	52	PHE	CZ-CE2-CD2	-6.10	112.78	120.10
19	Z	1	MET	CG-SD-CE	-6.10	90.44	100.20
4	D	114	THR	CA-CB-CG2	-6.10	103.86	112.40
11	4	70	ARG	NE-CZ-NH1	6.10	123.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	110	MET	N-CA-C	-6.10	94.53	111.00
16	V	46	ARG	NE-CZ-NH2	6.10	123.35	120.30
4	D	17	PHE	CB-CG-CD2	-6.10	116.53	120.80
25	U	167	ALA	N-CA-CB	6.09	118.63	110.10
30	L	308	ARG	NH1-CZ-NH2	6.09	126.10	119.40
2	B	155	TYR	CB-CG-CD1	6.09	124.65	121.00
30	L	20	ASP	CB-CG-OD2	6.09	123.78	118.30
24	R	295	TYR	CG-CD2-CE2	6.09	126.17	121.30
23	Q	232	PHE	CB-CG-CD1	6.08	125.06	120.80
7	G	59	TYR	CB-CG-CD2	-6.08	117.35	121.00
24	R	337	PHE	CB-CG-CD2	-6.08	116.54	120.80
32	J	302	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	A	120	ASP	CB-CG-OD2	6.08	123.77	118.30
14	7	153	THR	CA-CB-OG1	6.08	121.77	109.00
30	L	331	ALA	N-CA-CB	6.08	118.61	110.10
14	7	236	VAL	CA-CB-CG2	6.08	120.01	110.90
31	M	423	TYR	CB-CG-CD1	6.07	124.64	121.00
6	F	62	LYS	N-CA-CB	6.07	121.53	110.60
12	5	84	TYR	CD1-CG-CD2	6.07	124.58	117.90
20	N	245	ALA	CB-CA-C	-6.07	100.99	110.10
31	M	88	THR	CA-CB-CG2	-6.07	103.90	112.40
21	S	298	TYR	CG-CD2-CE2	6.07	126.16	121.30
32	J	383	PHE	CD1-CG-CD2	6.07	126.19	118.30
31	M	109	GLU	N-CA-CB	6.06	121.51	110.60
8	1	41	PHE	CB-CG-CD1	6.06	125.04	120.80
5	E	131	GLY	O-C-N	-6.06	113.01	122.70
17	T	136	GLY	N-CA-C	-6.06	97.96	113.10
3	C	49	ARG	CD-NE-CZ	-6.05	115.13	123.60
1	A	241	ALA	CB-CA-C	-6.05	101.03	110.10
31	M	161	TYR	CB-CG-CD2	6.05	124.63	121.00
29	K	29	PHE	CG-CD2-CE2	-6.05	114.15	120.80
13	6	238	ARG	NE-CZ-NH2	6.04	123.32	120.30
22	P	369	TYR	CA-CB-CG	-6.04	101.91	113.40
4	D	226	LEU	CB-CG-CD1	6.04	121.28	111.00
10	3	110	ALA	CB-CA-C	-6.04	101.03	110.10
20	N	658	VAL	CA-CB-CG2	6.04	119.96	110.90
17	T	305	TYR	CB-CG-CD1	-6.04	117.38	121.00
24	R	259	TYR	CD1-CG-CD2	6.04	124.55	117.90
11	4	59	TYR	CG-CD1-CE1	-6.04	116.47	121.30
24	R	143	TYR	CZ-CE2-CD2	6.04	125.23	119.80
19	Z	313	GLU	N-CA-CB	6.03	121.46	110.60
20	N	883	ARG	NE-CZ-NH2	6.03	123.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	51	ASN	CA-CB-CG	-6.03	100.14	113.40
16	V	36	LEU	CB-CG-CD2	6.03	121.25	111.00
26	O	106	SER	N-CA-CB	6.03	119.54	110.50
19	Z	819	TYR	CB-CG-CD1	-6.03	117.38	121.00
10	3	147	TYR	CB-CG-CD2	-6.02	117.39	121.00
20	N	653	ALA	CB-CA-C	-6.02	101.06	110.10
24	R	38	ARG	NE-CZ-NH1	6.02	123.31	120.30
19	Z	326	LEU	CB-CG-CD1	6.02	121.23	111.00
20	N	575	ASP	CB-CG-OD2	6.02	123.72	118.30
23	Q	90	ARG	NE-CZ-NH2	-6.02	117.29	120.30
15	W	28	ALA	CB-CA-C	-6.02	101.08	110.10
2	B	130	PHE	CG-CD1-CE1	-6.01	114.19	120.80
9	2	85	TYR	CB-CG-CD2	6.01	124.61	121.00
6	F	157	ARG	NE-CZ-NH1	6.01	123.31	120.30
17	T	177	TYR	CB-CG-CD2	6.01	124.61	121.00
20	N	682	TYR	CB-CG-CD2	6.01	124.61	121.00
22	P	142	ARG	NE-CZ-NH1	6.01	123.31	120.30
22	P	182	ARG	NE-CZ-NH1	-6.01	117.30	120.30
22	P	314	LEU	CB-CG-CD1	6.01	121.22	111.00
27	H	97	ARG	CB-CA-C	-6.01	98.38	110.40
7	G	54	VAL	CA-CB-CG2	-6.01	101.89	110.90
29	K	352	MET	CB-CA-C	-6.00	98.39	110.40
19	Z	456	ARG	N-CA-C	-6.00	94.80	111.00
13	6	97	ALA	N-CA-CB	6.00	118.50	110.10
23	Q	143	TYR	CG-CD1-CE1	-6.00	116.50	121.30
23	Q	308	ASP	CB-CG-OD2	-6.00	112.90	118.30
25	U	169	GLU	OE1-CD-OE2	5.99	130.49	123.30
26	O	342	ASP	CB-CG-OD1	-5.99	112.91	118.30
3	C	60	PHE	CB-CG-CD2	5.99	124.99	120.80
17	T	267	LEU	CB-CG-CD1	5.99	121.18	111.00
20	N	74	PHE	CB-CG-CD2	-5.99	116.61	120.80
22	P	392	PHE	CZ-CE2-CD2	-5.99	112.91	120.10
17	T	311	TRP	CB-CG-CD2	-5.99	118.81	126.60
23	Q	201	TYR	CZ-CE2-CD2	5.99	125.19	119.80
2	B	79	MET	CG-SD-CE	-5.99	90.62	100.20
13	6	162	PHE	CB-CG-CD1	-5.99	116.61	120.80
12	5	184	ALA	N-CA-CB	5.98	118.48	110.10
18	Y	57	ARG	NH1-CZ-NH2	-5.98	112.82	119.40
24	R	233	ARG	NE-CZ-NH2	5.98	123.29	120.30
27	H	97	ARG	NE-CZ-NH1	5.98	123.29	120.30
4	D	115	ARG	NE-CZ-NH2	5.98	123.29	120.30
5	E	95	GLU	CB-CA-C	-5.97	98.46	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	157	ASP	CB-CG-OD1	-5.97	112.93	118.30
21	S	415	LEU	CB-CG-CD2	5.97	121.15	111.00
25	U	51	SER	CB-CA-C	-5.97	98.76	110.10
29	K	366	ARG	NE-CZ-NH2	-5.97	117.32	120.30
3	C	130	PHE	CB-CG-CD2	-5.97	116.62	120.80
11	4	55	GLN	CB-CA-C	-5.97	98.47	110.40
29	K	167	ILE	C-N-CA	5.97	134.83	122.30
30	L	328	LYS	CB-CA-C	-5.97	98.47	110.40
17	T	98	TYR	CD1-CE1-CZ	-5.96	114.43	119.80
24	R	174	TRP	CZ3-CH2-CZ2	-5.96	114.44	121.60
29	K	139	LEU	CB-CG-CD2	5.96	121.14	111.00
21	S	281	TRP	CB-CG-CD1	5.96	134.75	127.00
25	U	45	LYS	N-CA-C	-5.96	94.90	111.00
30	L	85	VAL	CA-CB-CG1	5.96	119.84	110.90
3	C	57	ASP	CB-CG-OD2	-5.96	112.94	118.30
23	Q	74	ARG	NE-CZ-NH1	-5.96	117.32	120.30
31	M	91	TYR	N-CA-CB	5.96	121.33	110.60
2	B	229	TYR	CG-CD1-CE1	5.96	126.06	121.30
23	Q	389	ASP	N-CA-CB	5.96	121.32	110.60
12	5	147	TYR	CB-CG-CD1	-5.95	117.43	121.00
14	7	151	TRP	N-CA-CB	5.95	121.32	110.60
5	E	162	PHE	CB-CG-CD1	-5.95	116.64	120.80
19	Z	196	MET	CG-SD-CE	-5.95	90.68	100.20
26	O	330	ARG	NE-CZ-NH1	-5.95	117.33	120.30
5	E	124	GLY	N-CA-C	-5.95	98.24	113.10
18	Y	52	PHE	CG-CD2-CE2	5.95	127.34	120.80
28	I	242	GLN	N-CA-CB	5.95	121.30	110.60
19	Z	645	ASP	CB-CG-OD2	5.94	123.65	118.30
4	D	133	PHE	CB-CG-CD2	-5.94	116.64	120.80
8	1	62	ARG	NE-CZ-NH2	-5.94	117.33	120.30
28	I	259	TYR	CZ-CE2-CD2	-5.94	114.45	119.80
23	Q	310	ARG	NE-CZ-NH1	5.94	123.27	120.30
20	N	21	GLU	OE1-CD-OE2	-5.94	116.18	123.30
24	R	1	MET	CG-SD-CE	5.94	109.70	100.20
23	Q	33	ARG	NE-CZ-NH2	-5.93	117.33	120.30
19	Z	805	ASP	CB-CG-OD2	-5.93	112.96	118.30
19	Z	160	ARG	NE-CZ-NH1	-5.93	117.33	120.30
9	2	66	GLY	N-CA-C	-5.93	98.28	113.10
21	S	70	ASP	CB-CG-OD2	5.93	123.64	118.30
20	N	54	PHE	CB-CG-CD1	5.93	124.95	120.80
30	L	255	ARG	NE-CZ-NH2	-5.92	117.34	120.30
25	U	79	TYR	CD1-CE1-CZ	5.92	125.13	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	185	PHE	N-CA-CB	5.92	121.25	110.60
14	7	139	ALA	CB-CA-C	-5.92	101.23	110.10
23	Q	75	PRO	CA-N-CD	-5.91	103.22	111.50
23	Q	415	TYR	CB-CG-CD2	5.91	124.55	121.00
4	D	144	PHE	CB-CG-CD1	5.91	124.94	120.80
31	M	160	SER	CB-CA-C	-5.91	98.88	110.10
19	Z	434	TYR	CZ-CE2-CD2	5.91	125.12	119.80
31	M	49	ARG	NE-CZ-NH1	-5.91	117.35	120.30
24	R	311	TYR	CB-CG-CD2	-5.91	117.46	121.00
19	Z	787	LEU	N-CA-CB	5.90	122.20	110.40
26	O	295	GLU	N-CA-CB	5.90	121.23	110.60
1	A	21	ARG	NE-CZ-NH2	-5.90	117.35	120.30
4	D	123	ARG	NE-CZ-NH2	-5.90	117.35	120.30
20	N	557	TYR	CA-CB-CG	-5.90	102.19	113.40
3	C	148	TYR	CA-CB-CG	-5.90	102.20	113.40
16	V	208	ARG	N-CA-C	-5.89	95.09	111.00
24	R	268	TYR	CA-CB-CG	-5.89	102.20	113.40
24	R	277	VAL	CA-CB-CG1	5.89	119.74	110.90
24	R	85	ASP	CB-CG-OD1	-5.89	113.00	118.30
7	G	48	PHE	CD1-CE1-CZ	5.88	127.16	120.10
8	1	229	LYS	CD-CE-NZ	5.88	125.23	111.70
30	L	305	ARG	NE-CZ-NH2	5.88	123.24	120.30
24	R	267	ARG	N-CA-CB	5.88	121.18	110.60
12	5	204	TYR	CG-CD2-CE2	-5.88	116.60	121.30
22	P	213	PHE	CD1-CE1-CZ	5.88	127.15	120.10
23	Q	138	PHE	CB-CG-CD1	5.88	124.91	120.80
28	I	115	ILE	CA-CB-CG1	5.88	122.17	111.00
4	D	60	ARG	NE-CZ-NH1	5.88	123.24	120.30
9	2	121	THR	CA-CB-CG2	5.88	120.62	112.40
11	4	36	PHE	CG-CD2-CE2	-5.88	114.34	120.80
26	O	308	GLU	N-CA-CB	5.87	121.17	110.60
27	H	69	ASP	CB-CG-OD2	-5.87	113.02	118.30
10	3	53	LEU	CB-CA-C	-5.87	99.05	110.20
13	6	65	ARG	NE-CZ-NH1	-5.87	117.36	120.30
23	Q	29	SER	N-CA-CB	5.87	119.30	110.50
4	D	5	ARG	NE-CZ-NH1	-5.87	117.37	120.30
17	T	133	PRO	C-N-CA	5.87	136.36	121.70
24	R	128	TYR	CB-CG-CD1	-5.87	117.48	121.00
4	D	131	ARG	NE-CZ-NH2	-5.86	117.37	120.30
31	M	39	MET	CG-SD-CE	-5.86	90.82	100.20
19	Z	344	VAL	CA-CB-CG2	-5.86	102.11	110.90
7	G	162	TRP	N-CA-CB	5.86	121.14	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	J	157	GLN	O-C-N	5.85	132.06	122.70
9	2	241	ARG	NE-CZ-NH1	5.85	123.22	120.30
8	1	98	PHE	CB-CG-CD1	5.85	124.89	120.80
27	H	351	ARG	NE-CZ-NH2	-5.85	117.38	120.30
20	N	361	ARG	NE-CZ-NH1	-5.84	117.38	120.30
21	S	388	TYR	CD1-CE1-CZ	-5.84	114.54	119.80
14	7	159	TYR	CZ-CE2-CD2	-5.84	114.54	119.80
18	Y	69	THR	CA-CB-CG2	-5.84	104.22	112.40
27	H	212	VAL	CG1-CB-CG2	5.84	120.24	110.90
25	U	116	CYS	CA-CB-SG	-5.84	103.49	114.00
10	3	80	ARG	NE-CZ-NH2	-5.83	117.38	120.30
20	N	375	PHE	CB-CG-CD1	5.83	124.88	120.80
21	S	286	TYR	CB-CG-CD1	5.83	124.50	121.00
27	H	180	CYS	C-N-CA	5.83	136.27	121.70
32	J	266	ASP	O-C-N	-5.83	113.37	122.70
21	S	290	ARG	NE-CZ-NH2	5.83	123.21	120.30
13	6	131	TYR	N-CA-C	-5.83	95.27	111.00
23	Q	137	TYR	CZ-CE2-CD2	-5.83	114.56	119.80
31	M	277	LEU	CB-CG-CD1	5.83	120.90	111.00
13	6	61	SER	N-CA-C	-5.82	95.28	111.00
3	C	202	ASP	CB-CG-OD1	5.82	123.54	118.30
20	N	572	ARG	NE-CZ-NH2	-5.82	117.39	120.30
12	5	178	ASN	C-N-CA	5.82	136.24	121.70
25	U	69	PHE	CB-CG-CD2	-5.82	116.73	120.80
21	S	424	LEU	CB-CG-CD2	5.81	120.88	111.00
15	W	7	MET	CA-CB-CG	5.81	123.18	113.30
6	F	96	ARG	NE-CZ-NH1	-5.81	117.39	120.30
26	O	373	ASP	CB-CG-OD1	5.81	123.53	118.30
30	L	60	ASP	CB-CA-C	-5.81	98.78	110.40
30	L	308	ARG	NE-CZ-NH1	5.81	123.20	120.30
27	H	161	VAL	CA-CB-CG2	5.81	119.61	110.90
21	S	492	PHE	CA-C-N	5.80	133.35	117.10
17	T	163	ASP	CB-CA-C	-5.80	98.79	110.40
28	I	334	ILE	CA-CB-CG1	5.80	122.01	111.00
6	F	239	ARG	NE-CZ-NH2	-5.79	117.40	120.30
20	N	394	ALA	N-CA-CB	5.79	118.21	110.10
26	O	213	PHE	CD1-CG-CD2	-5.79	110.77	118.30
31	M	391	THR	CA-CB-CG2	-5.79	104.29	112.40
23	Q	212	MET	CA-CB-CG	-5.79	103.45	113.30
8	1	219	ARG	NH1-CZ-NH2	5.79	125.77	119.40
20	N	758	PRO	N-CD-CG	5.79	111.88	103.20
31	M	347	ARG	NE-CZ-NH1	5.79	123.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	M	160	SER	N-CA-CB	5.79	119.18	110.50
23	Q	33	ARG	NE-CZ-NH1	5.78	123.19	120.30
20	N	573	ASP	CB-CG-OD1	5.78	123.50	118.30
22	P	123	ARG	NH1-CZ-NH2	-5.78	113.04	119.40
30	L	293	THR	CA-CB-OG1	5.78	121.13	109.00
14	7	210	ARG	NE-CZ-NH1	-5.77	117.41	120.30
9	2	115	ARG	NH1-CZ-NH2	-5.77	113.05	119.40
22	P	270	VAL	CA-CB-CG1	5.77	119.56	110.90
27	H	422	LYS	CB-CA-C	-5.77	98.86	110.40
25	U	228	TYR	CB-CG-CD1	-5.77	117.54	121.00
26	O	185	ILE	N-CA-C	-5.77	95.43	111.00
7	G	118	MET	CA-CB-CG	-5.77	103.50	113.30
30	L	185	LEU	CB-CG-CD2	-5.76	101.20	111.00
26	O	249	GLN	N-CA-CB	5.76	120.97	110.60
11	4	157	VAL	CA-CB-CG1	5.76	119.54	110.90
32	J	160	GLU	OE1-CD-OE2	-5.76	116.39	123.30
14	7	130	ARG	NE-CZ-NH1	5.76	123.18	120.30
26	O	211	PHE	CB-CG-CD1	-5.75	116.77	120.80
14	7	168	TYR	CG-CD1-CE1	-5.75	116.70	121.30
27	H	428	ARG	NE-CZ-NH1	5.75	123.18	120.30
28	I	303	ARG	CB-CA-C	-5.75	98.89	110.40
19	Z	392	THR	CA-CB-OG1	5.75	121.08	109.00
21	S	432	PHE	CB-CG-CD2	-5.75	116.78	120.80
30	L	20	ASP	CB-CA-C	-5.75	98.90	110.40
31	M	381	ASP	CB-CG-OD1	-5.75	113.12	118.30
19	Z	785	ARG	NE-CZ-NH2	5.75	123.17	120.30
8	1	123	TYR	CB-CG-CD1	5.75	124.45	121.00
31	M	402	VAL	CA-CB-CG1	5.75	119.52	110.90
1	A	49	VAL	CA-CB-CG2	5.75	119.52	110.90
24	R	386	VAL	CA-CB-CG2	-5.74	102.29	110.90
20	N	765	VAL	CB-CA-C	5.74	122.31	111.40
15	W	10	VAL	CA-CB-CG2	5.74	119.51	110.90
31	M	222	PRO	N-CA-CB	5.74	110.19	103.30
19	Z	363	SER	N-CA-CB	5.74	119.11	110.50
11	4	181	ARG	CA-CB-CG	5.74	126.02	113.40
29	K	338	ARG	NE-CZ-NH1	-5.73	117.43	120.30
15	W	138	VAL	CG1-CB-CG2	-5.73	101.73	110.90
21	S	464	SER	N-CA-CB	5.73	119.10	110.50
31	M	276	ALA	N-CA-CB	5.73	118.12	110.10
4	D	82	LEU	N-CA-C	-5.73	95.53	111.00
19	Z	265	ALA	CB-CA-C	-5.73	101.51	110.10
28	I	273	VAL	CA-CB-CG2	-5.73	102.31	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	O	232	TRP	CB-CG-CD1	5.73	134.44	127.00
30	L	346	VAL	CA-CB-CG2	-5.72	102.31	110.90
29	K	302	ASN	N-CA-CB	5.72	120.90	110.60
20	N	695	MET	CG-SD-CE	-5.72	91.05	100.20
30	L	396	SER	N-CA-CB	5.72	119.08	110.50
27	H	432	TYR	CB-CG-CD2	-5.72	117.57	121.00
4	D	177	PHE	CB-CG-CD2	5.71	124.80	120.80
10	3	25	ASP	N-CA-CB	5.71	120.88	110.60
20	N	783	TYR	CG-CD2-CE2	5.71	125.87	121.30
23	Q	283	GLN	N-CA-CB	5.71	120.88	110.60
32	J	35	VAL	CA-CB-CG1	5.71	119.47	110.90
7	G	30	ALA	CB-CA-C	-5.71	101.54	110.10
20	N	492	ASP	CB-CG-OD2	5.71	123.44	118.30
24	R	150	PHE	CG-CD2-CE2	5.71	127.08	120.80
7	G	103	PHE	CG-CD2-CE2	5.70	127.07	120.80
30	L	381	PHE	CB-CG-CD1	5.70	124.79	120.80
20	N	524	LYS	CA-CB-CG	5.70	125.94	113.40
22	P	392	PHE	CG-CD2-CE2	5.70	127.07	120.80
3	C	225	ILE	CA-CB-CG1	5.70	121.82	111.00
20	N	113	VAL	CA-CB-CG2	-5.70	102.36	110.90
20	N	577	ILE	CA-CB-CG1	5.70	121.82	111.00
11	4	18	ASP	N-CA-CB	5.69	120.85	110.60
18	Y	61	GLU	O-C-N	5.69	131.81	122.70
20	N	756	HIS	N-CA-C	-5.69	95.63	111.00
26	O	323	SER	N-CA-CB	5.68	119.03	110.50
12	5	142	LEU	CB-CG-CD1	5.68	120.66	111.00
21	S	395	ARG	NE-CZ-NH2	-5.68	117.46	120.30
22	P	118	LEU	CB-CG-CD2	5.67	120.65	111.00
26	O	255	TRP	CB-CG-CD1	-5.67	119.62	127.00
1	A	99	ALA	CB-CA-C	-5.67	101.59	110.10
30	L	85	VAL	CG1-CB-CG2	-5.67	101.83	110.90
21	S	89	PHE	CB-CG-CD2	-5.67	116.83	120.80
24	R	304	TYR	CB-CG-CD2	-5.67	117.60	121.00
3	C	116	ASP	CB-CG-OD2	5.67	123.40	118.30
12	5	76	ASP	CB-CG-OD1	5.67	123.40	118.30
9	2	198	VAL	CA-CB-CG1	5.66	119.39	110.90
22	P	144	ARG	NH1-CZ-NH2	5.66	125.63	119.40
27	H	143	ASP	CB-CG-OD2	5.66	123.40	118.30
7	G	243	SER	CB-CA-C	-5.66	99.34	110.10
8	1	42	ASP	CB-CG-OD1	5.66	123.39	118.30
24	R	68	ASP	N-CA-CB	5.66	120.79	110.60
4	D	116	TYR	CZ-CE2-CD2	5.66	124.89	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	67	LEU	CB-CG-CD1	5.66	120.62	111.00
24	R	215	ASP	CB-CG-OD1	-5.66	113.21	118.30
3	C	115	CYS	CA-CB-SG	5.66	124.19	114.00
28	I	434	THR	CA-C-N	5.66	132.93	117.10
20	N	813	TYR	CD1-CG-CD2	5.65	124.11	117.90
28	I	173	VAL	CA-CB-CG2	-5.65	102.43	110.90
32	J	351	MET	CG-SD-CE	-5.65	91.17	100.20
19	Z	232	TYR	CB-CG-CD1	5.64	124.39	121.00
16	V	266	THR	CA-CB-CG2	-5.64	104.50	112.40
25	U	214	LYS	CB-CA-C	-5.64	99.12	110.40
13	6	35	ASN	CB-CA-C	-5.64	99.13	110.40
19	Z	323	ASN	CB-CG-OD1	5.64	132.87	121.60
25	U	184	VAL	N-CA-CB	5.64	123.90	111.50
19	Z	162	LEU	CB-CG-CD1	5.63	120.58	111.00
30	L	352	PHE	CB-CG-CD2	-5.63	116.86	120.80
3	C	102	GLN	N-CA-CB	5.63	120.74	110.60
20	N	772	TRP	CD2-CE2-CZ2	-5.63	115.54	122.30
22	P	201	ARG	NE-CZ-NH1	-5.63	117.49	120.30
27	H	312	ARG	NE-CZ-NH2	-5.63	117.49	120.30
22	P	198	ASP	CB-CG-OD2	-5.63	113.23	118.30
26	O	198	PHE	CG-CD1-CE1	-5.62	114.61	120.80
4	D	216	VAL	CA-CB-CG2	-5.62	102.47	110.90
22	P	341	PHE	CB-CG-CD1	5.62	124.73	120.80
27	H	111	TYR	CG-CD1-CE1	-5.62	116.80	121.30
13	6	206	PHE	CB-CG-CD1	5.62	124.73	120.80
4	D	9	VAL	N-CA-C	-5.62	95.84	111.00
20	N	751	ARG	NE-CZ-NH1	5.62	123.11	120.30
6	F	221	PHE	CB-CG-CD2	-5.61	116.87	120.80
28	I	438	LEU	CB-CG-CD1	5.61	120.54	111.00
25	U	283	ARG	NE-CZ-NH1	5.61	123.11	120.30
16	V	58	LEU	N-CA-CB	5.61	121.62	110.40
20	N	246	TYR	CG-CD1-CE1	-5.61	116.81	121.30
26	O	127	ASP	CB-CG-OD2	5.61	123.35	118.30
19	Z	866	GLN	CG-CD-OE1	-5.61	110.39	121.60
21	S	281	TRP	CB-CG-CD2	-5.61	119.31	126.60
27	H	395	PHE	CB-CG-CD2	-5.60	116.88	120.80
25	U	232	ASP	CB-CG-OD1	5.60	123.34	118.30
19	Z	718	ASP	CA-C-O	-5.60	108.34	120.10
30	L	239	HIS	CA-CB-CG	-5.59	104.09	113.60
31	M	441	TYR	CB-CG-CD1	-5.59	117.64	121.00
19	Z	45	LEU	CB-CG-CD1	-5.59	101.49	111.00
20	N	723	ASP	CB-CG-OD2	5.59	123.33	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	861	THR	CA-CB-CG2	-5.59	104.57	112.40
23	Q	88	LEU	CB-CA-C	-5.59	99.58	110.20
28	I	417	GLU	OE1-CD-OE2	5.59	130.01	123.30
11	4	120	TYR	CG-CD1-CE1	-5.59	116.83	121.30
15	W	1	MET	CG-SD-CE	-5.59	91.26	100.20
4	D	112	TYR	CB-CG-CD2	5.58	124.35	121.00
32	J	78	ARG	NE-CZ-NH1	5.58	123.09	120.30
6	F	6	TYR	CD1-CE1-CZ	-5.58	114.78	119.80
6	F	122	ARG	NE-CZ-NH2	5.58	123.09	120.30
16	V	263	ASP	CB-CG-OD1	5.58	123.32	118.30
31	M	209	MET	CB-CA-C	-5.58	99.24	110.40
11	4	117	TYR	CB-CG-CD2	-5.58	117.65	121.00
7	G	22	PHE	CB-CG-CD2	-5.58	116.90	120.80
27	H	226	ALA	N-CA-CB	5.58	117.91	110.10
26	O	226	ARG	NE-CZ-NH2	-5.58	117.51	120.30
31	M	412	ARG	NE-CZ-NH2	-5.58	117.51	120.30
30	L	150	GLY	CA-C-O	5.57	130.63	120.60
6	F	51	ARG	NE-CZ-NH1	5.57	123.08	120.30
26	O	138	VAL	CA-CB-CG1	5.57	119.25	110.90
30	L	238	ASP	CB-CA-C	-5.57	99.26	110.40
14	7	101	TYR	N-CA-CB	5.57	120.62	110.60
14	7	121	PHE	CB-CG-CD2	-5.57	116.90	120.80
19	Z	250	ARG	NE-CZ-NH2	-5.57	117.52	120.30
14	7	104	PHE	CZ-CE2-CD2	-5.56	113.42	120.10
31	M	74	ASP	CB-CG-OD1	5.56	123.31	118.30
2	B	163	MET	C-N-CA	5.56	133.98	122.30
26	O	363	MET	CA-CB-CG	5.56	122.75	113.30
23	Q	411	VAL	CG1-CB-CG2	5.56	119.79	110.90
12	5	74	ALA	CB-CA-C	-5.56	101.77	110.10
15	W	57	ASP	CB-CG-OD1	-5.55	113.30	118.30
20	N	92	ASP	CB-CG-OD2	-5.55	113.30	118.30
24	R	155	ASP	CB-CG-OD2	-5.55	113.30	118.30
6	F	224	TYR	CB-CG-CD1	-5.55	117.67	121.00
13	6	102	TYR	CB-CG-CD1	-5.55	117.67	121.00
3	C	9	THR	CA-CB-CG2	-5.55	104.63	112.40
20	N	144	ASP	CB-CA-C	-5.55	99.30	110.40
23	Q	397	TYR	CZ-CE2-CD2	5.55	124.79	119.80
19	Z	515	ALA	N-CA-CB	-5.54	102.34	110.10
24	R	192	ARG	NH1-CZ-NH2	5.54	125.50	119.40
28	I	184	TYR	CB-CG-CD1	-5.54	117.67	121.00
19	Z	646	MET	CG-SD-CE	-5.54	91.33	100.20
5	E	146	VAL	CA-CB-CG1	5.54	119.21	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	M	234	THR	CA-CB-CG2	-5.54	104.64	112.40
25	U	203	SER	O-C-N	5.54	131.56	122.70
26	O	96	PHE	CB-CG-CD1	-5.54	116.92	120.80
27	H	43	ARG	NE-CZ-NH1	5.54	123.07	120.30
7	G	72	ARG	NE-CZ-NH1	5.54	123.07	120.30
9	2	167	TYR	CZ-CE2-CD2	-5.54	114.82	119.80
22	P	156	ASN	N-CA-CB	5.53	120.56	110.60
23	Q	187	ARG	NE-CZ-NH2	-5.53	117.53	120.30
9	2	220	VAL	N-CA-C	-5.53	96.07	111.00
23	Q	263	THR	N-CA-C	-5.53	96.06	111.00
28	I	275	GLU	OE1-CD-OE2	5.53	129.94	123.30
9	2	245	TYR	CG-CD2-CE2	5.53	125.72	121.30
31	M	373	SER	C-N-CA	5.53	135.52	121.70
14	7	154	LYS	N-CA-C	-5.53	96.08	111.00
16	V	245	VAL	CA-CB-CG1	-5.53	102.61	110.90
6	F	81	ALA	CB-CA-C	-5.52	101.81	110.10
2	B	54	SER	O-C-N	5.52	131.54	122.70
5	E	15	PHE	CB-CG-CD2	-5.52	116.93	120.80
20	N	770	TRP	CB-CG-CD2	-5.52	119.42	126.60
27	H	310	ASP	O-C-N	-5.52	110.61	121.10
26	O	118	ILE	CA-CB-CG1	5.52	121.49	111.00
3	C	184	MET	CG-SD-CE	-5.52	91.38	100.20
21	S	437	ALA	CB-CA-C	5.51	118.37	110.10
13	6	170	ALA	N-CA-CB	5.51	117.82	110.10
14	7	115	VAL	O-C-N	-5.51	113.88	122.70
20	N	246	TYR	CB-CG-CD1	-5.51	117.69	121.00
7	G	186	THR	CA-CB-CG2	-5.51	104.69	112.40
19	Z	232	TYR	CG-CD1-CE1	-5.51	116.89	121.30
19	Z	314	TYR	CA-CB-CG	-5.51	102.93	113.40
7	G	9	ASP	CB-CG-OD2	-5.51	113.34	118.30
9	2	251	THR	N-CA-CB	5.51	120.76	110.30
22	P	131	VAL	CG1-CB-CG2	-5.51	102.09	110.90
30	L	107	LYS	CB-CA-C	-5.51	99.39	110.40
30	L	247	ASP	CB-CG-OD1	-5.51	113.34	118.30
20	N	129	ARG	NE-CZ-NH2	-5.50	117.55	120.30
12	5	163	TRP	CA-CB-CG	5.50	124.16	113.70
20	N	744	VAL	CA-CB-CG2	-5.50	102.65	110.90
5	E	29	GLU	CB-CA-C	5.50	121.41	110.40
19	Z	137	ARG	NE-CZ-NH1	5.50	123.05	120.30
20	N	395	ARG	NE-CZ-NH1	5.50	123.05	120.30
12	5	172	TYR	CG-CD1-CE1	-5.50	116.90	121.30
28	I	376	ASP	CB-CG-OD2	5.50	123.25	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	U	106	ILE	O-C-N	5.50	131.50	122.70
2	B	177	ARG	NE-CZ-NH2	5.50	123.05	120.30
14	7	202	PRO	N-CA-CB	5.49	109.89	103.30
16	V	224	SER	CB-CA-C	-5.49	99.66	110.10
22	P	289	ARG	NE-CZ-NH2	5.49	123.05	120.30
7	G	60	GLU	N-CA-C	-5.49	96.17	111.00
20	N	636	VAL	CA-CB-CG2	-5.49	102.66	110.90
4	D	74	ALA	C-N-CA	5.49	135.42	121.70
13	6	52	SER	N-CA-CB	5.49	118.73	110.50
13	6	153	PRO	N-CD-CG	5.49	111.43	103.20
18	Y	65	TYR	CG-CD2-CE2	-5.49	116.91	121.30
8	1	58	TYR	CB-CG-CD1	5.49	124.29	121.00
12	5	148	GLN	CB-CA-C	-5.49	99.43	110.40
16	V	235	SER	N-CA-CB	5.48	118.73	110.50
21	S	485	MET	CA-CB-CG	5.48	122.62	113.30
26	O	72	ASN	N-CA-CB	5.48	120.47	110.60
32	J	370	ALA	CB-CA-C	-5.48	101.88	110.10
1	A	191	PHE	CB-CG-CD1	-5.48	116.96	120.80
22	P	340	VAL	CA-CB-CG1	5.48	119.12	110.90
32	J	271	ARG	NE-CZ-NH2	-5.48	117.56	120.30
2	B	102	GLN	N-CA-CB	5.48	120.46	110.60
8	1	153	MET	CG-SD-CE	-5.48	91.43	100.20
1	A	212	PRO	CA-C-N	5.48	129.25	117.20
12	5	236	TYR	CB-CG-CD1	5.48	124.29	121.00
21	S	260	TYR	CB-CG-CD1	5.48	124.29	121.00
23	Q	389	ASP	CB-CA-C	-5.48	99.44	110.40
25	U	242	LEU	CB-CG-CD1	5.48	120.31	111.00
25	U	249	PHE	CB-CG-CD2	-5.48	116.97	120.80
32	J	231	VAL	CA-CB-CG2	5.48	119.12	110.90
6	F	9	ASP	CA-CB-CG	-5.47	101.36	113.40
11	4	57	ALA	CB-CA-C	-5.47	101.89	110.10
17	T	266	LEU	CB-CG-CD1	5.47	120.31	111.00
19	Z	158	TYR	CB-CG-CD1	5.47	124.28	121.00
28	I	210	TYR	CG-CD1-CE1	5.47	125.68	121.30
3	C	207	SER	N-CA-CB	5.47	118.71	110.50
20	N	394	ALA	CB-CA-C	-5.47	101.89	110.10
15	W	143	PHE	CB-CG-CD1	-5.47	116.97	120.80
29	K	250	VAL	CA-CB-CG1	5.47	119.11	110.90
27	H	76	ALA	N-CA-CB	5.47	117.76	110.10
12	5	141	LEU	CB-CG-CD1	5.47	120.29	111.00
5	E	20	ARG	CG-CD-NE	-5.46	100.33	111.80
20	N	474	ARG	NE-CZ-NH1	5.46	123.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	124	ILE	CA-CB-CG1	5.46	121.38	111.00
27	H	310	ASP	CB-CG-OD1	-5.46	113.39	118.30
17	T	296	PHE	CB-CG-CD2	5.46	124.62	120.80
19	Z	416	MET	CA-CB-CG	5.46	122.58	113.30
5	E	18	GLU	C-N-CA	5.46	133.76	122.30
11	4	19	ARG	NE-CZ-NH1	5.46	123.03	120.30
12	5	63	LEU	CB-CG-CD1	5.46	120.28	111.00
19	Z	366	ASP	C-N-CA	5.46	135.35	121.70
17	T	318	TYR	CG-CD1-CE1	-5.46	116.94	121.30
20	N	224	ASP	CB-CG-OD2	-5.45	113.39	118.30
28	I	206	THR	CA-CB-CG2	-5.45	104.77	112.40
16	V	207	TYR	CB-CG-CD1	5.45	124.27	121.00
12	5	258	TYR	CZ-CE2-CD2	5.45	124.70	119.80
5	E	24	VAL	CA-CB-CG2	-5.45	102.73	110.90
20	N	453	HIS	CA-CB-CG	-5.45	104.34	113.60
27	H	391	GLU	C-N-CA	5.45	135.32	121.70
19	Z	715	HIS	C-N-CA	5.45	135.32	121.70
31	M	441	TYR	CD1-CG-CD2	5.45	123.89	117.90
22	P	415	PHE	CB-CG-CD1	-5.45	116.99	120.80
24	R	245	GLU	N-CA-CB	5.45	120.40	110.60
2	B	101	TYR	CA-CB-CG	-5.44	103.06	113.40
12	5	128	ARG	NH1-CZ-NH2	-5.44	113.42	119.40
22	P	436	MET	CB-CA-C	-5.44	99.52	110.40
7	G	103	PHE	CD1-CG-CD2	-5.44	111.23	118.30
26	O	122	LYS	N-CA-CB	5.44	120.39	110.60
29	K	191	TYR	CB-CG-CD1	5.44	124.26	121.00
10	3	45	MET	C-N-CA	-5.44	110.89	122.30
12	5	171	TYR	CB-CG-CD1	-5.44	117.74	121.00
20	N	254	GLU	OE1-CD-OE2	-5.44	116.78	123.30
19	Z	554	TYR	CG-CD1-CE1	-5.43	116.95	121.30
12	5	116	ARG	CG-CD-NE	-5.43	100.39	111.80
30	L	170	PRO	N-CA-CB	-5.43	96.62	102.60
19	Z	505	MET	N-CA-CB	5.43	120.38	110.60
27	H	227	ARG	NE-CZ-NH2	5.43	123.02	120.30
28	I	377	ASP	CB-CG-OD1	-5.43	113.41	118.30
24	R	226	VAL	CA-CB-CG2	5.43	119.05	110.90
8	1	221	VAL	N-CA-C	-5.43	96.34	111.00
22	P	198	ASP	CB-CG-OD1	5.43	123.19	118.30
25	U	68	TRP	CE2-CD2-CE3	5.43	125.21	118.70
3	C	214	ALA	CB-CA-C	-5.43	101.96	110.10
20	N	778	PHE	CB-CG-CD1	-5.43	117.00	120.80
29	K	394	VAL	CA-CB-CG2	-5.42	102.77	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
19	Z	445	LEU	CB-CG-CD2	5.42	120.22	111.00
21	S	129	PRO	O-C-N	5.42	131.37	122.70
24	R	311	TYR	CG-CD2-CE2	-5.42	116.96	121.30
19	Z	757	ASN	C-N-CA	5.42	135.25	121.70
4	D	123	ARG	NE-CZ-NH1	5.42	123.01	120.30
11	4	48	GLY	O-C-N	5.42	131.37	122.70
23	Q	175	LYS	N-CA-CB	5.42	120.35	110.60
23	Q	201	TYR	CB-CG-CD2	5.42	124.25	121.00
31	M	389	ARG	CA-CB-CG	-5.42	101.48	113.40
7	G	103	PHE	CB-CG-CD1	5.42	124.59	120.80
22	P	369	TYR	CD1-CE1-CZ	-5.41	114.93	119.80
5	E	129	ASP	CB-CG-OD2	-5.41	113.43	118.30
8	1	147	VAL	CA-CB-CG2	5.41	119.02	110.90
21	S	144	ARG	NE-CZ-NH2	-5.41	117.59	120.30
10	3	187	VAL	CG1-CB-CG2	-5.41	102.25	110.90
24	R	68	ASP	CA-CB-CG	-5.41	101.50	113.40
25	U	151	THR	CA-CB-CG2	-5.41	104.83	112.40
31	M	418	LEU	N-CA-CB	5.41	121.21	110.40
8	1	162	GLY	O-C-N	5.41	131.35	122.70
24	R	153	ASP	O-C-N	5.41	131.35	122.70
27	H	130	ALA	CB-CA-C	-5.41	101.99	110.10
27	H	234	ASP	CB-CG-OD1	5.41	123.16	118.30
16	V	104	ARG	NE-CZ-NH2	-5.40	117.60	120.30
6	F	224	TYR	CB-CG-CD2	5.40	124.24	121.00
19	Z	875	ALA	N-CA-CB	5.40	117.66	110.10
5	E	156	MET	CG-SD-CE	-5.40	91.56	100.20
11	4	85	ARG	NE-CZ-NH1	5.40	123.00	120.30
31	M	257	PRO	N-CA-CB	5.40	109.78	103.30
31	M	313	MET	CG-SD-CE	-5.40	91.56	100.20
20	N	772	TRP	NE1-CE2-CZ2	5.40	136.34	130.40
20	N	253	TYR	CZ-CE2-CD2	5.39	124.66	119.80
13	6	149	TYR	CB-CG-CD2	-5.39	117.76	121.00
20	N	325	MET	C-N-CA	5.39	135.18	121.70
29	K	302	ASN	CA-CB-CG	5.39	125.26	113.40
11	4	161	ARG	NE-CZ-NH2	-5.39	117.61	120.30
31	M	374	ARG	NE-CZ-NH1	5.39	122.99	120.30
20	N	425	THR	CA-CB-OG1	5.39	120.31	109.00
24	R	364	TRP	CB-CG-CD2	-5.39	119.60	126.60
20	N	158	ARG	NE-CZ-NH2	-5.38	117.61	120.30
27	H	43	ARG	CA-CB-CG	5.38	125.25	113.40
27	H	133	ASP	CB-CG-OD1	5.38	123.15	118.30
20	N	769	PHE	CB-CG-CD2	5.38	124.57	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	916	ASP	CB-CG-OD1	-5.38	113.46	118.30
21	S	64	ASP	N-CA-CB	5.38	120.29	110.60
19	Z	300	ARG	N-CA-CB	-5.38	100.91	110.60
26	O	67	PHE	N-CA-CB	5.38	120.29	110.60
3	C	215	THR	OG1-CB-CG2	-5.38	97.63	110.00
10	3	112	LEU	N-CA-C	-5.38	96.48	111.00
20	N	341	PHE	CB-CG-CD2	-5.38	117.04	120.80
29	K	175	GLN	CG-CD-OE1	-5.38	110.85	121.60
10	3	51	ILE	N-CA-CB	5.38	123.16	110.80
27	H	123	VAL	CA-CB-CG1	-5.38	102.84	110.90
13	6	190	HIS	CA-CB-CG	5.37	122.73	113.60
29	K	403	TYR	CZ-CE2-CD2	-5.37	114.96	119.80
31	M	378	VAL	O-C-N	5.37	131.30	122.70
11	4	84	THR	N-CA-CB	5.37	120.51	110.30
17	T	170	TYR	CB-CG-CD2	5.37	124.22	121.00
21	S	207	TYR	CB-CG-CD2	-5.37	117.78	121.00
29	K	315	ASP	CB-CG-OD1	5.37	123.13	118.30
17	T	262	PHE	CB-CG-CD1	5.37	124.56	120.80
24	R	247	LEU	N-CA-CB	5.37	121.14	110.40
3	C	69	ASN	CB-CG-OD1	-5.37	110.86	121.60
20	N	900	TYR	CD1-CG-CD2	5.37	123.80	117.90
20	N	598	ALA	CB-CA-C	-5.37	102.05	110.10
22	P	270	VAL	CA-CB-CG2	-5.37	102.85	110.90
24	R	340	ALA	CB-CA-C	-5.37	102.05	110.10
28	I	82	GLN	O-C-N	-5.37	114.12	122.70
20	N	128	GLN	CA-CB-CG	5.36	125.20	113.40
27	H	121	PHE	CB-CG-CD1	5.36	124.55	120.80
14	7	74	TYR	CB-CG-CD1	-5.36	117.78	121.00
17	T	117	GLU	O-C-N	5.36	131.28	122.70
20	N	890	LYS	N-CA-CB	5.36	120.25	110.60
3	C	159	TRP	CG-CD2-CE3	-5.36	129.08	133.90
28	I	166	ASP	C-N-CA	5.36	135.09	121.70
11	4	128	PRO	N-CD-CG	5.36	111.23	103.20
14	7	253	TRP	CB-CG-CD1	5.36	133.96	127.00
22	P	224	LEU	CB-CG-CD2	5.36	120.10	111.00
21	S	316	THR	CA-CB-CG2	-5.35	104.91	112.40
3	C	132	VAL	CB-CA-C	-5.35	101.24	111.40
19	Z	432	TYR	CB-CG-CD1	5.35	124.21	121.00
25	U	232	ASP	CB-CG-OD2	-5.35	113.49	118.30
27	H	403	ILE	CA-CB-CG1	5.35	121.16	111.00
8	1	177	ARG	NH1-CZ-NH2	-5.35	113.52	119.40
13	6	213	ASP	CB-CG-OD1	5.34	123.11	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	264	ASP	CB-CG-OD1	5.34	123.11	118.30
19	Z	357	ARG	NE-CZ-NH1	5.34	122.97	120.30
20	N	590	TYR	CG-CD2-CE2	5.34	125.58	121.30
21	S	216	PHE	CB-CG-CD1	-5.34	117.06	120.80
30	L	63	ALA	N-CA-CB	5.34	117.58	110.10
23	Q	231	TYR	CB-CG-CD2	-5.34	117.79	121.00
19	Z	801	VAL	C-N-CA	5.34	135.06	121.70
20	N	713	TYR	CG-CD1-CE1	5.34	125.57	121.30
27	H	80	LEU	CB-CG-CD2	-5.34	101.92	111.00
31	M	419	THR	CA-CB-OG1	5.34	120.22	109.00
5	E	20	ARG	NE-CZ-NH2	-5.34	117.63	120.30
7	G	125	LEU	CB-CG-CD2	5.34	120.08	111.00
29	K	411	GLU	CA-CB-CG	5.34	125.15	113.40
19	Z	858	LYS	CA-C-O	-5.34	108.89	120.10
28	I	259	TYR	CG-CD2-CE2	5.34	125.57	121.30
3	C	194	VAL	CG1-CB-CG2	5.33	119.43	110.90
14	7	222	TYR	CD1-CG-CD2	5.33	123.77	117.90
26	O	206	LEU	CB-CA-C	-5.33	100.06	110.20
21	S	124	ARG	C-N-CA	5.33	135.03	121.70
5	E	208	GLU	OE1-CD-OE2	-5.33	116.91	123.30
6	F	35	THR	CA-CB-CG2	-5.33	104.94	112.40
7	G	173	ALA	N-CA-CB	5.33	117.56	110.10
17	T	232	PRO	N-CD-CG	5.33	111.19	103.20
19	Z	539	LEU	CB-CG-CD2	5.33	120.06	111.00
7	G	48	PHE	CB-CG-CD2	-5.33	117.07	120.80
26	O	137	ASP	CB-CG-OD2	-5.33	113.51	118.30
6	F	214	ILE	CA-CB-CG1	5.32	121.12	111.00
13	6	199	MET	CG-SD-CE	-5.32	91.68	100.20
24	R	337	PHE	CG-CD2-CE2	-5.32	114.94	120.80
10	3	1	MET	CG-SD-CE	-5.32	91.68	100.20
23	Q	302	PHE	CB-CG-CD1	-5.32	117.07	120.80
15	W	165	GLY	CA-C-O	-5.32	111.02	120.60
31	M	171	TYR	CD1-CE1-CZ	-5.32	115.01	119.80
2	B	222	THR	CA-CB-OG1	5.32	120.17	109.00
22	P	407	ASP	CB-CG-OD1	-5.32	113.52	118.30
29	K	417	TYR	CB-CA-C	-5.32	99.76	110.40
23	Q	85	ALA	CB-CA-C	-5.32	102.13	110.10
5	E	32	LYS	N-CA-CB	5.31	120.17	110.60
9	2	49	VAL	N-CA-C	-5.31	96.66	111.00
28	I	191	ASP	CB-CG-OD1	5.31	123.08	118.30
19	Z	600	TYR	CD1-CG-CD2	5.31	123.74	117.90
20	N	220	LEU	CB-CG-CD2	5.31	120.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	410	VAL	CA-CB-CG2	-5.31	102.94	110.90
23	Q	34	ASP	N-CA-CB	5.31	120.16	110.60
8	1	225	ASP	CB-CG-OD1	-5.31	113.52	118.30
26	O	85	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
21	S	145	PRO	N-CA-CB	5.31	109.67	103.30
19	Z	533	ASP	N-CA-CB	5.30	120.15	110.60
22	P	4	GLY	N-CA-C	-5.30	99.84	113.10
32	J	63	LEU	CB-CG-CD2	5.30	120.02	111.00
20	N	815	ALA	N-CA-C	5.30	125.31	111.00
28	I	359	LYS	N-CA-CB	5.30	120.14	110.60
14	7	228	TYR	CB-CG-CD1	-5.30	117.82	121.00
21	S	165	LEU	CB-CG-CD2	5.30	120.01	111.00
23	Q	55	SER	CB-CA-C	-5.30	100.03	110.10
27	H	304	ASN	CB-CA-C	-5.30	99.80	110.40
29	K	339	ARG	NE-CZ-NH1	5.30	122.95	120.30
30	L	247	ASP	CB-CG-OD2	5.30	123.07	118.30
8	1	206	VAL	C-N-CA	5.30	134.94	121.70
20	N	882	ALA	N-CA-CB	5.30	117.52	110.10
9	2	228	PHE	CB-CG-CD2	-5.30	117.09	120.80
14	7	253	TRP	CB-CG-CD2	-5.30	119.72	126.60
26	O	244	ASP	CB-CG-OD2	-5.30	113.53	118.30
29	K	287	ARG	CD-NE-CZ	-5.30	116.19	123.60
32	J	250	GLU	N-CA-C	-5.29	96.70	111.00
8	1	209	LEU	N-CA-C	-5.29	96.71	111.00
13	6	146	GLY	C-N-CA	5.29	134.93	121.70
17	T	188	SER	CB-CA-C	-5.29	100.05	110.10
2	B	185	GLU	OE1-CD-OE2	5.29	129.65	123.30
15	W	21	PHE	CG-CD1-CE1	-5.29	114.98	120.80
19	Z	380	PHE	CB-CG-CD2	-5.29	117.10	120.80
2	B	147	PHE	CB-CG-CD2	5.29	124.50	120.80
1	A	125	TYR	CZ-CE2-CD2	5.29	124.56	119.80
13	6	53	ASP	CB-CG-OD1	-5.29	113.54	118.30
9	2	255	LEU	CB-CG-CD2	5.28	119.98	111.00
20	N	109	THR	O-C-N	-5.28	114.25	122.70
22	P	450	GLU	OE1-CD-OE2	5.28	129.64	123.30
20	N	138	PHE	CB-CG-CD2	5.28	124.50	120.80
21	S	82	VAL	CG1-CB-CG2	-5.28	102.45	110.90
21	S	176	ARG	NE-CZ-NH1	5.28	122.94	120.30
26	O	156	TYR	CB-CG-CD2	-5.28	117.83	121.00
26	O	220	PRO	CA-N-CD	-5.28	104.11	111.50
12	5	208	VAL	CG1-CB-CG2	-5.28	102.46	110.90
32	J	226	GLU	O-C-N	-5.27	114.23	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	G	31	VAL	CA-CB-CG2	5.27	118.81	110.90
13	6	85	HIS	N-CA-CB	5.27	120.09	110.60
14	7	175	ALA	N-CA-CB	5.27	117.48	110.10
31	M	292	ASP	CB-CG-OD2	-5.27	113.56	118.30
6	F	82	ARG	NE-CZ-NH1	5.27	122.94	120.30
11	4	177	THR	CA-CB-CG2	-5.27	105.02	112.40
9	2	221	ILE	N-CA-C	-5.27	96.78	111.00
16	V	121	TRP	CB-CG-CD2	-5.27	119.75	126.60
26	O	172	TYR	CB-CG-CD2	-5.27	117.84	121.00
27	H	292	ASP	CB-CG-OD2	5.27	123.04	118.30
19	Z	143	ARG	N-CA-CB	5.27	120.08	110.60
12	5	241	ASP	CA-CB-CG	-5.26	101.82	113.40
22	P	12	ARG	NE-CZ-NH2	-5.26	117.67	120.30
9	2	129	MET	CG-SD-CE	-5.26	91.78	100.20
10	3	193	ASP	CB-CG-OD2	-5.26	113.56	118.30
3	C	211	VAL	CG1-CB-CG2	5.26	119.32	110.90
21	S	376	ASP	CB-CG-OD2	-5.26	113.57	118.30
22	P	75	TYR	CB-CG-CD1	5.26	124.16	121.00
14	7	123	ASP	CB-CG-OD1	-5.26	113.57	118.30
23	Q	203	PRO	N-CD-CG	5.26	111.09	103.20
3	C	156	TYR	CB-CG-CD2	-5.26	117.85	121.00
10	3	155	GLU	CA-C-N	5.26	131.82	117.10
24	R	23	ARG	NE-CZ-NH2	-5.26	117.67	120.30
20	N	675	MET	CG-SD-CE	-5.25	91.79	100.20
19	Z	432	TYR	CB-CG-CD2	-5.25	117.85	121.00
19	Z	803	PHE	CB-CG-CD2	-5.25	117.12	120.80
22	P	88	MET	CG-SD-CE	-5.25	91.80	100.20
24	R	253	LEU	CB-CG-CD1	5.25	119.93	111.00
31	M	418	LEU	CB-CG-CD1	5.25	119.93	111.00
3	C	227	VAL	N-CA-C	-5.25	96.82	111.00
14	7	201	GLN	N-CA-CB	5.25	120.05	110.60
20	N	916	ASP	CB-CG-OD2	5.25	123.03	118.30
22	P	97	LEU	N-CA-CB	5.25	120.90	110.40
28	I	419	PHE	CB-CG-CD2	-5.25	117.12	120.80
2	B	47	ALA	O-C-N	5.25	131.10	122.70
3	C	179	TYR	CZ-CE2-CD2	-5.25	115.08	119.80
9	2	232	TYR	CB-CG-CD2	-5.25	117.85	121.00
17	T	148	ARG	CB-CA-C	-5.25	99.90	110.40
21	S	414	SER	N-CA-CB	5.25	118.37	110.50
22	P	277	ALA	N-CA-CB	5.25	117.45	110.10
25	U	125	ASP	C-N-CA	5.25	134.82	121.70
6	F	138	ASP	CB-CG-OD2	-5.25	113.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
17	T	340	ARG	CD-NE-CZ	-5.25	116.26	123.60
19	Z	225	ALA	CB-CA-C	-5.25	102.23	110.10
32	J	398	ASN	CB-CG-OD1	-5.25	111.11	121.60
12	5	63	LEU	N-CA-C	5.25	125.16	111.00
28	I	146	PRO	C-N-CA	5.25	133.31	122.30
21	S	479	CYS	N-CA-CB	5.24	120.04	110.60
20	N	812	ALA	C-N-CA	5.24	134.81	121.70
3	C	73	ALA	N-CA-CB	5.24	117.44	110.10
27	H	289	ALA	N-CA-CB	5.24	117.44	110.10
2	B	199	PHE	CG-CD1-CE1	5.24	126.56	120.80
8	1	54	THR	N-CA-C	-5.24	96.85	111.00
15	W	49	VAL	CA-CB-CG2	-5.24	103.04	110.90
5	E	116	VAL	CA-CB-CG1	5.24	118.76	110.90
30	L	44	ARG	NE-CZ-NH1	5.24	122.92	120.30
16	V	60	GLU	CG-CD-OE2	-5.24	107.83	118.30
1	A	239	LEU	CB-CG-CD1	5.23	119.90	111.00
29	K	153	MET	CG-SD-CE	-5.23	91.83	100.20
26	O	220	PRO	N-CD-CG	5.23	111.05	103.20
28	I	176	VAL	CA-CB-CG1	-5.23	103.05	110.90
20	N	770	TRP	CA-CB-CG	5.23	123.63	113.70
30	L	134	TYR	CG-CD1-CE1	5.23	125.48	121.30
2	B	229	TYR	CD1-CE1-CZ	-5.23	115.10	119.80
6	F	157	ARG	NE-CZ-NH2	-5.22	117.69	120.30
23	Q	382	GLU	CA-CB-CG	5.22	124.89	113.40
32	J	386	ALA	CB-CA-C	-5.22	102.27	110.10
13	6	55	ARG	NE-CZ-NH2	-5.22	117.69	120.30
24	R	261	PHE	CD1-CE1-CZ	-5.22	113.83	120.10
4	D	218	ARG	CD-NE-CZ	5.22	130.91	123.60
6	F	10	VAL	CB-CA-C	5.22	121.32	111.40
19	Z	32	GLU	OE1-CD-OE2	5.22	129.56	123.30
19	Z	304	PHE	CB-CA-C	-5.22	99.96	110.40
21	S	94	LEU	CB-CG-CD1	5.22	119.87	111.00
21	S	110	TYR	CG-CD2-CE2	-5.22	117.12	121.30
27	H	300	LEU	CB-CG-CD1	5.22	119.87	111.00
29	K	171	ASP	CB-CG-OD1	-5.22	113.60	118.30
24	R	174	TRP	CB-CG-CD2	-5.22	119.82	126.60
11	4	104	LEU	N-CA-C	-5.21	96.92	111.00
14	7	138	ARG	CG-CD-NE	-5.21	100.85	111.80
27	H	74	PRO	N-CD-CG	5.21	111.02	103.20
11	4	182	VAL	CA-CB-CG1	-5.21	103.08	110.90
7	G	99	PHE	CB-CG-CD1	5.21	124.45	120.80
20	N	96	TYR	CG-CD2-CE2	-5.21	117.13	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
21	S	167	MET	CA-CB-CG	5.21	122.16	113.30
10	3	205	ASP	N-CA-CB	5.21	119.97	110.60
14	7	195	ARG	NE-CZ-NH2	5.21	122.91	120.30
19	Z	803	PHE	CB-CG-CD1	5.21	124.45	120.80
25	U	190	ARG	NE-CZ-NH1	-5.21	117.69	120.30
29	K	398	ASP	CB-CG-OD2	-5.21	113.61	118.30
4	D	155	PRO	N-CA-CB	5.21	109.55	103.30
9	2	229	LEU	N-CA-C	-5.21	96.94	111.00
19	Z	332	ALA	N-CA-C	-5.21	96.94	111.00
18	Y	65	TYR	CB-CG-CD2	-5.21	117.88	121.00
12	5	195	PHE	CD1-CE1-CZ	-5.20	113.86	120.10
19	Z	45	LEU	CB-CA-C	-5.20	100.31	110.20
19	Z	716	ASP	CB-CG-OD1	5.20	122.98	118.30
21	S	197	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
27	H	41	TYR	CB-CG-CD2	5.20	124.12	121.00
8	1	221	VAL	CG1-CB-CG2	5.20	119.22	110.90
11	4	117	TYR	CA-CB-CG	-5.20	103.52	113.40
4	D	16	LEU	CB-CG-CD1	-5.20	102.16	111.00
13	6	238	ARG	NH1-CZ-NH2	-5.20	113.68	119.40
19	Z	688	ARG	CG-CD-NE	-5.20	100.88	111.80
20	N	250	PHE	CB-CG-CD1	5.20	124.44	120.80
10	3	62	THR	N-CA-CB	5.19	120.17	110.30
28	I	426	VAL	CA-CB-CG2	-5.19	103.11	110.90
12	5	222	ALA	CB-CA-C	-5.19	102.31	110.10
27	H	111	TYR	CB-CG-CD1	5.19	124.12	121.00
27	H	339	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
32	J	306	LEU	O-C-N	-5.19	114.39	122.70
12	5	92	LYS	N-CA-CB	5.19	119.94	110.60
31	M	384	TYR	CG-CD1-CE1	-5.19	117.15	121.30
10	3	31	GLN	N-CA-CB	5.19	119.94	110.60
19	Z	842	VAL	CA-CB-CG1	-5.19	103.12	110.90
21	S	346	GLN	CG-CD-OE1	-5.19	111.22	121.60
23	Q	278	ARG	NE-CZ-NH1	5.19	122.89	120.30
5	E	217	LEU	CB-CA-C	-5.19	100.34	110.20
8	1	112	ALA	CB-CA-C	-5.19	102.32	110.10
16	V	82	VAL	CA-CB-CG2	5.19	118.68	110.90
23	Q	238	GLY	O-C-N	5.19	131.00	122.70
27	H	285	PHE	CB-CG-CD2	5.19	124.43	120.80
31	M	229	TYR	CG-CD1-CE1	-5.19	117.15	121.30
13	6	54	THR	N-CA-C	-5.18	97.00	111.00
14	7	169	VAL	CA-CB-CG1	5.18	118.68	110.90
21	S	385	ASP	CB-CG-OD2	-5.18	113.63	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	76	ALA	N-CA-CB	5.18	117.36	110.10
26	O	319	LEU	CB-CA-C	-5.18	100.35	110.20
27	H	217	PRO	N-CA-CB	5.18	109.52	103.30
32	J	43	ARG	O-C-N	-5.18	114.41	122.70
13	6	140	LEU	N-CA-C	-5.18	97.01	111.00
13	6	200	ARG	CD-NE-CZ	-5.18	116.35	123.60
22	P	261	ASP	CB-CG-OD2	-5.18	113.64	118.30
4	D	73	PHE	CG-CD1-CE1	-5.18	115.10	120.80
5	E	230	THR	CA-CB-CG2	-5.18	105.15	112.40
6	F	18	ARG	O-C-N	-5.18	114.41	122.70
5	E	126	GLU	N-CA-CB	5.18	119.92	110.60
19	Z	878	GLU	CB-CG-CD	-5.18	100.21	114.20
21	S	359	LEU	CB-CG-CD1	5.18	119.81	111.00
28	I	290	ILE	CA-CB-CG1	5.18	120.84	111.00
17	T	96	GLY	N-CA-C	-5.18	100.16	113.10
19	Z	564	LEU	CB-CA-C	-5.18	100.36	110.20
13	6	215	TYR	CD1-CE1-CZ	-5.18	115.14	119.80
26	O	289	ARG	NE-CZ-NH2	-5.18	117.71	120.30
32	J	113	ARG	NE-CZ-NH2	-5.18	117.71	120.30
4	D	159	TYR	CB-CG-CD1	5.17	124.11	121.00
18	Y	70	SER	N-CA-CB	5.17	118.26	110.50
20	N	899	ARG	C-N-CA	5.17	134.63	121.70
27	H	105	ASP	CB-CG-OD1	5.17	122.96	118.30
5	E	87	THR	CA-CB-CG2	-5.17	105.16	112.40
1	A	86	ASP	CB-CG-OD1	-5.17	113.65	118.30
2	B	161	THR	N-CA-CB	5.17	120.12	110.30
19	Z	349	TYR	CB-CG-CD2	5.17	124.10	121.00
22	P	45	GLU	N-CA-CB	5.17	119.90	110.60
24	R	143	TYR	CG-CD2-CE2	-5.17	117.17	121.30
32	J	226	GLU	CA-C-N	5.17	126.53	116.20
13	6	102	TYR	CG-CD1-CE1	-5.17	117.17	121.30
25	U	267	ARG	NE-CZ-NH1	5.17	122.88	120.30
15	W	42	ARG	C-N-CA	5.16	134.61	121.70
17	T	302	MET	CA-CB-CG	5.16	122.08	113.30
26	O	321	ARG	NE-CZ-NH1	-5.16	117.72	120.30
30	L	331	ALA	C-N-CA	5.16	133.14	122.30
32	J	148	TYR	CB-CG-CD2	-5.16	117.90	121.00
28	I	295	TYR	CA-CB-CG	-5.16	103.59	113.40
29	K	342	ARG	NE-CZ-NH1	5.16	122.88	120.30
12	5	224	TYR	CB-CG-CD2	5.16	124.09	121.00
20	N	51	ASP	CB-CG-OD1	5.16	122.94	118.30
20	N	471	ASP	CB-CG-OD2	5.16	122.94	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	O	366	LEU	CB-CG-CD1	-5.16	102.23	111.00
32	J	402	LYS	CA-CB-CG	5.16	124.75	113.40
27	H	121	PHE	CB-CG-CD2	-5.16	117.19	120.80
29	K	287	ARG	O-C-N	5.16	130.95	122.70
22	P	453	HIS	O-C-N	5.16	130.95	122.70
3	C	103	GLU	N-CA-C	-5.15	97.08	111.00
9	2	187	PRO	C-N-CA	5.15	134.58	121.70
17	T	206	ASN	CA-CB-CG	-5.15	102.06	113.40
5	E	91	LYS	CB-CA-C	-5.15	100.10	110.40
6	F	139	ASP	CB-CG-OD2	5.15	122.94	118.30
17	T	295	PHE	CB-CG-CD1	-5.15	117.19	120.80
24	R	13	LYS	CB-CA-C	-5.15	100.10	110.40
28	I	348	ASP	CB-CG-OD2	-5.15	113.66	118.30
30	L	315	ILE	N-CA-C	-5.15	97.10	111.00
30	L	138	HIS	N-CA-CB	5.15	119.87	110.60
19	Z	267	ARG	CD-NE-CZ	-5.15	116.39	123.60
27	H	39	SER	N-CA-CB	5.15	118.22	110.50
20	N	851	GLU	C-N-CA	5.14	134.56	121.70
24	R	351	ASN	C-N-CA	5.14	134.56	121.70
27	H	394	MET	N-CA-CB	5.14	119.86	110.60
30	L	286	ARG	NE-CZ-NH1	5.14	122.87	120.30
8	1	42	ASP	CB-CG-OD2	-5.14	113.67	118.30
9	2	81	SER	CB-CA-C	5.14	119.86	110.10
17	T	340	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
20	N	639	LEU	CB-CA-C	-5.14	100.44	110.20
24	R	354	VAL	CA-CB-CG2	5.14	118.60	110.90
1	A	23	TYR	CD1-CG-CD2	5.13	123.55	117.90
26	O	294	GLU	OE1-CD-OE2	5.13	129.46	123.30
19	Z	349	TYR	CB-CG-CD1	-5.13	117.92	121.00
22	P	314	LEU	N-CA-CB	5.13	120.66	110.40
2	B	203	MET	O-C-N	5.13	130.91	122.70
6	F	48	ALA	CB-CA-C	-5.13	102.41	110.10
11	4	136	ALA	C-N-CA	5.13	134.53	121.70
7	G	199	TYR	CA-CB-CG	-5.13	103.65	113.40
21	S	465	THR	CA-CB-CG2	-5.13	105.22	112.40
30	L	36	ILE	CA-CB-CG2	-5.13	100.64	110.90
1	A	124	VAL	CA-CB-CG2	-5.13	103.21	110.90
19	Z	420	TRP	N-CA-CB	5.13	119.83	110.60
14	7	213	VAL	CA-CB-CG2	5.12	118.58	110.90
30	L	94	VAL	N-CA-C	-5.12	97.17	111.00
32	J	211	PHE	CB-CG-CD1	-5.12	117.21	120.80
15	W	94	HIS	N-CA-CB	5.12	119.82	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
16	V	174	PRO	N-CD-CG	5.12	110.88	103.20
19	Z	430	ASP	CB-CG-OD1	-5.12	113.69	118.30
24	R	53	TYR	CG-CD1-CE1	-5.12	117.20	121.30
25	U	81	MET	CG-SD-CE	-5.12	92.01	100.20
25	U	120	VAL	CG1-CB-CG2	-5.12	102.71	110.90
20	N	172	ASP	CB-CG-OD1	-5.12	113.69	118.30
25	U	135	THR	N-CA-CB	5.12	120.02	110.30
3	C	136	TYR	CG-CD1-CE1	-5.12	117.21	121.30
5	E	135	ARG	N-CA-CB	5.12	119.81	110.60
7	G	1	MET	CG-SD-CE	-5.12	92.02	100.20
17	T	304	ASP	CB-CG-OD1	-5.12	113.70	118.30
20	N	800	VAL	CG1-CB-CG2	5.12	119.08	110.90
28	I	124	SER	N-CA-C	-5.12	97.19	111.00
31	M	86	ASN	CB-CG-ND2	5.11	128.97	116.70
31	M	241	ARG	NE-CZ-NH1	-5.11	117.74	120.30
7	G	236	ALA	CB-CA-C	-5.11	102.43	110.10
9	2	245	TYR	CB-CG-CD2	5.11	124.07	121.00
22	P	236	HIS	CA-CB-CG	5.11	122.29	113.60
27	H	432	TYR	CG-CD1-CE1	-5.11	117.21	121.30
23	Q	327	TYR	CZ-CE2-CD2	5.11	124.40	119.80
26	O	325	ASP	CB-CA-C	-5.11	100.18	110.40
22	P	350	ARG	NH1-CZ-NH2	5.11	125.02	119.40
32	J	145	ASP	N-CA-CB	5.11	119.79	110.60
19	Z	385	PHE	N-CA-CB	5.10	119.79	110.60
22	P	436	MET	CG-SD-CE	-5.10	92.03	100.20
19	Z	652	VAL	CA-CB-CG2	-5.10	103.25	110.90
23	Q	84	LYS	CA-CB-CG	5.10	124.62	113.40
1	A	9	PHE	CD1-CE1-CZ	5.10	126.22	120.10
14	7	154	LYS	N-CA-CB	5.10	119.78	110.60
16	V	74	ALA	N-CA-CB	5.10	117.24	110.10
31	M	365	ARG	NE-CZ-NH1	-5.10	117.75	120.30
31	M	381	ASP	CB-CG-OD2	5.10	122.89	118.30
28	I	123	VAL	CG1-CB-CG2	-5.10	102.74	110.90
1	A	71	LYS	N-CA-C	-5.10	97.24	111.00
23	Q	401	LEU	N-CA-CB	5.10	120.59	110.40
2	B	155	TYR	CB-CG-CD2	-5.09	117.94	121.00
17	T	327	LYS	CA-C-N	5.09	131.37	117.10
28	I	112	LEU	CB-CG-CD2	-5.09	102.34	111.00
21	S	234	ALA	N-CA-CB	5.09	117.23	110.10
24	R	385	ARG	NE-CZ-NH1	5.09	122.85	120.30
31	M	424	MET	CG-SD-CE	-5.09	92.06	100.20
21	S	445	ALA	O-C-N	5.09	130.84	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
23	Q	69	LEU	CB-CG-CD1	5.09	119.65	111.00
5	E	42	THR	N-CA-C	-5.08	97.27	111.00
22	P	199	TYR	CZ-CE2-CD2	-5.08	115.23	119.80
29	K	205	TYR	CG-CD1-CE1	-5.08	117.23	121.30
5	E	97	GLN	CA-CB-CG	5.08	124.58	113.40
24	R	36	ALA	N-CA-CB	5.08	117.21	110.10
19	Z	494	ARG	N-CA-C	-5.08	97.29	111.00
24	R	49	ASN	C-N-CA	5.08	134.40	121.70
25	U	38	VAL	CB-CA-C	-5.08	101.75	111.40
7	G	207	ASP	CB-CG-OD1	-5.08	113.73	118.30
10	3	151	GLU	OE1-CD-OE2	5.08	129.39	123.30
19	Z	90	THR	CA-CB-CG2	-5.08	105.29	112.40
3	C	51	ASN	N-CA-CB	5.08	119.73	110.60
16	V	207	TYR	CB-CG-CD2	-5.08	117.95	121.00
19	Z	130	ALA	CB-CA-C	-5.08	102.49	110.10
21	S	454	VAL	N-CA-C	-5.08	97.30	111.00
28	I	249	ARG	CG-CD-NE	-5.08	101.14	111.80
31	M	263	PHE	CB-CG-CD2	5.08	124.35	120.80
20	N	181	LEU	CB-CA-C	-5.07	100.56	110.20
32	J	189	TYR	N-CA-CB	5.07	119.73	110.60
1	A	120	ASP	CB-CG-OD1	-5.07	113.74	118.30
9	2	261	PRO	O-C-N	5.07	130.81	122.70
20	N	460	TYR	CA-CB-CG	5.07	123.03	113.40
21	S	290	ARG	NE-CZ-NH1	5.07	122.84	120.30
23	Q	390	GLU	OE1-CD-OE2	-5.07	117.22	123.30
31	M	112	ALA	N-CA-CB	5.07	117.20	110.10
31	M	120	ARG	NH1-CZ-NH2	5.07	124.98	119.40
4	D	190	ASP	CB-CG-OD2	-5.07	113.74	118.30
19	Z	161	HIS	N-CA-CB	5.07	119.72	110.60
6	F	77	LEU	CB-CG-CD2	5.07	119.61	111.00
16	V	224	SER	C-N-CA	5.07	134.36	121.70
19	Z	675	PHE	CG-CD1-CE1	-5.07	115.23	120.80
31	M	226	VAL	CB-CA-C	5.07	121.02	111.40
31	M	394	PHE	N-CA-CB	5.07	119.72	110.60
19	Z	240	VAL	CG1-CB-CG2	-5.06	102.80	110.90
25	U	25	ARG	NE-CZ-NH1	5.06	122.83	120.30
19	Z	42	GLU	C-N-CA	5.06	134.35	121.70
30	L	107	LYS	N-CA-CB	5.06	119.71	110.60
1	A	95	ARG	NE-CZ-NH2	-5.06	117.77	120.30
7	G	199	TYR	CD1-CE1-CZ	5.06	124.35	119.80
31	M	306	ASP	CB-CG-OD2	-5.06	113.75	118.30
2	B	220	ARG	CD-NE-CZ	-5.06	116.52	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	5	TYR	CD1-CE1-CZ	5.06	124.35	119.80
3	C	226	ARG	NE-CZ-NH1	5.06	122.83	120.30
14	7	188	TYR	CD1-CE1-CZ	5.06	124.35	119.80
28	I	197	ILE	CB-CA-C	-5.06	101.49	111.60
3	C	145	PHE	CB-CA-C	-5.05	100.29	110.40
19	Z	386	GLY	N-CA-C	-5.05	100.46	113.10
20	N	344	ARG	NE-CZ-NH1	-5.05	117.77	120.30
12	5	66	LYS	N-CA-CB	5.05	119.69	110.60
7	G	68	PHE	CB-CG-CD2	5.05	124.34	120.80
30	L	19	ARG	NE-CZ-NH2	-5.05	117.77	120.30
30	L	132	LEU	CB-CG-CD1	5.05	119.59	111.00
6	F	57	ALA	N-CA-CB	5.05	117.17	110.10
21	S	419	ALA	N-CA-CB	5.05	117.17	110.10
21	S	122	ALA	N-CA-CB	5.05	117.17	110.10
31	M	49	ARG	NE-CZ-NH2	5.05	122.82	120.30
6	F	101	ARG	NE-CZ-NH1	-5.04	117.78	120.30
13	6	83	GLY	N-CA-C	-5.04	100.49	113.10
17	T	121	ARG	NH1-CZ-NH2	5.04	124.95	119.40
23	Q	72	TYR	CD1-CG-CD2	5.04	123.45	117.90
12	5	220	TYR	CZ-CE2-CD2	5.04	124.34	119.80
20	N	575	ASP	N-CA-CB	5.04	119.68	110.60
23	Q	416	ASN	O-C-N	-5.04	114.63	122.70
1	A	191	PHE	CG-CD1-CE1	-5.04	115.26	120.80
4	D	101	ARG	NE-CZ-NH2	-5.04	117.78	120.30
11	4	27	GLN	CA-CB-CG	5.04	124.48	113.40
16	V	61	PHE	CB-CG-CD2	5.04	124.33	120.80
19	Z	159	VAL	CA-CB-CG2	5.04	118.46	110.90
28	I	208	PRO	N-CD-CG	5.04	110.76	103.20
17	T	184	GLN	CG-CD-OE1	-5.04	111.53	121.60
27	H	392	ALA	N-CA-CB	5.04	117.15	110.10
24	R	298	GLU	OE1-CD-OE2	5.04	129.34	123.30
29	K	69	LYS	CB-CG-CD	5.04	124.69	111.60
13	6	80	GLY	N-CA-C	-5.03	100.51	113.10
19	Z	723	TYR	CG-CD2-CE2	-5.03	117.27	121.30
25	U	257	MET	CG-SD-CE	5.03	108.25	100.20
30	L	27	ARG	NE-CZ-NH1	-5.03	117.78	120.30
31	M	225	GLY	N-CA-C	-5.03	100.52	113.10
2	B	7	SER	N-CA-C	-5.03	97.42	111.00
20	N	502	TYR	CG-CD2-CE2	-5.03	117.28	121.30
20	N	742	HIS	CA-CB-CG	5.03	122.15	113.60
14	7	191	GLN	N-CA-C	5.03	124.58	111.00
16	V	175	ARG	NE-CZ-NH2	-5.03	117.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	122	LEU	CB-CA-C	-5.03	100.64	110.20
2	B	89	ARG	NE-CZ-NH1	-5.03	117.79	120.30
3	C	130	PHE	C-N-CA	5.03	132.86	122.30
10	3	74	TYR	CB-CG-CD1	-5.03	117.98	121.00
12	5	184	ALA	CB-CA-C	-5.03	102.56	110.10
14	7	69	ASP	C-N-CA	5.03	134.27	121.70
19	Z	323	ASN	CB-CG-ND2	-5.03	104.63	116.70
20	N	887	ALA	O-C-N	-5.03	114.66	122.70
31	M	418	LEU	CB-CG-CD2	-5.03	102.45	111.00
19	Z	784	ASP	CB-CG-OD1	-5.03	113.78	118.30
22	P	357	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
24	R	271	PHE	CB-CG-CD2	5.03	124.32	120.80
20	N	911	ILE	N-CA-C	-5.02	97.44	111.00
6	F	161	ILE	CA-CB-CG2	-5.02	100.86	110.90
9	2	115	ARG	CB-CA-C	5.02	120.45	110.40
17	T	331	SER	N-CA-CB	5.02	118.03	110.50
19	Z	865	PHE	CG-CD1-CE1	5.02	126.32	120.80
23	Q	411	VAL	CA-CB-CG1	-5.02	103.37	110.90
27	H	102	ILE	N-CA-CB	5.02	122.35	110.80
27	H	379	ASN	CA-CB-CG	-5.02	102.35	113.40
30	L	257	PHE	CG-CD2-CE2	-5.02	115.28	120.80
21	S	459	MET	CB-CA-C	-5.02	100.36	110.40
24	R	53	TYR	CB-CG-CD2	-5.02	117.99	121.00
2	B	166	ASN	CA-C-N	-5.02	106.16	117.20
4	D	74	ALA	N-CA-CB	5.02	117.13	110.10
10	3	164	PHE	CB-CG-CD1	5.02	124.31	120.80
19	Z	298	LEU	CB-CG-CD1	5.02	119.53	111.00
32	J	4	ASP	CB-CG-OD1	-5.02	113.78	118.30
13	6	215	TYR	CG-CD2-CE2	-5.02	117.29	121.30
26	O	282	PHE	CB-CG-CD2	-5.02	117.29	120.80
12	5	239	ARG	NE-CZ-NH2	-5.01	117.79	120.30
16	V	162	LEU	CB-CG-CD2	-5.01	102.47	111.00
23	Q	314	ARG	NH1-CZ-NH2	-5.01	113.88	119.40
7	G	145	ASP	CB-CG-OD2	5.01	122.81	118.30
19	Z	590	PHE	CB-CG-CD2	5.01	124.31	120.80
26	O	218	MET	CG-SD-CE	-5.01	92.18	100.20
5	E	229	PHE	N-CA-CB	5.01	119.62	110.60
6	F	153	TYR	CB-CG-CD1	5.01	124.01	121.00
10	3	48	ARG	NE-CZ-NH2	5.01	122.81	120.30
14	7	170	ASP	C-N-CA	5.01	134.23	121.70
12	5	80	THR	N-CA-CB	5.01	119.82	110.30
21	S	112	ALA	N-CA-CB	5.01	117.11	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	P	248	ARG	NE-CZ-NH2	5.01	122.81	120.30
30	L	278	MET	CG-SD-CE	-5.01	92.18	100.20
1	A	10	ASP	CB-CA-C	-5.01	100.38	110.40
26	O	255	TRP	CB-CG-CD2	5.01	133.11	126.60
11	4	153	ARG	NE-CZ-NH1	5.00	122.80	120.30
13	6	203	LYS	CB-CA-C	-5.00	100.39	110.40
8	1	152	MET	CG-SD-CE	-5.00	92.19	100.20
11	4	160	LEU	CB-CG-CD1	5.00	119.51	111.00
22	P	384	LEU	CB-CG-CD2	5.00	119.51	111.00
5	E	103	TYR	CD1-CE1-CZ	5.00	124.30	119.80
24	R	304	TYR	CD1-CG-CD2	5.00	123.40	117.90

There are no chirality outliers.

All (291) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	122	ARG	Sidechain
8	1	123	TYR	Sidechain
8	1	124	ARG	Sidechain
8	1	169	TYR	Sidechain
8	1	199	ARG	Sidechain
8	1	94	TYR	Sidechain
9	2	118	ARG	Sidechain
9	2	124	ARG	Sidechain
9	2	154	TYR	Sidechain
9	2	157	TYR	Sidechain
9	2	167	TYR	Sidechain
9	2	85	TYR	Sidechain
10	3	104	TYR	Sidechain
10	3	129	CYS	Peptide
10	3	136	PHE	Sidechain
10	3	147	TYR	Sidechain
10	3	48	ARG	Sidechain
10	3	5	SER	Peptide
10	3	6	TYR	Sidechain
10	3	74	TYR	Sidechain
10	3	80	ARG	Sidechain
11	4	120	TYR	Sidechain
11	4	137	PHE	Sidechain
11	4	153	ARG	Sidechain
11	4	67	TYR	Sidechain
12	5	113	PHE	Sidechain

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Mol	Chain	Res	Type	Group
12	5	116	ARG	Sidechain
12	5	120	ARG	Sidechain
12	5	125	TYR	Sidechain
12	5	128	ARG	Sidechain
12	5	171	TYR	Sidechain
12	5	220	TYR	Sidechain
12	5	236	TYR	Sidechain
12	5	239	ARG	Sidechain
12	5	258	TYR	Sidechain
12	5	62	THR	Peptide
13	6	124	TYR	Sidechain
13	6	131	TYR	Sidechain
13	6	149	TYR	Sidechain
13	6	157	TYR	Sidechain
13	6	159	ARG	Sidechain
13	6	182	PHE	Sidechain
13	6	215	TYR	Sidechain
13	6	29	PHE	Sidechain
13	6	55	ARG	Sidechain
14	7	138	ARG	Sidechain
14	7	168	TYR	Sidechain
14	7	80	PHE	Sidechain
14	7	88	ARG	Sidechain
1	A	103	TYR	Sidechain
1	A	160	TYR	Sidechain
1	A	210	PHE	Sidechain
1	A	227	PHE	Sidechain
1	A	228	ARG	Sidechain
1	A	23	TYR	Sidechain
1	A	88	ARG	Sidechain
1	A	93	ARG	Sidechain
2	B	101	TYR	Sidechain
2	B	128	ARG	Sidechain
2	B	145	TYR	Sidechain
2	B	167	TYR	Sidechain
2	B	197	GLU	Mainchain
2	B	218	PHE	Sidechain
2	B	220	ARG	Sidechain
2	B	229	TYR	Sidechain
2	B	4	ARG	Sidechain
2	B	6	TYR	Sidechain
2	B	76	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	C	101	TYR	Sidechain
3	C	143	TYR	Sidechain
3	C	179	TYR	Sidechain
3	C	226	ARG	Sidechain
3	C	66	TYR	Sidechain
3	C	97	TYR	Sidechain
4	D	10	PHE	Sidechain
4	D	112	TYR	Sidechain
4	D	130	ARG	Sidechain
4	D	144	PHE	Sidechain
4	D	149	ARG	Sidechain
4	D	151	TYR	Sidechain
4	D	218	ARG	Sidechain
4	D	234	TYR	Sidechain
5	E	15	PHE	Sidechain
5	E	185	TYR	Sidechain
6	F	107	ARG	Sidechain
6	F	122	ARG	Sidechain
6	F	137	TYR	Sidechain
6	F	171	TYR	Sidechain
6	F	193	ARG	Sidechain
6	F	239	ARG	Sidechain
6	F	87	PHE	Sidechain
6	F	96	ARG	Sidechain
7	G	115	ARG	Sidechain
7	G	121	HIS	Sidechain
7	G	141	TYR	Sidechain
7	G	15	PHE	Sidechain
7	G	26	TYR	Sidechain
7	G	41	ARG	Sidechain
7	G	68	PHE	Sidechain
7	G	8	TYR	Sidechain
27	H	188	ARG	Sidechain
27	H	258	ARG	Sidechain
27	H	284	ARG	Sidechain
27	H	297	ARG	Sidechain
27	H	323	ARG	Sidechain
27	H	336	ARG	Sidechain
27	H	353	HIS	Sidechain
27	H	386	ARG	Sidechain
27	H	420	TYR	Sidechain
27	H	43	ARG	Sidechain

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Mol	Chain	Res	Type	Group
27	H	97	ARG	Sidechain
28	I	132	TYR	Sidechain
28	I	184	TYR	Sidechain
28	I	259	TYR	Sidechain
28	I	294	ARG	Sidechain
28	I	295	TYR	Sidechain
28	I	322	ARG	Sidechain
28	I	349	ARG	Sidechain
28	I	408	ARG	Sidechain
28	I	439	TYR	Sidechain
28	I	59	ARG	Sidechain
28	I	71	TYR	Sidechain
28	I	80	ARG	Sidechain
32	J	121	TYR	Sidechain
32	J	211	PHE	Sidechain
32	J	213	ARG	Sidechain
32	J	23	TYR	Sidechain
32	J	307	ARG	Sidechain
32	J	310	ARG	Sidechain
32	J	334	ARG	Sidechain
32	J	353	GLY	Peptide
32	J	369	TYR	Sidechain
32	J	383	PHE	Sidechain
32	J	95	PHE	Sidechain
29	K	111	TYR	Sidechain
29	K	188	PHE	Sidechain
29	K	205	TYR	Sidechain
29	K	245	ARG	Sidechain
29	K	287	ARG	Sidechain
29	K	299	PHE	Sidechain
29	K	313	ARG	Sidechain
29	K	366	ARG	Sidechain
29	K	388	ARG	Sidechain
29	K	392	TYR	Sidechain
29	K	403	TYR	Sidechain
30	L	175	ARG	Sidechain
30	L	187	TYR	Sidechain
30	L	199	ARG	Sidechain
30	L	233	PHE	Sidechain
30	L	305	ARG	Sidechain
30	L	311	ARG	Sidechain
30	L	323	ARG	Sidechain

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Mol	Chain	Res	Type	Group
30	L	54	TYR	Sidechain
30	L	92	ARG	Sidechain
30	L	93	TYR	Sidechain
30	L	98	ARG	Sidechain
31	M	160	SER	Peptide
31	M	161	TYR	Sidechain
31	M	183	ARG	Sidechain
31	M	251	PHE	Sidechain
31	M	307	ARG	Sidechain,Peptide
31	M	365	ARG	Sidechain
31	M	91	TYR	Sidechain
20	N	205	TYR	Sidechain
20	N	25	HIS	Sidechain
20	N	253	TYR	Sidechain
20	N	361	ARG	Sidechain
20	N	494	TYR	Sidechain
20	N	502	TYR	Sidechain
20	N	584	TYR	Sidechain
20	N	601	ARG	Sidechain
20	N	627	PHE	Sidechain
20	N	647	HIS	Sidechain
20	N	710	ARG	Sidechain
20	N	751	ARG	Sidechain
20	N	783	TYR	Sidechain
20	N	813	TYR	Sidechain
20	N	931	HIS	Sidechain
20	N	950	TYR	Sidechain
20	N	96	TYR	Sidechain
26	O	155	PHE	Sidechain
26	O	172	TYR	Sidechain
26	O	198	PHE	Sidechain
26	O	211	PHE	Sidechain
26	O	213	PHE	Sidechain
26	O	24	ARG	Sidechain
26	O	352	ARG	Sidechain
26	O	60	TYR	Sidechain
26	O	85	ARG	Sidechain
22	P	12	ARG	Sidechain
22	P	123	ARG	Sidechain
22	P	137	TYR	Sidechain
22	P	142	ARG	Sidechain
22	P	144	ARG	Sidechain

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Mol	Chain	Res	Type	Group
22	P	199	TYR	Sidechain
22	P	324	TYR	Sidechain
22	P	341	PHE	Sidechain
22	P	372	ARG	Sidechain
22	P	65	ARG	Sidechain
22	P	75	TYR	Sidechain
22	P	93	ARG	Sidechain
23	Q	122	ARG	Sidechain
23	Q	231	TYR	Sidechain
23	Q	239	TYR	Sidechain
23	Q	253	TYR	Sidechain
23	Q	337	ARG	Sidechain
23	Q	363	ARG	Sidechain
23	Q	397	TYR	Sidechain
23	Q	415	TYR	Sidechain
23	Q	76	PHE	Sidechain
23	Q	9	PHE	Sidechain
24	R	125	ARG	Sidechain
24	R	128	TYR	Sidechain
24	R	216	TYR	Sidechain
24	R	257	ARG	Sidechain
24	R	259	TYR	Sidechain
24	R	264	TYR	Sidechain
24	R	268	TYR	Sidechain
24	R	304	TYR	Sidechain
24	R	311	TYR	Sidechain
24	R	318	TYR	Sidechain
24	R	379	ARG	Sidechain
24	R	54	TYR	Sidechain
21	S	107	TYR	Sidechain
21	S	124	ARG	Sidechain
21	S	130	PHE	Sidechain
21	S	177	TYR	Sidechain
21	S	196	ARG	Sidechain
21	S	214	TYR	Sidechain
21	S	254	TYR	Sidechain
21	S	257	TYR	Sidechain
21	S	283	ARG	Sidechain
21	S	284	TYR	Sidechain
21	S	286	TYR	Sidechain
21	S	287	TYR	Sidechain
21	S	298	TYR	Sidechain

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Mol	Chain	Res	Type	Group
21	S	303	ARG	Sidechain
21	S	388	TYR	Sidechain
21	S	393	ARG	Sidechain
21	S	432	PHE	Sidechain
21	S	463	TYR	Sidechain
21	S	466	ARG	Sidechain
21	S	475	ARG	Sidechain
21	S	61	ARG	Sidechain
21	S	88	ARG	Sidechain
17	T	107	ARG	Sidechain
17	T	148	ARG	Sidechain
17	T	169	ARG	Sidechain
17	T	170	TYR	Sidechain
17	T	190	TYR	Sidechain
17	T	244	TYR	Sidechain
17	T	282	TYR	Sidechain
17	T	287	PHE	Sidechain
17	T	309	ARG	Sidechain
17	T	319	TYR	Sidechain
17	T	321	PHE	Sidechain
25	U	115	TYR	Sidechain
25	U	12	HIS	Sidechain
25	U	190	ARG	Sidechain
25	U	228	TYR	Sidechain
25	U	245	PHE	Sidechain
25	U	250	TYR	Sidechain
16	V	112	TYR	Sidechain
16	V	207	TYR	Sidechain
16	V	208	ARG	Sidechain
16	V	234	TYR	Sidechain
16	V	65	TYR	Sidechain
15	W	108	ARG	Sidechain
15	W	130	ARG	Sidechain
15	W	70	ARG	Sidechain
18	Y	57	ARG	Sidechain
19	Z	142	TYR	Sidechain
19	Z	181	ARG	Sidechain
19	Z	232	TYR	Sidechain
19	Z	250	ARG	Sidechain
19	Z	261	ARG	Sidechain
19	Z	300	ARG	Sidechain
19	Z	314	TYR	Sidechain

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Mol	Chain	Res	Type	Group
19	Z	33	ARG	Sidechain
19	Z	349	TYR	Sidechain
19	Z	434	TYR	Sidechain
19	Z	489	TYR	Sidechain
19	Z	494	ARG	Sidechain
19	Z	554	TYR	Sidechain
19	Z	680	ARG	Sidechain
19	Z	751	TYR	Sidechain
19	Z	79	ARG	Sidechain
19	Z	807	ARG	Sidechain
19	Z	83	ARG	Sidechain
19	Z	838	ARG	Sidechain

5.2 Too-close contacts ⓘ

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	1920	0	1927	0	0
2	B	1828	0	1823	0	0
3	C	1960	0	1983	0	0
4	D	1926	0	1955	0	0
5	E	1778	0	1756	0	0
6	F	1871	0	1856	0	0
7	G	1912	0	1907	0	0
8	1	1516	0	1485	0	0
9	2	1651	0	1674	0	0
10	3	1600	0	1621	0	0
11	4	1572	0	1575	0	0
12	5	1560	0	1519	0	0
13	6	1659	0	1654	0	0
14	7	1686	0	1662	0	0
15	W	1480	0	1522	0	0
16	V	2272	0	2288	0	0
17	T	2149	0	2170	0	0
18	Y	199	0	180	0	0
19	Z	6913	0	6910	0	0
20	N	7082	0	7121	0	0
21	S	3844	0	3888	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
22	P	3706	0	3817	0	0
23	Q	3335	0	3435	0	0
24	R	3204	0	3204	0	0
25	U	2299	0	2334	0	0
26	O	3011	0	3042	0	0
27	H	3113	0	3162	0	0
28	I	3042	0	3098	0	0
29	K	3125	0	3151	0	0
30	L	3098	0	3171	0	0
31	M	3252	0	3321	0	0
32	J	3194	0	3311	0	0
All	All	82757	0	83522	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

There are no symmetry-related clashes.

5.3 Torsion angles ⓘ

5.3.1 Protein backbone ⓘ

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the backbone conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	244/246 (99%)	233 (96%)	7 (3%)	4 (2%)	11	51
2	B	232/234 (99%)	217 (94%)	13 (6%)	2 (1%)	20	63
3	C	247/261 (95%)	238 (96%)	8 (3%)	1 (0%)	38	77
4	D	244/254 (96%)	230 (94%)	11 (4%)	3 (1%)	15	57
5	E	231/241 (96%)	222 (96%)	9 (4%)	0	100	100
6	F	236/263 (90%)	216 (92%)	18 (8%)	2 (1%)	22	67
7	G	243/255 (95%)	225 (93%)	14 (6%)	4 (2%)	11	51
8	1	200/238 (84%)	169 (84%)	19 (10%)	12 (6%)	2	23

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
9	2	217/277 (78%)	184 (85%)	19 (9%)	14 (6%)	1	22
10	3	203/205 (99%)	167 (82%)	19 (9%)	17 (8%)	1	15
11	4	194/201 (96%)	172 (89%)	12 (6%)	10 (5%)	2	26
12	5	199/263 (76%)	179 (90%)	15 (8%)	5 (2%)	6	41
13	6	211/240 (88%)	182 (86%)	21 (10%)	8 (4%)	4	32
14	7	214/263 (81%)	188 (88%)	18 (8%)	8 (4%)	4	33
15	W	193/377 (51%)	171 (89%)	15 (8%)	7 (4%)	4	33
16	V	287/310 (93%)	264 (92%)	15 (5%)	8 (3%)	6	39
17	T	261/353 (74%)	234 (90%)	23 (9%)	4 (2%)	12	53
18	Y	22/70 (31%)	21 (96%)	1 (4%)	0	100	100
19	Z	894/908 (98%)	805 (90%)	64 (7%)	25 (3%)	6	39
20	N	901/953 (94%)	827 (92%)	50 (6%)	24 (3%)	6	40
21	S	474/530 (89%)	438 (92%)	24 (5%)	12 (2%)	6	41
22	P	454/456 (100%)	422 (93%)	23 (5%)	9 (2%)	9	46
23	Q	420/422 (100%)	390 (93%)	19 (4%)	11 (3%)	6	40
24	R	387/389 (100%)	367 (95%)	15 (4%)	5 (1%)	14	56
25	U	286/320 (89%)	263 (92%)	14 (5%)	9 (3%)	5	37
26	O	374/376 (100%)	346 (92%)	19 (5%)	9 (2%)	7	42
27	H	394/433 (91%)	348 (88%)	38 (10%)	8 (2%)	9	46
28	I	383/440 (87%)	349 (91%)	20 (5%)	14 (4%)	4	33
29	K	389/418 (93%)	356 (92%)	30 (8%)	3 (1%)	22	67
30	L	387/403 (96%)	359 (93%)	21 (5%)	7 (2%)	10	49
31	M	413/442 (93%)	380 (92%)	25 (6%)	8 (2%)	9	47
32	J	404/406 (100%)	369 (91%)	27 (7%)	8 (2%)	9	46
All	All	10438/11447 (91%)	9531 (91%)	646 (6%)	261 (2%)	10	41

All (261) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	D	75	VAL
8	1	45	VAL
8	1	81	SER
8	1	105	GLU
8	1	163	SER

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Mol	Chain	Res	Type
8	1	206	VAL
9	2	75	SER
9	2	81	SER
9	2	91	THR
9	2	172	SER
9	2	189	MET
9	2	251	THR
10	3	31	GLN
10	3	57	ALA
10	3	142	CYS
11	4	3	TYR
11	4	50	ALA
12	5	179	ARG
13	6	85	HIS
13	6	129	PHE
13	6	147	ALA
13	6	168	ALA
14	7	56	LEU
14	7	176	TYR
14	7	242	GLU
16	V	147	PRO
16	V	189	ILE
16	V	219	ASN
19	Z	2	GLU
19	Z	24	ALA
19	Z	175	ASP
19	Z	261	ARG
19	Z	330	PHE
19	Z	332	ALA
19	Z	384	ALA
19	Z	457	ASN
19	Z	802	SER
19	Z	810	ILE
20	N	172	ASP
20	N	701	ILE
20	N	899	ARG
20	N	912	ILE
21	S	55	ALA
21	S	111	LYS
21	S	296	LEU
22	P	335	THR
22	P	340	VAL

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Mol	Chain	Res	Type
22	P	342	SER
23	Q	37	GLU
23	Q	43	VAL
24	R	208	PHE
25	U	5	ALA
25	U	126	VAL
25	U	180	LYS
25	U	184	VAL
26	O	286	ALA
27	H	181	LYS
27	H	248	LYS
28	I	86	LYS
28	I	373	THR
28	I	391	SER
29	K	406	VAL
31	M	282	ALA
2	B	59	GLU
4	D	47	LYS
6	F	151	ALA
8	1	44	GLY
8	1	72	ASP
8	1	143	GLN
8	1	152	MET
8	1	207	ILE
8	1	233	SER
9	2	55	ILE
9	2	150	GLY
9	2	188	ASP
9	2	253	ALA
10	3	30	ILE
10	3	116	THR
10	3	158	MET
10	3	185	VAL
11	4	27	GLN
11	4	131	ALA
12	5	62	THR
13	6	39	VAL
13	6	220	LEU
14	7	65	VAL
14	7	101	TYR
14	7	175	ALA
15	W	188	ILE

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Mol	Chain	Res	Type
16	V	199	HIS
17	T	183	GLU
17	T	258	SER
17	T	340	ARG
19	Z	293	GLN
19	Z	601	ALA
19	Z	773	LYS
20	N	126	ILE
20	N	488	THR
20	N	772	TRP
20	N	806	CYS
20	N	812	ALA
21	S	462	ILE
22	P	93	ARG
22	P	452	ILE
23	Q	17	SER
23	Q	274	LYS
23	Q	375	HIS
24	R	52	PRO
24	R	211	TYR
24	R	344	HIS
25	U	31	ASN
25	U	243	GLN
26	O	49	CYS
27	H	269	ALA
27	H	276	GLU
27	H	308	GLY
27	H	400	ARG
28	I	87	PRO
28	I	127	VAL
28	I	167	THR
28	I	389	ASP
28	I	410	ARG
31	M	108	GLU
31	M	114	ILE
31	M	301	SER
31	M	347	ARG
32	J	9	MET
32	J	120	SER
32	J	228	ALA
32	J	281	ASP
1	A	55	LYS

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Mol	Chain	Res	Type
1	A	65	THR
2	B	199	PHE
4	D	53	LEU
6	F	200	PRO
7	G	8	TYR
7	G	185	MET
8	1	136	TRP
9	2	67	MET
10	3	11	VAL
10	3	41	LYS
11	4	5	ILE
11	4	22	ALA
11	4	177	THR
12	5	108	ALA
12	5	155	SER
12	5	157	GLY
13	6	31	PRO
13	6	48	SER
15	W	18	ASN
15	W	114	GLY
15	W	178	SER
16	V	179	SER
16	V	262	GLU
17	T	96	GLY
19	Z	151	LEU
19	Z	314	TYR
19	Z	508	SER
19	Z	604	GLY
19	Z	703	ARG
19	Z	721	VAL
20	N	471	ASP
20	N	769	PHE
20	N	872	GLU
20	N	873	PRO
20	N	880	ASN
21	S	125	ASP
21	S	464	SER
22	P	6	SER
22	P	115	ILE
23	Q	58	ALA
24	R	49	ASN
25	U	134	PRO

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Mol	Chain	Res	Type
25	U	186	THR
26	O	263	ALA
26	O	303	THR
27	H	106	SER
28	I	185	ALA
28	I	229	GLY
28	I	433	GLY
29	K	334	PRO
30	L	372	ASP
32	J	119	ASP
32	J	121	TYR
1	A	57	PRO
3	C	206	LEU
7	G	145	ASP
9	2	161	SER
10	3	130	PRO
10	3	186	ILE
14	7	77	LEU
14	7	258	MET
15	W	148	VAL
16	V	116	PRO
16	V	155	VAL
19	Z	738	ASN
19	Z	892	PRO
20	N	363	SER
21	S	73	GLU
21	S	82	VAL
21	S	195	ASN
21	S	501	LEU
23	Q	19	ASP
23	Q	297	ARG
23	Q	391	PRO
28	I	432	GLU
29	K	369	LYS
30	L	144	VAL
30	L	341	ASP
31	M	306	ASP
1	A	10	ASP
9	2	63	ALA
10	3	29	GLY
10	3	85	TYR
11	4	32	HIS

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Mol	Chain	Res	Type
15	W	177	PRO
19	Z	178	LYS
19	Z	837	LEU
20	N	854	MET
21	S	127	LEU
21	S	134	PRO
22	P	136	ILE
23	Q	4	ALA
25	U	244	GLU
26	O	48	PRO
26	O	104	VAL
26	O	262	ALA
26	O	371	ALA
28	I	179	ALA
28	I	189	GLY
30	L	143	ASN
30	L	319	ASN
30	L	396	SER
31	M	112	ALA
32	J	104	ASP
32	J	262	GLY
10	3	43	PHE
15	W	175	PRO
19	Z	114	ALA
20	N	29	ALA
20	N	849	LYS
20	N	852	GLU
20	N	883	ARG
20	N	926	GLU
22	P	97	LEU
23	Q	63	ALA
31	M	182	GLU
10	3	137	VAL
11	4	26	VAL
19	Z	365	VAL
20	N	813	TYR
30	L	141	PRO
7	G	217	VAL
9	2	173	GLY
10	3	195	ILE
20	N	487	GLY
10	3	119	PRO

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Mol	Chain	Res	Type
11	4	148	THR
20	N	118	LEU
26	O	183	VAL
27	H	65	ILE

5.3.2 Protein sidechains ⓘ

In the following table, the Percentiles column shows the percent sidechain outliers of the chain as a percentile score with respect to all PDB entries followed by that with respect to all EM entries.

The Analysed column shows the number of residues for which the sidechain conformation was analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	210/210 (100%)	198 (94%)	12 (6%)	24	56
2	B	191/191 (100%)	186 (97%)	5 (3%)	51	75
3	C	209/221 (95%)	192 (92%)	17 (8%)	14	44
4	D	208/215 (97%)	199 (96%)	9 (4%)	33	64
5	E	195/203 (96%)	184 (94%)	11 (6%)	25	57
6	F	204/224 (91%)	196 (96%)	8 (4%)	37	66
7	G	202/212 (95%)	196 (97%)	6 (3%)	46	72
8	1	160/185 (86%)	146 (91%)	14 (9%)	12	39
9	2	180/227 (79%)	160 (89%)	20 (11%)	7	29
10	3	175/175 (100%)	160 (91%)	15 (9%)	12	42
11	4	167/172 (97%)	149 (89%)	18 (11%)	7	31
12	5	158/205 (77%)	139 (88%)	19 (12%)	6	27
13	6	179/200 (90%)	167 (93%)	12 (7%)	19	51
14	7	178/215 (83%)	159 (89%)	19 (11%)	8	31
15	W	168/312 (54%)	156 (93%)	12 (7%)	17	49
16	V	253/268 (94%)	237 (94%)	16 (6%)	21	53
17	T	233/298 (78%)	222 (95%)	11 (5%)	30	62
18	Y	22/63 (35%)	22 (100%)	0	100	100
19	Z	753/765 (98%)	708 (94%)	45 (6%)	22	55
20	N	776/814 (95%)	738 (95%)	38 (5%)	29	61

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	S	414/458 (90%)	390 (94%)	24 (6%)	23	56
22	P	419/419 (100%)	401 (96%)	18 (4%)	33	64
23	Q	362/362 (100%)	345 (95%)	17 (5%)	30	62
24	R	345/345 (100%)	325 (94%)	20 (6%)	23	56
25	U	259/289 (90%)	246 (95%)	13 (5%)	28	60
26	O	334/334 (100%)	320 (96%)	14 (4%)	34	64
27	H	341/372 (92%)	325 (95%)	16 (5%)	30	62
28	I	341/385 (89%)	327 (96%)	14 (4%)	35	65
29	K	343/367 (94%)	325 (95%)	18 (5%)	27	59
30	L	341/353 (97%)	321 (94%)	20 (6%)	23	55
31	M	357/382 (94%)	348 (98%)	9 (2%)	53	77
32	J	352/352 (100%)	337 (96%)	15 (4%)	33	64
All	All	9029/9793 (92%)	8524 (94%)	505 (6%)	29	57

All (505) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	62	ASP
1	A	93	ARG
1	A	103	TYR
1	A	111	VAL
1	A	112	ASP
1	A	118	ILE
1	A	172	GLN
1	A	207	SER
1	A	223	GLU
1	A	224	ASN
1	A	228	ARG
1	A	239	LEU
2	B	19	LEU
2	B	71	HIS
2	B	147	PHE
2	B	205	GLU
2	B	220	ARG
3	C	3	ARG
3	C	12	PHE
3	C	40	ASN
3	C	43	VAL

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Mol	Chain	Res	Type
3	C	44	LEU
3	C	60	PHE
3	C	86	LEU
3	C	114	LEU
3	C	137	ILE
3	C	141	LYS
3	C	143	TYR
3	C	148	TYR
3	C	164	ILE
3	C	178	ASP
3	C	188	SER
3	C	225	ILE
3	C	240	HIS
4	D	43	LEU
4	D	57	ARG
4	D	60	ARG
4	D	68	ASN
4	D	154	ASP
4	D	205	VAL
4	D	214	LEU
4	D	219	ARG
4	D	245	ASN
5	E	31	HIS
5	E	33	LEU
5	E	66	LYS
5	E	100	TRP
5	E	105	GLU
5	E	135	ARG
5	E	146	VAL
5	E	209	LYS
5	E	210	LEU
5	E	215	ILE
5	E	231	LYS
6	F	66	VAL
6	F	104	PRO
6	F	107	ARG
6	F	138	ASP
6	F	146	GLN
6	F	166	GLN
6	F	200	PRO
6	F	214	ILE
7	G	56	SER

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Mol	Chain	Res	Type
7	G	154	PRO
7	G	180	LEU
7	G	182	MET
7	G	191	VAL
7	G	235	GLU
8	1	36	ILE
8	1	37	MET
8	1	47	LEU
8	1	92	VAL
8	1	103	LEU
8	1	108	LEU
8	1	122	ARG
8	1	147	VAL
8	1	149	MET
8	1	177	ARG
8	1	187	GLN
8	1	206	VAL
8	1	219	ARG
8	1	235	LEU
9	2	50	VAL
9	2	51	TYR
9	2	62	ARG
9	2	72	LYS
9	2	77	ILE
9	2	82	PRO
9	2	100	GLN
9	2	120	VAL
9	2	136	TYR
9	2	167	TYR
9	2	168	VAL
9	2	169	THR
9	2	181	PHE
9	2	184	LYS
9	2	185	PHE
9	2	196	LYS
9	2	222	SER
9	2	238	LYS
9	2	246	ARG
9	2	255	LEU
10	3	15	LYS
10	3	25	ASP
10	3	27	ARG

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Mol	Chain	Res	Type
10	3	45	MET
10	3	70	ARG
10	3	71	LEU
10	3	97	GLU
10	3	112	LEU
10	3	113	ASP
10	3	141	THR
10	3	147	TYR
10	3	164	PHE
10	3	183	MET
10	3	189	ILE
10	3	192	LYS
11	4	4	LEU
11	4	19	ARG
11	4	24	ASN
11	4	43	LEU
11	4	60	ILE
11	4	62	LYS
11	4	66	LEU
11	4	69	MET
11	4	102	LEU
11	4	108	ASP
11	4	124	LEU
11	4	138	LEU
11	4	140	LEU
11	4	143	LEU
11	4	150	THR
11	4	172	ILE
11	4	181	ARG
11	4	192	GLU
12	5	61	THR
12	5	67	PHE
12	5	99	TYR
12	5	103	THR
12	5	104	MET
12	5	113	PHE
12	5	114	TRP
12	5	125	TYR
12	5	126	GLU
12	5	145	MET
12	5	159	MET
12	5	170	LEU

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Mol	Chain	Res	Type
12	5	173	VAL
12	5	180	ILE
12	5	195	PHE
12	5	204	TYR
12	5	236	TYR
12	5	249	ASP
12	5	254	LEU
13	6	31	PRO
13	6	42	ILE
13	6	101	MET
13	6	103	LYS
13	6	159	ARG
13	6	172	LEU
13	6	180	VAL
13	6	200	ARG
13	6	212	ARG
13	6	224	ILE
13	6	227	LYS
13	6	238	ARG
14	7	56	LEU
14	7	74	TYR
14	7	81	ARG
14	7	108	LYS
14	7	113	GLN
14	7	120	LEU
14	7	121	PHE
14	7	136	LEU
14	7	140	MET
14	7	154	LYS
14	7	170	ASP
14	7	183	THR
14	7	194	LEU
14	7	216	CYS
14	7	218	ARG
14	7	231	PHE
14	7	236	VAL
14	7	243	ILE
14	7	258	MET
15	W	57	ASP
15	W	62	THR
15	W	63	THR
15	W	71	ILE

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Mol	Chain	Res	Type
15	W	72	LEU
15	W	75	LEU
15	W	78	VAL
15	W	85	THR
15	W	110	ILE
15	W	124	LEU
15	W	160	LEU
15	W	188	ILE
16	V	65	TYR
16	V	73	PHE
16	V	77	GLN
16	V	91	PHE
16	V	139	ARG
16	V	163	ILE
16	V	177	THR
16	V	185	ASN
16	V	196	LEU
16	V	203	ILE
16	V	210	ASN
16	V	231	LEU
16	V	234	TYR
16	V	255	TYR
16	V	266	THR
16	V	268	GLU
17	T	132	LEU
17	T	164	ILE
17	T	185	LEU
17	T	258	SER
17	T	259	TYR
17	T	293	ILE
17	T	302	MET
17	T	305	TYR
17	T	319	TYR
17	T	321	PHE
17	T	350	GLU
19	Z	16	PRO
19	Z	28	SER
19	Z	31	LYS
19	Z	34	ARG
19	Z	83	ARG
19	Z	86	THR
19	Z	103	TYR

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Mol	Chain	Res	Type
19	Z	110	TYR
19	Z	119	LYS
19	Z	158	TYR
19	Z	189	LYS
19	Z	192	VAL
19	Z	193	PRO
19	Z	202	HIS
19	Z	209	MET
19	Z	210	GLU
19	Z	238	ASN
19	Z	241	PRO
19	Z	251	CYS
19	Z	291	GLN
19	Z	294	MET
19	Z	309	GLU
19	Z	333	LEU
19	Z	340	MET
19	Z	349	TYR
19	Z	398	TRP
19	Z	416	MET
19	Z	455	VAL
19	Z	492	SER
19	Z	508	SER
19	Z	553	THR
19	Z	590	PHE
19	Z	632	LYS
19	Z	652	VAL
19	Z	684	PRO
19	Z	704	LEU
19	Z	715	HIS
19	Z	738	ASN
19	Z	740	ARG
19	Z	760	PHE
19	Z	800	LEU
19	Z	809	ILE
19	Z	866	GLN
19	Z	868	HIS
19	Z	872	VAL
20	N	43	ASP
20	N	82	LEU
20	N	127	ASP
20	N	128	GLN

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Mol	Chain	Res	Type
20	N	142	LEU
20	N	167	ILE
20	N	188	MET
20	N	206	MET
20	N	232	ILE
20	N	236	LEU
20	N	243	LEU
20	N	247	GLN
20	N	262	SER
20	N	356	THR
20	N	418	GLU
20	N	422	LEU
20	N	459	ASP
20	N	470	ASN
20	N	524	LYS
20	N	583	MET
20	N	602	LEU
20	N	608	SER
20	N	612	ASP
20	N	627	PHE
20	N	629	THR
20	N	644	TYR
20	N	701	ILE
20	N	720	LYS
20	N	751	ARG
20	N	788	ILE
20	N	809	SER
20	N	813	TYR
20	N	861	LYS
20	N	880	ASN
20	N	891	VAL
20	N	908	ILE
20	N	921	ILE
20	N	949	GLU
21	S	45	SER
21	S	92	ARG
21	S	117	PHE
21	S	124	ARG
21	S	125	ASP
21	S	128	LEU
21	S	140	ASP
21	S	145	PRO

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Mol	Chain	Res	Type
21	S	169	ILE
21	S	176	ARG
21	S	216	PHE
21	S	269	LYS
21	S	271	VAL
21	S	274	GLU
21	S	302	ARG
21	S	330	VAL
21	S	342	LEU
21	S	343	GLN
21	S	348	SER
21	S	389	THR
21	S	399	ILE
21	S	410	TYR
21	S	425	ASP
21	S	463	TYR
22	P	8	ARG
22	P	50	LEU
22	P	83	LEU
22	P	90	LEU
22	P	104	MET
22	P	131	VAL
22	P	136	ILE
22	P	140	ILE
22	P	145	LEU
22	P	149	LEU
22	P	194	LEU
22	P	202	THR
22	P	211	THR
22	P	230	MET
22	P	247	TYR
22	P	289	ARG
22	P	314	LEU
22	P	393	LEU
23	Q	21	GLU
23	Q	26	ILE
23	Q	57	LEU
23	Q	109	LEU
23	Q	122	ARG
23	Q	158	LYS
23	Q	172	LEU
23	Q	214	SER

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Mol	Chain	Res	Type
23	Q	242	ILE
23	Q	243	ASP
23	Q	263	THR
23	Q	314	ARG
23	Q	330	LEU
23	Q	352	SER
23	Q	356	LEU
23	Q	365	LEU
23	Q	392	PRO
24	R	16	ASP
24	R	23	ARG
24	R	25	LEU
24	R	35	THR
24	R	37	VAL
24	R	73	MET
24	R	75	LYS
24	R	88	LEU
24	R	134	LEU
24	R	143	TYR
24	R	151	TYR
24	R	199	GLU
24	R	208	PHE
24	R	217	LYS
24	R	267	ARG
24	R	292	TYR
24	R	296	VAL
24	R	329	PHE
24	R	356	THR
24	R	360	ASP
25	U	4	LEU
25	U	33	LYS
25	U	82	PHE
25	U	106	ILE
25	U	128	PRO
25	U	135	THR
25	U	145	HIS
25	U	162	ILE
25	U	192	THR
25	U	237	LEU
25	U	250	TYR
25	U	273	HIS
25	U	286	GLU

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Mol	Chain	Res	Type
26	O	50	PHE
26	O	68	GLU
26	O	152	HIS
26	O	160	SER
26	O	184	ASP
26	O	222	LEU
26	O	240	PHE
26	O	249	GLN
26	O	253	SER
26	O	272	ILE
26	O	353	LEU
26	O	359	ASP
26	O	363	MET
26	O	372	GLN
27	H	43	ARG
27	H	69	ASP
27	H	98	CYS
27	H	102	ILE
27	H	125	LEU
27	H	150	HIS
27	H	164	MET
27	H	182	GLU
27	H	263	MET
27	H	280	ILE
27	H	310	ASP
27	H	312	ARG
27	H	333	ARG
27	H	336	ARG
27	H	346	PRO
27	H	428	ARG
28	I	58	CYS
28	I	73	LEU
28	I	90	GLU
28	I	115	ILE
28	I	135	ILE
28	I	156	VAL
28	I	164	MET
28	I	178	LYS
28	I	294	ARG
28	I	297	SER
28	I	309	MET
28	I	368	HIS

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Mol	Chain	Res	Type
28	I	438	LEU
28	I	440	LEU
29	K	30	LEU
29	K	68	LEU
29	K	80	LYS
29	K	81	ARG
29	K	113	VAL
29	K	119	ILE
29	K	121	ARG
29	K	140	VAL
29	K	157	ASP
29	K	167	ILE
29	K	191	TYR
29	K	203	LEU
29	K	239	TYR
29	K	246	MET
29	K	272	THR
29	K	309	MET
29	K	336	PRO
29	K	411	GLU
30	L	31	LEU
30	L	34	LYS
30	L	59	ASN
30	L	80	GLU
30	L	85	VAL
30	L	106	LEU
30	L	114	LEU
30	L	132	LEU
30	L	155	GLN
30	L	178	ILE
30	L	187	TYR
30	L	220	LYS
30	L	232	MET
30	L	244	ILE
30	L	265	ARG
30	L	266	GLU
30	L	308	ARG
30	L	319	ASN
30	L	327	LEU
30	L	356	ASP
31	M	101	ASP
31	M	184	PRO

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Mol	Chain	Res	Type
31	M	201	LEU
31	M	213	GLU
31	M	218	LEU
31	M	313	MET
31	M	316	LEU
31	M	363	GLU
31	M	384	TYR
32	J	15	LYS
32	J	20	LEU
32	J	22	GLN
32	J	25	LEU
32	J	87	VAL
32	J	88	LYS
32	J	98	ASP
32	J	123	LEU
32	J	132	ASP
32	J	196	LYS
32	J	226	GLU
32	J	245	ILE
32	J	251	ILE
32	J	276	LEU
32	J	280	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains ⓘ

There are no non-standard protein/DNA/RNA residues in this entry.

5.5 Carbohydrates ⓘ

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.