



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:02 PM BST

PDB ID : 3J9T
EMDB ID: : EMD-6284
Title : Yeast V-ATPase state 1
Authors : Zhao, J.; Benlekbir, S.; Rubinstein, J.L.
Deposited on : 2015-02-23
Resolution : 6.90 Å(reported)
Based on PDB ID : 4DL0, 4RND, 1HO8, 1U7L

This is a wwPDB EM Map/Model Validation Report for a publicly released PDB/EMDB entry.
For rigid body fitted models, validation errors reported here could stem from errors in the original structure(s) used in the fitting.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
<http://wwpdb.org/validation/2016/EMValidationReportHelp>

MolProbity : 4.02b-467
Mogul : unknown
Percentile statistics : 20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : trunk27241

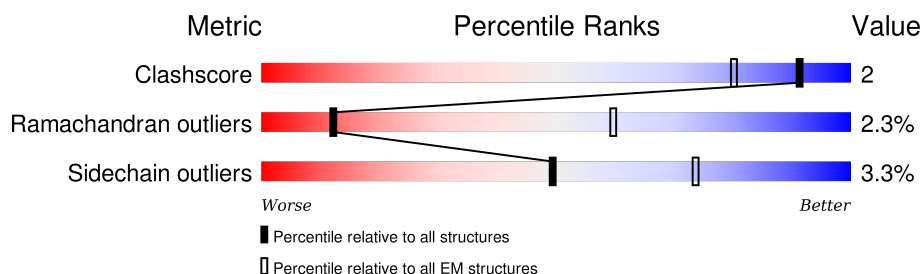
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 6.90 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.















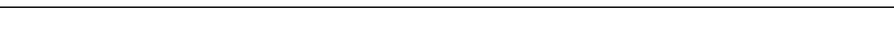

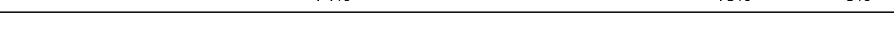




Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	M	256	59% 20% • 18%
2	N	118	77% 19% • •
3	A	616	67% 26% • •
3	C	616	72% 20% • •
3	E	616	68% 24% • •
4	B	517	61% 23% • 12%
4	D	517	64% 21% • • 12%
4	F	517	59% 25% • 12%
5	Q	345	73% 22% 5%

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Mol	Chain	Length	Quality of chain
6	H	114	 74%18%8%
6	J	114	 72%19%8%
6	L	114	 76%14%8%
7	G	233	 73%18%7%
7	I	233	 76%14%7%
7	K	233	 75%16%7%
8	P	478	 78%15%7%
9	b	840	 28%8%63%
10	O	392	 73%22%5%
11	R	160	 69%23%6%
11	S	160	 74%18%6%
11	T	160	 78%14%6%
11	U	160	 71%21%6%
11	V	160	 74%16%6%
11	W	160	 73%18%6%
11	X	160	 73%20%6%
11	Y	160	 74%19%6%
11	Z	160	 78%13%6%
11	a	160	 77%15%6%

2 Entry composition

There are 11 unique types of molecules in this entry. The entry contains 57659 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 V-type proton ATPase subunit D.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	M	210	Total	C	N	O	S	0	0
			1691	1061	305	321	4		

- Molecule 2 is a protein called V-type proton ATPase subunit F.

Mol	Chain	Residues	Atoms				AltConf	Trace
2	N	115	Total	C	N	O	0	0
			928	589	157	182		

- Molecule 3 is a protein called V-type proton ATPase catalytic subunit A.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	A	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		
3	C	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		
3	E	593	Total	C	N	O	S	0	0
			4578	2904	760	894	20		

- Molecule 4 is a protein called V-type proton ATPase subunit B.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	B	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		
4	D	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		
4	F	457	Total	C	N	O	S	0	0
			3585	2266	612	695	12		

- Molecule 5 is a protein called V-type proton ATPase subunit d.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	Q	345	Total	C	N	O	S	0	0
			2802	1779	454	555	14		

- Molecule 6 is a protein called V-type proton ATPase subunit G.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	L	105	Total	C	N	O		0	0
			824	517	144	163			
6	H	105	Total	C	N	O		0	0
			824	517	144	163			
6	J	105	Total	C	N	O		0	0
			824	517	144	163			

- Molecule 7 is a protein called V-type proton ATPase subunit E.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	K	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		
7	G	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		
7	I	217	Total	C	N	O	S	0	0
			1731	1083	296	347	5		

- Molecule 8 is a protein called V-type proton ATPase subunit H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	P	461	Total	C	N	O	S	0	0
			3712	2373	623	704	12		

- Molecule 9 is a protein called V-type proton ATPase subunit a, vacuolar isoform.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	b	312	Total	C	N	O	S	0	0
			2540	1614	434	489	3		

- Molecule 10 is a protein called V-type proton ATPase subunit C.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	O	392	Total	C	N	O	S	0	0
			3122	2005	516	596	5		

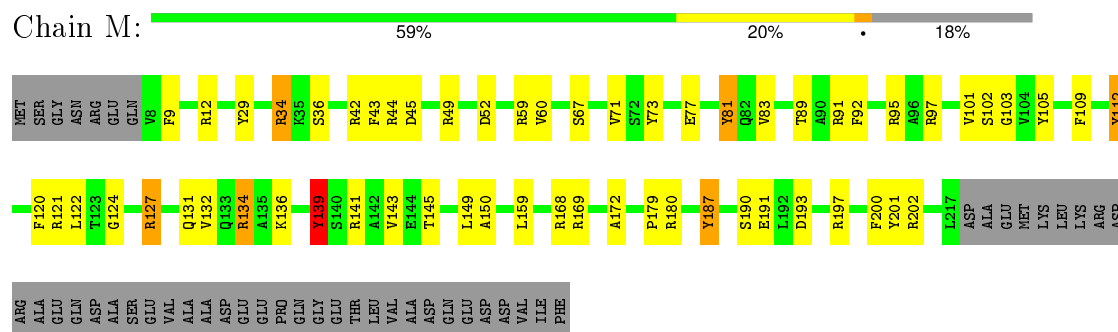
- Molecule 11 is a protein called V-type proton ATPase subunit c.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	Y	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	R	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	U	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	V	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	T	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	W	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	S	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	X	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	Z	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	a	150	Total 1071	C 704	N 173	O 187	S 7	0	0

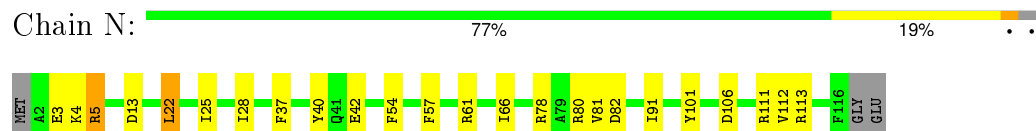
3 Residue-property plots

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors 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.

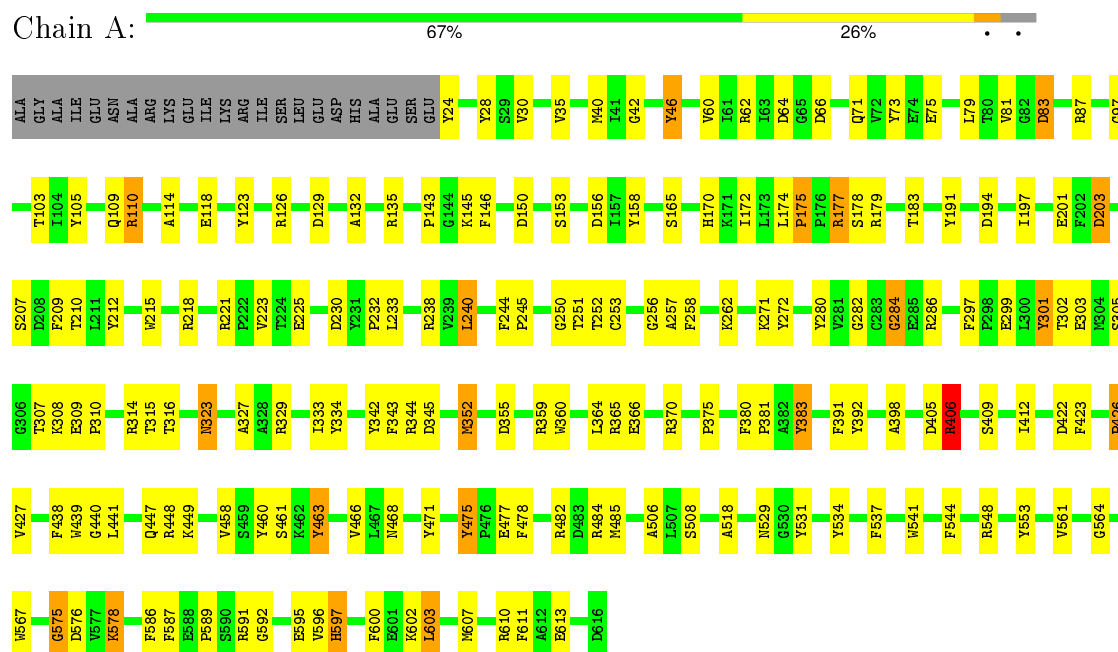
• Molecule 1: V-type proton ATPase subunit D



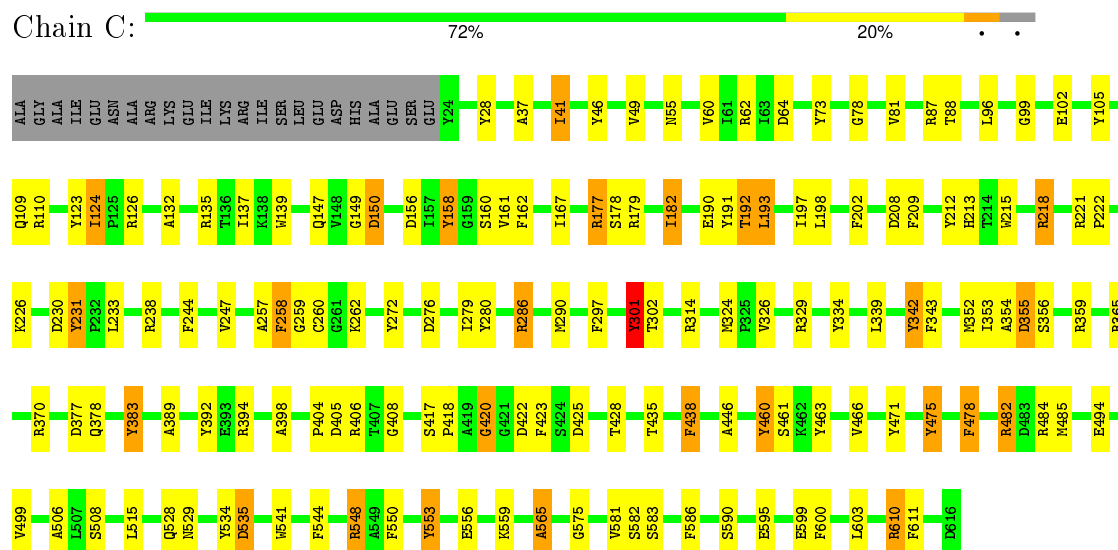
• Molecule 2: V-type proton ATPase subunit F



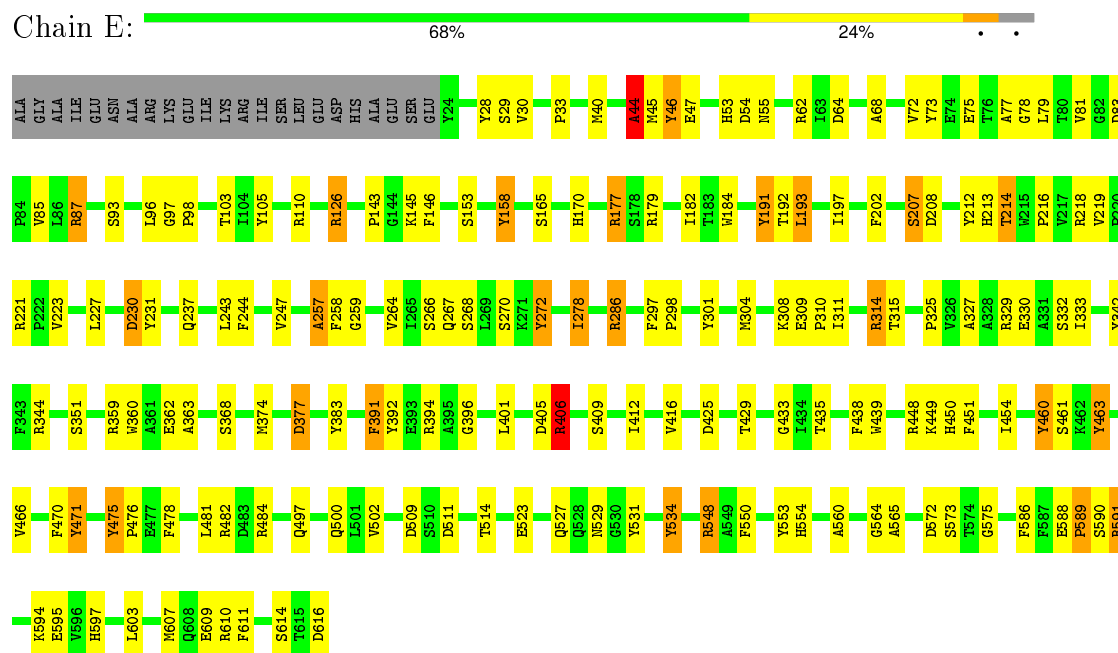
• Molecule 3: V-type proton ATPase catalytic subunit A



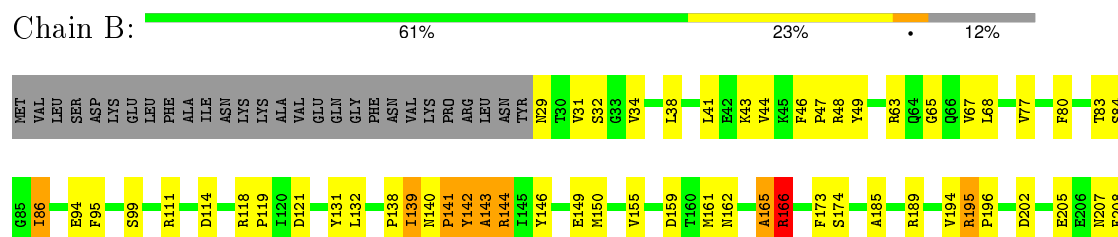
- Molecule 3: V-type proton ATPase catalytic subunit A

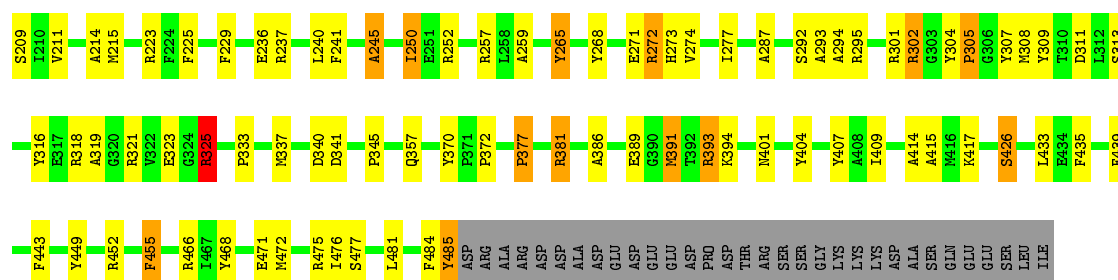


- Molecule 3: V-type proton ATPase catalytic subunit A

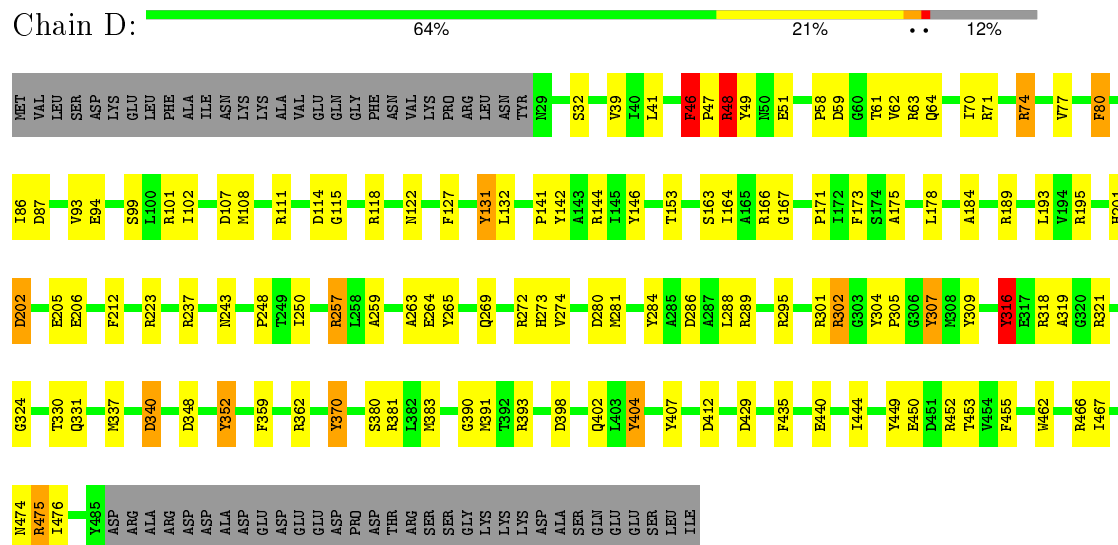


- Molecule 4: V-type proton ATPase subunit B

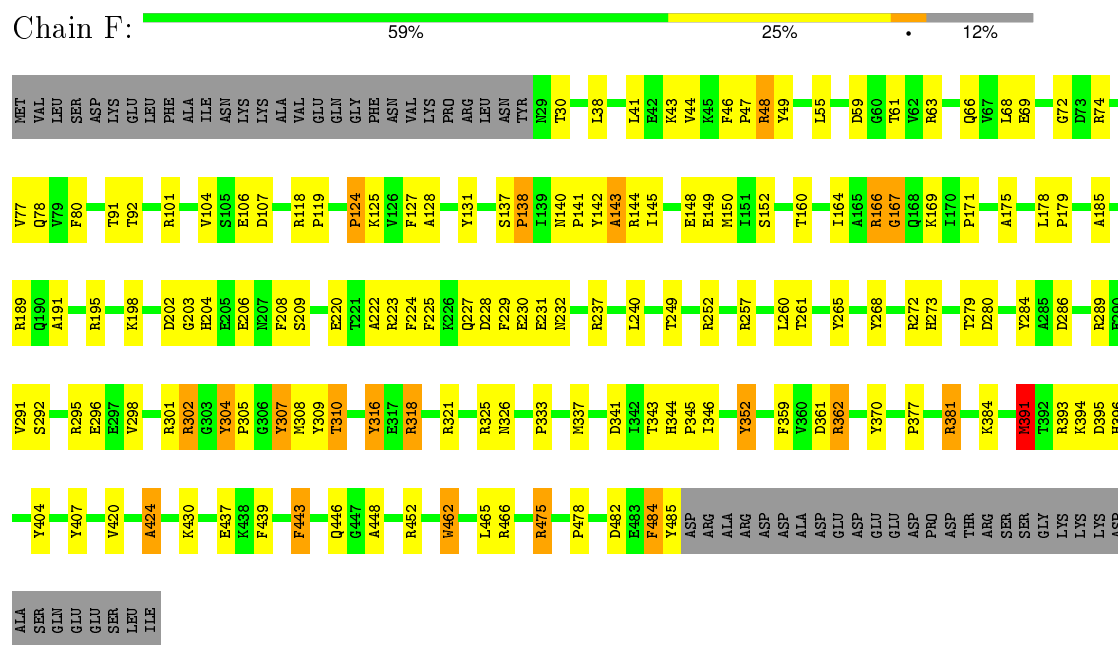




• Molecule 4: V-type proton ATPase subunit B

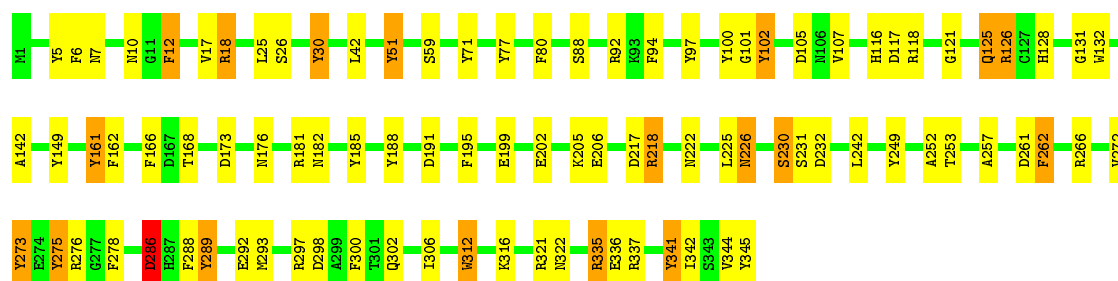


• Molecule 4: V-type proton ATPase subunit B



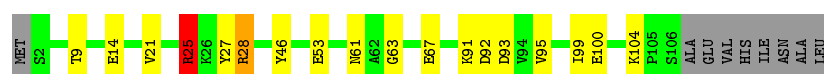
• Molecule 5: V-type proton ATPase subunit d

Chain Q: 



- Molecule 6: V-type proton ATPase subunit G

Chain L: 



- Molecule 6: V-type proton ATPase subunit G

Chain H: 



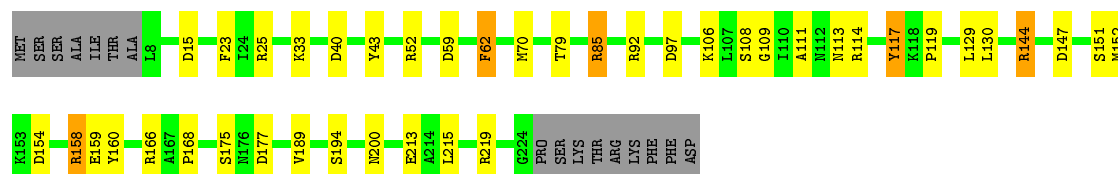
- Molecule 6: V-type proton ATPase subunit G

Chain J: 



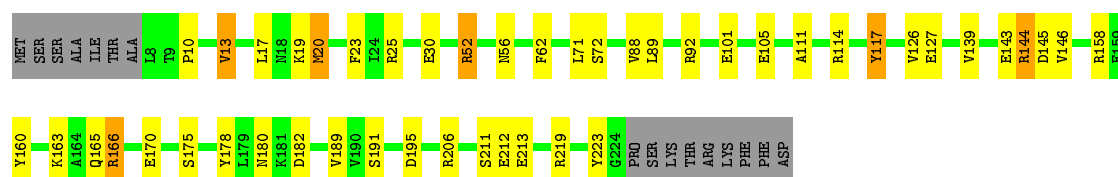
- Molecule 7: V-type proton ATPase subunit E

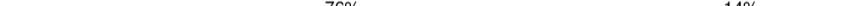
Chain K: 



- Molecule 7: V-type proton ATPase subunit E

Chain G: 



Chain I: 

Chain P: 

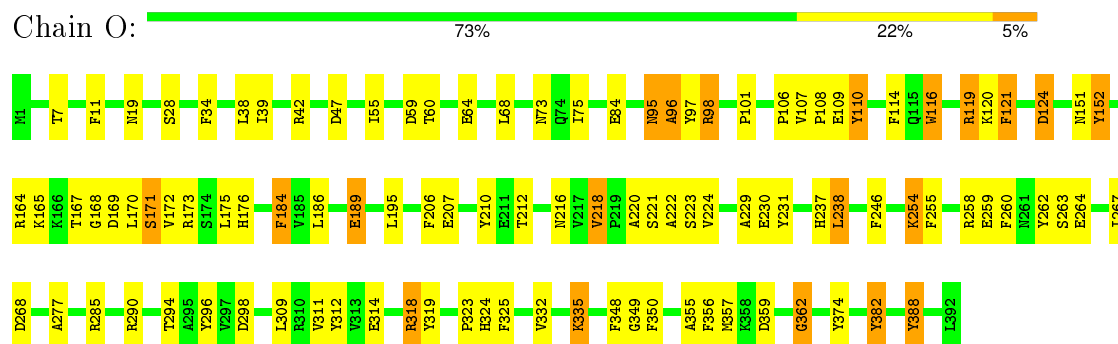
A318	A322	K329	Y330	S331	D332	Y350	Y359	L368	C369	P372	F379	M380	D390	Y391	Y392	F395	K396	R407	D410	V411	N412	S437	I438	D439	L440	L441	D449	M455	H456	S457	S459	R460	Y463	A468	T469	F477	K478
D120	F128	K133	G134	D135	F136	F144	V147	G154	L155	H156	V161	E178	Y184	E192	L193	I196	V202	E207	R220	A221	V231	N236	H237	Y244	H245	F255	F259	Y267	D273	L274	L282	K285	R288	R301			

Chain b: 28% 8% 63%

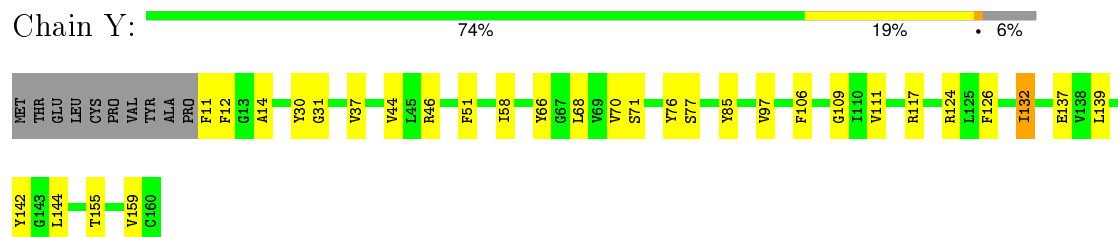
Position	Amino Acid	Region
1	GLY	Red
2	LEU	Red
3	PRO	Red
4	THR	Red
5	PHE	Red
6	VAL	Red
7	GLY	Red
8	THR	Red
9	ILE	Red
10	VAL	Red
11	ASN	Red
12	LYS	Red
13	TRP	Red
14	ALA	Red
15	THR	Red
16	VAL	Red
17	LYS	Red
18	GLY	Red
19	PHE	Red
20	THR	Red
21	LEU	Red
22	THR	Red
23	ASN	Red
24	ILE	Red
25	GLY	Red
26	ILE	Red
27	ASP	Red
28	VAL	Red
29	PRO	Yellow
30	VAL	Yellow
31	LYS	Yellow
32	ARG	Yellow
33	GLY	Yellow
34	THR	Yellow
35	LYS	Yellow
36	ILE	Yellow
37	LYS	Yellow
38	LEU	Green
39	ASP	Green
40	THR	Green
41	ALA	Green
42	ALA	Green
43	THR	Green
44	PRO	Green
45	THR	Green
46	PRO	Green
47	THR	Green
48	VAL	Green
49	THR	Green
50	LEU	Green
51	ASN	Green
52	GLY	Green
53	LYS	Green
54	ILE	Green
55	THR	Green
56	ALA	Green
57	ALA	Green
58	THR	Green
59	MET	Green
60	ILE	Green
61	THR	Green
62	LYS	Green
63	VAL	Green
64	GLY	Green
65	THR	Green
66	ILE	Green
67	THR	Green
68	PRO	Green
69	GLY	Green
70	LEU	Green
71	LEU	Green
72	PHE	Green
73	LEU	Green
74	VAL	Green
75	GLN	Green
76	MET	Green
77	ALA	Green
78	GLY	Green
79	ILE	Green
80	PHE	Green
81	THR	Green
82	ASP	Green
83	GLY	Green
84	THR	Green
85	ILE	Green
86	THR	Green
87	ASP	Green
88	ALA	Green
89	ALA	Green
90	LYS	Green
91	ASP	Green
92	VAL	Green
93	GLN	Green
94	VAL	Green
95	GLY	Green
96	GLU	Green
97	GLU	Green
98	VAL	Green
99	GLY	Green
100	SER	Green

PHE	GLY	ASP	ILE	MET	ILE	HIS	GLN	VAL	VAL	ILE	HIS	THR	ILE	GLU	PHE	CYS	ASN	CYS	VAL	SER	THR	ALA	SER	THR	LEU	ARG	LEU	TRP	ALA	LEU	SER	SER	VAL	LEU	TRP	THR	MET	THR	ILE	GLN	ILE	ALA	PHE	GLY	PHE	ARG	PHE	GLY	ASP	VAL		
PHE	MET	THR	VAL	ALA	LEU	PHE	ALA	ALA	MET	TRP	PHE	ALA	LEU	THR	CYS	ALA	VAL	VAL	LEU	MET	GLU	GLY	THR	SER	LEU	HIS	SER	LEU	ARG	LEU	SER	LYS	PHE	PHE	VAL	GLY	GLY	LEU	PRO	TYR	GLU	PRO	PHE	ALA	PHE	ARG	GLY	TYR	LYS	VAL	GLY	MET
GLU	VAL	ALA	VAL	VAL	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER	SER		

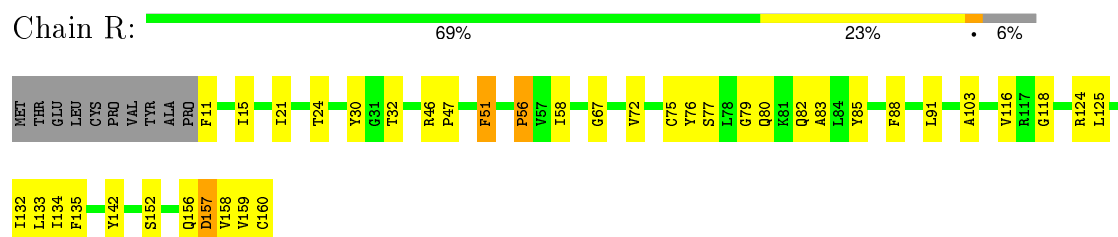
• Molecule 10: V-type proton ATPase subunit C



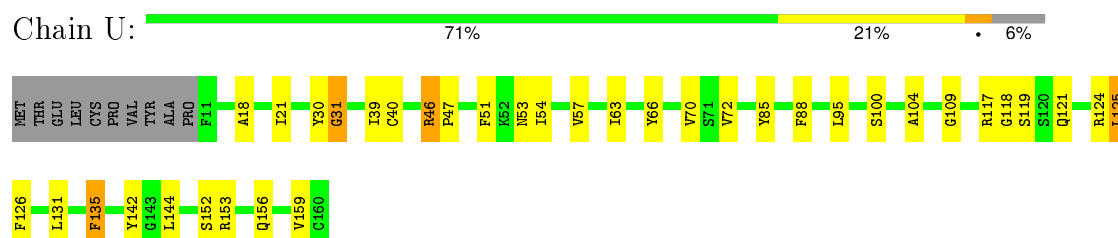
• Molecule 11: V-type proton ATPase subunit c



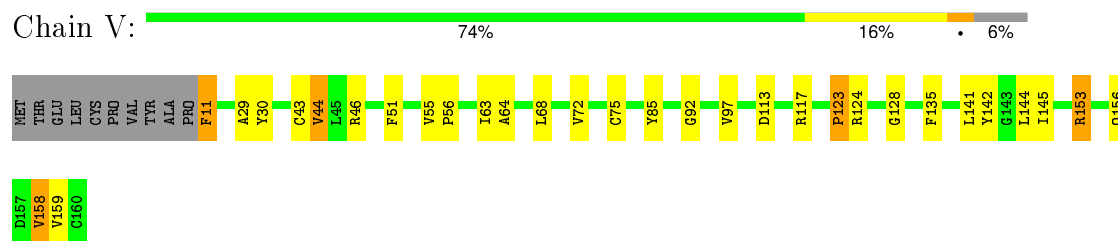
• Molecule 11: V-type proton ATPase subunit c



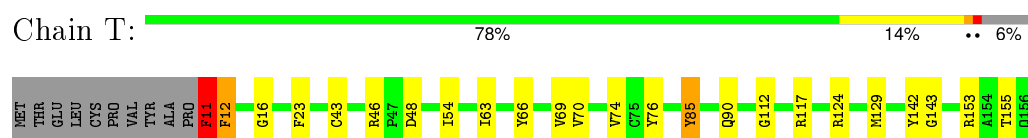
• Molecule 11: V-type proton ATPase subunit c



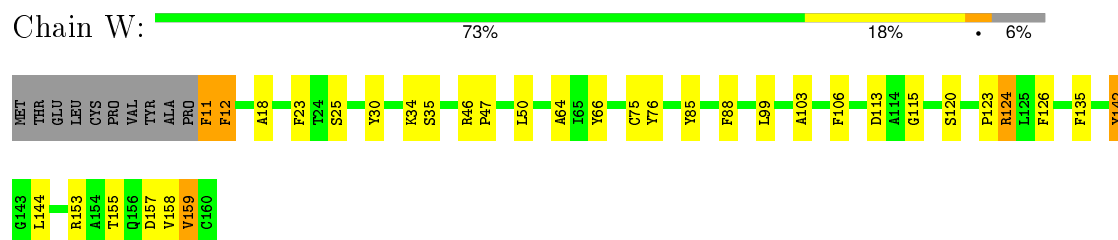
- Molecule 11: V-type proton ATPase subunit c



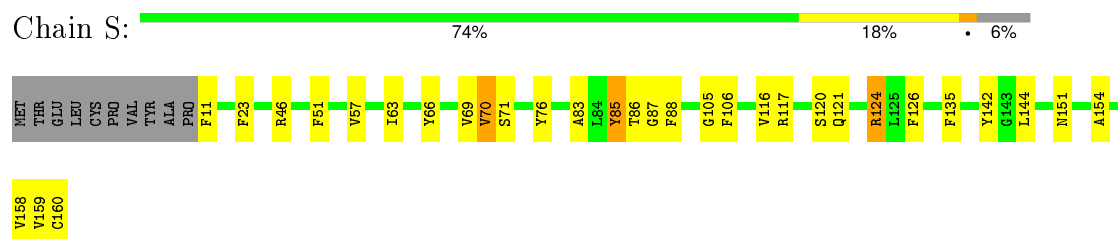
- Molecule 11: V-type proton ATPase subunit c



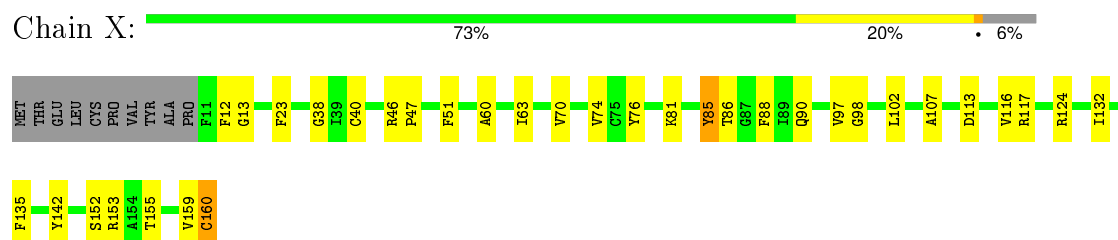
- Molecule 11: V-type proton ATPase subunit c



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● Molecule 11: V-type proton ATPase subunit c



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	50503	Depositor
Resolution determination method	FSC 0.143	Depositor
CTF correction method	Each particle	Depositor
Microscope	FEI TECNAI F20	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	30	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	7000	Depositor
Magnification	34483	Depositor
Image detector	GATAN K2 (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	M	1.76	20/1710 (1.2%)	1.95	49/2295 (2.1%)
10	O	1.69	25/3185 (0.8%)	1.95	81/4314 (1.9%)
11	R	1.65	8/1086 (0.7%)	1.96	26/1472 (1.8%)
11	S	1.67	10/1086 (0.9%)	1.89	21/1472 (1.4%)
11	T	1.65	9/1086 (0.8%)	1.89	27/1472 (1.8%)
11	U	1.65	7/1086 (0.6%)	1.91	19/1472 (1.3%)
11	V	1.68	6/1086 (0.6%)	1.94	22/1472 (1.5%)
11	W	1.69	7/1086 (0.6%)	2.07	36/1472 (2.4%)
11	X	1.72	15/1086 (1.4%)	1.87	20/1472 (1.4%)
11	Y	1.64	6/1086 (0.6%)	1.93	26/1472 (1.8%)
11	Z	1.65	7/1086 (0.6%)	1.85	18/1472 (1.2%)
11	a	1.68	10/1086 (0.9%)	1.87	24/1472 (1.6%)
2	N	1.68	7/944 (0.7%)	1.85	21/1277 (1.6%)
3	A	1.75	44/4677 (0.9%)	2.02	134/6339 (2.1%)
3	C	1.71	34/4677 (0.7%)	1.91	109/6339 (1.7%)
3	E	1.78	53/4677 (1.1%)	1.96	122/6339 (1.9%)
4	B	1.72	27/3654 (0.7%)	1.99	99/4953 (2.0%)
4	D	1.72	40/3654 (1.1%)	2.00	78/4953 (1.6%)
4	F	1.74	34/3654 (0.9%)	2.02	109/4953 (2.2%)
5	Q	1.75	23/2861 (0.8%)	1.99	73/3880 (1.9%)
6	H	1.58	2/828 (0.2%)	1.76	14/1098 (1.3%)
6	J	1.62	3/828 (0.4%)	1.85	20/1098 (1.8%)
6	L	1.65	6/828 (0.7%)	1.69	10/1098 (0.9%)
7	G	1.72	21/1743 (1.2%)	1.82	30/2338 (1.3%)
7	I	1.70	18/1743 (1.0%)	1.82	30/2338 (1.3%)
7	K	1.71	17/1743 (1.0%)	1.77	31/2338 (1.3%)
8	P	1.65	21/3766 (0.6%)	1.85	63/5087 (1.2%)
9	b	1.73	18/2578 (0.7%)	2.03	81/3479 (2.3%)
All	All	1.71	498/58610 (0.8%)	1.93	1393/79236 (1.8%)

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	M	0	7
10	O	0	12
11	S	0	1
11	T	0	4
11	U	0	2
11	V	0	2
11	W	0	4
11	X	0	1
11	Z	0	2
11	a	0	2
2	N	0	2
3	A	0	11
3	C	0	14
3	E	0	12
4	B	0	13
4	D	0	13
4	F	0	11
5	Q	0	14
6	L	0	2
7	G	0	4
7	I	0	3
7	K	0	5
8	P	0	9
9	b	0	14
All	All	0	164

All (498) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	X	160	CYS	CB-SG	11.36	2.01	1.82
8	P	392	TYR	CG-CD2	9.03	1.50	1.39
3	E	268	SER	CA-CB	8.92	1.66	1.52
9	b	248	ARG	NE-CZ	8.29	1.43	1.33
3	C	110	ARG	CD-NE	8.22	1.60	1.46
3	E	461	SER	CA-CB	8.11	1.65	1.52
3	A	359	ARG	CZ-NH1	7.99	1.43	1.33
3	A	179	ARG	CZ-NH1	7.99	1.43	1.33
7	G	101	GLU	CD-OE1	7.92	1.34	1.25
5	Q	249	TYR	CZ-OH	7.82	1.51	1.37
3	E	110	ARG	CD-NE	7.70	1.59	1.46
4	B	426	SER	CA-CB	7.68	1.64	1.52
5	Q	71	TYR	CE1-CZ	7.66	1.48	1.38
1	M	42	ARG	CZ-NH2	7.46	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	I	206	ARG	NE-CZ	7.32	1.42	1.33
7	I	160	TYR	CE1-CZ	7.31	1.48	1.38
11	X	152	SER	CA-CB	7.28	1.63	1.52
4	B	304	TYR	CE1-CZ	7.28	1.48	1.38
1	M	180	ARG	CZ-NH2	7.24	1.42	1.33
3	C	471	TYR	CZ-OH	7.20	1.50	1.37
9	b	31	TYR	CE2-CZ	7.18	1.47	1.38
3	E	231	TYR	CB-CG	7.14	1.62	1.51
3	C	383	TYR	CB-CG	7.12	1.62	1.51
11	X	117	ARG	CZ-NH2	7.09	1.42	1.33
7	I	25	ARG	NE-CZ	7.08	1.42	1.33
4	D	212	PHE	CG-CD2	7.06	1.49	1.38
4	F	485	TYR	CG-CD1	7.05	1.48	1.39
3	E	531	TYR	CZ-OH	7.03	1.49	1.37
11	S	87	GLY	CA-C	-7.03	1.40	1.51
7	G	211	SER	CA-CB	6.95	1.63	1.52
10	O	109	GLU	CD-OE2	6.94	1.33	1.25
3	A	553	TYR	CG-CD2	6.92	1.48	1.39
3	E	218	ARG	CZ-NH2	6.90	1.42	1.33
4	D	74	ARG	CD-NE	6.90	1.58	1.46
3	A	592	GLY	CA-C	-6.85	1.40	1.51
9	b	328	TYR	CG-CD2	6.85	1.48	1.39
4	F	265	TYR	CG-CD2	6.83	1.48	1.39
8	P	23	ARG	CZ-NH2	6.79	1.41	1.33
7	K	52	ARG	CZ-NH2	6.79	1.41	1.33
9	b	27	ARG	CD-NE	6.78	1.57	1.46
3	E	110	ARG	CZ-NH2	6.77	1.41	1.33
5	Q	88	SER	CA-CB	6.76	1.63	1.52
11	S	23	PHE	CG-CD1	6.74	1.48	1.38
4	F	272	ARG	CZ-NH1	6.73	1.41	1.33
11	a	124	ARG	CZ-NH1	6.73	1.41	1.33
3	E	28	TYR	CE1-CZ	6.72	1.47	1.38
3	A	409	SER	CA-CB	6.70	1.62	1.52
11	X	13	GLY	CA-C	-6.67	1.41	1.51
4	D	201	HIS	CB-CG	-6.67	1.38	1.50
7	I	114	ARG	N-CA	-6.66	1.33	1.46
4	B	370	TYR	CE2-CZ	6.65	1.47	1.38
5	Q	321	ARG	CZ-NH1	6.64	1.41	1.33
1	M	12	ARG	CZ-NH1	6.64	1.41	1.33
11	X	153	ARG	CZ-NH2	6.64	1.41	1.33
9	b	332	ARG	NE-CZ	6.60	1.41	1.33
4	D	264	GLU	CD-OE2	6.59	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	M	121	ARG	NE-CZ	6.57	1.41	1.33
11	X	142	TYR	CE2-CZ	6.55	1.47	1.38
1	M	197	ARG	CZ-NH1	6.55	1.41	1.33
11	a	124	ARG	CD-NE	6.55	1.57	1.46
4	D	289	ARG	CZ-NH2	6.55	1.41	1.33
3	A	258	PHE	CB-CG	-6.50	1.40	1.51
4	D	393	ARG	CZ-NH1	6.49	1.41	1.33
7	K	219	ARG	CZ-NH2	6.48	1.41	1.33
3	E	553	TYR	CE1-CZ	6.47	1.47	1.38
4	F	321	ARG	CZ-NH2	6.47	1.41	1.33
3	E	191	TYR	CZ-OH	6.46	1.48	1.37
11	R	56	PRO	CA-CB	-6.46	1.40	1.53
7	G	206	ARG	CZ-NH2	6.45	1.41	1.33
7	I	170	GLU	CG-CD	6.45	1.61	1.51
4	D	272	ARG	NE-CZ	6.44	1.41	1.33
10	O	223	SER	CA-CB	6.43	1.62	1.52
10	O	258	ARG	CZ-NH1	6.43	1.41	1.33
3	E	392	TYR	CE1-CZ	6.43	1.47	1.38
10	O	84	GLU	CD-OE2	6.42	1.32	1.25
10	O	207	GLU	CG-CD	6.42	1.61	1.51
1	M	36	SER	CA-CB	6.42	1.62	1.52
3	E	611	PHE	CG-CD2	6.41	1.48	1.38
3	C	314	ARG	CZ-NH2	6.41	1.41	1.33
11	X	12	PHE	C-N	6.39	1.44	1.33
7	I	72	SER	CA-CB	6.38	1.62	1.52
8	P	359	TYR	CG-CD2	6.37	1.47	1.39
1	M	34	ARG	NE-CZ	6.35	1.41	1.33
10	O	210	TYR	CZ-OH	6.35	1.48	1.37
3	A	344	ARG	CZ-NH1	6.35	1.41	1.33
3	E	342	TYR	CZ-OH	6.34	1.48	1.37
3	E	46	TYR	CZ-OH	6.34	1.48	1.37
3	A	343	PHE	CG-CD2	6.33	1.48	1.38
4	D	475	ARG	CZ-NH2	6.33	1.41	1.33
8	P	301	ARG	CD-NE	6.32	1.57	1.46
4	F	137	SER	CA-CB	6.32	1.62	1.52
4	F	362	ARG	NE-CZ	6.31	1.41	1.33
7	G	160	TYR	C-N	6.29	1.44	1.33
3	E	46	TYR	CE2-CZ	6.29	1.46	1.38
11	W	120	SER	CA-CB	6.27	1.62	1.52
1	M	91	ARG	CZ-NH2	6.27	1.41	1.33
2	N	111	ARG	NE-CZ	6.27	1.41	1.33
11	Y	14	ALA	CA-CB	6.26	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	T	12	PHE	CG-CD1	6.25	1.48	1.38
1	M	201	TYR	CE2-CZ	6.24	1.46	1.38
8	P	178	GLU	CG-CD	-6.24	1.42	1.51
11	Y	70	VAL	CB-CG2	6.24	1.66	1.52
4	B	131	TYR	CZ-OH	6.24	1.48	1.37
10	O	152	TYR	CB-CG	-6.23	1.42	1.51
1	M	169	ARG	CZ-NH2	6.23	1.41	1.33
3	E	529	ASN	C-N	6.22	1.44	1.33
10	O	318	ARG	CZ-NH2	6.21	1.41	1.33
4	D	407	TYR	CZ-OH	6.20	1.48	1.37
3	C	417	SER	CA-CB	6.18	1.62	1.52
7	I	204	GLU	CD-OE1	6.17	1.32	1.25
3	E	33	PRO	N-CD	-6.16	1.39	1.47
4	B	144	ARG	CZ-NH2	6.16	1.41	1.33
7	I	114	ARG	CZ-NH2	6.15	1.41	1.33
4	F	284	TYR	CG-CD1	-6.15	1.31	1.39
3	A	392	TYR	CG-CD2	6.14	1.47	1.39
3	C	478	PHE	CG-CD2	6.14	1.48	1.38
9	b	151	PHE	CG-CD1	6.14	1.48	1.38
2	N	78	ARG	NE-CZ	6.13	1.41	1.33
3	C	392	TYR	CB-CG	6.13	1.60	1.51
4	B	302	ARG	CZ-NH1	6.11	1.41	1.33
3	E	314	ARG	CD-NE	6.11	1.56	1.46
7	I	8	LEU	N-CA	6.10	1.58	1.46
4	D	205	GLU	CD-OE2	6.10	1.32	1.25
3	A	591	ARG	CZ-NH2	6.10	1.41	1.33
3	C	460	TYR	CG-CD1	6.10	1.47	1.39
11	a	46	ARG	CZ-NH2	6.09	1.41	1.33
4	B	325	ARG	CZ-NH1	6.09	1.41	1.33
4	F	295	ARG	NE-CZ	6.09	1.41	1.33
8	P	288	ARG	CZ-NH2	6.08	1.41	1.33
10	O	356	PHE	CG-CD1	6.08	1.47	1.38
6	J	53	GLU	CG-CD	6.08	1.61	1.51
3	E	332	SER	CA-CB	6.07	1.62	1.52
3	A	105	TYR	CE2-CZ	6.07	1.46	1.38
1	M	190	SER	CB-OG	6.07	1.50	1.42
3	A	314	ARG	NE-CZ	6.07	1.41	1.33
4	B	325	ARG	CD-NE	6.07	1.56	1.46
10	O	238	LEU	N-CA	-6.06	1.34	1.46
9	b	193	ARG	CD-NE	6.06	1.56	1.46
11	S	117	ARG	CD-NE	6.06	1.56	1.46
3	A	177	ARG	CZ-NH2	6.05	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Z	153	ARG	CZ-NH2	6.05	1.41	1.33
10	O	388	TYR	CE2-CZ	6.04	1.46	1.38
4	D	318	ARG	CZ-NH2	6.02	1.40	1.33
3	E	362	GLU	CG-CD	-6.02	1.43	1.51
5	Q	249	TYR	CG-CD2	6.02	1.47	1.39
4	D	302	ARG	NE-CZ	6.02	1.40	1.33
4	F	381	ARG	CZ-NH1	6.02	1.40	1.33
3	A	105	TYR	CE1-CZ	6.01	1.46	1.38
9	b	248	ARG	CD-NE	6.00	1.56	1.46
3	A	329	ARG	CZ-NH2	5.99	1.40	1.33
11	X	23	PHE	CB-CG	5.99	1.61	1.51
5	Q	100	TYR	CE1-CZ	5.98	1.46	1.38
11	U	117	ARG	CZ-NH2	5.97	1.40	1.33
3	A	613	GLU	CD-OE1	5.96	1.32	1.25
10	O	264	GLU	CG-CD	5.95	1.60	1.51
11	a	35	SER	C-N	5.94	1.43	1.33
4	F	232	ASN	C-N	5.94	1.43	1.33
7	G	30	GLU	CB-CG	5.93	1.63	1.52
11	X	88	PHE	CB-CG	5.92	1.61	1.51
11	X	98	GLY	N-CA	-5.91	1.37	1.46
4	B	196	PRO	N-CD	-5.91	1.39	1.47
4	F	101	ARG	CZ-NH1	5.90	1.40	1.33
4	D	248	PRO	N-CD	-5.89	1.39	1.47
7	G	144	ARG	CZ-NH2	5.89	1.40	1.33
3	C	482	ARG	CD-NE	5.88	1.56	1.46
4	D	257	ARG	NE-CZ	5.88	1.40	1.33
3	E	221	ARG	CZ-NH1	5.87	1.40	1.33
11	W	153	ARG	CD-NE	5.87	1.56	1.46
3	C	595	GLU	CD-OE2	-5.87	1.19	1.25
11	V	56	PRO	N-CD	-5.86	1.39	1.47
4	F	289	ARG	NE-CZ	5.86	1.40	1.33
3	E	145	LYS	N-CA	-5.85	1.34	1.46
8	P	455	ASN	CA-CB	5.85	1.68	1.53
4	F	407	TYR	CG-CD2	5.84	1.46	1.39
7	K	117	TYR	CE2-CZ	5.84	1.46	1.38
9	b	305	GLU	CD-OE2	5.83	1.32	1.25
11	Y	77	SER	CA-CB	5.82	1.61	1.52
11	Y	124	ARG	NE-CZ	5.82	1.40	1.33
1	M	67	SER	CA-CB	5.82	1.61	1.52
3	E	392	TYR	CB-CG	-5.82	1.43	1.51
7	G	52	ARG	CZ-NH2	5.82	1.40	1.33
11	T	16	GLY	C-N	5.81	1.47	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	179	ARG	CZ-NH2	5.81	1.40	1.33
7	G	158	ARG	NE-CZ	5.81	1.40	1.33
7	I	198	GLU	CB-CG	5.81	1.63	1.52
11	V	117	ARG	NE-CZ	5.80	1.40	1.33
4	D	455	PHE	CB-CG	5.80	1.61	1.51
5	Q	218	ARG	CZ-NH1	5.79	1.40	1.33
7	G	213	GLU	CD-OE2	5.79	1.32	1.25
7	K	43	TYR	CB-CG	-5.78	1.43	1.51
4	B	268	TYR	CZ-OH	5.77	1.47	1.37
3	E	97	GLY	N-CA	5.77	1.54	1.46
7	K	151	SER	CA-CB	5.76	1.61	1.52
11	W	124	ARG	CD-NE	5.75	1.56	1.46
4	B	215	MET	C-N	5.75	1.43	1.33
11	X	76	TYR	CG-CD1	5.74	1.46	1.39
9	b	27	ARG	CZ-NH1	5.74	1.40	1.33
7	K	166	ARG	CZ-NH1	5.74	1.40	1.33
7	G	178	TYR	CB-CG	5.74	1.60	1.51
11	T	124	ARG	CZ-NH2	5.74	1.40	1.33
1	M	127	ARG	CZ-NH1	5.74	1.40	1.33
11	S	76	TYR	CG-CD1	5.73	1.46	1.39
11	W	85	TYR	CG-CD2	5.73	1.46	1.39
3	C	62	ARG	NE-CZ	5.72	1.40	1.33
4	D	111	ARG	CZ-NH2	5.72	1.40	1.33
3	E	267	GLN	CG-CD	5.72	1.64	1.51
3	A	215	TRP	NE1-CE2	-5.72	1.30	1.37
7	I	166	ARG	CD-NE	5.71	1.56	1.46
3	E	126	ARG	CZ-NH2	5.71	1.40	1.33
4	F	466	ARG	CZ-NH1	5.71	1.40	1.33
1	M	49	ARG	NE-CZ	5.71	1.40	1.33
11	W	76	TYR	CB-CG	5.71	1.60	1.51
11	S	121	GLN	N-CA	-5.71	1.34	1.46
11	a	46	ARG	CD-NE	5.71	1.56	1.46
11	V	55	VAL	CB-CG1	5.70	1.64	1.52
4	B	99	SER	CA-CB	5.69	1.61	1.52
11	Y	117	ARG	CZ-NH2	5.69	1.40	1.33
7	K	114	ARG	CZ-NH1	5.69	1.40	1.33
11	X	38	GLY	CA-C	-5.69	1.42	1.51
4	B	407	TYR	CD2-CE2	5.68	1.47	1.39
6	J	2	SER	CB-OG	5.68	1.49	1.42
5	Q	77	TYR	CD1-CE1	5.68	1.47	1.39
10	O	374	TYR	CE1-CZ	5.68	1.46	1.38
7	G	223	TYR	CB-CG	-5.68	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	Q	337	ARG	CD-NE	5.67	1.56	1.46
5	Q	341	TYR	CE1-CZ	5.67	1.46	1.38
7	G	182	ASP	CA-C	-5.67	1.38	1.52
3	A	212	TYR	CD2-CE2	5.66	1.47	1.39
3	E	286	ARG	CD-NE	5.66	1.56	1.46
7	K	85	ARG	CZ-NH1	5.66	1.40	1.33
7	G	143	GLU	N-CA	-5.66	1.35	1.46
11	a	135	PHE	CE2-CZ	5.66	1.48	1.37
3	A	477	GLU	CD-OE1	5.65	1.31	1.25
6	L	25	ARG	NE-CZ	5.65	1.40	1.33
11	a	124	ARG	NE-CZ	5.65	1.40	1.33
3	E	394	ARG	CZ-NH2	5.65	1.40	1.33
10	O	28	SER	CA-CB	5.65	1.61	1.52
3	E	165	SER	CA-CB	5.64	1.61	1.52
3	E	158	TYR	CD2-CE2	5.64	1.47	1.39
3	E	406	ARG	CZ-NH2	5.64	1.40	1.33
3	A	468	ASN	CB-CG	5.64	1.64	1.51
3	A	62	ARG	CZ-NH1	5.63	1.40	1.33
3	A	250	GLY	CA-C	-5.63	1.42	1.51
8	P	32	ARG	CZ-NH1	5.62	1.40	1.33
8	P	73	ASN	C-N	5.61	1.43	1.33
11	S	124	ARG	CD-NE	5.61	1.55	1.46
4	F	309	TYR	CZ-OH	5.61	1.47	1.37
7	I	92	ARG	CZ-NH2	5.60	1.40	1.33
4	B	333	PRO	CA-C	5.59	1.64	1.52
3	A	359	ARG	CD-NE	5.59	1.55	1.46
11	S	71	SER	CA-CB	5.59	1.61	1.52
3	E	351	SER	CA-CB	5.59	1.61	1.52
9	b	42	ARG	NE-CZ	5.58	1.40	1.33
4	F	220	GLU	CD-OE2	5.58	1.31	1.25
11	V	113	ASP	CA-CB	5.57	1.66	1.53
11	a	118	GLY	CA-C	-5.57	1.43	1.51
3	C	102	GLU	CD-OE1	5.55	1.31	1.25
3	A	24	TYR	CB-CG	5.55	1.59	1.51
4	B	205	GLU	CD-OE2	5.55	1.31	1.25
11	R	82	GLN	CG-CD	5.55	1.63	1.51
3	A	126	ARG	NE-CZ	5.55	1.40	1.33
11	S	105	GLY	CA-C	-5.55	1.43	1.51
11	U	119	SER	CA-CB	5.54	1.61	1.52
4	F	465	LEU	N-CA	-5.54	1.35	1.46
7	G	158	ARG	CD-NE	5.54	1.55	1.46
3	A	225	GLU	CG-CD	5.53	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	171	PRO	N-CD	-5.53	1.40	1.47
3	E	179	ARG	CD-NE	5.53	1.55	1.46
11	U	46	ARG	CZ-NH2	5.53	1.40	1.33
5	Q	118	ARG	CD-NE	5.53	1.55	1.46
3	E	609	GLU	CB-CG	5.53	1.62	1.52
11	R	118	GLY	N-CA	-5.53	1.37	1.46
7	I	219	ARG	CZ-NH2	5.53	1.40	1.33
7	G	163	LYS	CA-CB	5.52	1.66	1.53
7	I	85	ARG	NE-CZ	5.52	1.40	1.33
8	P	220	ARG	NE-CZ	5.51	1.40	1.33
9	b	268	GLU	CG-CD	5.51	1.60	1.51
4	F	80	PHE	CG-CD2	5.50	1.47	1.38
9	b	343	ARG	CZ-NH2	5.50	1.40	1.33
7	G	175	SER	CB-OG	5.50	1.49	1.42
2	N	54	PHE	CG-CD2	5.49	1.47	1.38
7	K	194	SER	CA-CB	5.49	1.61	1.52
3	C	556	GLU	CD-OE2	5.49	1.31	1.25
4	F	230	GLU	CG-CD	5.49	1.60	1.51
7	K	213	GLU	CD-OE2	5.48	1.31	1.25
4	F	119	PRO	N-CD	-5.48	1.40	1.47
11	Z	153	ARG	NE-CZ	5.47	1.40	1.33
4	D	370	TYR	CG-CD2	5.47	1.46	1.39
4	F	167	GLY	CA-C	-5.47	1.43	1.51
8	P	460	ARG	NE-CZ	5.47	1.40	1.33
10	O	152	TYR	CZ-OH	5.47	1.47	1.37
3	E	363	ALA	CA-CB	5.46	1.64	1.52
8	P	477	PHE	CE2-CZ	5.45	1.47	1.37
3	A	73	TYR	CE1-CZ	5.45	1.45	1.38
3	C	212	TYR	CG-CD2	5.45	1.46	1.39
11	a	27	GLY	N-CA	5.44	1.54	1.46
4	F	144	ARG	CD-NE	5.44	1.55	1.46
7	K	158	ARG	NE-CZ	5.44	1.40	1.33
3	C	286	ARG	CZ-NH1	5.43	1.40	1.33
3	C	215	TRP	CG-CD1	5.43	1.44	1.36
4	F	437	GLU	CB-CG	5.43	1.62	1.52
10	O	382	TYR	CZ-OH	5.42	1.47	1.37
11	U	85	TYR	CD1-CE1	5.42	1.47	1.39
3	C	599	GLU	CA-CB	5.41	1.65	1.53
11	U	142	TYR	CG-CD1	5.41	1.46	1.39
11	T	142	TYR	CG-CD2	5.41	1.46	1.39
4	D	318	ARG	CD-NE	5.41	1.55	1.46
4	D	450	GLU	CG-CD	5.41	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	b	70	ARG	CD-NE	5.41	1.55	1.46
3	C	126	ARG	CZ-NH1	5.41	1.40	1.33
6	L	46	TYR	CE2-CZ	5.41	1.45	1.38
4	D	449	TYR	CE2-CZ	5.40	1.45	1.38
11	T	66	TYR	C-N	5.40	1.42	1.33
8	P	110	GLY	CA-C	-5.40	1.43	1.51
4	F	284	TYR	CG-CD2	5.40	1.46	1.39
7	G	223	TYR	CG-CD2	5.39	1.46	1.39
3	E	396	GLY	CA-C	-5.39	1.43	1.51
11	Z	12	PHE	N-CA	-5.38	1.35	1.46
3	A	309	GLU	CD-OE2	5.38	1.31	1.25
11	a	43	CYS	CB-SG	-5.37	1.73	1.81
5	Q	105	ASP	CA-CB	5.37	1.65	1.53
4	F	284	TYR	CB-CG	5.37	1.59	1.51
11	R	160	CYS	CB-SG	-5.36	1.73	1.81
11	U	31	GLY	N-CA	-5.36	1.38	1.46
4	F	106	GLU	CD-OE1	5.35	1.31	1.25
5	Q	276	ARG	NE-CZ	5.35	1.40	1.33
3	C	343	PHE	CG-CD1	5.34	1.46	1.38
3	C	478	PHE	CE1-CZ	5.34	1.47	1.37
7	K	144	ARG	CD-NE	5.34	1.55	1.46
11	X	46	ARG	NE-CZ	5.34	1.40	1.33
1	M	179	PRO	N-CD	-5.34	1.40	1.47
11	V	92	GLY	CA-C	-5.34	1.43	1.51
3	C	209	PHE	CG-CD1	5.34	1.46	1.38
3	E	46	TYR	CA-CB	5.34	1.65	1.53
8	P	192	GLU	CD-OE2	5.33	1.31	1.25
4	D	71	ARG	CZ-NH2	5.33	1.40	1.33
3	E	29	SER	CA-CB	5.33	1.60	1.52
11	R	47	PRO	N-CD	-5.33	1.40	1.47
1	M	169	ARG	CZ-NH1	5.33	1.40	1.33
3	A	191	TYR	CE1-CZ	5.33	1.45	1.38
4	F	395	ASP	CA-CB	5.33	1.65	1.53
3	A	610	ARG	N-CA	-5.32	1.35	1.46
7	G	114	ARG	NE-CZ	5.32	1.40	1.33
7	I	223	TYR	CG-CD1	5.32	1.46	1.39
3	C	326	VAL	CB-CG1	5.31	1.64	1.52
9	b	180	ILE	C-N	5.31	1.42	1.33
3	A	143	PRO	N-CD	-5.31	1.40	1.47
9	b	217	GLU	CD-OE2	-5.31	1.19	1.25
11	T	124	ARG	CD-NE	5.31	1.55	1.46
4	F	370	TYR	CG-CD2	5.31	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	25	ARG	NE-CZ	5.31	1.40	1.33
9	b	139	GLU	CB-CG	5.30	1.62	1.52
3	A	564	GLY	CA-C	-5.30	1.43	1.51
11	S	135	PHE	CG-CD1	5.30	1.46	1.38
1	M	112	TYR	CZ-OH	5.30	1.46	1.37
11	X	124	ARG	CD-NE	5.30	1.55	1.46
7	I	43	TYR	CE1-CZ	5.29	1.45	1.38
3	A	575	GLY	CA-C	-5.29	1.43	1.51
11	U	117	ARG	CD-NE	5.29	1.55	1.46
5	Q	336	GLU	CD-OE1	5.29	1.31	1.25
3	E	223	VAL	CB-CG1	5.28	1.64	1.52
3	E	344	ARG	CZ-NH2	5.28	1.40	1.33
3	E	475	TYR	CA-CB	5.27	1.65	1.53
4	D	48	ARG	CZ-NH1	5.27	1.39	1.33
3	E	433	GLY	N-CA	-5.27	1.38	1.46
3	C	73	TYR	CB-CG	5.26	1.59	1.51
4	D	61	THR	N-CA	-5.26	1.35	1.46
4	B	433	LEU	N-CA	-5.26	1.35	1.46
11	T	23	PHE	CG-CD1	5.26	1.46	1.38
11	W	113	ASP	CB-CG	5.26	1.62	1.51
3	A	97	GLY	N-CA	-5.26	1.38	1.46
4	B	323	GLU	CD-OE2	5.26	1.31	1.25
11	Z	76	TYR	CE1-CZ	5.25	1.45	1.38
3	A	471	TYR	CZ-OH	5.25	1.46	1.37
4	D	173	PHE	CG-CD2	5.25	1.46	1.38
3	E	586	PHE	CG-CD1	5.25	1.46	1.38
11	R	67	GLY	CA-C	-5.25	1.43	1.51
3	E	237	GLN	CG-CD	5.24	1.63	1.51
6	J	12	GLN	N-CA	5.24	1.56	1.46
4	F	316	TYR	CE2-CZ	5.24	1.45	1.38
3	C	383	TYR	CG-CD1	5.24	1.46	1.39
5	Q	80	PHE	CD2-CE2	5.24	1.49	1.39
10	O	362	GLY	CA-C	-5.23	1.43	1.51
7	I	43	TYR	CE2-CZ	5.23	1.45	1.38
3	E	383	TYR	CD1-CE1	-5.23	1.31	1.39
4	D	223	ARG	CZ-NH1	5.23	1.39	1.33
2	N	37	PHE	CG-CD1	5.22	1.46	1.38
4	D	316	TYR	CE2-CZ	5.22	1.45	1.38
4	D	402	GLN	CA-CB	-5.22	1.42	1.53
5	Q	297	ARG	NE-CZ	5.22	1.39	1.33
3	A	343	PHE	CD1-CE1	5.22	1.49	1.39
11	W	25	SER	CA-C	-5.22	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	O	119	ARG	NE-CZ	5.22	1.39	1.33
6	H	25	ARG	CD-NE	5.22	1.55	1.46
3	E	325	PRO	N-CA	-5.22	1.38	1.47
3	A	40	MET	CG-SD	5.21	1.94	1.81
4	F	227	GLN	CA-CB	5.21	1.65	1.53
11	Z	153	ARG	CZ-NH1	5.21	1.39	1.33
8	P	245	HIS	CB-CG	-5.20	1.40	1.50
4	D	449	TYR	CE1-CZ	5.20	1.45	1.38
4	B	268	TYR	CG-CD1	5.20	1.46	1.39
4	F	140	ASN	CB-CG	5.20	1.63	1.51
8	P	154	GLY	N-CA	-5.20	1.38	1.46
3	C	167	ILE	N-CA	-5.20	1.35	1.46
3	A	518	ALA	CA-CB	5.19	1.63	1.52
4	D	237	ARG	NE-CZ	5.19	1.39	1.33
6	H	56	GLU	CG-CD	5.19	1.59	1.51
8	P	332	ASP	CA-CB	5.19	1.65	1.53
7	K	160	TYR	CE1-CZ	5.18	1.45	1.38
1	M	97	ARG	CD-NE	5.18	1.55	1.46
7	K	92	ARG	CD-NE	5.18	1.55	1.46
3	A	484	ARG	CZ-NH2	5.18	1.39	1.33
4	D	167	GLY	N-CA	-5.18	1.38	1.46
4	F	152	SER	CA-CB	5.17	1.60	1.52
5	Q	217	ASP	CA-CB	5.17	1.65	1.53
4	D	321	ARG	CZ-NH1	5.17	1.39	1.33
8	P	128	PHE	CG-CD2	5.17	1.46	1.38
11	V	85	TYR	CB-CG	-5.17	1.43	1.51
10	O	324	HIS	CB-CG	5.17	1.59	1.50
1	M	103	GLY	N-CA	5.17	1.53	1.46
7	G	170	GLU	CD-OE1	5.17	1.31	1.25
3	A	218	ARG	NE-CZ	5.17	1.39	1.33
6	L	100	GLU	CD-OE2	-5.16	1.20	1.25
11	X	23	PHE	CG-CD2	5.16	1.46	1.38
8	P	21	ARG	CZ-NH2	5.16	1.39	1.33
6	L	67	GLU	CB-CG	5.16	1.61	1.52
3	C	610	ARG	CZ-NH1	5.16	1.39	1.33
4	B	321	ARG	CZ-NH2	5.15	1.39	1.33
11	R	152	SER	C-N	5.15	1.45	1.34
3	E	301	TYR	CG-CD2	5.15	1.45	1.39
5	Q	51	TYR	CG-CD1	5.15	1.45	1.39
6	L	28	ARG	CZ-NH2	5.15	1.39	1.33
3	E	359	ARG	NE-CZ	5.14	1.39	1.33
4	D	166	ARG	CD-NE	5.13	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	Z	23	PHE	CG-CD2	5.13	1.46	1.38
3	E	266	SER	CB-OG	5.13	1.49	1.42
3	C	365	ARG	CD-NE	5.13	1.55	1.46
1	M	191	GLU	CD-OE1	5.13	1.31	1.25
4	F	252	ARG	NE-CZ	5.12	1.39	1.33
3	A	123	TYR	CE1-CZ	5.12	1.45	1.38
10	O	97	TYR	CG-CD1	5.12	1.45	1.39
4	B	305	PRO	C-N	5.11	1.42	1.33
7	K	159	GLU	CD-OE2	5.11	1.31	1.25
7	G	127	GLU	CD-OE1	5.11	1.31	1.25
3	E	359	ARG	CZ-NH1	5.10	1.39	1.33
3	C	99	GLY	CA-C	-5.10	1.43	1.51
11	T	46	ARG	CZ-NH2	5.10	1.39	1.33
4	F	195	ARG	NE-CZ	5.09	1.39	1.33
4	D	381	ARG	CZ-NH2	5.08	1.39	1.33
3	A	297	PHE	CE2-CZ	5.08	1.47	1.37
3	C	149	GLY	CA-C	5.08	1.59	1.51
2	N	80	ARG	CZ-NH2	5.07	1.39	1.33
4	D	301	ARG	NE-CZ	5.07	1.39	1.33
4	D	307	TYR	CG-CD2	5.07	1.45	1.39
4	B	94	GLU	CA-C	-5.07	1.39	1.52
10	O	98	ARG	CZ-NH1	5.07	1.39	1.33
10	O	349	GLY	CA-C	-5.07	1.43	1.51
11	S	126	PHE	CB-CG	5.07	1.59	1.51
2	N	80	ARG	CZ-NH1	5.07	1.39	1.33
7	I	85	ARG	CZ-NH1	5.07	1.39	1.33
4	D	195	ARG	CD-NE	5.07	1.55	1.46
4	D	32	SER	C-N	5.06	1.42	1.33
3	E	573	SER	CA-CB	5.06	1.60	1.52
5	Q	292	GLU	CG-CD	5.06	1.59	1.51
10	O	121	PHE	CB-CG	-5.06	1.42	1.51
3	C	190	GLU	CG-CD	5.06	1.59	1.51
7	K	109	GLY	CA-C	-5.06	1.43	1.51
10	O	312	TYR	CG-CD2	5.06	1.45	1.39
11	Y	30	TYR	CZ-OH	5.05	1.46	1.37
3	A	426	PRO	N-CD	-5.05	1.40	1.47
3	C	135	ARG	CZ-NH2	5.05	1.39	1.33
3	C	160	SER	CA-CB	5.05	1.60	1.52
9	b	142	ARG	CZ-NH2	5.05	1.39	1.33
4	B	207	ASN	N-CA	-5.05	1.36	1.46
4	D	163	SER	CA-CB	5.05	1.60	1.52
6	L	53	GLU	CG-CD	5.04	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	K	108	SER	CA-CB	5.04	1.60	1.52
8	P	17	ARG	CZ-NH1	5.04	1.39	1.33
4	D	352	TYR	CE2-CZ	5.04	1.45	1.38
3	E	439	TRP	CB-CG	5.04	1.59	1.50
5	Q	181	ARG	NE-CZ	5.04	1.39	1.33
11	Z	51	PHE	CG-CD1	5.04	1.46	1.38
11	T	112	GLY	CA-C	5.04	1.59	1.51
5	Q	132	TRP	CZ2-CH2	5.03	1.47	1.37
10	O	230	GLU	CD-OE2	5.03	1.31	1.25
2	N	3	GLU	CB-CG	5.03	1.61	1.52
4	B	146	TYR	CD1-CE1	5.03	1.46	1.39
5	Q	312	TRP	CE2-CZ2	-5.03	1.31	1.39
4	B	63	ARG	CZ-NH1	5.03	1.39	1.33
8	P	329	LYS	N-CA	-5.02	1.36	1.46
3	C	482	ARG	NE-CZ	5.02	1.39	1.33
4	B	477	SER	CA-CB	5.01	1.60	1.52
11	R	79	GLY	CA-C	-5.01	1.43	1.51
3	A	272	TYR	N-CA	-5.01	1.36	1.46
3	E	62	ARG	CZ-NH2	5.00	1.39	1.33
4	B	119	PRO	N-CD	-5.00	1.40	1.47
4	B	272	ARG	NE-CZ	5.00	1.39	1.33
5	Q	202	GLU	CD-OE1	5.00	1.31	1.25

All (1393) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	406	ARG	NE-CZ-NH1	17.62	129.11	120.30
1	M	91	ARG	NE-CZ-NH1	17.37	128.98	120.30
4	B	485	TYR	CB-CG-CD1	17.28	131.37	121.00
4	D	111	ARG	NE-CZ-NH1	16.88	128.74	120.30
3	E	329	ARG	NE-CZ-NH1	16.34	128.47	120.30
11	W	124	ARG	NE-CZ-NH1	-16.22	112.19	120.30
5	Q	266	ARG	NE-CZ-NH2	-15.46	112.57	120.30
8	P	255	PHE	CB-CG-CD1	15.44	131.61	120.80
10	O	34	PHE	CB-CG-CD2	-15.29	110.10	120.80
11	U	88	PHE	CB-CG-CD2	-15.26	110.12	120.80
4	F	404	TYR	CB-CG-CD2	-15.16	111.90	121.00
3	A	177	ARG	NE-CZ-NH1	14.87	127.73	120.30
10	O	319	TYR	CB-CG-CD2	-14.77	112.14	121.00
9	b	69	TYR	CB-CG-CD2	-14.62	112.23	121.00
4	D	111	ARG	NE-CZ-NH2	-14.54	113.03	120.30
11	V	30	TYR	CB-CG-CD2	-14.53	112.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	46	ARG	NE-CZ-NH2	-14.38	113.11	120.30
6	J	46	TYR	CB-CG-CD1	-14.31	112.42	121.00
4	B	485	TYR	CB-CG-CD2	-14.26	112.44	121.00
9	b	69	TYR	CB-CG-CD1	14.11	129.47	121.00
3	A	46	TYR	CB-CG-CD1	14.07	129.44	121.00
1	M	92	PHE	CB-CG-CD1	13.94	130.56	120.80
3	C	334	TYR	CB-CG-CD2	-13.47	112.92	121.00
4	D	272	ARG	NE-CZ-NH2	-13.28	113.66	120.30
3	A	406	ARG	NE-CZ-NH2	-13.22	113.69	120.30
3	C	550	PHE	CB-CG-CD2	-13.19	111.57	120.80
5	Q	30	TYR	CB-CG-CD1	-13.16	113.10	121.00
3	E	314	ARG	NE-CZ-NH1	13.14	126.87	120.30
4	F	257	ARG	NE-CZ-NH1	12.98	126.79	120.30
2	N	113	ARG	NE-CZ-NH1	12.96	126.78	120.30
4	D	118	ARG	NE-CZ-NH2	-12.81	113.89	120.30
9	b	151	PHE	CB-CG-CD2	-12.66	111.94	120.80
3	E	484	ARG	NE-CZ-NH1	12.61	126.61	120.30
11	U	88	PHE	CB-CG-CD1	12.51	129.56	120.80
3	E	553	TYR	CB-CG-CD2	-12.48	113.52	121.00
5	Q	6	PHE	CB-CG-CD2	12.38	129.46	120.80
11	Z	11	PHE	CB-CG-CD2	12.30	129.41	120.80
8	P	255	PHE	CB-CG-CD2	-12.30	112.19	120.80
3	E	218	ARG	NE-CZ-NH1	12.27	126.44	120.30
3	C	553	TYR	CB-CG-CD1	-12.18	113.69	121.00
11	R	85	TYR	CB-CG-CD1	12.17	128.30	121.00
4	D	309	TYR	CB-CG-CD2	-12.16	113.70	121.00
3	A	548	ARG	NE-CZ-NH2	-12.16	114.22	120.30
5	Q	289	TYR	CB-CG-CD2	-12.05	113.77	121.00
11	W	135	PHE	CB-CG-CD2	-12.04	112.37	120.80
3	C	135	ARG	NE-CZ-NH2	-11.97	114.32	120.30
11	W	30	TYR	CB-CG-CD1	11.92	128.15	121.00
10	O	260	PHE	CB-CG-CD1	-11.87	112.49	120.80
9	b	31	TYR	CB-CG-CD1	-11.83	113.90	121.00
3	A	314	ARG	NE-CZ-NH2	-11.80	114.40	120.30
10	O	210	TYR	CB-CG-CD1	-11.77	113.94	121.00
4	D	316	TYR	CB-CG-CD1	11.75	128.05	121.00
8	P	288	ARG	NE-CZ-NH2	-11.74	114.43	120.30
4	F	237	ARG	NE-CZ-NH2	-11.71	114.44	120.30
11	T	124	ARG	NE-CZ-NH2	-11.59	114.50	120.30
5	Q	249	TYR	CB-CG-CD2	-11.46	114.12	121.00
6	H	30	ASP	CB-CG-OD2	-11.43	108.01	118.30
4	D	118	ARG	NE-CZ-NH1	11.40	126.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	224	PHE	CB-CG-CD2	-11.37	112.84	120.80
4	F	252	ARG	NE-CZ-NH1	11.33	125.97	120.30
11	X	142	TYR	CB-CG-CD2	-11.31	114.22	121.00
3	A	158	TYR	CB-CG-CD1	-11.24	114.25	121.00
4	F	304	TYR	CB-CG-CD2	-11.21	114.27	121.00
3	A	46	TYR	CB-CG-CD2	-11.20	114.28	121.00
4	D	435	PHE	CB-CG-CD1	11.20	128.64	120.80
4	F	237	ARG	NE-CZ-NH1	11.19	125.90	120.30
8	P	109	TYR	CB-CG-CD1	-11.18	114.29	121.00
3	E	87	ARG	NE-CZ-NH2	-11.14	114.73	120.30
9	b	343	ARG	NE-CZ-NH2	-11.13	114.74	120.30
3	E	286	ARG	NE-CZ-NH2	11.12	125.86	120.30
11	V	85	TYR	CB-CG-CD1	-11.11	114.33	121.00
11	a	46	ARG	NE-CZ-NH1	11.10	125.85	120.30
11	Y	46	ARG	NE-CZ-NH2	-11.08	114.76	120.30
5	Q	97	TYR	CB-CG-CD2	-11.08	114.35	121.00
11	T	142	TYR	CB-CG-CD2	-11.02	114.39	121.00
3	A	365	ARG	NE-CZ-NH2	11.01	125.80	120.30
7	I	158	ARG	NE-CZ-NH1	10.99	125.80	120.30
3	A	553	TYR	CB-CG-CD1	10.87	127.52	121.00
7	G	117	TYR	CB-CG-CD1	-10.86	114.48	121.00
11	W	30	TYR	CB-CG-CD2	-10.85	114.49	121.00
4	F	475	ARG	NE-CZ-NH1	10.85	125.72	120.30
4	F	131	TYR	CB-CG-CD1	10.84	127.51	121.00
4	D	173	PHE	CB-CG-CD1	10.81	128.37	120.80
4	F	63	ARG	NE-CZ-NH1	10.77	125.68	120.30
11	V	30	TYR	CB-CG-CD1	10.71	127.43	121.00
9	b	332	ARG	NE-CZ-NH2	-10.68	114.96	120.30
7	I	25	ARG	NE-CZ-NH2	-10.66	114.97	120.30
9	b	60	ARG	NE-CZ-NH1	10.63	125.62	120.30
3	A	87	ARG	NE-CZ-NH1	10.63	125.61	120.30
5	Q	321	ARG	NE-CZ-NH1	10.59	125.59	120.30
9	b	42	ARG	NE-CZ-NH2	-10.59	115.01	120.30
3	A	380	PHE	CB-CG-CD2	-10.58	113.39	120.80
3	C	221	ARG	NE-CZ-NH1	10.56	125.58	120.30
4	D	362	ARG	NE-CZ-NH2	-10.56	115.02	120.30
7	I	117	TYR	CB-CG-CD2	-10.50	114.70	121.00
10	O	260	PHE	CB-CG-CD2	10.42	128.10	120.80
9	b	285	TYR	CB-CG-CD1	10.41	127.25	121.00
7	I	206	ARG	NE-CZ-NH1	10.38	125.49	120.30
9	b	120	ARG	NE-CZ-NH2	-10.35	115.12	120.30
9	b	151	PHE	CB-CG-CD1	10.34	128.04	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	267	TYR	CB-CG-CD2	-10.33	114.80	121.00
3	A	87	ARG	NE-CZ-NH2	-10.31	115.14	120.30
3	C	212	TYR	CB-CG-CD1	10.31	127.18	121.00
11	S	88	PHE	CB-CG-CD2	-10.31	113.59	120.80
8	P	109	TYR	CB-CG-CD2	10.29	127.17	121.00
4	D	173	PHE	CB-CG-CD2	-10.22	113.64	120.80
11	W	23	PHE	CB-CG-CD2	-10.16	113.69	120.80
4	D	257	ARG	NE-CZ-NH2	-10.16	115.22	120.30
11	S	51	PHE	CB-CG-CD2	-10.14	113.70	120.80
4	F	195	ARG	NE-CZ-NH2	10.13	125.36	120.30
11	Y	124	ARG	NE-CZ-NH2	-10.10	115.25	120.30
11	V	51	PHE	CB-CG-CD2	-10.06	113.76	120.80
10	O	356	PHE	CB-CG-CD2	-10.05	113.77	120.80
4	B	208	PHE	CB-CG-CD1	10.05	127.83	120.80
3	A	342	TYR	CB-CG-CD2	-10.04	114.98	121.00
5	Q	289	TYR	CB-CG-CD1	10.04	127.02	121.00
4	B	121	ASP	CB-CG-OD2	-10.02	109.28	118.30
9	b	208	ARG	NE-CZ-NH2	-10.01	115.30	120.30
4	F	316	TYR	CB-CG-CD1	10.01	127.00	121.00
4	F	286	ASP	CB-CG-OD2	-10.00	109.30	118.30
3	C	135	ARG	NE-CZ-NH1	9.99	125.30	120.30
4	F	485	TYR	CB-CG-CD1	9.98	126.99	121.00
7	I	223	TYR	CB-CG-CD2	-9.98	115.01	121.00
11	a	126	PHE	CB-CG-CD1	9.95	127.76	120.80
1	M	9	PHE	CB-CG-CD2	-9.95	113.84	120.80
8	P	267	TYR	CB-CG-CD1	9.94	126.97	121.00
4	F	46	PHE	CB-CG-CD1	9.93	127.75	120.80
7	I	206	ARG	NE-CZ-NH2	-9.92	115.34	120.30
5	Q	77	TYR	CB-CG-CD2	-9.90	115.06	121.00
4	B	452	ARG	NE-CZ-NH1	9.87	125.23	120.30
3	C	471	TYR	CB-CG-CD2	9.87	126.92	121.00
5	Q	335	ARG	NE-CZ-NH2	-9.85	115.38	120.30
8	P	301	ARG	NE-CZ-NH1	9.83	125.22	120.30
11	Z	11	PHE	CB-CG-CD1	-9.83	113.92	120.80
10	O	356	PHE	CB-CG-CD1	9.81	127.67	120.80
7	K	62	PHE	CB-CG-CD1	-9.80	113.94	120.80
4	F	223	ARG	NE-CZ-NH1	-9.79	115.41	120.30
8	P	184	TYR	CB-CG-CD1	9.75	126.85	121.00
11	Y	85	TYR	CB-CG-CD2	-9.72	115.17	121.00
11	Y	51	PHE	CB-CG-CD1	9.72	127.60	120.80
4	B	316	TYR	CB-CG-CD2	-9.70	115.18	121.00
10	O	231	TYR	CB-CG-CD2	-9.69	115.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	N	61	ARG	NE-CZ-NH2	9.67	125.14	120.30
10	O	34	PHE	CB-CG-CD1	9.67	127.57	120.80
3	C	238	ARG	NE-CZ-NH1	9.66	125.13	120.30
1	M	12	ARG	NE-CZ-NH1	-9.65	115.47	120.30
11	X	76	TYR	CB-CG-CD2	-9.65	115.21	121.00
11	T	23	PHE	CB-CG-CD1	9.64	127.55	120.80
4	D	101	ARG	NE-CZ-NH1	-9.63	115.48	120.30
3	E	448	ARG	NE-CZ-NH2	-9.63	115.48	120.30
6	J	46	TYR	CG-CD2-CE2	-9.62	113.61	121.30
9	b	53	ARG	NE-CZ-NH2	9.57	125.09	120.30
9	b	141	TYR	CB-CG-CD1	9.56	126.74	121.00
7	I	43	TYR	CG-CD1-CE1	-9.55	113.66	121.30
4	B	46	PHE	CB-CG-CD2	-9.53	114.13	120.80
4	B	466	ARG	NE-CZ-NH2	-9.53	115.54	120.30
4	F	189	ARG	NE-CZ-NH1	9.53	125.06	120.30
11	a	106	PHE	CB-CG-CD2	-9.50	114.15	120.80
4	B	370	TYR	CB-CG-CD1	-9.47	115.32	121.00
9	b	20	TYR	CB-CG-CD2	-9.47	115.32	121.00
4	F	59	ASP	CB-CG-OD1	-9.46	109.79	118.30
11	Z	76	TYR	CB-CG-CD2	-9.45	115.33	121.00
5	Q	266	ARG	NE-CZ-NH1	9.42	125.01	120.30
4	F	166	ARG	NE-CZ-NH1	-9.42	115.59	120.30
4	D	309	TYR	CB-CG-CD1	9.39	126.64	121.00
4	D	316	TYR	CB-CG-CD2	-9.37	115.38	121.00
11	U	153	ARG	NE-CZ-NH1	9.35	124.98	120.30
10	O	169	ASP	CB-CG-OD1	-9.32	109.91	118.30
9	b	208	ARG	NE-CZ-NH1	9.32	124.96	120.30
11	R	85	TYR	CB-CG-CD2	-9.29	115.42	121.00
4	D	307	TYR	CB-CG-CD1	9.29	126.57	121.00
4	F	321	ARG	NE-CZ-NH1	9.28	124.94	120.30
4	D	407	TYR	CB-CG-CD2	-9.28	115.43	121.00
4	F	362	ARG	NE-CZ-NH2	-9.27	115.67	120.30
4	F	466	ARG	NE-CZ-NH2	-9.27	115.67	120.30
11	Y	51	PHE	CB-CG-CD2	-9.26	114.32	120.80
3	A	380	PHE	CB-CG-CD1	9.23	127.26	120.80
7	G	219	ARG	NE-CZ-NH2	-9.22	115.69	120.30
4	B	307	TYR	CG-CD2-CE2	-9.20	113.94	121.30
4	B	466	ARG	NE-CZ-NH1	9.19	124.90	120.30
3	A	123	TYR	CB-CG-CD2	-9.18	115.49	121.00
11	Z	88	PHE	CB-CG-CD1	9.17	127.22	120.80
11	X	135	PHE	CB-CG-CD2	-9.17	114.38	120.80
3	A	334	TYR	CB-CG-CD2	9.15	126.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	158	TYR	CB-CG-CD1	-9.14	115.51	121.00
11	X	135	PHE	CB-CG-CD1	9.13	127.19	120.80
1	M	120	PHE	CB-CG-CD2	-9.12	114.42	120.80
3	C	46	TYR	CB-CG-CD1	9.12	126.47	121.00
8	P	458	ASP	CB-CG-OD1	-9.10	110.11	118.30
4	F	223	ARG	NE-CZ-NH2	9.04	124.82	120.30
4	B	150	MET	CG-SD-CE	-9.03	85.76	100.20
11	Y	124	ARG	NE-CZ-NH1	9.03	124.81	120.30
4	F	302	ARG	NE-CZ-NH1	9.01	124.80	120.30
11	T	85	TYR	CB-CG-CD1	-9.01	115.60	121.00
4	F	46	PHE	CB-CG-CD2	-8.98	114.51	120.80
10	O	319	TYR	CB-CG-CD1	8.96	126.38	121.00
3	E	553	TYR	CG-CD2-CE2	-8.96	114.14	121.30
11	X	85	TYR	CB-CG-CD2	8.95	126.37	121.00
4	B	435	PHE	CB-CG-CD2	8.95	127.07	120.80
9	b	51	PHE	CB-CG-CD1	8.94	127.06	120.80
9	b	70	ARG	NE-CZ-NH1	8.90	124.75	120.30
7	G	166	ARG	NE-CZ-NH2	-8.89	115.85	120.30
4	B	325	ARG	NE-CZ-NH2	-8.89	115.85	120.30
7	G	23	PHE	CB-CG-CD2	8.88	127.02	120.80
8	P	359	TYR	CB-CG-CD1	-8.88	115.67	121.00
4	F	307	TYR	CB-CG-CD1	8.87	126.32	121.00
3	C	212	TYR	CG-CD1-CE1	8.87	128.39	121.30
4	B	443	PHE	CB-CG-CD2	8.81	126.97	120.80
11	R	135	PHE	CB-CG-CD2	-8.80	114.64	120.80
3	A	177	ARG	NE-CZ-NH2	-8.79	115.90	120.30
4	F	359	PHE	CB-CG-CD2	-8.77	114.66	120.80
9	b	285	TYR	CB-CG-CD2	-8.77	115.74	121.00
3	E	272	TYR	CB-CG-CD2	-8.66	115.80	121.00
3	C	276	ASP	CB-CG-OD1	-8.65	110.51	118.30
10	O	116	TRP	N-CA-CB	8.64	126.16	110.60
8	P	379	PHE	CB-CG-CD2	-8.64	114.75	120.80
11	W	18	ALA	N-CA-CB	8.64	122.20	110.10
4	F	424	ALA	N-CA-CB	8.63	122.18	110.10
4	B	257	ARG	NE-CZ-NH2	-8.61	116.00	120.30
5	Q	6	PHE	CB-CG-CD1	-8.59	114.79	120.80
10	O	325	PHE	CB-CG-CD2	-8.59	114.79	120.80
7	G	160	TYR	CB-CG-CD1	-8.59	115.85	121.00
8	P	288	ARG	NE-CZ-NH1	8.55	124.58	120.30
7	K	177	ASP	CB-CG-OD1	-8.55	110.61	118.30
11	U	18	ALA	N-CA-CB	-8.55	98.13	110.10
4	B	155	VAL	CA-CB-CG2	-8.54	98.10	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	280	TYR	CB-CG-CD2	-8.54	115.88	121.00
11	S	85	TYR	CB-CG-CD2	-8.53	115.88	121.00
7	I	158	ARG	NE-CZ-NH2	-8.51	116.04	120.30
11	X	153	ARG	NE-CZ-NH2	-8.51	116.04	120.30
3	E	616	ASP	CB-CG-OD1	8.51	125.96	118.30
5	Q	51	TYR	CB-CG-CD2	8.51	126.11	121.00
3	E	202	PHE	CB-CG-CD1	-8.49	114.86	120.80
1	M	134	ARG	NE-CZ-NH1	8.48	124.54	120.30
11	a	12	PHE	CB-CG-CD2	8.47	126.73	120.80
11	T	12	PHE	CB-CG-CD1	-8.46	114.88	120.80
3	E	257	ALA	N-CA-CB	8.45	121.94	110.10
9	b	72	PHE	CB-CG-CD2	8.43	126.70	120.80
11	S	124	ARG	NE-CZ-NH1	8.42	124.51	120.30
4	D	48	ARG	NE-CZ-NH2	8.38	124.49	120.30
6	L	27	TYR	CB-CG-CD1	8.38	126.03	121.00
4	F	362	ARG	NE-CZ-NH1	8.37	124.49	120.30
3	A	83	ASP	CB-CG-OD1	-8.33	110.80	118.30
11	R	76	TYR	CG-CD2-CE2	8.33	127.97	121.30
4	B	307	TYR	CB-CG-CD2	-8.32	116.01	121.00
11	W	142	TYR	CB-CG-CD1	8.31	125.99	121.00
3	A	123	TYR	CB-CG-CD1	8.30	125.98	121.00
3	C	482	ARG	NE-CZ-NH1	-8.30	116.15	120.30
5	Q	77	TYR	CB-CG-CD1	8.29	125.98	121.00
1	M	141	ARG	NE-CZ-NH1	8.29	124.44	120.30
3	E	177	ARG	NE-CZ-NH2	-8.28	116.16	120.30
3	A	209	PHE	CB-CG-CD1	8.28	126.60	120.80
4	F	304	TYR	CG-CD1-CE1	-8.26	114.69	121.30
7	I	76	THR	CA-CB-CG2	-8.26	100.83	112.40
7	G	206	ARG	NE-CZ-NH1	8.23	124.42	120.30
1	M	97	ARG	NE-CZ-NH1	-8.23	116.19	120.30
6	H	30	ASP	CB-CG-OD1	8.22	125.70	118.30
3	A	531	TYR	CB-CG-CD2	-8.20	116.08	121.00
3	E	451	PHE	CB-CG-CD2	-8.19	115.07	120.80
3	C	600	PHE	CB-CG-CD1	8.18	126.53	120.80
11	a	106	PHE	CB-CG-CD1	8.17	126.52	120.80
11	V	135	PHE	CB-CG-CD1	8.17	126.52	120.80
10	O	312	TYR	CB-CG-CD2	-8.12	116.13	121.00
4	F	393	ARG	NE-CZ-NH2	8.11	124.36	120.30
10	O	96	ALA	N-CA-CB	8.09	121.43	110.10
4	B	307	TYR	CD1-CG-CD2	8.09	126.80	117.90
3	C	423	PHE	CB-CG-CD1	-8.07	115.15	120.80
3	E	392	TYR	CG-CD1-CE1	8.06	127.75	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	112	ARG	NE-CZ-NH2	-8.05	116.28	120.30
4	F	225	PHE	CB-CG-CD1	8.04	126.43	120.80
4	D	429	ASP	CB-CG-OD2	-8.04	111.07	118.30
8	P	128	PHE	CB-CG-CD2	-8.02	115.19	120.80
3	A	534	TYR	CB-CG-CD1	8.00	125.80	121.00
7	I	43	TYR	CB-CG-CD1	-8.00	116.20	121.00
9	b	110	TYR	CB-CG-CD2	-7.98	116.21	121.00
3	E	392	TYR	CB-CG-CD1	7.97	125.78	121.00
9	b	141	TYR	CB-CG-CD2	-7.97	116.22	121.00
8	P	407	ARG	NE-CZ-NH1	-7.96	116.32	120.30
4	B	468	TYR	CB-CG-CD1	7.93	125.76	121.00
11	W	135	PHE	CB-CG-CD1	7.93	126.35	120.80
3	E	342	TYR	CG-CD2-CE2	-7.92	114.96	121.30
11	Z	12	PHE	CB-CG-CD1	7.89	126.32	120.80
4	F	257	ARG	NE-CZ-NH2	-7.88	116.36	120.30
2	N	61	ARG	NH1-CZ-NH2	-7.88	110.73	119.40
11	Y	142	TYR	CB-CG-CD1	7.88	125.73	121.00
10	O	42	ARG	NE-CZ-NH1	7.87	124.24	120.30
4	D	452	ARG	NE-CZ-NH1	7.87	124.23	120.30
4	F	404	TYR	CG-CD1-CE1	-7.84	115.02	121.30
11	V	135	PHE	CB-CG-CD2	-7.83	115.32	120.80
11	R	30	TYR	CB-CG-CD2	-7.83	116.30	121.00
4	B	472	MET	CG-SD-CE	7.82	112.72	100.20
3	E	460	TYR	CB-CG-CD1	7.82	125.69	121.00
3	E	314	ARG	NE-CZ-NH2	-7.82	116.39	120.30
3	E	406	ARG	NE-CZ-NH1	7.82	124.21	120.30
3	C	179	ARG	NE-CZ-NH2	-7.81	116.39	120.30
11	V	64	ALA	N-CA-CB	7.80	121.02	110.10
3	E	329	ARG	NE-CZ-NH2	-7.80	116.40	120.30
4	B	295	ARG	NE-CZ-NH2	-7.79	116.40	120.30
11	V	51	PHE	CB-CG-CD1	7.79	126.25	120.80
3	A	587	PHE	CB-CG-CD1	7.79	126.25	120.80
8	P	128	PHE	CB-CG-CD1	7.78	126.24	120.80
4	B	165	ALA	CB-CA-C	-7.77	98.45	110.10
4	F	208	PHE	CB-CG-CD1	-7.76	115.36	120.80
3	E	614	SER	N-CA-CB	7.74	122.12	110.50
10	O	164	ARG	NE-CZ-NH1	7.74	124.17	120.30
11	W	142	TYR	CB-CG-CD2	-7.74	116.35	121.00
3	E	425	ASP	CB-CG-OD1	7.72	125.25	118.30
11	a	12	PHE	CB-CG-CD1	-7.71	115.40	120.80
11	U	124	ARG	NE-CZ-NH2	-7.70	116.45	120.30
3	C	46	TYR	CB-CG-CD2	-7.70	116.38	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	L	27	TYR	CB-CG-CD2	-7.69	116.39	121.00
11	W	23	PHE	CB-CG-CD1	7.69	126.18	120.80
3	E	257	ALA	CB-CA-C	-7.69	98.57	110.10
4	D	462	TRP	CH2-CZ2-CE2	7.68	125.08	117.40
4	D	265	TYR	CG-CD1-CE1	-7.68	115.16	121.30
1	M	139	TYR	CB-CG-CD2	7.68	125.61	121.00
7	K	52	ARG	NE-CZ-NH1	7.67	124.14	120.30
3	E	218	ARG	NE-CZ-NH2	-7.67	116.46	120.30
11	X	142	TYR	CB-CG-CD1	7.67	125.60	121.00
4	B	166	ARG	NE-CZ-NH1	7.67	124.13	120.30
11	R	124	ARG	NE-CZ-NH2	-7.65	116.47	120.30
3	C	553	TYR	CG-CD1-CE1	-7.65	115.18	121.30
11	Y	11	PHE	CB-CG-CD1	7.64	126.15	120.80
11	Z	85	TYR	CB-CG-CD1	-7.63	116.42	121.00
9	b	205	ARG	NE-CZ-NH1	-7.63	116.48	120.30
3	A	221	ARG	NE-CZ-NH1	7.61	124.11	120.30
5	Q	217	ASP	CB-CG-OD1	7.61	125.14	118.30
11	S	46	ARG	NE-CZ-NH1	7.60	124.10	120.30
3	A	314	ARG	NE-CZ-NH1	7.60	124.10	120.30
5	Q	300	PHE	CB-CG-CD1	7.60	126.12	120.80
11	Z	30	TYR	CB-CG-CD2	-7.59	116.45	121.00
4	B	318	ARG	NE-CZ-NH1	7.58	124.09	120.30
4	D	114	ASP	CB-CG-OD2	-7.58	111.48	118.30
7	K	117	TYR	CB-CG-CD2	-7.58	116.45	121.00
4	B	381	ARG	NE-CZ-NH1	-7.57	116.51	120.30
3	C	392	TYR	CG-CD1-CE1	-7.57	115.24	121.30
1	M	91	ARG	NE-CZ-NH2	-7.57	116.52	120.30
3	A	158	TYR	CZ-CE2-CD2	-7.56	112.99	119.80
3	A	66	ASP	CB-CG-OD1	7.55	125.09	118.30
11	W	12	PHE	CB-CG-CD1	-7.55	115.52	120.80
4	B	159	ASP	CB-CG-OD2	-7.54	111.51	118.30
4	B	414	ALA	N-CA-CB	7.54	120.66	110.10
3	E	591	ARG	NE-CZ-NH2	-7.54	116.53	120.30
11	W	88	PHE	CB-CG-CD1	7.54	126.08	120.80
3	A	383	TYR	CG-CD2-CE2	-7.54	115.27	121.30
4	B	455	PHE	CB-CG-CD1	-7.53	115.53	120.80
6	L	28	ARG	NE-CZ-NH2	-7.53	116.53	120.30
7	G	160	TYR	CB-CG-CD2	7.52	125.52	121.00
5	Q	51	TYR	CB-CG-CD1	-7.52	116.49	121.00
5	Q	30	TYR	CB-CG-CD2	7.52	125.51	121.00
4	F	478	PRO	N-CA-CB	7.51	112.32	103.30
9	b	343	ARG	NE-CZ-NH1	7.51	124.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	157	ASP	CB-CG-OD1	-7.50	111.55	118.30
3	E	548	ARG	NE-CZ-NH2	-7.50	116.55	120.30
3	E	40	MET	CG-SD-CE	-7.49	88.21	100.20
11	X	76	TYR	CB-CG-CD1	7.48	125.49	121.00
4	B	245	ALA	CB-CA-C	-7.47	98.89	110.10
11	X	124	ARG	NE-CZ-NH2	-7.47	116.56	120.30
4	F	49	TYR	CB-CG-CD1	7.46	125.48	121.00
11	W	113	ASP	CB-CG-OD2	-7.45	111.59	118.30
3	A	460	TYR	CB-CG-CD1	-7.44	116.53	121.00
8	P	259	PHE	CB-CG-CD1	7.44	126.01	120.80
4	B	49	TYR	CZ-CE2-CD2	-7.43	113.11	119.80
4	B	452	ARG	NE-CZ-NH2	-7.42	116.59	120.30
7	I	43	TYR	CD1-CG-CD2	7.41	126.06	117.90
4	F	49	TYR	CB-CG-CD2	-7.40	116.56	121.00
11	T	11	PHE	CB-CG-CD1	7.39	125.97	120.80
7	G	144	ARG	NE-CZ-NH1	7.38	123.99	120.30
10	O	246	PHE	CB-CG-CD2	-7.38	115.63	120.80
3	A	129	ASP	CB-CG-OD2	-7.36	111.67	118.30
3	A	191	TYR	CB-CG-CD2	-7.35	116.59	121.00
9	b	352	ARG	NE-CZ-NH1	-7.35	116.63	120.30
11	V	85	TYR	CB-CG-CD2	7.35	125.41	121.00
11	a	85	TYR	CB-CG-CD2	-7.35	116.59	121.00
5	Q	71	TYR	CB-CG-CD1	7.34	125.41	121.00
3	E	610	ARG	NE-CZ-NH1	-7.34	116.63	120.30
8	P	439	ASP	CB-CG-OD2	7.33	124.90	118.30
3	A	126	ARG	NE-CZ-NH2	-7.33	116.64	120.30
11	Y	142	TYR	CB-CG-CD2	-7.33	116.60	121.00
8	P	244	TYR	CG-CD2-CE2	-7.33	115.44	121.30
9	b	116	TYR	CB-CG-CD1	7.32	125.39	121.00
7	K	92	ARG	NE-CZ-NH2	-7.32	116.64	120.30
3	C	208	ASP	CB-CG-OD1	-7.31	111.72	118.30
3	C	392	TYR	CB-CG-CD2	-7.30	116.62	121.00
6	J	27	TYR	CB-CG-CD2	-7.30	116.62	121.00
3	A	24	TYR	CB-CG-CD2	-7.29	116.63	121.00
5	Q	7	ASN	O-C-N	7.28	134.34	122.70
2	N	40	TYR	CB-CG-CD2	-7.25	116.65	121.00
3	C	534	TYR	CB-CG-CD2	-7.23	116.66	121.00
3	E	342	TYR	CB-CG-CD1	-7.22	116.67	121.00
3	E	297	PHE	CB-CG-CD2	-7.22	115.74	120.80
4	D	466	ARG	NE-CZ-NH2	-7.22	116.69	120.30
2	N	113	ARG	NH1-CZ-NH2	-7.22	111.46	119.40
4	D	114	ASP	CB-CG-OD1	7.21	124.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	117	ARG	NE-CZ-NH1	7.20	123.90	120.30
4	B	302	ARG	NE-CZ-NH1	7.20	123.90	120.30
3	E	75	GLU	N-CA-CB	7.20	123.56	110.60
5	Q	286	ASP	CB-CG-OD2	-7.19	111.83	118.30
7	G	62	PHE	CB-CG-CD2	-7.18	115.78	120.80
11	R	88	PHE	CB-CG-CD2	-7.18	115.78	120.80
3	C	425	ASP	CB-CG-OD1	-7.17	111.84	118.30
11	T	46	ARG	NE-CZ-NH2	-7.15	116.72	120.30
11	R	135	PHE	CB-CG-CD1	7.15	125.81	120.80
3	E	191	TYR	CB-CG-CD2	-7.15	116.71	121.00
3	E	191	TYR	CB-CG-CD1	7.13	125.28	121.00
2	N	40	TYR	CB-CG-CD1	7.13	125.28	121.00
5	Q	262	PHE	CB-CG-CD2	-7.13	115.81	120.80
4	D	265	TYR	CB-CG-CD2	-7.12	116.73	121.00
11	T	142	TYR	CD1-CE1-CZ	7.12	126.21	119.80
11	V	44	VAL	CA-CB-CG1	-7.11	100.24	110.90
3	C	182	ILE	CA-CB-CG2	-7.09	96.71	110.90
6	H	27	TYR	CG-CD2-CE2	-7.08	115.64	121.30
3	C	581	VAL	CG1-CB-CG2	7.08	122.23	110.90
5	Q	297	ARG	NE-CZ-NH2	-7.07	116.76	120.30
4	D	281	MET	CA-CB-CG	7.07	125.31	113.30
10	O	97	TYR	CB-CG-CD1	7.05	125.23	121.00
3	C	370	ARG	NE-CZ-NH1	7.05	123.82	120.30
3	A	132	ALA	N-CA-CB	7.04	119.96	110.10
2	N	82	ASP	N-CA-CB	7.04	123.26	110.60
8	P	76	THR	CA-CB-CG2	-7.03	102.56	112.40
2	N	101	TYR	CB-CG-CD2	-7.03	116.78	121.00
4	F	268	TYR	CG-CD2-CE2	7.02	126.92	121.30
3	A	129	ASP	CB-CG-OD1	7.02	124.62	118.30
8	P	220	ARG	NE-CZ-NH1	7.01	123.81	120.30
4	F	104	VAL	N-CA-C	-7.01	92.08	111.00
4	F	407	TYR	CB-CG-CD1	7.00	125.20	121.00
3	E	64	ASP	CB-CG-OD2	-7.00	112.00	118.30
8	P	350	TYR	CG-CD2-CE2	-7.00	115.70	121.30
3	A	297	PHE	CB-CG-CD2	-6.99	115.90	120.80
4	F	430	LYS	N-CA-CB	6.98	123.16	110.60
4	F	74	ARG	NE-CZ-NH1	6.97	123.79	120.30
11	V	97	VAL	CG1-CB-CG2	6.97	122.06	110.90
9	b	177	ALA	N-CA-CB	6.97	119.86	110.10
6	H	44	ASP	CB-CG-OD1	6.97	124.58	118.30
4	D	49	TYR	CB-CG-CD2	-6.96	116.82	121.00
3	A	610	ARG	NE-CZ-NH2	-6.96	116.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	A	146	PHE	CB-CG-CD2	-6.95	115.93	120.80
11	R	77	SER	CB-CA-C	-6.95	96.89	110.10
3	A	355	ASP	N-CA-C	-6.95	92.24	111.00
3	A	576	ASP	CB-CG-OD2	6.95	124.55	118.30
5	Q	249	TYR	CG-CD2-CE2	-6.95	115.74	121.30
4	F	224	PHE	CB-CG-CD1	6.93	125.66	120.80
3	C	600	PHE	CB-CG-CD2	-6.93	115.95	120.80
2	N	61	ARG	NE-CZ-NH1	6.93	123.76	120.30
4	D	321	ARG	NE-CZ-NH1	6.93	123.76	120.30
11	Y	85	TYR	CB-CG-CD1	6.92	125.15	121.00
4	B	140	ASN	N-CA-CB	6.92	123.05	110.60
7	K	92	ARG	NE-CZ-NH1	6.91	123.76	120.30
10	O	222	ALA	N-CA-CB	6.91	119.77	110.10
2	N	37	PHE	CB-CG-CD1	-6.89	115.98	120.80
7	K	152	MET	CG-SD-CE	-6.87	89.21	100.20
11	W	11	PHE	CB-CG-CD2	6.87	125.61	120.80
8	P	380	TRP	CE3-CZ3-CH2	-6.87	113.65	121.20
3	A	591	ARG	NE-CZ-NH1	6.87	123.73	120.30
9	b	110	TYR	CB-CG-CD1	6.87	125.12	121.00
10	O	332	VAL	CA-CB-CG2	-6.87	100.60	110.90
3	A	553	TYR	CB-CG-CD2	-6.86	116.88	121.00
7	K	97	ASP	CB-CG-OD1	-6.85	112.13	118.30
3	E	244	PHE	CB-CG-CD2	-6.85	116.00	120.80
11	Y	12	PHE	CB-CG-CD2	-6.85	116.00	120.80
11	T	48	ASP	CB-CG-OD2	-6.85	112.14	118.30
5	Q	126	ARG	NE-CZ-NH1	6.84	123.72	120.30
10	O	348	PHE	CB-CG-CD2	-6.84	116.01	120.80
11	T	124	ARG	NE-CZ-NH1	6.84	123.72	120.30
3	C	334	TYR	CG-CD2-CE2	-6.84	115.83	121.30
11	W	46	ARG	NE-CZ-NH1	6.83	123.72	120.30
3	A	253	CYS	CA-CB-SG	-6.83	101.70	114.00
3	C	105	TYR	CB-CG-CD1	-6.83	116.90	121.00
6	L	25	ARG	NE-CZ-NH1	-6.83	116.88	120.30
3	C	156	ASP	CB-CG-OD2	-6.83	112.15	118.30
4	D	280	ASP	CB-CG-OD1	6.83	124.45	118.30
5	Q	166	PHE	CD1-CE1-CZ	6.83	128.29	120.10
11	R	32	THR	CA-CB-CG2	-6.82	102.86	112.40
11	W	23	PHE	CZ-CE2-CD2	6.82	128.28	120.10
10	O	231	TYR	CB-CG-CD1	6.81	125.09	121.00
7	I	160	TYR	CG-CD1-CE1	6.81	126.75	121.30
10	O	335	LYS	N-CA-CB	6.81	122.85	110.60
3	C	484	ARG	NE-CZ-NH1	6.80	123.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	71	TYR	CB-CG-CD2	-6.80	116.92	121.00
6	J	68	LEU	CB-CG-CD1	6.79	122.55	111.00
3	E	377	ASP	CB-CG-OD1	6.79	124.41	118.30
10	O	290	ARG	NE-CZ-NH2	-6.79	116.90	120.30
11	T	76	TYR	CB-CG-CD2	-6.79	116.92	121.00
9	b	359	ARG	NE-CZ-NH2	-6.79	116.91	120.30
3	A	342	TYR	CB-CG-CD1	6.78	125.07	121.00
10	O	246	PHE	CB-CG-CD1	6.78	125.55	120.80
3	C	221	ARG	NH1-CZ-NH2	-6.77	111.95	119.40
10	O	169	ASP	CB-CG-OD2	6.77	124.39	118.30
5	Q	230	SER	N-CA-CB	6.77	120.66	110.50
5	Q	191	ASP	CB-CG-OD2	-6.76	112.22	118.30
6	H	44	ASP	CB-CG-OD2	-6.76	112.22	118.30
4	D	49	TYR	CB-CG-CD1	6.75	125.05	121.00
3	E	64	ASP	CB-CG-OD1	6.74	124.37	118.30
11	S	106	PHE	CB-CG-CD2	-6.74	116.08	120.80
3	A	370	ARG	NE-CZ-NH2	-6.73	116.94	120.30
4	D	63	ARG	NE-CZ-NH2	6.73	123.67	120.30
8	P	120	ASP	CB-CG-OD2	-6.73	112.25	118.30
4	B	161	MET	CB-CA-C	-6.73	96.95	110.40
10	O	206	PHE	CB-CG-CD2	-6.72	116.09	120.80
3	E	511	ASP	CB-CG-OD2	-6.71	112.26	118.30
4	B	46	PHE	CB-CG-CD1	6.71	125.50	120.80
3	E	54	ASP	CB-CG-OD1	6.71	124.34	118.30
3	E	105	TYR	CB-CG-CD2	6.71	125.03	121.00
3	C	334	TYR	CB-CG-CD1	6.70	125.02	121.00
8	P	468	ALA	CB-CA-C	-6.70	100.05	110.10
4	B	404	TYR	CB-CG-CD1	6.69	125.01	121.00
3	E	534	TYR	CB-CG-CD2	-6.68	116.99	121.00
10	O	258	ARG	NE-CZ-NH2	-6.67	116.96	120.30
3	A	301	TYR	CB-CG-CD1	-6.67	117.00	121.00
9	b	205	ARG	NE-CZ-NH2	6.66	123.63	120.30
11	T	85	TYR	CG-CD2-CE2	-6.65	115.98	121.30
3	A	548	ARG	NE-CZ-NH1	6.65	123.62	120.30
3	E	460	TYR	CB-CG-CD2	-6.64	117.01	121.00
11	Z	142	TYR	CB-CG-CD1	6.64	124.99	121.00
3	E	449	LYS	N-CA-CB	6.64	122.55	110.60
6	J	76	VAL	CA-CB-CG2	-6.63	100.95	110.90
3	C	324	MET	CG-SD-CE	6.63	110.80	100.20
4	D	195	ARG	NE-CZ-NH1	-6.62	116.99	120.30
3	E	429	THR	CA-CB-CG2	-6.62	103.13	112.40
6	J	37	THR	CA-CB-CG2	-6.61	103.15	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	5	TYR	CB-CG-CD1	-6.60	117.04	121.00
8	P	86	THR	CA-CB-CG2	-6.60	103.16	112.40
9	b	236	PHE	CB-CG-CD2	-6.60	116.18	120.80
11	T	11	PHE	CB-CG-CD2	-6.60	116.18	120.80
11	W	126	PHE	CB-CG-CD2	-6.60	116.18	120.80
2	N	37	PHE	CB-CG-CD2	6.60	125.42	120.80
11	W	155	THR	CA-CB-CG2	-6.60	103.17	112.40
4	F	318	ARG	NE-CZ-NH1	-6.59	117.00	120.30
3	E	425	ASP	CB-CG-OD2	-6.58	112.37	118.30
3	C	218	ARG	NE-CZ-NH1	-6.58	117.01	120.30
3	A	230	ASP	CB-CG-OD2	-6.57	112.39	118.30
3	C	586	PHE	CB-CG-CD2	-6.57	116.20	120.80
6	L	46	TYR	CB-CG-CD2	6.57	124.94	121.00
10	O	318	ARG	NE-CZ-NH2	6.57	123.58	120.30
11	W	106	PHE	CB-CG-CD2	-6.57	116.20	120.80
10	O	110	TYR	CB-CG-CD1	-6.55	117.07	121.00
4	F	307	TYR	CB-CG-CD2	-6.55	117.07	121.00
3	C	515	LEU	CB-CG-CD2	6.54	122.13	111.00
3	E	438	PHE	CB-CG-CD1	-6.54	116.22	120.80
5	Q	337	ARG	NE-CZ-NH2	6.52	123.56	120.30
6	J	38	ASP	CB-CG-OD2	-6.52	112.43	118.30
1	M	168	ARG	NE-CZ-NH1	-6.52	117.04	120.30
3	A	178	SER	N-CA-CB	6.52	120.28	110.50
6	J	46	TYR	CZ-CE2-CD2	6.51	125.66	119.80
3	A	183	THR	CA-CB-CG2	-6.51	103.28	112.40
4	D	475	ARG	NE-CZ-NH1	6.51	123.56	120.30
11	T	153	ARG	NE-CZ-NH2	-6.51	117.04	120.30
5	Q	275	TYR	CZ-CE2-CD2	6.50	125.65	119.80
3	E	565	ALA	N-CA-CB	6.50	119.20	110.10
11	W	11	PHE	CB-CG-CD1	-6.50	116.25	120.80
11	W	12	PHE	CB-CG-CD2	6.50	125.35	120.80
3	A	150	ASP	CB-CA-C	-6.50	97.41	110.40
9	b	20	TYR	CG-CD2-CE2	-6.49	116.10	121.30
7	G	25	ARG	NE-CZ-NH2	-6.49	117.06	120.30
7	K	144	ARG	NE-CZ-NH1	-6.49	117.06	120.30
7	K	219	ARG	NE-CZ-NH1	6.48	123.54	120.30
5	Q	5	TYR	CG-CD2-CE2	-6.47	116.12	121.30
4	D	74	ARG	NE-CZ-NH2	-6.47	117.07	120.30
4	B	307	TYR	CB-CG-CD1	-6.46	117.12	121.00
3	C	534	TYR	CB-CG-CD1	6.46	124.88	121.00
10	O	277	ALA	CB-CA-C	-6.46	100.40	110.10
4	B	48	ARG	NE-CZ-NH2	-6.46	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	S	135	PHE	CB-CG-CD1	6.46	125.32	120.80
1	M	97	ARG	NE-CZ-NH2	6.46	123.53	120.30
4	D	39	VAL	CA-CB-CG2	-6.46	101.22	110.90
3	C	314	ARG	NE-CZ-NH2	-6.45	117.07	120.30
10	O	382	TYR	CZ-CE2-CD2	-6.45	113.99	119.80
4	F	272	ARG	NE-CZ-NH1	6.45	123.53	120.30
3	C	408	GLY	N-CA-C	-6.45	96.98	113.10
4	D	305	PRO	N-CD-CG	6.45	112.87	103.20
11	V	153	ARG	N-CA-CB	6.44	122.20	110.60
7	I	223	TYR	CB-CG-CD1	6.44	124.86	121.00
3	C	548	ARG	NE-CZ-NH1	6.44	123.52	120.30
3	A	64	ASP	CB-CG-OD1	-6.44	112.51	118.30
3	E	471	TYR	CB-CG-CD1	6.44	124.86	121.00
3	E	550	PHE	CB-CG-CD1	-6.43	116.30	120.80
1	M	202	ARG	NE-CZ-NH2	6.43	123.52	120.30
1	M	73	TYR	CD1-CE1-CZ	-6.43	114.01	119.80
11	R	125	LEU	CB-CG-CD1	6.43	121.93	111.00
4	D	175	ALA	N-CA-C	-6.41	93.68	111.00
8	P	392	TYR	CB-CG-CD1	6.41	124.85	121.00
3	A	271	LYS	N-CA-CB	-6.41	99.06	110.60
4	F	127	PHE	CB-CG-CD2	-6.41	116.31	120.80
4	F	443	PHE	CD1-CE1-CZ	6.41	127.79	120.10
5	Q	92	ARG	NE-CZ-NH1	6.40	123.50	120.30
5	Q	257	ALA	N-CA-CB	6.40	119.06	110.10
3	E	553	TYR	CZ-CE2-CD2	6.40	125.56	119.80
7	I	100	PHE	CB-CG-CD2	-6.40	116.32	120.80
11	T	85	TYR	CG-CD1-CE1	-6.39	116.19	121.30
1	M	169	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	M	172	ALA	CB-CA-C	-6.39	100.52	110.10
3	E	309	GLU	N-CA-CB	6.39	122.09	110.60
3	A	333	ILE	CA-CB-CG1	6.38	123.12	111.00
11	X	88	PHE	CB-CG-CD2	-6.38	116.33	120.80
4	D	46	PHE	CB-CG-CD1	6.38	125.26	120.80
1	M	143	VAL	CA-CB-CG1	6.38	120.46	110.90
9	b	291	THR	CA-CB-CG2	-6.37	103.48	112.40
1	M	81	TYR	CB-CG-CD1	-6.37	117.18	121.00
3	A	194	ASP	CB-CG-OD1	-6.37	112.57	118.30
8	P	161	VAL	CA-CB-CG2	-6.37	101.35	110.90
3	C	272	TYR	CB-CG-CD1	6.36	124.82	121.00
4	F	191	ALA	N-CA-CB	6.35	118.99	110.10
3	A	212	TYR	CB-CG-CD1	6.35	124.81	121.00
4	D	286	ASP	CB-CG-OD2	-6.35	112.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	438	PHE	CB-CG-CD2	6.35	125.24	120.80
11	V	11	PHE	CB-CG-CD2	-6.34	116.36	120.80
1	M	197	ARG	NE-CZ-NH2	-6.34	117.13	120.30
2	N	42	GLU	OE1-CD-OE2	-6.34	115.69	123.30
3	C	463	TYR	CB-CG-CD1	6.33	124.80	121.00
10	O	151	ASN	CA-CB-CG	-6.33	99.47	113.40
3	E	110	ARG	NE-CZ-NH2	-6.33	117.14	120.30
3	A	534	TYR	CB-CG-CD2	-6.33	117.20	121.00
8	P	350	TYR	CZ-CE2-CD2	6.33	125.50	119.80
4	F	391	MET	CG-SD-CE	-6.33	90.08	100.20
7	G	88	VAL	CA-CB-CG2	-6.33	101.41	110.90
5	Q	102	TYR	CB-CG-CD2	-6.32	117.21	121.00
3	E	401	LEU	CB-CG-CD1	6.32	121.74	111.00
11	U	30	TYR	CB-CG-CD1	-6.31	117.21	121.00
11	W	64	ALA	CB-CA-C	-6.31	100.64	110.10
4	D	453	THR	CA-CB-CG2	-6.30	103.58	112.40
9	b	212	PHE	CB-CG-CD2	6.30	125.21	120.80
4	F	485	TYR	CB-CG-CD2	-6.30	117.22	121.00
3	A	201	GLU	N-CA-CB	6.29	121.92	110.60
11	W	88	PHE	CB-CG-CD2	-6.29	116.40	120.80
9	b	31	TYR	CB-CG-CD2	6.29	124.77	121.00
11	W	76	TYR	CB-CG-CD2	-6.29	117.23	121.00
10	O	98	ARG	NE-CZ-NH1	-6.28	117.16	120.30
4	D	193	LEU	CB-CG-CD1	-6.26	100.35	111.00
3	A	567	TRP	CG-CD2-CE3	-6.26	128.26	133.90
4	D	178	LEU	CB-CA-C	-6.26	98.30	110.20
4	B	229	PHE	CB-CG-CD2	6.26	125.18	120.80
3	C	463	TYR	CZ-CE2-CD2	6.26	125.43	119.80
5	Q	105	ASP	CB-CG-OD1	-6.26	112.67	118.30
8	P	28	ASP	CB-CG-OD1	6.26	123.93	118.30
3	A	327	ALA	CB-CA-C	-6.25	100.72	110.10
3	C	88	THR	CA-CB-CG2	-6.24	103.66	112.40
11	V	123	PRO	N-CA-CB	-6.24	95.73	102.60
3	A	534	TYR	CZ-CE2-CD2	-6.24	114.18	119.80
3	E	202	PHE	CB-CG-CD2	6.24	125.17	120.80
3	E	342	TYR	CZ-CE2-CD2	6.24	125.41	119.80
11	U	117	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	M	169	ARG	NE-CZ-NH1	-6.23	117.18	120.30
8	P	34	GLU	N-CA-CB	6.23	121.82	110.60
9	b	93	ASP	CB-CG-OD2	-6.23	112.69	118.30
9	b	332	ARG	NH1-CZ-NH2	6.23	126.26	119.40
4	D	108	MET	CG-SD-CE	6.23	110.16	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	b	213	PHE	N-CA-C	-6.22	94.21	111.00
11	T	46	ARG	NE-CZ-NH1	6.22	123.41	120.30
11	a	117	ARG	NE-CZ-NH2	-6.22	117.19	120.30
5	Q	345	TYR	CB-CG-CD2	6.21	124.73	121.00
4	B	118	ARG	NE-CZ-NH1	6.21	123.40	120.30
5	Q	217	ASP	CB-CG-OD2	-6.21	112.71	118.30
5	Q	322	ASN	N-CA-CB	6.21	121.78	110.60
4	D	404	TYR	CB-CG-CD1	-6.21	117.28	121.00
8	P	412	ASN	N-CA-CB	6.20	121.75	110.60
10	O	382	TYR	CG-CD1-CE1	-6.20	116.34	121.30
6	J	46	TYR	CB-CG-CD2	6.20	124.72	121.00
9	b	310	PHE	CB-CG-CD1	-6.19	116.46	120.80
3	A	463	TYR	CG-CD2-CE2	-6.19	116.34	121.30
11	W	35	SER	O-C-N	6.19	133.72	123.20
4	D	348	ASP	CB-CG-OD1	6.18	123.86	118.30
4	F	308	MET	CA-CB-CG	6.18	123.80	113.30
9	b	236	PHE	CB-CG-CD1	6.18	125.12	120.80
11	W	124	ARG	NE-CZ-NH2	6.17	123.39	120.30
11	U	104	ALA	N-CA-CB	6.15	118.72	110.10
4	F	309	TYR	CG-CD1-CE1	-6.15	116.38	121.30
1	M	12	ARG	CD-NE-CZ	6.15	132.21	123.60
3	E	44	ALA	CB-CA-C	6.15	119.32	110.10
4	F	124	PRO	N-CD-CG	6.14	112.42	103.20
3	C	238	ARG	NE-CZ-NH2	-6.14	117.23	120.30
3	E	153	SER	N-CA-C	-6.13	94.44	111.00
4	F	482	ASP	N-CA-CB	6.13	121.63	110.60
11	S	124	ARG	NE-CZ-NH2	-6.13	117.24	120.30
4	B	80	PHE	CB-CG-CD1	-6.12	116.51	120.80
4	B	229	PHE	CB-CG-CD1	-6.12	116.51	120.80
8	P	136	PHE	CB-CG-CD1	-6.12	116.51	120.80
3	A	24	TYR	CG-CD2-CE2	-6.12	116.40	121.30
7	G	191	SER	N-CA-CB	6.12	119.68	110.50
1	M	105	TYR	CB-CG-CD2	6.12	124.67	121.00
7	K	117	TYR	CB-CG-CD1	6.12	124.67	121.00
4	F	321	ARG	NE-CZ-NH2	-6.12	117.24	120.30
9	b	261	TYR	CB-CG-CD1	6.11	124.67	121.00
7	G	178	TYR	N-CA-CB	6.11	121.60	110.60
3	C	28	TYR	CB-CG-CD2	6.11	124.66	121.00
3	C	280	TYR	CB-CG-CD1	6.10	124.66	121.00
3	C	87	ARG	NE-CZ-NH1	-6.10	117.25	120.30
4	B	241	PHE	CB-CA-C	-6.10	98.20	110.40
3	C	162	PHE	CB-CG-CD1	6.10	125.07	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	102	TYR	CB-CG-CD1	6.10	124.66	121.00
4	D	383	MET	CB-CA-C	-6.10	98.21	110.40
1	M	44	ARG	CB-CA-C	-6.09	98.21	110.40
10	O	382	TYR	CG-CD2-CE2	6.09	126.17	121.30
4	B	119	PRO	N-CD-CG	6.09	112.34	103.20
9	b	310	PHE	CB-CG-CD2	6.09	125.06	120.80
11	R	157	ASP	N-CA-CB	6.09	121.56	110.60
7	G	126	VAL	CA-CB-CG1	6.09	120.03	110.90
7	I	89	LEU	CB-CG-CD1	6.09	121.35	111.00
1	M	42	ARG	NE-CZ-NH2	6.08	123.34	120.30
4	B	189	ARG	NE-CZ-NH2	6.08	123.34	120.30
5	Q	191	ASP	CB-CG-OD1	6.08	123.77	118.30
3	A	383	TYR	CB-CG-CD1	-6.07	117.36	121.00
6	J	34	GLN	CG-CD-OE1	-6.07	109.46	121.60
5	Q	88	SER	N-CA-CB	6.07	119.61	110.50
3	A	307	THR	CA-CB-CG2	-6.06	103.92	112.40
11	Y	97	VAL	CB-CA-C	-6.06	99.89	111.40
3	E	214	THR	CA-CB-CG2	6.06	120.88	112.40
4	B	111	ARG	NE-CZ-NH2	-6.05	117.27	120.30
4	F	484	PHE	CB-CG-CD2	-6.05	116.56	120.80
3	C	28	TYR	CG-CD2-CE2	6.05	126.14	121.30
3	E	451	PHE	CB-CG-CD1	6.05	125.04	120.80
3	C	73	TYR	CB-CG-CD2	-6.05	117.37	121.00
10	O	318	ARG	NH1-CZ-NH2	-6.05	112.75	119.40
3	A	531	TYR	CG-CD1-CE1	-6.04	116.47	121.30
3	C	471	TYR	CG-CD2-CE2	6.04	126.13	121.30
11	a	133	LEU	CB-CG-CD1	-6.04	100.74	111.00
6	L	92	ASP	CB-CG-OD1	-6.03	112.87	118.30
8	P	410	ASP	CB-CA-C	6.03	122.46	110.40
11	U	40	CYS	N-CA-CB	6.03	121.46	110.60
4	D	87	ASP	CB-CG-OD2	-6.03	112.87	118.30
5	Q	26	SER	N-CA-CB	6.03	119.54	110.50
9	b	336	ILE	N-CA-C	-6.03	94.72	111.00
3	E	416	VAL	CA-CB-CG1	-6.03	101.86	110.90
7	K	130	LEU	N-CA-CB	-6.03	98.34	110.40
3	A	24	TYR	CG-CD1-CE1	-6.03	116.48	121.30
3	E	264	VAL	CA-CB-CG2	6.03	119.94	110.90
11	Z	76	TYR	CG-CD2-CE2	-6.02	116.48	121.30
3	A	177	ARG	N-CA-CB	6.02	121.44	110.60
8	P	369	CYS	N-CA-CB	6.02	121.43	110.60
8	P	32	ARG	NE-CZ-NH1	6.02	123.31	120.30
6	J	19	GLU	OE1-CD-OE2	6.01	130.52	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	435	PHE	CB-CG-CD2	-6.01	116.59	120.80
4	F	189	ARG	NH1-CZ-NH2	-6.00	112.80	119.40
5	Q	232	ASP	CB-CG-OD1	6.00	123.70	118.30
1	M	172	ALA	N-CA-CB	6.00	118.50	110.10
10	O	350	PHE	CB-CG-CD2	6.00	125.00	120.80
7	I	52	ARG	NE-CZ-NH2	5.99	123.30	120.30
3	A	447	GLN	CB-CA-C	-5.99	98.42	110.40
9	b	120	ARG	NH1-CZ-NH2	5.99	125.98	119.40
11	T	12	PHE	CB-CG-CD2	5.99	124.99	120.80
2	N	13	ASP	N-CA-CB	5.98	121.36	110.60
3	A	209	PHE	CB-CG-CD2	-5.98	116.61	120.80
4	F	359	PHE	CB-CG-CD1	5.98	124.99	120.80
11	R	46	ARG	NE-CZ-NH2	-5.98	117.31	120.30
11	W	103	ALA	CB-CA-C	-5.97	101.14	110.10
8	P	147	VAL	CA-CB-CG2	-5.97	101.95	110.90
11	Z	76	TYR	CD1-CE1-CZ	-5.97	114.43	119.80
3	C	280	TYR	CG-CD2-CE2	-5.96	116.53	121.30
9	b	243	ASP	CB-CG-OD1	-5.96	112.94	118.30
11	X	40	CYS	CA-CB-SG	-5.96	103.27	114.00
11	T	43	CYS	O-C-N	-5.95	113.17	122.70
11	R	83	ALA	CB-CA-C	-5.95	101.17	110.10
3	A	600	PHE	CB-CG-CD1	-5.95	116.64	120.80
1	M	112	TYR	CG-CD2-CE2	-5.95	116.54	121.30
4	D	184	ALA	N-CA-CB	5.94	118.42	110.10
11	S	116	VAL	CG1-CB-CG2	-5.94	101.39	110.90
11	Y	85	TYR	CG-CD2-CE2	-5.94	116.55	121.30
1	M	112	TYR	N-CA-CB	5.94	121.28	110.60
3	E	230	ASP	CB-CG-OD1	5.93	123.64	118.30
3	A	438	PHE	CB-CG-CD2	-5.93	116.65	120.80
8	P	396	ARG	NE-CZ-NH1	-5.93	117.34	120.30
8	P	231	VAL	CA-CB-CG1	5.93	119.79	110.90
10	O	382	TYR	CB-CG-CD1	-5.93	117.44	121.00
10	O	95	ASN	N-CA-CB	5.92	121.26	110.60
7	K	43	TYR	CB-CG-CD1	-5.92	117.45	121.00
9	b	186	TYR	CG-CD2-CE2	-5.92	116.56	121.30
3	A	352	MET	CG-SD-CE	-5.91	90.74	100.20
3	C	359	ARG	NE-CZ-NH2	5.91	123.25	120.30
10	O	259	GLU	OE1-CD-OE2	5.91	130.39	123.30
11	T	142	TYR	CB-CG-CD1	5.91	124.55	121.00
10	O	323	PRO	O-C-N	5.91	132.15	122.70
9	b	66	GLU	N-CA-CB	5.91	121.23	110.60
2	N	106	ASP	CB-CG-OD2	-5.91	112.98	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	I	160	TYR	CB-CG-CD1	5.91	124.54	121.00
7	I	12	GLN	N-CA-CB	5.90	121.22	110.60
4	D	80	PHE	CB-CG-CD2	-5.90	116.67	120.80
1	M	92	PHE	CB-CG-CD2	-5.89	116.67	120.80
4	F	304	TYR	CD1-CG-CD2	5.89	124.38	117.90
3	E	394	ARG	NE-CZ-NH1	5.89	123.25	120.30
11	X	142	TYR	CG-CD1-CE1	-5.89	116.59	121.30
9	b	45	ASN	N-CA-C	-5.89	95.10	111.00
10	O	184	PHE	CB-CG-CD1	5.89	124.92	120.80
10	O	218	VAL	CA-CB-CG1	5.89	119.73	110.90
4	F	420	VAL	CA-CB-CG2	5.89	119.73	110.90
7	G	114	ARG	NE-CZ-NH1	5.89	123.24	120.30
7	G	139	VAL	CA-CB-CG2	-5.89	102.07	110.90
11	V	64	ALA	CB-CA-C	-5.88	101.28	110.10
4	F	381	ARG	NE-CZ-NH2	5.88	123.24	120.30
3	C	297	PHE	CB-CG-CD2	-5.87	116.69	120.80
3	C	258	PHE	CB-CG-CD1	-5.87	116.69	120.80
3	A	422	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	M	34	ARG	NE-CZ-NH2	-5.87	117.37	120.30
3	E	327	ALA	CB-CA-C	-5.87	101.30	110.10
3	A	587	PHE	CB-CG-CD2	-5.87	116.69	120.80
11	Z	153	ARG	NE-CZ-NH1	5.86	123.23	120.30
3	A	506	ALA	N-CA-CB	5.86	118.31	110.10
4	F	310	THR	CA-CB-CG2	-5.86	104.19	112.40
11	Z	30	TYR	CG-CD1-CE1	-5.86	116.61	121.30
8	P	13	PHE	CB-CG-CD1	5.86	124.90	120.80
11	R	142	TYR	CB-CG-CD1	5.86	124.51	121.00
11	S	142	TYR	CG-CD1-CE1	-5.86	116.61	121.30
5	Q	128	HIS	CB-CA-C	-5.86	98.69	110.40
5	Q	94	PHE	CB-CG-CD2	5.84	124.89	120.80
11	R	103	ALA	CB-CA-C	-5.84	101.33	110.10
5	Q	262	PHE	CB-CG-CD1	5.84	124.89	120.80
6	H	82	GLU	N-CA-CB	5.84	121.12	110.60
11	V	158	VAL	N-CA-CB	5.84	124.35	111.50
4	B	381	ARG	NH1-CZ-NH2	5.84	125.82	119.40
5	Q	18	ARG	NE-CZ-NH1	-5.84	117.38	120.30
11	S	154	ALA	CB-CA-C	-5.84	101.35	110.10
3	A	537	PHE	CG-CD2-CE2	5.83	127.22	120.80
3	C	73	TYR	CB-CG-CD1	5.83	124.50	121.00
4	F	268	TYR	CZ-CE2-CD2	-5.83	114.55	119.80
7	K	70	MET	N-CA-CB	5.83	121.09	110.60
7	I	216	PRO	N-CA-CB	5.82	110.29	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Z	142	TYR	CD1-CE1-CZ	5.82	125.03	119.80
3	E	73	TYR	CB-CG-CD1	5.81	124.49	121.00
3	E	177	ARG	NE-CZ-NH1	5.81	123.21	120.30
4	B	162	ASN	CB-CG-OD1	5.81	133.22	121.60
5	Q	202	GLU	CA-C-N	5.81	133.37	117.10
3	C	55	ASN	N-CA-CB	5.81	121.05	110.60
3	E	146	PHE	CB-CG-CD2	-5.81	116.73	120.80
3	A	567	TRP	CE2-CD2-CE3	5.81	125.67	118.70
3	A	203	ASP	CB-CG-OD1	-5.80	113.08	118.30
4	B	308	MET	CG-SD-CE	-5.80	90.92	100.20
3	E	73	TYR	CB-CG-CD2	-5.80	117.52	121.00
5	Q	142	ALA	CB-CA-C	-5.80	101.41	110.10
11	W	99	LEU	CB-CG-CD2	5.80	120.86	111.00
3	E	212	TYR	CZ-CE2-CD2	5.79	125.02	119.80
4	B	63	ARG	NE-CZ-NH1	5.79	123.20	120.30
2	N	78	ARG	NE-CZ-NH1	-5.79	117.40	120.30
1	M	101	VAL	N-CA-C	-5.79	95.37	111.00
7	G	189	VAL	CA-CB-CG2	-5.79	102.22	110.90
3	A	158	TYR	CB-CG-CD2	5.79	124.47	121.00
4	D	132	LEU	CB-CG-CD2	5.79	120.83	111.00
6	J	102	VAL	CA-CB-CG1	5.78	119.58	110.90
3	A	110	ARG	NE-CZ-NH1	5.78	123.19	120.30
3	E	409	SER	CB-CA-C	-5.78	99.12	110.10
4	F	55	LEU	CB-CG-CD2	-5.78	101.18	111.00
9	b	19	PHE	CB-CG-CD1	5.77	124.84	120.80
3	C	355	ASP	CB-CG-OD1	-5.77	113.11	118.30
3	E	438	PHE	CB-CG-CD2	5.76	124.84	120.80
11	Z	74	VAL	CA-CB-CG2	-5.76	102.25	110.90
3	A	461	SER	N-CA-CB	5.76	119.14	110.50
3	C	475	TYR	N-CA-CB	5.76	120.96	110.60
7	G	206	ARG	NE-CZ-NH2	-5.76	117.42	120.30
3	A	240	LEU	O-C-N	5.75	131.91	122.70
11	S	83	ALA	N-CA-CB	5.75	118.15	110.10
3	E	509	ASP	CB-CG-OD1	5.75	123.48	118.30
3	E	158	TYR	CB-CG-CD2	-5.75	117.55	121.00
11	a	79	GLY	N-CA-C	-5.75	98.73	113.10
4	B	393	ARG	NE-CZ-NH2	-5.75	117.43	120.30
6	H	24	ALA	O-C-N	-5.74	113.51	122.70
10	O	164	ARG	NH1-CZ-NH2	-5.74	113.09	119.40
3	E	333	ILE	CA-CB-CG1	5.74	121.90	111.00
4	F	404	TYR	CD1-CG-CD2	5.74	124.21	117.90
4	B	443	PHE	CB-CG-CD1	-5.73	116.79	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	X	85	TYR	CG-CD2-CE2	5.73	125.89	121.30
11	a	129	MET	CG-SD-CE	-5.73	91.03	100.20
9	b	99	TYR	CG-CD1-CE1	-5.73	116.72	121.30
10	O	165	LYS	N-CA-CB	5.72	120.90	110.60
4	D	340	ASP	CB-CG-OD1	5.72	123.45	118.30
7	G	160	TYR	CG-CD2-CE2	-5.72	116.72	121.30
8	P	460	ARG	NE-CZ-NH2	-5.72	117.44	120.30
4	F	279	THR	O-C-N	-5.71	113.56	122.70
4	B	316	TYR	CB-CG-CD1	5.71	124.43	121.00
3	A	210	THR	CA-CB-CG2	-5.71	104.41	112.40
7	G	212	GLU	N-CA-CB	5.71	120.87	110.60
11	R	124	ARG	NE-CZ-NH1	5.71	123.16	120.30
4	D	455	PHE	CB-CG-CD2	-5.71	116.81	120.80
3	C	535	ASP	CB-CG-OD1	5.70	123.43	118.30
2	N	25	ILE	N-CA-CB	5.70	123.91	110.80
4	B	449	TYR	CG-CD1-CE1	-5.70	116.74	121.30
11	Z	88	PHE	CB-CG-CD2	-5.70	116.81	120.80
3	E	572	ASP	CB-CG-OD1	5.70	123.43	118.30
1	M	89	THR	N-CA-CB	5.69	121.11	110.30
10	O	210	TYR	CG-CD2-CE2	-5.69	116.75	121.30
4	F	298	VAL	CA-CB-CG2	5.69	119.43	110.90
10	O	229	ALA	CB-CA-C	-5.69	101.57	110.10
4	F	144	ARG	NE-CZ-NH1	-5.68	117.46	120.30
11	W	159	VAL	CG1-CB-CG2	-5.68	101.81	110.90
4	B	34	VAL	N-CA-C	-5.68	95.67	111.00
4	B	49	TYR	CB-CG-CD2	-5.68	117.59	121.00
9	b	70	ARG	CB-CA-C	-5.67	99.05	110.40
4	B	209	SER	N-CA-CB	5.67	119.01	110.50
11	U	46	ARG	CB-CA-C	-5.67	99.06	110.40
11	a	76	TYR	CB-CG-CD1	5.67	124.40	121.00
8	P	202	VAL	CA-CB-CG1	-5.67	102.40	110.90
3	E	392	TYR	CD1-CE1-CZ	-5.67	114.70	119.80
6	L	46	TYR	CB-CG-CD1	-5.66	117.60	121.00
3	E	607	MET	CG-SD-CE	-5.66	91.14	100.20
2	N	91	ILE	CA-CB-CG2	-5.66	99.58	110.90
7	G	195	ASP	CB-CG-OD1	-5.66	113.21	118.30
5	Q	162	PHE	CG-CD2-CE2	5.65	127.02	120.80
3	C	222	PRO	N-CA-CB	5.65	110.08	103.30
4	F	222	ALA	CB-CA-C	-5.65	101.62	110.10
7	G	144	ARG	NE-CZ-NH2	-5.65	117.47	120.30
4	D	70	ILE	CA-CB-CG1	5.65	121.73	111.00
4	D	94	GLU	N-CA-C	-5.65	95.75	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	273	TYR	CB-CG-CD2	-5.65	117.61	121.00
7	K	15	ASP	CB-CA-C	-5.65	99.11	110.40
11	X	107	ALA	N-CA-CB	5.64	118.00	110.10
4	D	302	ARG	NE-CZ-NH1	5.64	123.12	120.30
6	J	72	ALA	CB-CA-C	-5.64	101.64	110.10
7	G	72	SER	N-CA-CB	5.63	118.95	110.50
3	E	448	ARG	CG-CD-NE	-5.63	99.98	111.80
10	O	254	LYS	N-CA-CB	5.63	120.73	110.60
11	U	72	VAL	CA-CB-CG1	5.63	119.34	110.90
3	A	485	MET	CG-SD-CE	-5.63	91.20	100.20
11	a	97	VAL	CG1-CB-CG2	5.62	119.90	110.90
3	A	28	TYR	CB-CG-CD2	5.62	124.37	121.00
3	C	463	TYR	CB-CG-CD2	-5.62	117.63	121.00
10	O	11	PHE	CB-CG-CD1	5.62	124.73	120.80
3	C	423	PHE	CB-CG-CD2	5.62	124.73	120.80
3	E	330	GLU	N-CA-CB	5.61	120.70	110.60
3	A	118	GLU	CA-CB-CG	5.61	125.74	113.40
3	A	316	THR	N-CA-C	-5.61	95.85	111.00
3	A	596	VAL	CA-CB-CG1	-5.61	102.48	110.90
1	M	60	VAL	CA-CB-CG2	-5.61	102.49	110.90
3	A	284	GLY	N-CA-C	-5.61	99.08	113.10
5	Q	12	PHE	CB-CG-CD1	-5.61	116.88	120.80
5	Q	162	PHE	CB-CG-CD1	5.61	124.72	120.80
11	S	160	CYS	CA-CB-SG	-5.61	103.91	114.00
3	C	352	MET	CG-SD-CE	-5.61	91.23	100.20
4	F	142	TYR	CA-CB-CG	-5.61	102.75	113.40
9	b	53	ARG	NE-CZ-NH1	-5.60	117.50	120.30
3	E	207	SER	N-CA-CB	5.60	118.90	110.50
3	A	302	THR	CA-CB-CG2	-5.60	104.56	112.40
3	A	343	PHE	CB-CG-CD1	5.60	124.72	120.80
1	M	102	SER	N-CA-CB	5.60	118.90	110.50
7	K	113	ASN	N-CA-CB	5.60	120.68	110.60
11	a	158	VAL	CB-CA-C	5.60	122.04	111.40
4	B	237	ARG	CG-CD-NE	-5.60	100.05	111.80
1	M	132	VAL	CG1-CB-CG2	-5.59	101.95	110.90
5	Q	278	PHE	CB-CG-CD1	5.59	124.71	120.80
1	M	29	TYR	CZ-CE2-CD2	5.58	124.83	119.80
4	D	466	ARG	NE-CZ-NH1	5.58	123.09	120.30
10	O	359	ASP	CB-CG-OD2	-5.58	113.28	118.30
4	F	142	TYR	C-N-CA	5.57	135.63	121.70
11	R	21	ILE	CA-CB-CG2	-5.57	99.76	110.90
3	A	252	THR	N-CA-C	-5.57	95.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	P	318	ALA	CB-CA-C	-5.57	101.75	110.10
4	F	150	MET	CA-CB-CG	5.57	122.76	113.30
11	a	24	THR	O-C-N	-5.57	113.80	122.70
5	Q	30	TYR	CD1-CE1-CZ	5.56	124.81	119.80
11	U	153	ARG	NE-CZ-NH2	-5.56	117.52	120.30
11	U	54	ILE	CA-CB-CG2	5.56	122.02	110.90
3	E	406	ARG	NH1-CZ-NH2	-5.56	113.29	119.40
8	P	411	VAL	CB-CA-C	5.56	121.96	111.40
3	C	541	TRP	CH2-CZ2-CE2	5.56	122.96	117.40
9	b	72	PHE	CG-CD2-CE2	5.56	126.91	120.80
3	A	327	ALA	N-CA-CB	5.55	117.87	110.10
4	F	280	ASP	CB-CG-OD2	-5.54	113.31	118.30
3	A	303	GLU	OE1-CD-OE2	5.54	129.95	123.30
1	M	9	PHE	CB-CG-CD1	5.54	124.68	120.80
3	E	184	TRP	CB-CG-CD1	-5.54	119.80	127.00
5	Q	10	ASN	CB-CA-C	-5.53	99.33	110.40
4	F	224	PHE	CG-CD1-CE1	-5.53	114.72	120.80
3	A	567	TRP	CA-CB-CG	5.53	124.20	113.70
10	O	268	ASP	CB-CG-OD1	-5.53	113.33	118.30
3	A	24	TYR	CD1-CG-CD2	5.53	123.98	117.90
3	C	550	PHE	CB-CG-CD1	5.53	124.67	120.80
10	O	59	ASP	CB-CG-OD1	-5.53	113.33	118.30
11	W	157	ASP	CB-CG-OD2	5.53	123.27	118.30
3	A	126	ARG	NE-CZ-NH1	5.52	123.06	120.30
7	G	56	ASN	CB-CA-C	-5.52	99.37	110.40
11	Y	70	VAL	CA-CB-CG2	-5.52	102.62	110.90
3	E	79	LEU	CB-CG-CD1	5.52	120.38	111.00
3	C	41	ILE	C-N-CA	5.51	133.88	122.30
4	B	439	PHE	CB-CG-CD1	-5.51	116.94	120.80
8	P	273	ASP	CB-CG-OD2	-5.51	113.34	118.30
11	Y	37	VAL	CA-CB-CG2	-5.51	102.64	110.90
11	Y	126	PHE	CB-CG-CD1	5.51	124.66	120.80
2	N	28	ILE	N-CA-C	-5.51	96.13	111.00
3	C	544	PHE	CZ-CE2-CD2	5.50	126.70	120.10
9	b	193	ARG	NE-CZ-NH2	5.50	123.05	120.30
3	C	132	ALA	N-CA-CB	5.50	117.80	110.10
3	A	145	LYS	CA-CB-CG	5.50	125.50	113.40
1	M	109	PHE	CB-CG-CD2	-5.50	116.95	120.80
11	X	51	PHE	CB-CG-CD1	-5.50	116.95	120.80
8	P	221	ALA	N-CA-CB	5.50	117.79	110.10
11	a	102	LEU	CB-CG-CD1	5.50	120.34	111.00
8	P	372	PRO	N-CA-CB	5.49	109.89	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	374	TYR	CB-CG-CD2	5.49	124.29	121.00
3	C	202	PHE	CB-CG-CD2	-5.49	116.96	120.80
4	B	265	TYR	CD1-CE1-CZ	5.49	124.74	119.80
3	C	582	SER	N-CA-CB	5.49	118.73	110.50
3	E	360	TRP	CE2-CD2-CE3	5.49	125.28	118.70
9	b	33	LEU	C-N-CA	5.49	133.82	122.30
3	C	150	ASP	CB-CG-OD1	5.48	123.23	118.30
3	E	46	TYR	CG-CD1-CE1	5.48	125.69	121.30
4	F	225	PHE	CB-CG-CD2	-5.48	116.96	120.80
10	O	255	PHE	CB-CG-CD1	5.48	124.64	120.80
11	W	115	GLY	O-C-N	-5.48	113.93	122.70
3	A	282	GLY	N-CA-C	-5.48	99.40	113.10
5	Q	181	ARG	NE-CZ-NH1	5.48	123.04	120.30
7	K	33	LYS	N-CA-CB	5.48	120.46	110.60
9	b	215	THR	CA-CB-CG2	-5.48	104.73	112.40
7	K	111	ALA	CB-CA-C	-5.48	101.89	110.10
4	B	301	ARG	NE-CZ-NH2	5.47	123.04	120.30
10	O	319	TYR	CG-CD1-CE1	-5.47	116.92	121.30
4	B	435	PHE	CB-CG-CD1	-5.47	116.97	120.80
3	A	299	GLU	O-C-N	5.47	131.45	122.70
4	B	185	ALA	CB-CA-C	-5.47	101.89	110.10
3	C	231	TYR	CB-CG-CD1	-5.47	117.72	121.00
3	A	238	ARG	NE-CZ-NH1	-5.46	117.57	120.30
7	K	154	ASP	CB-CG-OD1	-5.46	113.38	118.30
9	b	71	TYR	CG-CD2-CE2	-5.46	116.93	121.30
10	O	298	ASP	CB-CG-OD1	5.46	123.22	118.30
5	Q	289	TYR	CG-CD1-CE1	-5.46	116.93	121.30
11	S	46	ARG	NE-CZ-NH2	-5.46	117.57	120.30
6	J	103	ILE	CB-CA-C	-5.46	100.68	111.60
3	C	354	ALA	N-CA-C	-5.46	96.27	111.00
10	O	263	SER	N-CA-CB	5.46	118.69	110.50
7	I	76	THR	N-CA-CB	5.46	120.67	110.30
7	I	139	VAL	CA-CB-CG2	-5.46	102.72	110.90
7	I	145	ASP	CB-CG-OD2	-5.46	113.39	118.30
4	F	208	PHE	CD1-CG-CD2	5.45	125.39	118.30
7	I	43	TYR	CB-CG-CD2	-5.45	117.73	121.00
4	B	165	ALA	N-CA-CB	5.45	117.73	110.10
7	K	129	LEU	CB-CG-CD2	5.45	120.27	111.00
11	Y	44	VAL	CA-CB-CG2	5.45	119.08	110.90
1	M	159	LEU	CB-CG-CD2	-5.45	101.74	111.00
4	F	337	MET	CG-SD-CE	-5.45	91.48	100.20
1	M	197	ARG	N-CA-CB	5.45	120.40	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	O	170	LEU	CB-CA-C	-5.45	99.85	110.20
5	Q	306	ILE	C-N-CA	5.44	135.31	121.70
6	J	68	LEU	CB-CA-C	5.44	120.54	110.20
7	I	143	GLU	OE1-CD-OE2	5.44	129.83	123.30
8	P	109	TYR	CG-CD1-CE1	-5.44	116.95	121.30
3	E	219	VAL	CG1-CB-CG2	5.44	119.60	110.90
6	L	93	ASP	CB-CG-OD2	-5.44	113.41	118.30
11	a	126	PHE	CG-CD1-CE1	5.44	126.78	120.80
11	V	75	CYS	N-CA-CB	5.44	120.38	110.60
4	D	359	PHE	CB-CG-CD2	-5.43	117.00	120.80
11	U	51	PHE	CB-CG-CD2	-5.43	117.00	120.80
3	A	391	PHE	CB-CG-CD2	-5.42	117.00	120.80
9	b	91	TYR	CB-CG-CD2	5.42	124.25	121.00
11	X	153	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	M	45	ASP	CB-CG-OD1	-5.42	113.42	118.30
4	B	381	ARG	NE-CZ-NH2	-5.42	117.59	120.30
7	K	158	ARG	NE-CZ-NH2	-5.42	117.59	120.30
11	T	155	THR	CA-CB-CG2	-5.42	104.81	112.40
10	O	116	TRP	CG-CD2-CE3	-5.42	129.02	133.90
4	B	65	GLY	N-CA-C	-5.42	99.56	113.10
3	E	126	ARG	NE-CZ-NH2	5.42	123.01	120.30
6	H	25	ARG	NE-CZ-NH2	5.42	123.01	120.30
3	C	583	SER	CB-CA-C	-5.42	99.81	110.10
3	E	311	ILE	C-N-CA	5.41	135.23	121.70
3	E	509	ASP	CB-CG-OD2	-5.40	113.44	118.30
10	O	116	TRP	N-CA-C	-5.40	96.42	111.00
4	B	274	VAL	CG1-CB-CG2	-5.40	102.26	110.90
11	R	75	CYS	C-N-CA	5.40	135.20	121.70
11	V	11	PHE	CB-CG-CD1	5.40	124.58	120.80
3	A	423	PHE	CG-CD2-CE2	-5.40	114.86	120.80
4	B	132	LEU	CB-CG-CD2	5.40	120.18	111.00
8	P	93	LYS	CB-CA-C	-5.39	99.61	110.40
10	O	325	PHE	CD1-CE1-CZ	-5.39	113.63	120.10
3	E	502	VAL	CA-CB-CG2	-5.39	102.81	110.90
8	P	78	ILE	CA-CB-CG1	-5.39	100.76	111.00
11	T	142	TYR	CG-CD1-CE1	-5.39	116.99	121.30
4	D	71	ARG	NE-CZ-NH2	-5.39	117.61	120.30
4	F	195	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
1	M	187	TYR	CB-CG-CD2	-5.38	117.77	121.00
3	A	81	VAL	CB-CA-C	-5.38	101.17	111.40
3	C	178	SER	N-CA-CB	5.38	118.58	110.50
11	V	46	ARG	NE-CZ-NH1	5.38	122.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	S	106	PHE	CD1-CE1-CZ	-5.38	113.64	120.10
4	B	214	ALA	CB-CA-C	-5.38	102.03	110.10
7	K	62	PHE	CB-CG-CD2	5.38	124.57	120.80
10	O	55	ILE	CA-CB-CG1	5.38	121.22	111.00
2	N	81	VAL	N-CA-CB	5.38	123.33	111.50
6	J	39	ALA	N-CA-CB	5.38	117.63	110.10
3	C	499	VAL	CG1-CB-CG2	-5.38	102.30	110.90
3	E	368	SER	N-CA-CB	5.38	118.56	110.50
4	F	352	TYR	CZ-CE2-CD2	-5.38	114.96	119.80
7	G	105	GLU	CB-CA-C	-5.38	99.65	110.40
10	O	116	TRP	CE2-CD2-CE3	5.37	125.15	118.70
8	P	458	ASP	N-CA-CB	5.37	120.26	110.60
9	b	60	ARG	NE-CZ-NH2	-5.37	117.61	120.30
3	E	259	GLY	C-N-CA	5.37	135.11	121.70
11	S	76	TYR	CB-CG-CD1	5.37	124.22	121.00
3	C	37	ALA	N-CA-CB	5.36	117.61	110.10
10	O	314	GLU	OE1-CD-OE2	-5.36	116.86	123.30
3	C	405	ASP	N-CA-CB	5.36	120.25	110.60
4	D	324	GLY	N-CA-C	-5.36	99.70	113.10
9	b	91	TYR	CD1-CG-CD2	-5.36	112.00	117.90
3	C	177	ARG	N-CA-CB	5.36	120.24	110.60
5	Q	121	GLY	N-CA-C	-5.36	99.70	113.10
9	b	195	LYS	N-CA-CB	5.36	120.25	110.60
4	B	409	ILE	CA-CB-CG1	-5.36	100.82	111.00
9	b	248	ARG	NE-CZ-NH2	-5.35	117.62	120.30
9	b	142	ARG	NE-CZ-NH2	-5.35	117.62	120.30
3	A	343	PHE	O-C-N	-5.35	114.14	122.70
10	O	38	LEU	C-N-CA	5.35	135.08	121.70
1	M	29	TYR	CG-CD2-CE2	-5.35	117.02	121.30
7	I	126	VAL	CA-CB-CG1	5.35	118.92	110.90
11	S	88	PHE	CB-CG-CD1	5.35	124.54	120.80
8	P	109	TYR	CA-CB-CG	-5.34	103.25	113.40
8	P	301	ARG	NE-CZ-NH2	-5.34	117.63	120.30
9	b	328	TYR	CB-CG-CD1	5.34	124.21	121.00
3	A	475	TYR	N-CA-CB	5.34	120.22	110.60
4	B	377	PRO	N-CD-CG	5.34	111.21	103.20
3	C	494	GLU	OE1-CD-OE2	5.34	129.71	123.30
4	F	107	ASP	CB-CG-OD1	-5.34	113.50	118.30
7	K	189	VAL	CA-CB-CG2	-5.34	102.89	110.90
4	B	449	TYR	CA-CB-CG	-5.33	103.27	113.40
11	S	11	PHE	CB-CG-CD2	-5.33	117.07	120.80
3	A	114	ALA	N-CA-CB	5.33	117.56	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	Q	288	PHE	CB-CG-CD2	5.33	124.53	120.80
7	G	180	ASN	CB-CG-OD1	-5.32	110.95	121.60
4	D	62	VAL	CG1-CB-CG2	5.32	119.41	110.90
4	F	448	ALA	CB-CA-C	-5.32	102.12	110.10
8	P	136	PHE	CG-CD1-CE1	-5.32	114.95	120.80
9	b	324	ASN	N-CA-CB	5.32	120.18	110.60
11	a	71	SER	N-CA-CB	5.32	118.47	110.50
2	N	5	ARG	NE-CZ-NH2	-5.31	117.64	120.30
4	B	309	TYR	CG-CD2-CE2	-5.31	117.05	121.30
6	H	27	TYR	CB-CG-CD1	-5.31	117.81	121.00
3	A	370	ARG	NH1-CZ-NH2	5.31	125.24	119.40
4	F	124	PRO	CA-N-CD	-5.30	104.08	111.50
4	B	131	TYR	CB-CG-CD2	-5.30	117.82	121.00
3	E	68	ALA	CB-CA-C	-5.30	102.15	110.10
7	I	166	ARG	NE-CZ-NH2	5.30	122.95	120.30
4	D	80	PHE	CB-CG-CD1	5.30	124.51	120.80
4	F	346	ILE	CA-C-O	-5.30	108.97	120.10
11	Z	76	TYR	CB-CG-CD1	5.30	124.18	121.00
3	E	266	SER	N-CA-CB	5.30	118.45	110.50
9	b	103	SER	C-N-CA	5.30	133.43	122.30
4	F	302	ARG	NE-CZ-NH2	-5.29	117.65	120.30
7	K	79	THR	CA-CB-CG2	-5.29	104.99	112.40
6	H	68	LEU	CB-CG-CD2	5.29	120.00	111.00
3	C	565	ALA	N-CA-CB	5.28	117.50	110.10
4	F	149	GLU	N-CA-CB	5.28	120.11	110.60
11	Y	97	VAL	CA-CB-CG2	-5.28	102.97	110.90
11	Y	68	LEU	CB-CG-CD1	5.28	119.98	111.00
3	E	344	ARG	NE-CZ-NH1	5.28	122.94	120.30
10	O	11	PHE	CZ-CE2-CD2	-5.28	113.77	120.10
10	O	294	THR	CA-CB-CG2	-5.28	105.01	112.40
3	C	485	MET	CG-SD-CE	-5.28	91.76	100.20
4	F	209	SER	N-CA-CB	5.28	118.41	110.50
11	S	85	TYR	CG-CD1-CE1	-5.28	117.08	121.30
6	H	11	LEU	CB-CG-CD2	5.27	119.96	111.00
9	b	133	VAL	CA-CB-CG1	5.27	118.80	110.90
4	F	249	THR	CA-CB-CG2	-5.27	105.03	112.40
9	b	53	ARG	CD-NE-CZ	-5.27	116.23	123.60
4	D	393	ARG	NE-CZ-NH2	-5.26	117.67	120.30
9	b	149	ASP	CB-CG-OD1	-5.26	113.56	118.30
4	D	144	ARG	NE-CZ-NH1	5.26	122.93	120.30
7	G	13	VAL	CA-CB-CG1	-5.26	103.01	110.90
10	O	374	TYR	CB-CG-CD1	-5.26	117.84	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	75	CYS	N-CA-CB	5.26	120.07	110.60
9	b	285	TYR	CB-CA-C	-5.26	99.89	110.40
4	B	252	ARG	NE-CZ-NH2	-5.26	117.67	120.30
3	E	182	ILE	CA-CB-CG2	-5.26	100.39	110.90
4	B	95	PHE	CB-CG-CD2	-5.25	117.12	120.80
9	b	28	ASP	CB-CG-OD2	5.25	123.03	118.30
11	W	157	ASP	CB-CG-OD1	-5.25	113.57	118.30
3	C	466	VAL	CA-CB-CG2	-5.25	103.03	110.90
3	C	212	TYR	CD1-CG-CD2	-5.25	112.13	117.90
9	b	67	ARG	NE-CZ-NH1	-5.25	117.68	120.30
11	U	135	PHE	CD1-CE1-CZ	-5.24	113.81	120.10
3	E	184	TRP	CB-CG-CD2	5.24	133.41	126.60
5	Q	252	ALA	CB-CA-C	-5.24	102.24	110.10
9	b	15	ALA	N-CA-CB	5.24	117.44	110.10
11	U	125	LEU	CB-CG-CD2	5.24	119.91	111.00
11	R	51	PHE	CB-CG-CD1	5.24	124.47	120.80
4	F	143	ALA	CB-CA-C	-5.24	102.25	110.10
10	O	73	ASN	CB-CG-OD1	-5.24	111.13	121.60
4	B	114	ASP	CA-CB-CG	5.23	124.91	113.40
3	A	109	GLN	N-CA-CB	5.23	120.01	110.60
3	A	578	LYS	O-C-N	-5.23	114.33	122.70
4	B	272	ARG	NE-CZ-NH2	5.23	122.92	120.30
10	O	221	SER	N-CA-CB	5.23	118.35	110.50
11	T	85	TYR	CD1-CG-CD2	5.23	123.65	117.90
1	M	73	TYR	CG-CD1-CE1	5.23	125.48	121.30
3	C	506	ALA	N-CA-CB	5.23	117.42	110.10
6	J	104	LYS	N-CA-C	-5.23	96.89	111.00
3	C	428	THR	CA-CB-CG2	-5.23	105.08	112.40
3	E	46	TYR	CD1-CE1-CZ	-5.23	115.10	119.80
7	I	10	PRO	N-CA-CB	5.22	109.57	103.30
7	I	16	GLU	CB-CG-CD	-5.22	100.09	114.20
3	A	370	ARG	NE-CZ-NH1	-5.22	117.69	120.30
4	D	49	TYR	CZ-CE2-CD2	5.22	124.50	119.80
4	D	380	SER	N-CA-C	-5.22	96.90	111.00
3	A	427	VAL	CA-CB-CG1	-5.22	103.07	110.90
4	B	287	ALA	N-CA-CB	5.22	117.41	110.10
3	C	377	ASP	CB-CG-OD2	-5.22	113.60	118.30
4	F	229	PHE	CD1-CE1-CZ	5.22	126.36	120.10
4	F	69	GLU	OE1-CD-OE2	5.21	129.56	123.30
3	A	360	TRP	CE2-CD2-CE3	5.21	124.95	118.70
11	X	102	LEU	CB-CG-CD1	5.21	119.86	111.00
11	a	43	CYS	CB-CA-C	-5.21	99.98	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	C	301	TYR	CZ-CE2-CD2	-5.21	115.11	119.80
3	C	342	TYR	CG-CD2-CE2	-5.21	117.13	121.30
3	C	581	VAL	CA-CB-CG1	-5.21	103.09	110.90
7	K	70	MET	CG-SD-CE	5.21	108.53	100.20
11	U	70	VAL	CA-CB-CG2	-5.21	103.09	110.90
11	a	85	TYR	CB-CG-CD1	5.21	124.12	121.00
4	B	143	ALA	CB-CA-C	-5.20	102.30	110.10
3	C	161	VAL	CG1-CB-CG2	-5.20	102.58	110.90
3	C	162	PHE	CB-CG-CD2	-5.20	117.16	120.80
7	K	160	TYR	CD1-CE1-CZ	-5.20	115.12	119.80
11	a	76	TYR	CB-CG-CD2	-5.20	117.88	121.00
3	A	544	PHE	CB-CG-CD1	-5.20	117.16	120.80
3	C	124	ILE	CA-CB-CG1	5.20	120.88	111.00
11	W	124	ARG	CA-CB-CG	5.20	124.83	113.40
10	O	220	ALA	N-CA-CB	5.20	117.38	110.10
3	E	553	TYR	CD1-CG-CD2	5.20	123.61	117.90
8	P	359	TYR	CB-CG-CD2	5.19	124.12	121.00
3	C	611	PHE	CB-CG-CD2	-5.19	117.17	120.80
4	D	259	ALA	O-C-N	5.19	131.01	122.70
3	A	482	ARG	NE-CZ-NH1	5.19	122.89	120.30
3	C	446	ALA	N-CA-CB	5.19	117.36	110.10
3	A	365	ARG	NE-CZ-NH1	-5.19	117.71	120.30
3	A	392	TYR	CB-CG-CD2	5.19	124.11	121.00
3	E	298	PRO	N-CD-CG	5.19	110.98	103.20
6	L	61	ASN	N-CA-CB	5.19	119.94	110.60
6	J	44	ASP	CB-CA-C	-5.19	100.03	110.40
11	R	157	ASP	CB-CG-OD2	-5.19	113.63	118.30
3	A	561	VAL	CA-CB-CG1	-5.18	103.12	110.90
8	P	244	TYR	CZ-CE2-CD2	5.18	124.47	119.80
11	Y	106	PHE	CB-CG-CD2	-5.18	117.17	120.80
3	A	541	TRP	CB-CG-CD1	5.18	133.74	127.00
1	M	193	ASP	N-CA-CB	5.18	119.92	110.60
4	D	269	GLN	CB-CA-C	-5.18	100.04	110.40
3	E	439	TRP	C-N-CA	5.18	133.18	122.30
4	F	301	ARG	NE-CZ-NH1	5.17	122.89	120.30
6	H	81	ALA	CB-CA-C	-5.17	102.34	110.10
11	R	11	PHE	CG-CD2-CE2	5.17	126.49	120.80
11	T	63	ILE	C-N-CA	5.17	134.62	121.70
3	E	531	TYR	CZ-CE2-CD2	5.16	124.45	119.80
7	K	119	PRO	N-CA-CB	5.16	109.50	103.30
1	M	52	ASP	CB-CG-OD2	-5.16	113.66	118.30
7	K	85	ARG	NE-CZ-NH2	5.16	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	24	THR	OG1-CB-CG2	-5.16	98.14	110.00
11	T	159	VAL	CG1-CB-CG2	5.16	119.15	110.90
4	B	277	ILE	CA-CB-CG1	5.15	120.79	111.00
6	H	38	ASP	CB-CG-OD2	5.15	122.94	118.30
5	Q	225	LEU	CB-CG-CD1	5.15	119.75	111.00
9	b	91	TYR	CG-CD1-CE1	5.15	125.42	121.30
3	A	71	GLN	N-CA-C	-5.14	97.11	111.00
4	F	370	TYR	CB-CG-CD2	-5.14	117.91	121.00
3	C	420	GLY	N-CA-C	-5.14	100.25	113.10
3	E	227	LEU	CB-CG-CD1	5.14	119.74	111.00
4	B	308	MET	CA-CB-CG	5.14	122.04	113.30
8	P	133	LYS	N-CA-C	-5.14	97.12	111.00
11	Y	71	SER	N-CA-CB	5.14	118.21	110.50
3	A	73	TYR	CB-CG-CD2	-5.14	117.92	121.00
8	P	322	VAL	CA-CB-CG2	-5.14	103.19	110.90
11	U	100	SER	N-CA-CB	5.14	118.21	110.50
3	E	391	PHE	CG-CD1-CE1	-5.13	115.15	120.80
4	B	49	TYR	CE1-CZ-CE2	5.13	128.01	119.80
10	O	64	GLU	OE1-CD-OE2	-5.13	117.14	123.30
10	O	357	MET	CA-CB-CG	5.13	122.03	113.30
4	B	38	LEU	CB-CG-CD1	5.13	119.72	111.00
4	F	228	ASP	CB-CG-OD2	-5.13	113.68	118.30
4	F	131	TYR	CG-CD2-CE2	5.13	125.40	121.30
4	B	173	PHE	CB-CG-CD1	5.13	124.39	120.80
4	D	189	ARG	NE-CZ-NH1	5.13	122.86	120.30
5	Q	5	TYR	CD1-CG-CD2	5.13	123.54	117.90
3	E	586	PHE	CB-CG-CD1	5.13	124.39	120.80
4	B	84	SER	N-CA-CB	5.12	118.19	110.50
4	F	101	ARG	NE-CZ-NH2	-5.12	117.74	120.30
11	R	72	VAL	CA-CB-CG2	-5.12	103.21	110.90
1	M	201	TYR	CB-CG-CD1	5.12	124.07	121.00
11	V	29	ALA	N-CA-CB	5.12	117.27	110.10
11	Z	46	ARG	NE-CZ-NH2	-5.12	117.74	120.30
10	O	195	LEU	O-C-N	5.12	130.88	122.70
4	B	31	VAL	O-C-N	5.11	130.88	122.70
6	J	39	ALA	O-C-N	5.11	130.88	122.70
4	F	291	VAL	O-C-N	-5.11	114.52	122.70
3	E	103	THR	N-CA-C	-5.11	97.20	111.00
3	E	560	ALA	CB-CA-C	-5.11	102.43	110.10
7	G	178	TYR	CB-CG-CD1	5.11	124.06	121.00
3	A	79	LEU	CB-CG-CD2	5.11	119.68	111.00
4	B	294	ALA	N-CA-CB	5.10	117.24	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	E	72	VAL	CA-CB-CG2	-5.10	103.25	110.90
3	A	156	ASP	CB-CG-OD1	-5.10	113.71	118.30
4	D	202	ASP	C-N-CA	5.10	133.01	122.30
5	Q	42	LEU	CB-CG-CD1	5.10	119.67	111.00
4	D	304	TYR	CG-CD2-CE2	-5.10	117.22	121.30
3	E	470	PHE	CB-CG-CD2	-5.10	117.23	120.80
11	X	60	ALA	CB-CA-C	-5.10	102.45	110.10
4	D	107	ASP	CB-CG-OD2	5.09	122.88	118.30
10	O	60	THR	CA-CB-CG2	-5.09	105.27	112.40
5	Q	293	MET	CA-CB-CG	5.09	121.95	113.30
10	O	97	TYR	N-CA-CB	5.09	119.76	110.60
11	S	70	VAL	CA-CB-CG2	-5.09	103.26	110.90
3	C	88	THR	CA-CB-OG1	5.09	119.69	109.00
4	D	412	ASP	CB-CG-OD1	5.09	122.88	118.30
4	F	61	THR	CA-CB-CG2	-5.09	105.27	112.40
4	F	452	ARG	NE-CZ-NH1	5.09	122.84	120.30
5	Q	344	VAL	C-N-CA	5.09	134.42	121.70
4	B	311	ASP	CB-CG-OD2	-5.09	113.72	118.30
3	E	208	ASP	CB-CG-OD1	-5.09	113.72	118.30
4	F	145	ILE	N-CA-C	-5.09	97.27	111.00
10	O	124	ASP	CB-CG-OD2	-5.09	113.72	118.30
7	I	17	LEU	CB-CG-CD2	-5.09	102.35	111.00
5	Q	337	ARG	N-CA-C	-5.08	97.27	111.00
11	Y	137	GLU	C-N-CA	5.08	134.41	121.70
11	T	69	VAL	CA-CB-CG2	-5.08	103.27	110.90
4	B	415	ALA	N-CA-CB	5.08	117.21	110.10
6	J	38	ASP	CB-CG-OD1	5.08	122.87	118.30
11	R	133	LEU	CB-CA-C	-5.08	100.55	110.20
11	V	117	ARG	NE-CZ-NH2	-5.08	117.76	120.30
11	S	69	VAL	CA-CB-CG2	5.08	118.52	110.90
3	E	77	ALA	C-N-CA	-5.08	111.63	122.30
11	R	51	PHE	CB-CG-CD2	-5.08	117.24	120.80
7	I	86	LEU	CB-CA-C	-5.08	100.55	110.20
6	L	92	ASP	CB-CA-C	-5.07	100.25	110.40
4	B	309	TYR	CB-CG-CD2	-5.07	117.96	121.00
4	B	43	LYS	C-N-CA	5.07	134.37	121.70
11	W	123	PRO	O-C-N	5.07	130.81	122.70
3	A	165	SER	CB-CA-C	-5.07	100.48	110.10
4	B	63	ARG	N-CA-C	-5.07	97.33	111.00
6	H	69	GLU	CA-CB-CG	5.07	124.55	113.40
3	C	478	PHE	CZ-CE2-CD2	-5.06	114.02	120.10
4	F	185	ALA	CB-CA-C	-5.06	102.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	F	48	ARG	CG-CD-NE	-5.06	101.18	111.80
3	A	280	TYR	CD1-CE1-CZ	5.05	124.35	119.80
3	E	344	ARG	NE-CZ-NH2	-5.05	117.77	120.30
3	E	471	TYR	CB-CG-CD2	-5.05	117.97	121.00
11	a	126	PHE	CB-CG-CD2	-5.05	117.26	120.80
3	A	508	SER	N-CA-CB	5.05	118.08	110.50
9	b	25	ILE	O-C-N	-5.05	114.61	122.70
3	E	85	VAL	N-CA-C	-5.05	97.36	111.00
8	P	274	LEU	CB-CG-CD1	5.05	119.58	111.00
11	Y	132	ILE	N-CA-CB	5.05	122.42	110.80
3	E	87	ARG	NE-CZ-NH1	5.05	122.82	120.30
3	E	315	THR	N-CA-CB	5.05	119.89	110.30
3	A	323	ASN	CB-CA-C	-5.04	100.31	110.40
3	C	329	ARG	NE-CZ-NH2	5.04	122.82	120.30
3	E	383	TYR	CZ-CE2-CD2	-5.04	115.26	119.80
4	D	288	LEU	CB-CA-C	-5.04	100.62	110.20
4	F	361	ASP	C-N-CA	5.04	134.31	121.70
11	Y	44	VAL	N-CA-CB	5.04	122.59	111.50
3	A	280	TYR	CG-CD1-CE1	-5.04	117.27	121.30
1	M	59	ARG	NE-CZ-NH2	5.04	122.82	120.30
4	B	307	TYR	CD1-CE1-CZ	-5.04	115.27	119.80
3	E	463	TYR	CB-CG-CD1	-5.04	117.98	121.00
11	a	159	VAL	CA-CB-CG2	-5.04	103.34	110.90
5	Q	253	THR	CA-CB-CG2	-5.04	105.35	112.40
11	a	28	ALA	CB-CA-C	-5.04	102.55	110.10
4	B	340	ASP	CB-CG-OD1	5.03	122.83	118.30
5	Q	226	ASN	CB-CA-C	-5.03	100.33	110.40
8	P	407	ARG	NE-CZ-NH2	5.03	122.82	120.30
9	b	71	TYR	CZ-CE2-CD2	5.03	124.33	119.80
7	G	145	ASP	C-N-CA	5.03	134.28	121.70
3	E	247	VAL	O-C-N	-5.03	114.65	122.70
11	X	155	THR	N-CA-CB	5.03	119.86	110.30
3	A	345	ASP	CB-CG-OD1	5.03	122.82	118.30
8	P	449	ASP	CB-CG-OD1	5.03	122.82	118.30
3	C	471	TYR	CD1-CG-CD2	-5.03	112.37	117.90
7	K	40	ASP	CB-CG-OD2	-5.03	113.78	118.30
9	b	356	MET	N-CA-CB	5.03	119.65	110.60
4	D	330	THR	CA-C-N	-5.02	106.15	117.20
3	E	416	VAL	CA-CB-CG2	5.02	118.44	110.90
3	C	209	PHE	CA-CB-CG	-5.02	101.84	113.90
4	D	93	VAL	N-CA-C	-5.02	97.44	111.00
1	M	77	GLU	N-CA-CB	5.02	119.64	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	D	284	TYR	CZ-CE2-CD2	-5.02	115.28	119.80
3	A	280	TYR	CB-CG-CD1	-5.02	117.99	121.00
4	F	118	ARG	NE-CZ-NH2	-5.02	117.79	120.30
10	O	311	VAL	CA-CB-CG1	5.02	118.43	110.90
5	Q	182	ASN	CA-CB-CG	-5.02	102.36	113.40
8	P	477	PHE	CG-CD2-CE2	5.02	126.32	120.80
3	C	49	VAL	CA-CB-CG1	-5.02	103.38	110.90
2	N	106	ASP	CB-CG-OD1	5.01	122.81	118.30
9	b	124	MET	CG-SD-CE	-5.01	92.18	100.20
7	G	111	ALA	N-CA-CB	5.01	117.12	110.10
9	b	45	ASN	CB-CA-C	5.01	120.43	110.40
10	O	75	ILE	CA-CB-CG2	-5.01	100.88	110.90
3	A	179	ARG	CB-CG-CD	5.01	124.63	111.60
4	F	305	PRO	N-CA-CB	5.01	109.31	103.30
4	F	384	LYS	CA-C-N	-5.01	106.17	117.20
11	U	95	LEU	CB-CG-CD2	5.01	119.52	111.00
1	M	95	ARG	NE-CZ-NH2	5.01	122.81	120.30
4	B	240	LEU	CB-CA-C	-5.01	100.68	110.20
11	T	11	PHE	CA-CB-CG	5.01	125.92	113.90
11	X	63	ILE	C-N-CA	5.01	134.22	121.70
8	P	463	TYR	CG-CD2-CE2	5.01	125.31	121.30
4	F	446	GLN	N-CA-C	-5.01	97.48	111.00
7	K	25	ARG	NE-CZ-NH1	5.01	122.80	120.30
7	K	200	ASN	CB-CG-OD1	-5.01	111.59	121.60
9	b	186	TYR	CZ-CE2-CD2	5.01	124.31	119.80
11	V	153	ARG	NE-CZ-NH1	-5.01	117.80	120.30
11	Z	32	THR	CA-CB-CG2	-5.00	105.39	112.40
4	B	142	TYR	CB-CG-CD1	5.00	124.00	121.00
4	B	401	ASN	CA-CB-CG	-5.00	102.39	113.40
4	F	204	HIS	N-CA-CB	5.00	119.61	110.60
3	A	366	GLU	OE1-CD-OE2	-5.00	117.30	123.30
3	C	213	HIS	CB-CG-ND1	5.00	135.70	123.20
11	Y	76	TYR	CB-CG-CD1	5.00	124.00	121.00

There are no chirality outliers.

All (164) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
3	A	110	ARG	Sidechain
3	A	135	ARG	Sidechain
3	A	153	SER	Mainchain
3	A	244	PHE	Sidechain

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Mol	Chain	Res	Type	Group
3	A	301	TYR	Sidechain
3	A	383	TYR	Sidechain
3	A	448	ARG	Sidechain
3	A	46	TYR	Sidechain
3	A	463	TYR	Sidechain
3	A	586	PHE	Sidechain
3	A	611	PHE	Sidechain
4	B	142	TYR	Sidechain
4	B	144	ARG	Sidechain
4	B	195	ARG	Sidechain
4	B	223	ARG	Sidechain
4	B	225	PHE	Sidechain
4	B	265	TYR	Sidechain
4	B	272	ARG	Sidechain
4	B	302	ARG	Sidechain
4	B	325	ARG	Sidechain
4	B	381	ARG	Sidechain
4	B	393	ARG	Sidechain
4	B	455	PHE	Sidechain
4	B	475	ARG	Sidechain
3	C	123	TYR	Sidechain
3	C	191	TYR	Sidechain
3	C	218	ARG	Sidechain
3	C	301	TYR	Sidechain
3	C	342	TYR	Sidechain
3	C	383	TYR	Sidechain
3	C	394	ARG	Sidechain
3	C	438	PHE	Sidechain
3	C	460	TYR	Sidechain
3	C	478	PHE	Sidechain
3	C	482	ARG	Sidechain
3	C	548	ARG	Sidechain
3	C	553	TYR	Sidechain
3	C	610	ARG	Sidechain
4	D	131	TYR	Sidechain
4	D	142	TYR	Sidechain
4	D	146	TYR	Sidechain
4	D	257	ARG	Sidechain
4	D	273	HIS	Sidechain
4	D	295	ARG	Sidechain
4	D	302	ARG	Sidechain
4	D	307	TYR	Sidechain

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Mol	Chain	Res	Type	Group
4	D	316	TYR	Sidechain
4	D	370	TYR	Sidechain
4	D	404	TYR	Sidechain
4	D	48	ARG	Sidechain
4	D	74	ARG	Sidechain
3	E	126	ARG	Sidechain
3	E	158	TYR	Sidechain
3	E	177	ARG	Sidechain
3	E	191	TYR	Sidechain
3	E	272	TYR	Sidechain
3	E	314	ARG	Sidechain
3	E	46	TYR	Sidechain
3	E	463	TYR	Sidechain
3	E	471	TYR	Sidechain
3	E	53	HIS	Sidechain
3	E	534	TYR	Sidechain
3	E	591	ARG	Sidechain
4	F	302	ARG	Sidechain
4	F	304	TYR	Sidechain
4	F	316	TYR	Sidechain
4	F	325	ARG	Sidechain
4	F	352	TYR	Sidechain
4	F	362	ARG	Sidechain
4	F	381	ARG	Sidechain
4	F	44	VAL	Peptide
4	F	475	ARG	Sidechain
4	F	48	ARG	Sidechain
4	F	484	PHE	Sidechain
7	G	117	TYR	Sidechain
7	G	166	ARG	Sidechain
7	G	52	ARG	Sidechain
7	G	92	ARG	Sidechain
7	I	160	TYR	Sidechain
7	I	219	ARG	Sidechain
7	I	92	ARG	Sidechain
7	K	117	TYR	Sidechain
7	K	144	ARG	Sidechain
7	K	158	ARG	Sidechain
7	K	62	PHE	Sidechain
7	K	85	ARG	Sidechain
6	L	25	ARG	Sidechain
6	L	28	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	M	112	TYR	Sidechain
1	M	134	ARG	Sidechain
1	M	139	TYR	Sidechain
1	M	187	TYR	Sidechain
1	M	200	PHE	Sidechain
1	M	34	ARG	Sidechain
1	M	81	TYR	Sidechain
2	N	5	ARG	Sidechain
2	N	57	PHE	Sidechain
10	O	110	TYR	Sidechain
10	O	114	PHE	Sidechain
10	O	119	ARG	Sidechain
10	O	121	PHE	Sidechain
10	O	152	TYR	Sidechain
10	O	173	ARG	Sidechain
10	O	285	ARG	Sidechain
10	O	296	TYR	Sidechain
10	O	318	ARG	Sidechain
10	O	382	TYR	Sidechain
10	O	388	TYR	Sidechain
10	O	98	ARG	Sidechain
8	P	144	PHE	Sidechain
8	P	156	HIS	Sidechain
8	P	184	TYR	Sidechain
8	P	21	ARG	Sidechain
8	P	237	HIS	Sidechain
8	P	32	ARG	Sidechain
8	P	330	TYR	Sidechain
8	P	359	TYR	Sidechain
8	P	396	ARG	Sidechain
5	Q	116	HIS	Sidechain
5	Q	12	PHE	Sidechain
5	Q	126	ARG	Sidechain
5	Q	149	TYR	Sidechain
5	Q	161	TYR	Sidechain
5	Q	18	ARG	Sidechain
5	Q	185	TYR	Sidechain
5	Q	273	TYR	Sidechain
5	Q	275	TYR	Sidechain
5	Q	289	TYR	Sidechain
5	Q	30	TYR	Sidechain
5	Q	335	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	Q	341	TYR	Sidechain
5	Q	51	TYR	Sidechain
11	S	85	TYR	Sidechain
11	T	11	PHE	Sidechain
11	T	117	ARG	Sidechain
11	T	12	PHE	Sidechain
11	T	85	TYR	Sidechain
11	U	126	PHE	Sidechain
11	U	46	ARG	Sidechain
11	V	124	ARG	Sidechain
11	V	142	TYR	Sidechain
11	W	11	PHE	Sidechain
11	W	12	PHE	Sidechain
11	W	124	ARG	Sidechain
11	W	142	TYR	Sidechain
11	X	85	TYR	Sidechain
11	Z	153	ARG	Sidechain
11	Z	76	TYR	Sidechain
11	a	12	PHE	Sidechain
11	a	142	TYR	Sidechain
9	b	112	ARG	Sidechain
9	b	193	ARG	Sidechain
9	b	208	ARG	Sidechain
9	b	236	PHE	Sidechain
9	b	241	HIS	Sidechain
9	b	250	ARG	Sidechain
9	b	268	GLU	Peptide
9	b	315	ARG	Sidechain
9	b	320	PHE	Sidechain
9	b	352	ARG	Sidechain
9	b	49	ARG	Sidechain
9	b	71	TYR	Sidechain
9	b	86	GLY	Peptide
9	b	91	TYR	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	M	1691	0	1740	8	0
2	N	928	0	926	4	0
3	A	4578	0	4519	13	0
3	C	4578	0	4519	11	0
3	E	4578	0	4519	15	0
4	B	3585	0	3567	16	0
4	D	3585	0	3567	12	0
4	F	3585	0	3567	16	0
5	Q	2802	0	2689	9	0
6	H	824	0	877	5	0
6	J	824	0	877	5	0
6	L	824	0	877	3	0
7	G	1731	0	1797	6	0
7	I	1731	0	1797	7	0
7	K	1731	0	1797	1	0
8	P	3712	0	3829	11	0
9	b	2540	0	2537	0	0
10	O	3122	0	3155	8	0
11	R	1071	0	1141	2	0
11	S	1071	0	1141	3	0
11	T	1071	0	1141	3	0
11	U	1071	0	1141	11	0
11	V	1071	0	1141	24	0
11	W	1071	0	1141	5	0
11	X	1071	0	1141	4	0
11	Y	1071	0	1141	6	0
11	Z	1071	0	1141	8	0
11	a	1071	0	1141	0	0
All	All	57659	0	58566	191	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (191) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:160:CYS:CB	11:X:160:CYS:SG	2.01	1.47
11:V:141:LEU:HA	11:V:144:LEU:CD2	1.71	1.21
11:V:141:LEU:O	11:V:144:LEU:HG	1.48	1.13
11:V:141:LEU:HA	11:V:144:LEU:HD21	1.23	1.08
11:Z:66:TYR:HB3	11:Z:144:LEU:HD22	1.33	1.05
11:V:144:LEU:HD12	11:V:145:ILE:N	1.78	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:Y:66:TYR:HB3	11:Y:144:LEU:HD22	1.61	0.82
11:V:141:LEU:O	11:V:144:LEU:CG	2.30	0.78
11:U:66:TYR:HB3	11:U:144:LEU:HD22	1.64	0.78
11:U:66:TYR:CB	11:U:144:LEU:HD22	2.18	0.73
11:V:141:LEU:HD23	11:V:144:LEU:HD21	1.72	0.72
11:V:141:LEU:C	11:V:144:LEU:HG	2.13	0.67
11:Z:66:TYR:CB	11:Z:144:LEU:HD22	2.17	0.66
11:W:66:TYR:HB3	11:W:144:LEU:HD22	1.77	0.66
11:U:66:TYR:HB3	11:U:144:LEU:CD2	2.25	0.66
4:B:86:ILE:H	4:B:86:ILE:HD13	1.61	0.66
11:Y:66:TYR:HB3	11:Y:144:LEU:CD2	2.26	0.65
4:B:41:LEU:HD12	4:B:77:VAL:HG21	1.77	0.65
3:E:270:SER:HA	3:E:278:ILE:HD13	1.80	0.64
11:V:141:LEU:CA	11:V:144:LEU:HD21	2.16	0.61
11:U:31:GLY:HA2	11:U:109:GLY:HA3	1.80	0.61
4:D:46:PHE:H	4:D:47:PRO:CD	2.14	0.61
4:D:46:PHE:H	4:D:47:PRO:HD3	1.66	0.60
4:D:440:GLU:HA	4:D:444:ILE:HD12	1.84	0.60
3:E:405:ASP:H	3:E:406:ARG:HH21	1.50	0.59
11:Y:66:TYR:CB	11:Y:144:LEU:HD22	2.30	0.59
11:U:66:TYR:CG	11:U:144:LEU:HD22	2.36	0.59
11:V:144:LEU:HD12	11:V:145:ILE:H	1.65	0.58
4:B:29:ASN:HD21	7:I:198:GLU:HG3	1.69	0.57
5:Q:25:LEU:H	5:Q:25:LEU:HD12	1.69	0.57
6:L:21:VAL:HG12	6:L:25:ARG:HE	1.70	0.57
11:V:141:LEU:HA	11:V:144:LEU:CG	2.32	0.57
4:D:263:ALA:HB1	4:D:274:VAL:HG11	1.87	0.57
11:V:141:LEU:HA	11:V:144:LEU:HD23	1.79	0.56
11:Z:20:ALA:HB2	11:Z:94:GLY:HA2	1.86	0.56
11:V:141:LEU:CD2	11:V:144:LEU:HD21	2.35	0.56
1:M:136:LYS:HB3	2:N:22:LEU:HD22	1.88	0.55
10:O:237:HIS:CD2	6:H:7:ILE:HD11	2.42	0.55
3:E:193:LEU:HD13	3:E:193:LEU:H	1.71	0.55
4:B:166:ARG:HG2	4:B:273:HIS:CE1	2.42	0.55
1:M:71:VAL:HG13	1:M:131:GLN:HB3	1.88	0.54
4:F:171:PRO:HB3	4:F:333:PRO:HG2	1.90	0.54
3:E:30:VAL:HG23	3:E:81:VAL:HG22	1.90	0.54
4:B:165:ALA:HB2	4:B:386:ALA:CB	2.38	0.54
8:P:368:LEU:H	8:P:368:LEU:HD12	1.73	0.53
3:C:158:TYR:CE1	3:C:198:LEU:HD13	2.44	0.53
3:C:258:PHE:CD2	4:D:352:TYR:CD1	2.97	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:W:66:TYR:CG	11:W:144:LEU:HD22	2.44	0.52
4:D:115:GLY:HA3	4:D:243:ASN:HD22	1.73	0.52
6:H:80:LEU:HA	6:H:83:ILE:HD12	1.91	0.52
11:U:21:ILE:HD11	11:T:143:GLY:HA2	1.92	0.52
4:F:462:TRP:CE3	4:F:462:TRP:HA	2.45	0.52
3:E:589:PRO:HA	3:E:597:HIS:CE1	2.45	0.52
1:M:43:PHE:CZ	2:N:112:VAL:HG13	2.45	0.51
4:B:165:ALA:HB2	4:B:386:ALA:HB2	1.92	0.51
11:Y:31:GLY:HA2	11:Y:109:GLY:HA3	1.93	0.51
3:E:450:HIS:CE1	3:E:523:GLU:HA	2.45	0.51
4:B:250:ILE:H	4:B:250:ILE:HD13	1.75	0.51
4:F:260:LEU:HB3	4:F:318:ARG:HH11	1.76	0.51
3:A:323:ASN:HD22	4:B:313:SER:HB3	1.77	0.50
4:F:439:PHE:CZ	4:F:443:PHE:CD2	2.99	0.50
11:X:113:ASP:O	11:X:116:VAL:HG22	2.12	0.50
11:Z:73:LEU:HD22	11:Z:148:LEU:HD23	1.94	0.50
4:F:198:LYS:HG3	4:F:203:GLY:HA3	1.93	0.50
6:L:91:LYS:O	6:L:95:VAL:HG23	2.11	0.50
11:Z:66:TYR:HB3	11:Z:144:LEU:CD2	2.24	0.49
5:Q:206:GLU:HB3	5:Q:302:GLN:HE22	1.77	0.49
7:I:143:GLU:H	7:I:143:GLU:CD	2.16	0.49
11:R:132:ILE:HG23	11:S:57:VAL:HG11	1.95	0.49
11:Y:66:TYR:CG	11:Y:144:LEU:HD22	2.48	0.49
3:A:174:LEU:HD12	3:A:175:PRO:HD2	1.95	0.49
4:D:153:THR:HG23	4:D:164:ILE:HD12	1.95	0.48
3:C:137:ILE:HD12	3:C:139:TRP:HE1	1.78	0.48
11:V:68:LEU:O	11:V:72:VAL:HG23	2.13	0.48
5:Q:286:ASP:OD1	5:Q:342:ILE:HG23	2.13	0.48
11:U:125:LEU:CD1	11:V:43:CYS:HB3	2.43	0.48
10:O:184:PHE:HB3	10:O:262:TYR:CD1	2.48	0.48
8:P:411:VAL:HG11	8:P:456:HIS:CE1	2.48	0.48
11:X:70:VAL:HG21	11:X:97:VAL:HG11	1.94	0.47
3:E:589:PRO:HA	3:E:597:HIS:HE1	1.79	0.47
5:Q:101:GLY:HA3	5:Q:188:TYR:CE1	2.49	0.47
11:U:118:GLY:HA2	11:V:44:VAL:CG1	2.44	0.47
11:V:141:LEU:O	11:V:144:LEU:CD1	2.62	0.47
11:X:74:VAL:HG13	11:X:90:GLN:HE21	1.78	0.47
4:F:124:PRO:HA	7:G:89:LEU:HD13	1.96	0.47
8:P:438:ILE:HA	8:P:441:LEU:HD12	1.97	0.47
4:F:175:ALA:H	4:F:178:LEU:HD12	1.78	0.47
6:L:99:ILE:HD11	7:K:106:LYS:HB2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:I:139:VAL:HG11	7:I:149:ILE:HD13	1.97	0.47
3:E:391:PHE:CZ	3:E:412:ILE:HD11	2.50	0.47
4:D:41:LEU:HD12	4:D:77:VAL:HG21	1.96	0.46
1:M:150:ALA:HB1	2:N:66:ILE:HD13	1.97	0.46
3:C:226:LYS:HD3	3:C:398:ALA:HB2	1.97	0.46
3:A:251:THR:HA	3:A:412:ILE:HG23	1.98	0.46
11:V:144:LEU:CD1	11:V:145:ILE:N	2.64	0.46
8:P:147:VAL:HG22	8:P:193:LEU:HD11	1.97	0.46
4:B:236:GLU:HG2	7:I:81:ALA:HB1	1.96	0.46
5:Q:17:VAL:HG13	5:Q:312:TRP:CD2	2.51	0.46
4:D:316:TYR:HA	4:D:331:GLN:HE22	1.80	0.46
3:A:223:VAL:HG21	3:A:398:ALA:HB1	1.97	0.46
11:Z:20:ALA:HB2	11:Z:94:GLY:CA	2.45	0.46
3:A:406:ARG:N	3:A:406:ARG:HE	2.15	0.45
3:E:44:ALA:H	3:E:47:GLU:HB2	1.82	0.45
3:A:170:HIS:CD2	3:A:172:ILE:HD13	2.51	0.45
11:W:66:TYR:CB	11:W:144:LEU:HD22	2.43	0.45
3:C:109:GLN:HE22	3:C:339:LEU:HD11	1.81	0.45
3:A:603:LEU:HD13	3:A:607:MET:HG3	1.97	0.45
3:C:231:TYR:O	3:C:247:VAL:HG23	2.17	0.45
11:Z:24:THR:HG23	11:Z:101:GLY:HA3	1.99	0.45
3:E:96:LEU:HB2	3:E:213:HIS:CE1	2.52	0.45
3:A:232:PRO:O	3:A:233:LEU:HD23	2.17	0.45
4:F:344:HIS:HA	4:F:345:PRO:HD3	1.87	0.45
3:E:514:THR:HA	3:E:554:HIS:HE1	1.82	0.45
3:E:93:SER:HA	3:E:216:PRO:HA	1.98	0.45
5:Q:195:PHE:O	5:Q:199:GLU:HG3	2.17	0.45
4:B:143:ALA:HB1	4:B:325:ARG:HH21	1.81	0.45
11:Z:117:ARG:HD2	11:Z:117:ARG:H	1.82	0.44
3:C:147:GLN:O	3:C:182:ILE:HD11	2.16	0.44
11:V:144:LEU:HD12	11:V:145:ILE:CA	2.46	0.44
5:Q:125:GLN:H	5:Q:125:GLN:CD	2.20	0.44
4:F:38:LEU:HG	4:F:78:GLN:HE22	1.80	0.44
8:P:395:PHE:CE2	8:P:437:SER:HB2	2.53	0.44
6:J:10:LEU:HA	6:J:10:LEU:HD12	1.82	0.44
4:F:125:LYS:H	7:G:89:LEU:HD13	1.82	0.44
10:O:218:VAL:HG13	6:H:10:LEU:HD12	1.98	0.44
3:C:192:THR:HG22	3:C:193:LEU:H	1.83	0.44
11:U:131:LEU:HG	11:U:135:PHE:CZ	2.53	0.44
1:M:124:GLY:HA2	5:Q:226:ASN:HD22	1.82	0.44
11:Y:111:VAL:HG11	11:Y:132:ILE:HG22	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:141:LEU:HD23	11:V:144:LEU:CD2	2.46	0.43
1:M:150:ALA:CB	2:N:66:ILE:HD13	2.48	0.43
11:T:70:VAL:O	11:T:74:VAL:HG23	2.17	0.43
8:P:368:LEU:HD12	8:P:368:LEU:N	2.33	0.43
3:E:497:GLN:HA	3:E:500:GLN:HE21	1.84	0.43
4:F:160:THR:HA	4:F:396:HIS:CE1	2.53	0.43
5:Q:168:THR:HG22	5:Q:173:ASP:HB2	2.01	0.43
7:G:10:PRO:HA	7:G:13:VAL:HG22	1.99	0.43
3:A:240:LEU:HD23	3:A:439:TRP:CZ3	2.54	0.43
11:V:128:GLY:HA3	11:W:50:LEU:HD21	2.01	0.43
3:A:440:GLY:O	3:A:441:LEU:HD23	2.18	0.43
8:P:196:ILE:HD13	8:P:196:ILE:HG21	1.84	0.43
8:P:161:VAL:HG21	8:P:193:LEU:HD13	2.01	0.43
6:J:99:ILE:HD13	6:J:99:ILE:HA	1.88	0.42
1:M:145:THR:HG22	1:M:149:LEU:HD12	1.99	0.42
4:F:341:ASP:HB3	4:F:343:THR:H	1.84	0.42
10:O:262:TYR:CD1	10:O:267:ILE:HD11	2.53	0.42
4:F:30:THR:HG22	4:F:92:THR:HG22	2.01	0.42
3:C:244:PHE:HB3	3:C:461:SER:HB2	2.01	0.42
4:B:476:ILE:HG21	4:B:481:LEU:HD13	2.01	0.42
11:S:66:TYR:HB3	11:S:144:LEU:HD22	2.01	0.42
4:B:67:VAL:HG12	4:B:77:VAL:HG22	2.01	0.42
6:J:87:ALA:O	6:J:91:LYS:HB2	2.19	0.42
11:U:39:ILE:HG23	11:U:53:ASN:HB3	2.00	0.42
6:J:17:ALA:HB2	7:I:24:ILE:HG22	2.01	0.42
3:A:256:GLY:HA3	3:A:262:LYS:HD3	2.02	0.42
4:B:139:ILE:HG13	4:B:141:PRO:HD3	2.02	0.42
4:B:68:LEU:HD22	4:B:68:LEU:N	2.33	0.42
4:F:166:ARG:CZ	4:F:273:HIS:NE2	2.83	0.41
4:F:41:LEU:CD1	4:F:77:VAL:HG21	2.51	0.41
6:H:9:THR:HB	7:G:17:LEU:HD11	2.02	0.41
11:W:66:TYR:HB3	11:W:144:LEU:CD2	2.47	0.41
4:F:138:PRO:HD3	4:F:318:ARG:HH21	1.84	0.41
1:M:83:VAL:HG22	1:M:122:LEU:HD13	2.02	0.41
3:E:481:LEU:HD21	3:E:548:ARG:HE	1.86	0.41
11:V:141:LEU:CA	11:V:144:LEU:HG	2.50	0.41
10:O:184:PHE:HB3	10:O:262:TYR:CG	2.56	0.41
4:D:64:GLN:HG3	4:D:80:PHE:CD2	2.55	0.41
8:P:80:LEU:HD22	8:P:96:VAL:HG13	2.02	0.41
11:V:144:LEU:C	11:V:144:LEU:HD12	2.37	0.41
4:D:51:GLU:HA	4:D:99:SER:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:A:589:PRO:HA	3:A:597:HIS:CG	2.55	0.41
11:S:70:VAL:HG13	11:S:151:ASN:HD21	1.85	0.41
8:P:161:VAL:CG2	8:P:193:LEU:HD13	2.50	0.41
6:H:10:LEU:HD21	7:G:20:MET:HB3	2.03	0.41
6:J:27:TYR:O	6:J:31:LYS:HG2	2.20	0.41
10:O:107:VAL:HB	10:O:108:PRO:HD3	2.02	0.41
10:O:216:ASN:H	7:G:19:LYS:HE2	1.85	0.41
4:B:211:VAL:CG1	4:B:259:ALA:HB1	2.51	0.41
3:C:355:ASP:HA	3:C:356:SER:HA	1.91	0.41
11:R:15:ILE:HB	11:R:91:LEU:HD13	2.02	0.41
7:I:142:LEU:HD11	7:I:186:GLY:HA2	2.03	0.41
10:O:68:LEU:HD21	10:O:309:LEU:HD23	2.03	0.41
11:T:74:VAL:HG13	11:T:90:GLN:HG2	2.03	0.40
3:E:98:PRO:HA	3:E:170:HIS:CD2	2.57	0.40
11:V:141:LEU:CA	11:V:144:LEU:CD2	2.67	0.40
11:U:118:GLY:HA2	11:V:44:VAL:HG11	2.03	0.40
3:A:30:VAL:HG13	3:A:35:VAL:HG22	2.04	0.40
7:I:121:LEU:HA	7:I:124:LEU:HD12	2.04	0.40
8:P:104:LEU:HD23	8:P:114:VAL:HG22	2.04	0.40
4:B:245:ALA:HB1	3:C:389:ALA:HB1	2.02	0.40
4:D:398:ASP:HB3	4:D:476:ILE:HD12	2.02	0.40

There are no symmetry-related clashes.

5.3 Torsion angles [i](#)

5.3.1 Protein backbone [i](#)

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	M	208/256 (81%)	206 (99%)	2 (1%)	0	100	100
2	N	113/118 (96%)	102 (90%)	10 (9%)	1 (1%)	21	67
3	A	591/616 (96%)	541 (92%)	31 (5%)	19 (3%)	5	41
3	C	591/616 (96%)	538 (91%)	37 (6%)	16 (3%)	6	45

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	E	591/616 (96%)	542 (92%)	32 (5%)	17 (3%)	6	43
4	B	455/517 (88%)	413 (91%)	27 (6%)	15 (3%)	5	40
4	D	455/517 (88%)	416 (91%)	25 (6%)	14 (3%)	5	42
4	F	455/517 (88%)	411 (90%)	30 (7%)	14 (3%)	5	42
5	Q	343/345 (99%)	318 (93%)	18 (5%)	7 (2%)	9	51
6	H	103/114 (90%)	99 (96%)	3 (3%)	1 (1%)	19	65
6	J	103/114 (90%)	100 (97%)	3 (3%)	0	100	100
6	L	103/114 (90%)	98 (95%)	4 (4%)	1 (1%)	19	65
7	G	215/233 (92%)	207 (96%)	7 (3%)	1 (0%)	34	77
7	I	215/233 (92%)	208 (97%)	6 (3%)	1 (0%)	34	77
7	K	215/233 (92%)	205 (95%)	9 (4%)	1 (0%)	34	77
8	P	457/478 (96%)	431 (94%)	18 (4%)	8 (2%)	11	53
9	b	306/840 (36%)	274 (90%)	25 (8%)	7 (2%)	8	48
10	O	390/392 (100%)	350 (90%)	21 (5%)	19 (5%)	3	31
11	R	148/160 (92%)	138 (93%)	6 (4%)	4 (3%)	6	45
11	S	148/160 (92%)	140 (95%)	6 (4%)	2 (1%)	14	58
11	T	148/160 (92%)	143 (97%)	5 (3%)	0	100	100
11	U	148/160 (92%)	140 (95%)	5 (3%)	3 (2%)	9	51
11	V	148/160 (92%)	139 (94%)	5 (3%)	4 (3%)	6	45
11	W	148/160 (92%)	137 (93%)	8 (5%)	3 (2%)	9	51
11	X	148/160 (92%)	138 (93%)	8 (5%)	2 (1%)	14	58
11	Y	148/160 (92%)	139 (94%)	8 (5%)	1 (1%)	26	71
11	Z	148/160 (92%)	136 (92%)	9 (6%)	3 (2%)	9	51
11	a	148/160 (92%)	138 (93%)	7 (5%)	3 (2%)	9	51
All	All	7389/8469 (87%)	6847 (93%)	375 (5%)	167 (2%)	12	48

All (167) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
3	A	257	ALA
3	A	475	TYR
4	B	292	SER
3	C	475	TYR
3	C	529	ASN

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Mol	Chain	Res	Type
3	C	565	ALA
4	D	46	PHE
4	D	467	ILE
3	E	257	ALA
3	E	308	LYS
3	E	475	TYR
4	F	143	ALA
4	F	377	PRO
8	P	53	LYS
8	P	390	ASP
9	b	49	ARG
9	b	178	ALA
10	O	116	TRP
10	O	254	LYS
11	U	156	GLN
11	X	47	PRO
2	N	4	LYS
3	A	529	ASN
3	A	575	GLY
4	B	83	THR
4	B	141	PRO
4	B	391	MET
3	C	259	GLY
3	C	378	GLN
3	C	528	GLN
3	C	535	ASP
3	C	575	GLY
4	D	59	ASP
4	D	127	PHE
3	E	230	ASP
3	E	575	GLY
3	E	590	SER
4	F	141	PRO
4	F	179	PRO
4	F	391	MET
5	Q	131	GLY
8	P	54	LYS
8	P	332	ASP
8	P	412	ASN
8	P	458	ASP
9	b	24	GLU
10	O	39	ILE

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Mol	Chain	Res	Type
10	O	172	VAL
6	H	77	GLN
7	G	144	ARG
11	Y	155	THR
11	R	157	ASP
11	V	123	PRO
11	V	156	GLN
11	V	158	VAL
11	S	158	VAL
11	Z	159	VAL
11	a	158	VAL
11	a	159	VAL
3	A	42	GLY
3	A	207	SER
3	A	245	PRO
3	A	308	LYS
3	A	405	ASP
3	A	449	LYS
3	A	595	GLU
4	B	44	VAL
4	B	293	ALA
4	B	305	PRO
4	B	319	ALA
4	B	372	PRO
4	B	377	PRO
3	C	508	SER
4	D	48	ARG
4	D	122	ASN
4	D	141	PRO
4	D	319	ALA
3	E	44	ALA
3	E	78	GLY
3	E	589	PRO
3	E	594	LYS
3	E	595	GLU
4	F	128	ALA
4	F	167	GLY
4	F	202	ASP
4	F	424	ALA
5	Q	176	ASN
5	Q	230	SER
5	Q	261	ASP

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Mol	Chain	Res	Type
6	L	63	GLY
8	P	410	ASP
9	b	46	SER
9	b	177	ALA
9	b	265	SER
10	O	7	THR
10	O	96	ALA
10	O	167	THR
10	O	171	SER
10	O	176	HIS
10	O	186	LEU
10	O	335	LYS
11	U	47	PRO
11	V	159	VAL
11	W	47	PRO
11	W	158	VAL
11	Z	46	ARG
11	Z	158	VAL
3	A	203	ASP
3	C	78	GLY
3	C	257	ALA
3	C	260	CYS
3	C	590	SER
4	D	202	ASP
4	D	340	ASP
4	D	390	GLY
4	D	474	ASN
3	E	45	MET
3	E	207	SER
3	E	310	PRO
4	F	148	GLU
4	F	326	ASN
5	Q	231	SER
10	O	95	ASN
11	R	156	GLN
11	S	159	VAL
11	X	159	VAL
3	A	75	GLU
3	A	177	ARG
3	A	305	SER
3	A	381	PRO
4	B	138	PRO

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Mol	Chain	Res	Type
4	B	149	GLU
4	B	202	ASP
4	B	271	GLU
3	C	177	ARG
3	C	230	ASP
3	E	55	ASN
4	F	292	SER
8	P	135	ASP
10	O	106	PRO
10	O	355	ALA
11	R	80	GLN
11	U	159	VAL
4	D	391	MET
5	Q	117	ASP
10	O	120	LYS
10	O	189	GLU
11	W	159	VAL
11	a	156	GLN
10	O	101	PRO
3	A	310	PRO
3	A	375	PRO
4	D	58	PRO
4	F	72	GLY
7	K	168	PRO
11	R	158	VAL
3	A	284	GLY
4	B	139	ILE
3	C	420	GLY
3	E	143	PRO
3	E	564	GLY
5	Q	272	VAL
9	b	48	VAL
10	O	362	GLY
7	I	168	PRO
4	F	138	PRO
10	O	168	GLY

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	M	183/221 (83%)	181 (99%)	2 (1%)	80	91
2	N	102/104 (98%)	101 (99%)	1 (1%)	82	92
3	A	497/515 (96%)	479 (96%)	18 (4%)	42	74
3	C	497/515 (96%)	472 (95%)	25 (5%)	30	66
3	E	497/515 (96%)	473 (95%)	24 (5%)	31	67
4	B	391/444 (88%)	370 (95%)	21 (5%)	27	64
4	D	391/444 (88%)	384 (98%)	7 (2%)	66	87
4	F	391/444 (88%)	374 (96%)	17 (4%)	35	70
5	Q	309/309 (100%)	296 (96%)	13 (4%)	36	70
6	H	87/94 (93%)	84 (97%)	3 (3%)	44	75
6	J	87/94 (93%)	87 (100%)	0	100	100
6	L	87/94 (93%)	84 (97%)	3 (3%)	44	75
7	G	194/208 (93%)	190 (98%)	4 (2%)	61	84
7	I	194/208 (93%)	189 (97%)	5 (3%)	54	80
7	K	194/208 (93%)	189 (97%)	5 (3%)	54	80
8	P	426/439 (97%)	417 (98%)	9 (2%)	61	84
9	b	275/728 (38%)	265 (96%)	10 (4%)	42	74
10	O	348/348 (100%)	339 (97%)	9 (3%)	54	80
11	R	110/119 (92%)	104 (94%)	6 (6%)	27	63
11	S	110/119 (92%)	106 (96%)	4 (4%)	42	74
11	T	110/119 (92%)	107 (97%)	3 (3%)	52	79
11	U	110/119 (92%)	106 (96%)	4 (4%)	42	74
11	V	110/119 (92%)	107 (97%)	3 (3%)	52	79
11	W	110/119 (92%)	109 (99%)	1 (1%)	84	93
11	X	110/119 (92%)	107 (97%)	3 (3%)	52	79
11	Y	110/119 (92%)	107 (97%)	3 (3%)	52	79
11	Z	110/119 (92%)	108 (98%)	2 (2%)	66	87
11	a	110/119 (92%)	108 (98%)	2 (2%)	66	87
All	All	6250/7122 (88%)	6043 (97%)	207 (3%)	49	76

All (207) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	M	127	ARG
1	M	139	TYR
2	N	22	LEU
3	A	60	VAL
3	A	83	ASP
3	A	103	THR
3	A	175	PRO
3	A	197	ILE
3	A	286	ARG
3	A	315	THR
3	A	352	MET
3	A	364	LEU
3	A	406	ARG
3	A	426	PRO
3	A	458	VAL
3	A	466	VAL
3	A	478	PHE
3	A	578	LYS
3	A	597	HIS
3	A	602	LYS
3	A	603	LEU
4	B	32	SER
4	B	47	PRO
4	B	86	ILE
4	B	166	ARG
4	B	174	SER
4	B	194	VAL
4	B	195	ARG
4	B	250	ILE
4	B	325	ARG
4	B	337	MET
4	B	341	ASP
4	B	345	PRO
4	B	357	GLN
4	B	389	GLU
4	B	391	MET
4	B	394	LYS
4	B	417	LYS
4	B	426	SER
4	B	471	GLU
4	B	484	PHE
4	B	485	TYR
3	C	41	ILE

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Mol	Chain	Res	Type
3	C	60	VAL
3	C	64	ASP
3	C	81	VAL
3	C	96	LEU
3	C	124	ILE
3	C	150	ASP
3	C	192	THR
3	C	193	LEU
3	C	197	ILE
3	C	233	LEU
3	C	262	LYS
3	C	279	ILE
3	C	286	ARG
3	C	290	MET
3	C	301	TYR
3	C	302	THR
3	C	353	ILE
3	C	404	PRO
3	C	406	ARG
3	C	418	PRO
3	C	422	ASP
3	C	435	THR
3	C	559	LYS
3	C	603	LEU
4	D	86	ILE
4	D	102	ILE
4	D	131	TYR
4	D	206	GLU
4	D	250	ILE
4	D	337	MET
4	D	475	ARG
3	E	83	ASP
3	E	87	ARG
3	E	192	THR
3	E	193	LEU
3	E	197	ILE
3	E	214	THR
3	E	243	LEU
3	E	258	PHE
3	E	278	ILE
3	E	286	ARG
3	E	304	MET

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Mol	Chain	Res	Type
3	E	374	MET
3	E	377	ASP
3	E	406	ARG
3	E	435	THR
3	E	454	ILE
3	E	460	TYR
3	E	466	VAL
3	E	476	PRO
3	E	478	PHE
3	E	482	ARG
3	E	527	GLN
3	E	588	GLU
3	E	603	LEU
4	F	43	LYS
4	F	47	PRO
4	F	66	GLN
4	F	68	LEU
4	F	91	THR
4	F	164	ILE
4	F	169	LYS
4	F	206	GLU
4	F	231	GLU
4	F	240	LEU
4	F	261	THR
4	F	296	GLU
4	F	307	TYR
4	F	310	THR
4	F	391	MET
4	F	394	LYS
4	F	462	TRP
5	Q	59	SER
5	Q	102	TYR
5	Q	107	VAL
5	Q	125	GLN
5	Q	161	TYR
5	Q	205	LYS
5	Q	218	ARG
5	Q	222	ASN
5	Q	242	LEU
5	Q	262	PHE
5	Q	286	ASP
5	Q	298	ASP

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Mol	Chain	Res	Type
5	Q	316	LYS
6	L	9	THR
6	L	14	GLU
6	L	104	LYS
7	K	23	PHE
7	K	59	ASP
7	K	147	ASP
7	K	175	SER
7	K	215	LEU
8	P	28	ASP
8	P	36	LEU
8	P	37	SER
8	P	207	GLU
8	P	236	ASN
8	P	282	ILE
8	P	285	LYS
8	P	368	LEU
8	P	469	THR
9	b	20	TYR
9	b	21	ILE
9	b	85	GLU
9	b	90	LYS
9	b	213	PHE
9	b	216	VAL
9	b	250	ARG
9	b	291	THR
9	b	331	ASN
9	b	341	ILE
10	O	19	ASN
10	O	47	ASP
10	O	124	ASP
10	O	171	SER
10	O	175	LEU
10	O	189	GLU
10	O	212	THR
10	O	224	VAL
10	O	238	LEU
6	H	50	LYS
6	H	76	VAL
6	H	85	LYS
7	G	20	MET
7	G	71	LEU

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Mol	Chain	Res	Type
7	G	146	VAL
7	G	165	GLN
7	I	25	ARG
7	I	86	LEU
7	I	104	LYS
7	I	126	VAL
7	I	201	ASN
11	Y	58	ILE
11	Y	139	LEU
11	Y	159	VAL
11	R	51	PHE
11	R	56	PRO
11	R	58	ILE
11	R	116	VAL
11	R	134	ILE
11	R	159	VAL
11	U	57	VAL
11	U	63	ILE
11	U	121	GLN
11	U	152	SER
11	V	11	PHE
11	V	63	ILE
11	V	153	ARG
11	T	11	PHE
11	T	54	ILE
11	T	129	MET
11	W	34	LYS
11	S	63	ILE
11	S	86	THR
11	S	120	SER
11	S	124	ARG
11	X	81	LYS
11	X	86	THR
11	X	132	ILE
11	Z	56	PRO
11	Z	73	LEU
11	a	56	PRO
11	a	59	MET

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (53) such sidechains are listed below:

Mol	Chain	Res	Type
1	M	212	ASN
3	A	170	HIS
3	A	320	ASN
3	A	323	ASN
3	A	474	ASN
3	A	529	ASN
4	B	218	ASN
4	B	273	HIS
4	B	396	HIS
3	C	109	GLN
3	C	164	ASN
3	C	170	HIS
3	C	450	HIS
4	D	201	HIS
4	D	243	ASN
4	D	273	HIS
4	D	331	GLN
4	D	363	GLN
3	E	151	HIS
3	E	170	HIS
3	E	213	HIS
3	E	450	HIS
3	E	500	GLN
3	E	554	HIS
3	E	608	GLN
4	F	269	GLN
5	Q	255	HIS
5	Q	283	ASN
5	Q	302	GLN
6	L	12	GLN
8	P	156	HIS
8	P	179	GLN
8	P	206	HIS
8	P	241	GLN
8	P	245	HIS
8	P	412	ASN
8	P	456	HIS
9	b	52	GLN
9	b	324	ASN
10	O	237	HIS
10	O	282	GLN
10	O	302	ASN
6	H	3	GLN

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Mol	Chain	Res	Type
6	H	59	GLN
7	G	41	GLN
7	G	94	GLN
7	G	112	ASN
7	I	61	ASN
11	Y	90	GLN
11	R	90	GLN
11	T	82	GLN
11	W	122	GLN
11	X	90	GLN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains [i](#)

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

5.5 Carbohydrates [i](#)

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.