



wwPDB EM Map/Model Validation Report ⓘ

Apr 10, 2016 – 02:03 PM BST

PDB ID : 3J9V
EMDB ID: : EMD-6286
Title : Yeast V-ATPase state 3
Authors : Zhao, J.; Benlekbir, S.; Rubinstein, J.L.
Deposited on : 2015-02-23
Resolution : 8.30 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

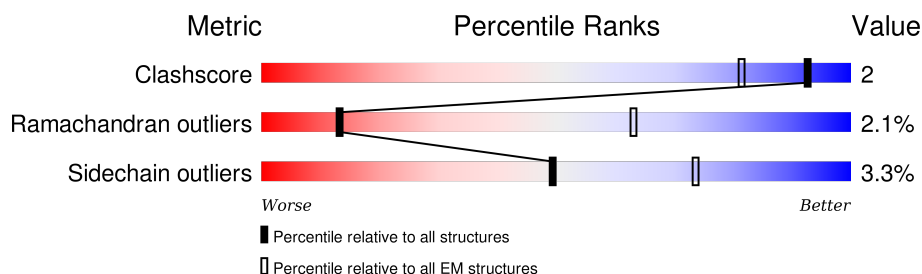
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

ELECTRON MICROSCOPY

The reported resolution of this entry is 8.30 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.













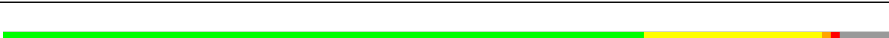


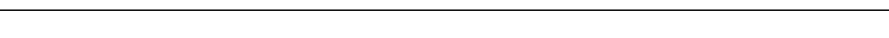
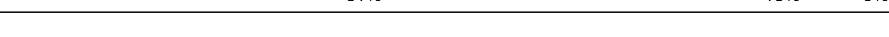
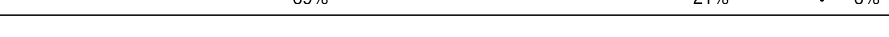



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	114402	924
Ramachandran outliers	111179	726
Sidechain outliers	111093	686

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	b	840	27% 9% • 63%
2	O	392	79% 17% •
3	M	256	61% 18% •• 18%
4	N	118	80% 16% ••
5	A	616	72% 21% ••
5	C	616	70% 22% ••
5	E	616	68% 22% 5% ••
6	B	517	65% 19% 5% 12%
6	D	517	65% 20% • 12%

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Mol	Chain	Length	Quality of chain
6	F	517	
7	Q	345	
8	H	114	
8	J	114	
8	L	114	
9	G	233	
9	I	233	
9	K	233	
10	P	478	
11	R	160	
11	S	160	
11	T	160	
11	U	160	
11	V	160	
11	W	160	
11	X	160	
11	Y	160	
11	Z	160	
11	a	160	

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 a, vacuolar isoform.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 9 is a protein called V-type proton ATPase subunit E.

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

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

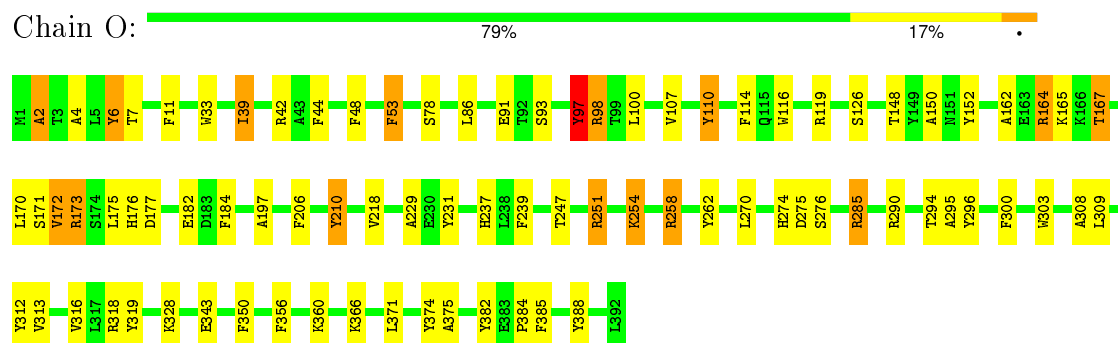
Mol	Chain	Residues	Atoms					AltConf	Trace
10	P	461	Total	C	N	O	S	0	0
			3712	2373	623	704	12		

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

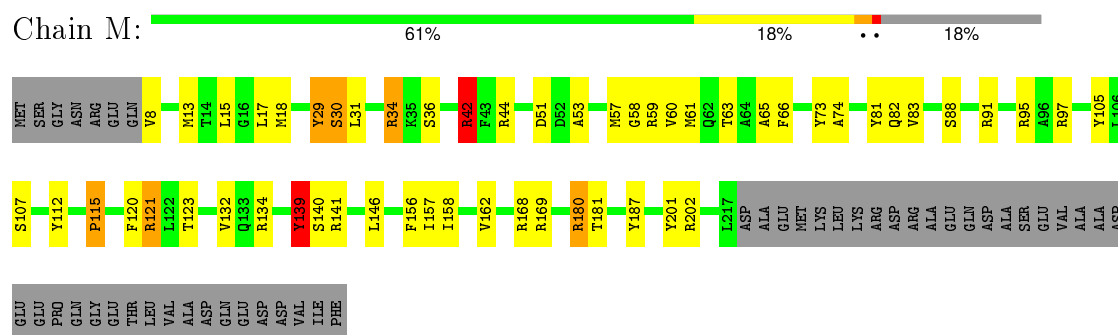
Mol	Chain	Residues	Atoms					AltConf	Trace
11	R	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	U	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	X	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	Y	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	W	150	Total 1071	C 704	N 173	O 187	S 7	0	0
11	Z	150	Total 1071	C 704	N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

- Molecule 1: V-type proton ATPase subunit a, vacuolar isoform

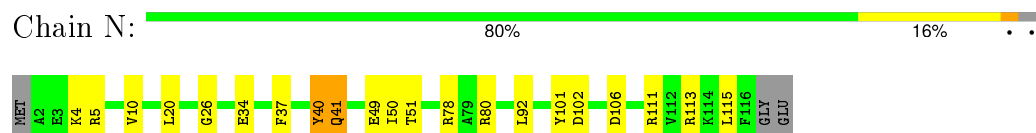
- Molecule 2: V-type proton ATPase subunit C



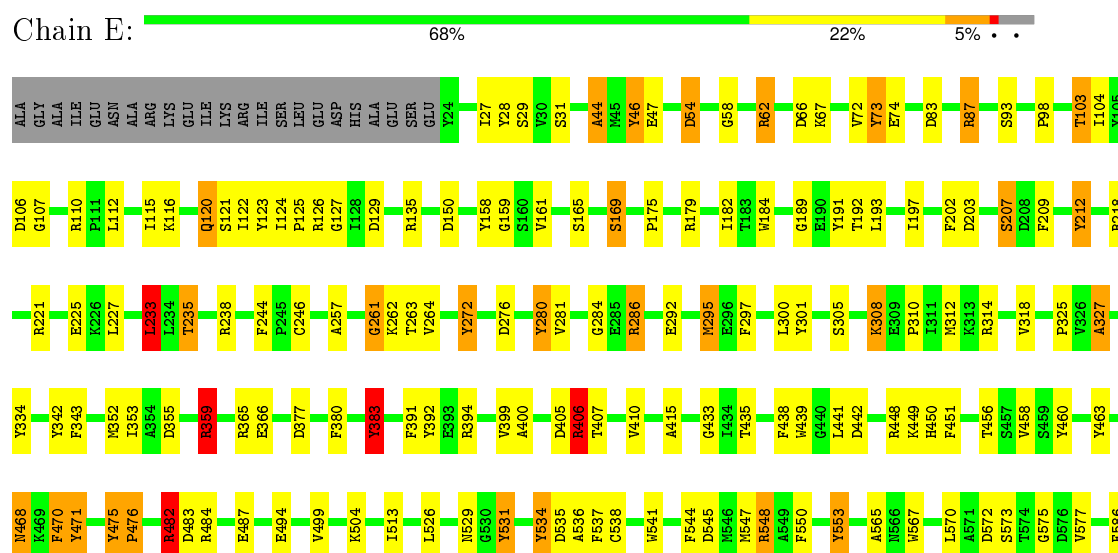
• Molecule 3: V-type proton ATPase subunit D



• Molecule 4: V-type proton ATPase subunit F



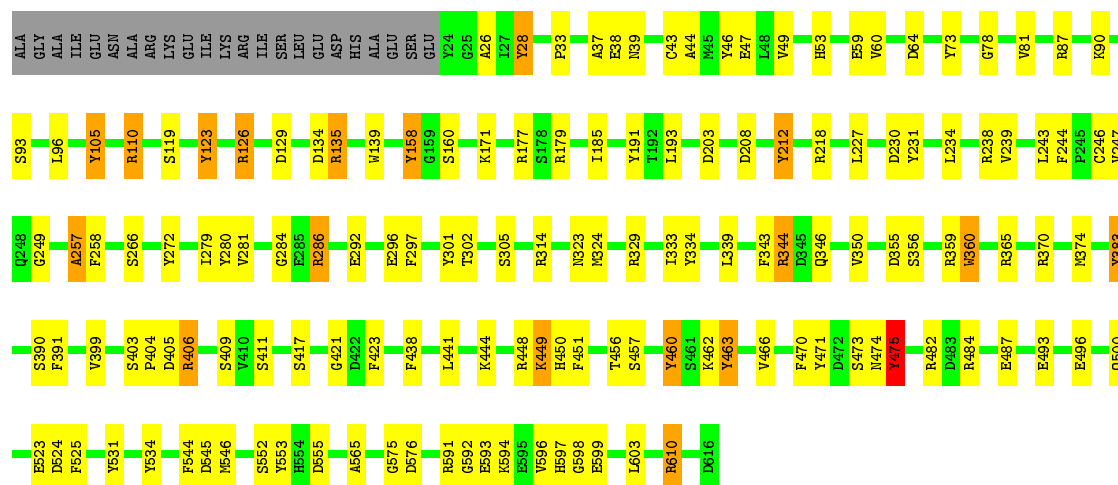
• Molecule 5: V-type proton ATPase catalytic subunit A





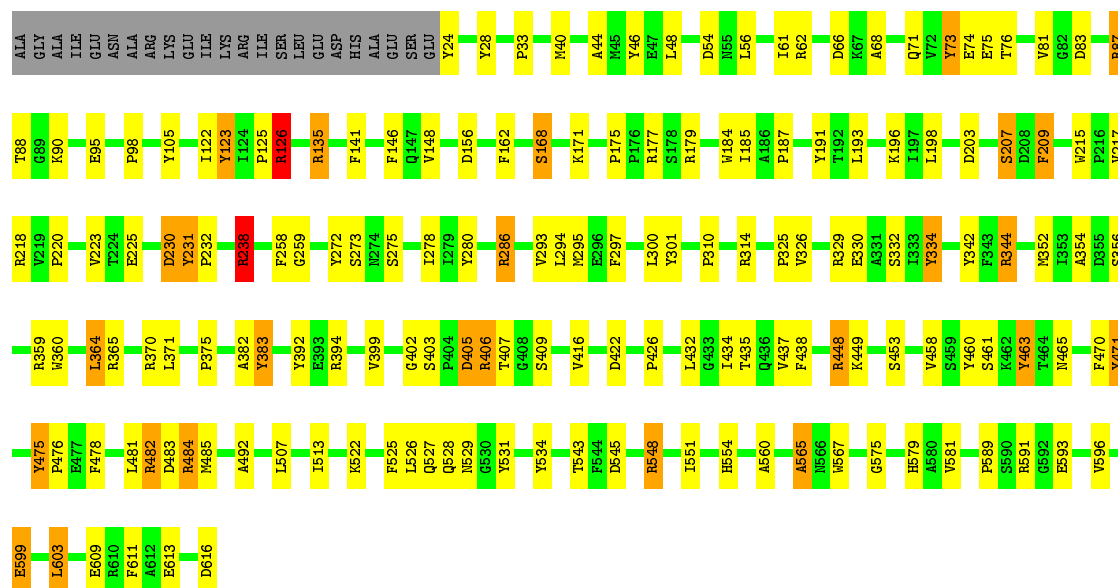
• Molecule 5: V-type proton ATPase catalytic subunit A

Chain A: 72% 21%



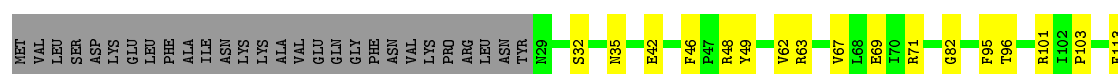
• Molecule 5: V-type proton ATPase catalytic subunit A

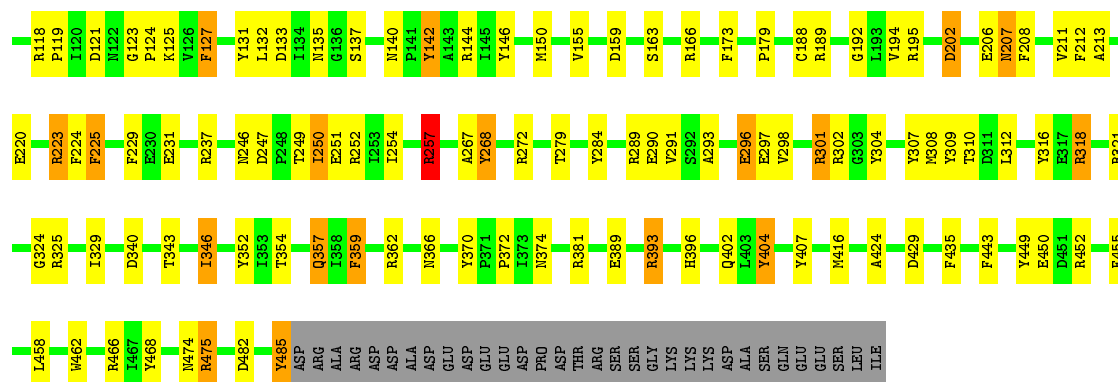
Chain C: 70% 22%



• Molecule 6: V-type proton ATPase subunit B

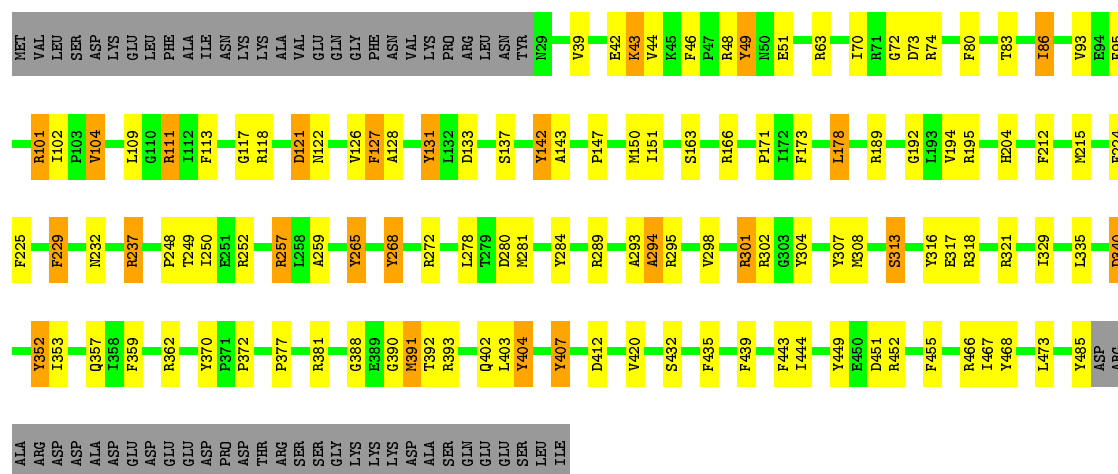
Chain F: 63% 21% 12%





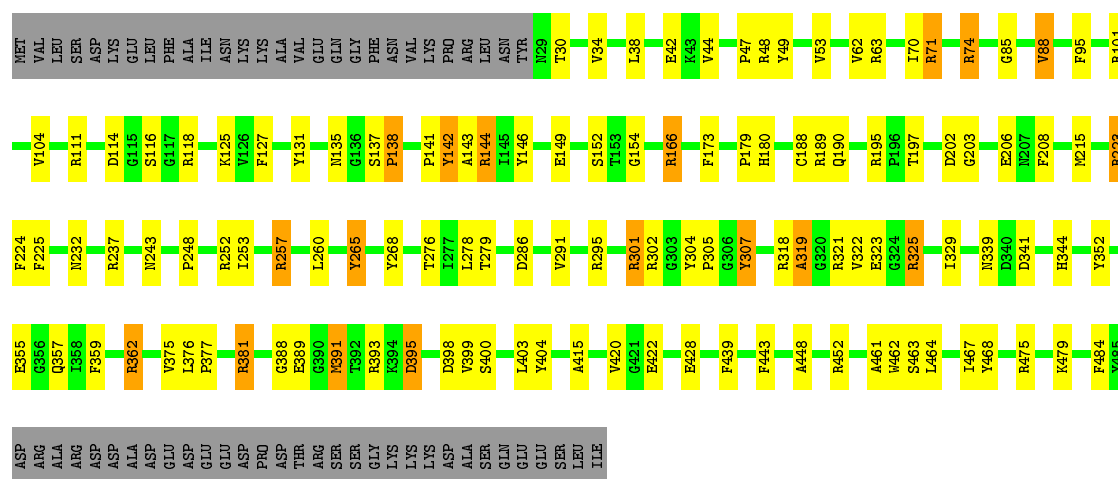
• Molecule 6: V-type proton ATPase subunit B

Chain B: 65% 19% 5% 12%

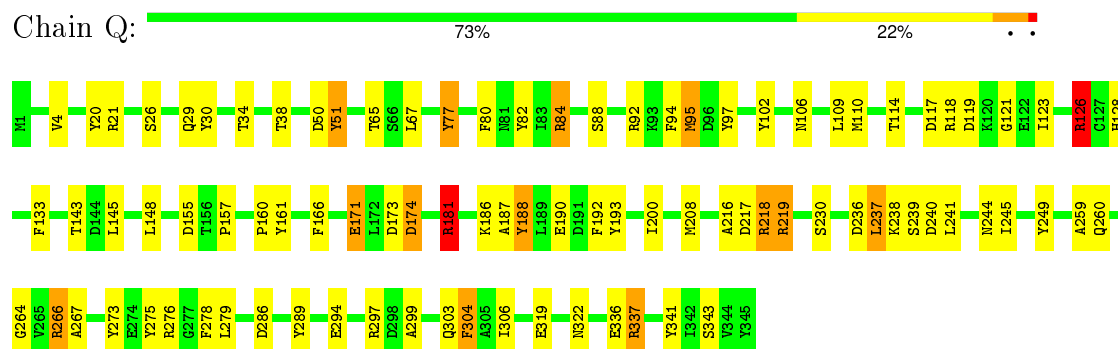


• Molecule 6: V-type proton ATPase subunit B

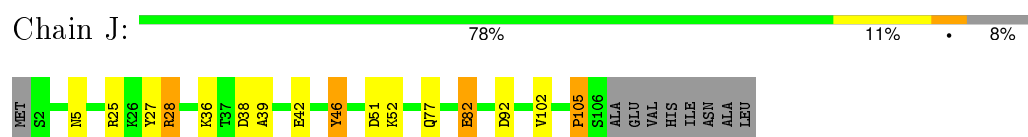
Chain D: 65% 20% 12%



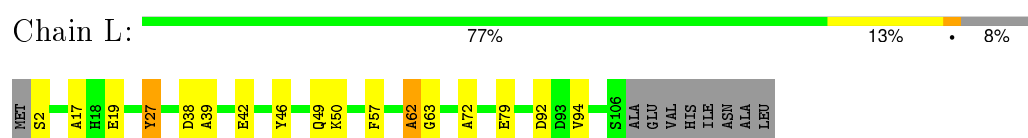
• Molecule 7: V-type proton ATPase subunit d



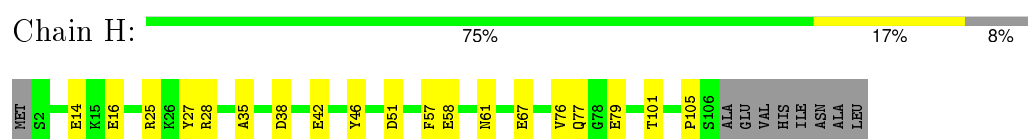
- Molecule 8: V-type proton ATPase subunit G



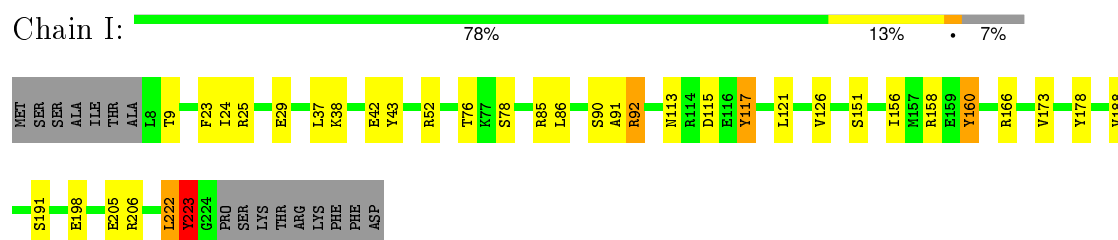
- Molecule 8: V-type proton ATPase subunit G



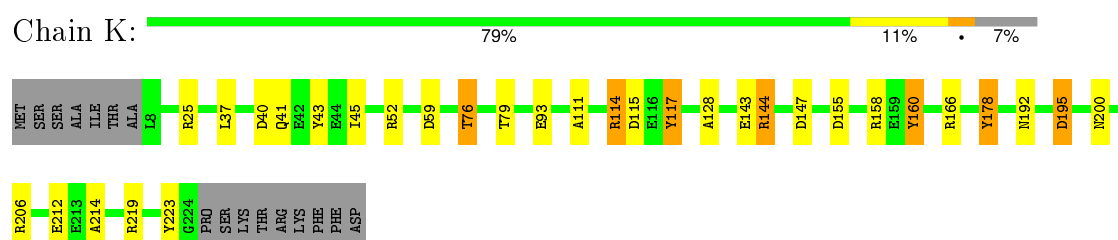
- Molecule 8: V-type proton ATPase subunit G



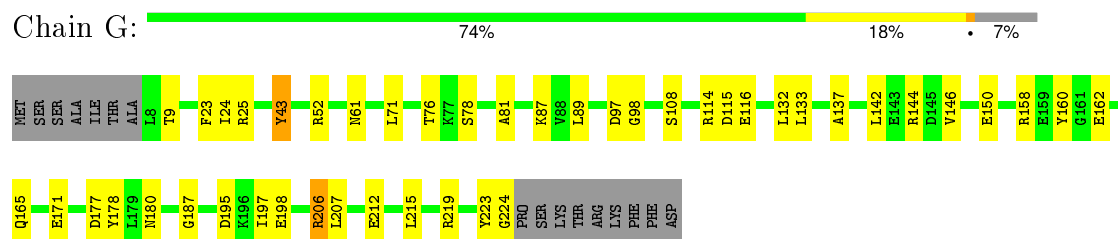
- Molecule 9: V-type proton ATPase subunit E



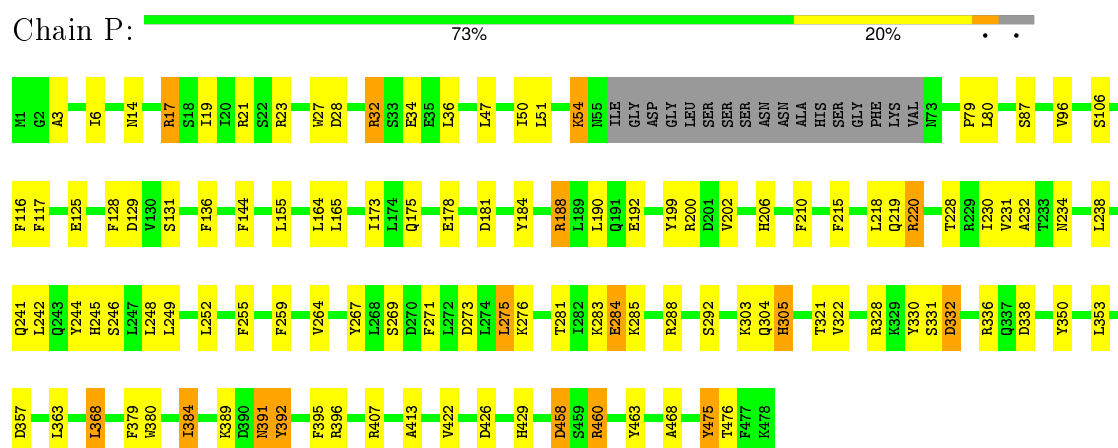
- Molecule 9: V-type proton ATPase subunit E



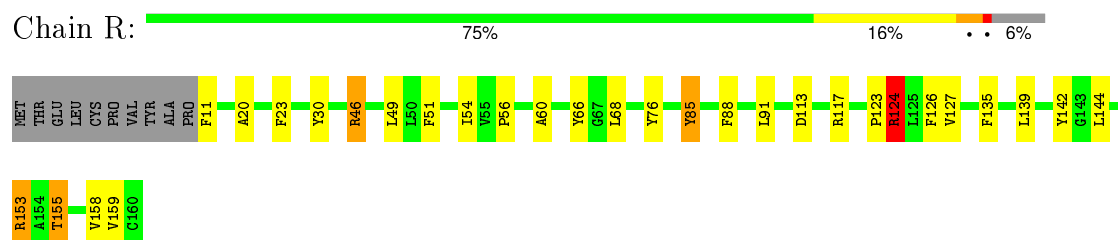
- Molecule 9: V-type proton ATPase subunit E



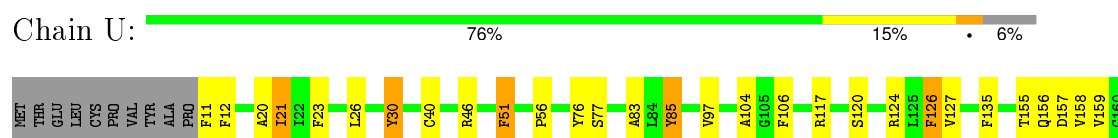
- Molecule 10: V-type proton ATPase subunit H



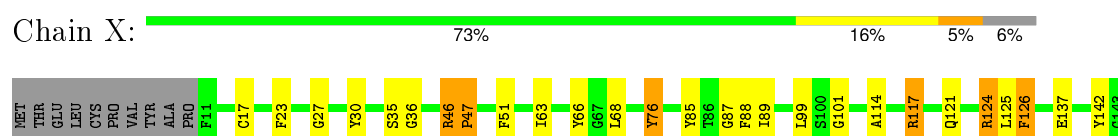
- Molecule 11: V-type proton ATPase subunit c



- Molecule 11: V-type proton ATPase subunit c



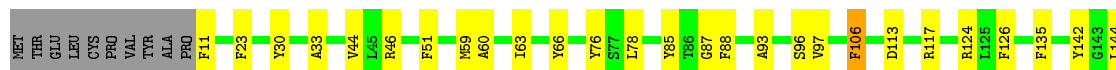
- Molecule 11: V-type proton ATPase subunit c





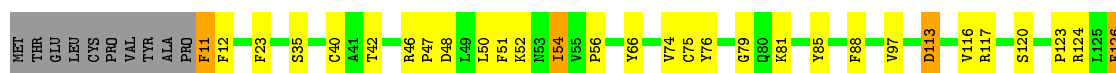
- Molecule 11: V-type proton ATPase subunit c

Chain Y: 75% 18% • 6%



- Molecule 11: V-type proton ATPase subunit c

Chain W: 69% 21% • 6%



- Molecule 11: V-type proton ATPase subunit c

Chain Z: 71% 21% • 6%



- Molecule 11: V-type proton ATPase subunit c

Chain V: 81% 13% • 6%



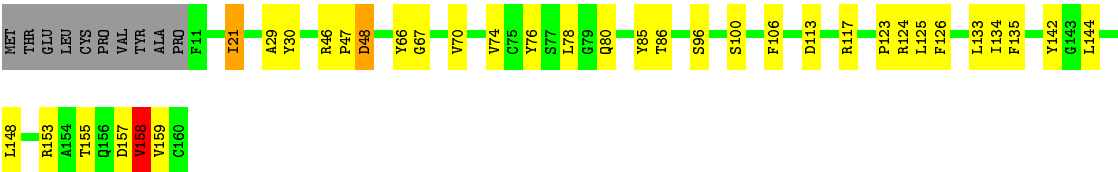
- Molecule 11: V-type proton ATPase subunit c

Chain a: 78% 14% • 6%



- Molecule 11: V-type proton ATPase subunit c

Chain S: 72% 20% • 6%



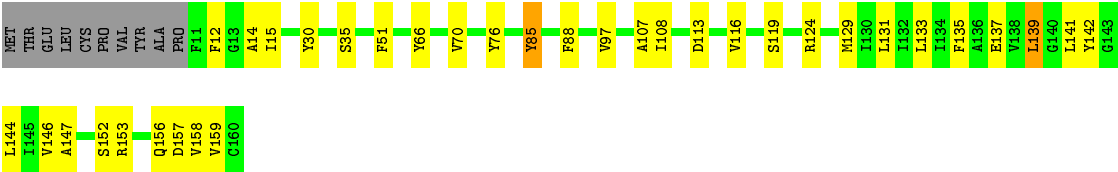
- Molecule 11: V-type proton ATPase subunit c

Chain T:

72%

21%

6%



4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	17595	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	b	1.76	22/2578 (0.9%)	2.07	83/3479 (2.4%)
10	P	1.68	25/3766 (0.7%)	1.87	74/5087 (1.5%)
11	R	1.63	3/1086 (0.3%)	2.03	30/1472 (2.0%)
11	S	1.77	7/1086 (0.6%)	1.79	19/1472 (1.3%)
11	T	1.60	4/1086 (0.4%)	1.97	25/1472 (1.7%)
11	U	1.65	6/1086 (0.6%)	2.05	23/1472 (1.6%)
11	V	1.67	4/1086 (0.4%)	1.84	17/1472 (1.2%)
11	W	1.67	9/1086 (0.8%)	1.95	30/1472 (2.0%)
11	X	1.72	7/1086 (0.6%)	1.86	22/1472 (1.5%)
11	Y	1.63	3/1086 (0.3%)	1.90	27/1472 (1.8%)
11	Z	1.68	7/1086 (0.6%)	1.87	18/1472 (1.2%)
11	a	1.68	7/1086 (0.6%)	1.97	24/1472 (1.6%)
2	O	1.68	27/3185 (0.8%)	1.90	63/4314 (1.5%)
3	M	1.76	16/1710 (0.9%)	1.87	43/2295 (1.9%)
4	N	1.68	8/944 (0.8%)	1.83	14/1277 (1.1%)
5	A	1.72	46/4677 (1.0%)	1.95	105/6339 (1.7%)
5	C	1.71	35/4677 (0.7%)	1.96	108/6339 (1.7%)
5	E	1.75	61/4677 (1.3%)	1.97	125/6339 (2.0%)
6	B	1.72	38/3654 (1.0%)	1.99	90/4953 (1.8%)
6	D	1.72	31/3654 (0.8%)	1.98	88/4953 (1.8%)
6	F	1.74	34/3654 (0.9%)	1.91	90/4953 (1.8%)
7	Q	1.74	28/2861 (1.0%)	1.96	78/3880 (2.0%)
8	H	1.70	8/828 (1.0%)	1.76	10/1098 (0.9%)
8	J	1.63	5/828 (0.6%)	1.72	9/1098 (0.8%)
8	L	1.59	3/828 (0.4%)	1.76	13/1098 (1.2%)
9	G	1.68	12/1743 (0.7%)	1.86	33/2338 (1.4%)
9	I	1.70	10/1743 (0.6%)	1.84	30/2338 (1.3%)
9	K	1.67	9/1743 (0.5%)	1.84	29/2338 (1.2%)
All	All	1.70	475/58610 (0.8%)	1.93	1320/79236 (1.7%)

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	b	0	11
10	P	0	9
11	R	0	3
11	S	0	1
11	T	0	1
11	U	0	3
11	W	0	1
11	X	0	7
11	Y	0	3
11	Z	0	2
11	a	0	3
2	O	0	10
3	M	0	4
5	A	0	14
5	C	0	17
5	E	0	19
6	B	0	20
6	D	0	8
6	F	0	11
7	Q	0	6
8	J	0	2
8	L	0	1
9	G	0	4
9	I	0	3
9	K	0	4
All	All	0	167

All (475) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	393	ARG	CZ-NH2	9.92	1.46	1.33
10	P	246	SER	CA-CB	9.62	1.67	1.52
6	B	257	ARG	NE-CZ	8.88	1.44	1.33
5	E	334	TYR	CE1-CZ	8.71	1.49	1.38
6	F	101	ARG	CZ-NH1	8.52	1.44	1.33
6	F	118	ARG	CD-NE	8.13	1.60	1.46
6	F	123	GLY	N-CA	-8.03	1.34	1.46
1	b	300	TYR	CD1-CE1	7.99	1.51	1.39
6	D	257	ARG	CZ-NH2	7.91	1.43	1.33
2	O	319	TYR	CG-CD1	7.90	1.49	1.39
5	E	573	SER	CA-CB	7.88	1.64	1.52
5	C	231	TYR	CG-CD2	7.62	1.49	1.39
6	D	463	SER	CA-CB	7.62	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	K	158	ARG	CD-NE	7.61	1.59	1.46
6	F	381	ARG	CZ-NH2	7.61	1.43	1.33
10	P	27	TRP	NE1-CE2	7.60	1.47	1.37
11	W	40	CYS	CB-SG	-7.53	1.69	1.82
10	P	178	GLU	CG-CD	7.52	1.63	1.51
1	b	112	ARG	NE-CZ	7.48	1.42	1.33
11	Y	117	ARG	CZ-NH1	7.46	1.42	1.33
11	U	85	TYR	CB-CG	-7.46	1.40	1.51
5	E	482	ARG	CZ-NH1	7.34	1.42	1.33
8	H	58	GLU	CG-CD	7.32	1.62	1.51
5	E	433	GLY	N-CA	-7.31	1.35	1.46
5	A	473	SER	CA-CB	7.30	1.64	1.52
2	O	251	ARG	NE-CZ	7.24	1.42	1.33
5	E	169	SER	CA-CB	7.18	1.63	1.52
5	E	225	GLU	CD-OE1	7.16	1.33	1.25
5	E	110	ARG	NE-CZ	7.16	1.42	1.33
5	A	218	ARG	CZ-NH2	7.12	1.42	1.33
5	A	314	ARG	NE-CZ	7.10	1.42	1.33
5	A	487	GLU	CG-CD	7.09	1.62	1.51
9	G	23	PHE	CG-CD1	7.06	1.49	1.38
6	F	362	ARG	CD-NE	7.05	1.58	1.46
5	E	207	SER	CA-CB	7.05	1.63	1.52
11	S	67	GLY	N-CA	-7.02	1.35	1.46
7	Q	264	GLY	CA-C	7.01	1.63	1.51
6	D	146	TYR	CE2-CZ	6.98	1.47	1.38
5	C	272	TYR	CE2-CZ	6.97	1.47	1.38
5	A	179	ARG	CZ-NH2	6.96	1.42	1.33
9	I	178	TYR	CE1-CZ	6.93	1.47	1.38
6	D	307	TYR	CG-CD2	6.92	1.48	1.39
5	A	360	TRP	NE1-CE2	6.90	1.46	1.37
7	Q	219	ARG	CZ-NH1	6.90	1.42	1.33
7	Q	266	ARG	CZ-NH2	6.89	1.42	1.33
5	E	391	PHE	CG-CD1	6.87	1.49	1.38
11	S	85	TYR	CZ-OH	6.86	1.49	1.37
6	B	289	ARG	CD-NE	6.84	1.58	1.46
10	P	188	ARG	CZ-NH1	6.82	1.42	1.33
6	D	393	ARG	CD-NE	6.82	1.58	1.46
6	F	166	ARG	CZ-NH2	6.78	1.41	1.33
9	I	206	ARG	CZ-NH1	6.78	1.41	1.33
11	a	76	TYR	CE1-CZ	6.77	1.47	1.38
7	Q	51	TYR	CE1-CZ	6.75	1.47	1.38
7	Q	92	ARG	CZ-NH1	6.75	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	46	TYR	CG-CD2	6.74	1.48	1.39
3	M	88	SER	CA-CB	6.74	1.63	1.52
9	K	144	ARG	CZ-NH2	6.72	1.41	1.33
2	O	173	ARG	NE-CZ	6.70	1.41	1.33
6	F	257	ARG	CZ-NH1	6.67	1.41	1.33
6	F	163	SER	CA-CB	6.66	1.62	1.52
2	O	119	ARG	CZ-NH2	6.66	1.41	1.33
5	E	191	TYR	CG-CD1	6.65	1.47	1.39
5	A	272	TYR	CE2-CZ	6.63	1.47	1.38
6	F	272	ARG	CZ-NH2	6.62	1.41	1.33
10	P	304	GLN	CA-CB	6.62	1.68	1.53
5	C	402	GLY	N-CA	-6.62	1.36	1.46
11	W	88	PHE	CG-CD2	6.61	1.48	1.38
9	I	29	GLU	CG-CD	6.61	1.61	1.51
4	N	49	GLU	CG-CD	6.60	1.61	1.51
4	N	40	TYR	CG-CD1	6.60	1.47	1.39
6	F	144	ARG	CZ-NH1	6.60	1.41	1.33
5	A	482	ARG	CZ-NH2	6.59	1.41	1.33
5	E	238	ARG	CZ-NH1	6.56	1.41	1.33
5	A	359	ARG	NE-CZ	6.53	1.41	1.33
6	B	295	ARG	NE-CZ	6.52	1.41	1.33
6	D	166	ARG	NE-CZ	6.52	1.41	1.33
11	S	117	ARG	NE-CZ	6.52	1.41	1.33
6	D	208	PHE	CG-CD2	6.51	1.48	1.38
2	O	91	GLU	CG-CD	6.50	1.61	1.51
5	A	552	SER	CA-CB	6.49	1.62	1.52
6	D	116	SER	CA-CB	6.49	1.62	1.52
5	A	280	TYR	CZ-OH	6.48	1.48	1.37
9	G	98	GLY	CA-C	-6.46	1.41	1.51
6	D	101	ARG	NE-CZ	6.45	1.41	1.33
5	A	471	TYR	CE1-CZ	6.45	1.47	1.38
4	N	26	GLY	CA-C	-6.44	1.41	1.51
5	E	567	TRP	CE3-CZ3	6.44	1.49	1.38
5	A	421	GLY	CA-C	-6.44	1.41	1.51
6	D	42	GLU	CD-OE2	6.43	1.32	1.25
2	O	318	ARG	CZ-NH2	6.42	1.41	1.33
6	F	268	TYR	CZ-OH	6.41	1.48	1.37
6	F	252	ARG	CD-NE	6.40	1.57	1.46
6	B	390	GLY	CA-C	-6.38	1.41	1.51
6	B	452	ARG	NE-CZ	6.38	1.41	1.33
6	B	449	TYR	CG-CD2	6.37	1.47	1.39
5	E	471	TYR	CE1-CZ	6.37	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	P	460	ARG	CA-CB	6.37	1.68	1.53
6	B	317	GLU	CG-CD	6.36	1.61	1.51
9	I	43	TYR	CG-CD2	6.36	1.47	1.39
10	P	350	TYR	CE2-CZ	6.35	1.46	1.38
6	D	135	ASN	C-N	6.35	1.44	1.33
8	L	42	GLU	CG-CD	6.34	1.61	1.51
5	A	59	GLU	CB-CG	6.34	1.64	1.52
11	R	11	PHE	CG-CD1	6.32	1.48	1.38
5	E	292	GLU	CD-OE2	6.29	1.32	1.25
6	D	224	PHE	CB-CG	-6.29	1.40	1.51
6	F	49	TYR	CG-CD1	6.28	1.47	1.39
7	Q	337	ARG	CD-NE	6.25	1.57	1.46
5	E	591	ARG	CZ-NH1	6.23	1.41	1.33
8	H	42	GLU	CG-CD	6.23	1.61	1.51
5	E	87	ARG	CZ-NH1	6.22	1.41	1.33
2	O	182	GLU	CG-CD	6.22	1.61	1.51
2	O	210	TYR	CD2-CE2	6.22	1.48	1.39
3	M	134	ARG	CD-NE	6.21	1.57	1.46
6	B	131	TYR	CG-CD2	6.21	1.47	1.39
6	D	321	ARG	CD-NE	6.20	1.56	1.46
2	O	98	ARG	CZ-NH2	6.20	1.41	1.33
9	K	212	GLU	CG-CD	6.20	1.61	1.51
5	C	177	ARG	CZ-NH2	6.19	1.41	1.33
9	I	78	SER	CA-CB	6.19	1.62	1.52
10	P	407	ARG	CZ-NH2	6.19	1.41	1.33
1	b	70	ARG	NE-CZ	6.19	1.41	1.33
7	Q	30	TYR	CD2-CE2	6.18	1.48	1.39
11	X	85	TYR	CE2-CZ	6.17	1.46	1.38
5	C	475	TYR	CE1-CZ	6.17	1.46	1.38
9	G	187	GLY	CA-C	-6.17	1.42	1.51
6	B	117	GLY	CA-C	-6.16	1.42	1.51
9	K	25	ARG	NE-CZ	6.13	1.41	1.33
11	Z	137	GLU	CD-OE1	6.12	1.32	1.25
2	O	262	TYR	CG-CD2	6.11	1.47	1.39
3	M	97	ARG	NE-CZ	6.10	1.41	1.33
6	D	268	TYR	CE2-CZ	6.10	1.46	1.38
9	K	114	ARG	CZ-NH2	6.09	1.41	1.33
5	C	135	ARG	CZ-NH1	6.09	1.41	1.33
6	D	74	ARG	CZ-NH1	6.09	1.41	1.33
9	I	78	SER	CB-OG	6.08	1.50	1.42
9	K	143	GLU	CG-CD	6.08	1.61	1.51
6	D	62	VAL	CB-CG2	6.07	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	127	GLY	CA-C	-6.06	1.42	1.51
6	F	309	TYR	CG-CD2	6.05	1.47	1.39
1	b	120	ARG	NE-CZ	6.05	1.41	1.33
6	F	32	SER	CA-CB	6.04	1.62	1.52
11	S	96	SER	CA-CB	6.04	1.62	1.52
6	B	393	ARG	CZ-NH2	6.04	1.40	1.33
1	b	70	ARG	CD-NE	6.02	1.56	1.46
10	P	21	ARG	CZ-NH2	6.01	1.40	1.33
11	W	117	ARG	CZ-NH2	6.01	1.40	1.33
5	A	110	ARG	CZ-NH2	6.00	1.40	1.33
7	Q	171	GLU	CG-CD	6.00	1.60	1.51
3	M	105	TYR	CE1-CZ	6.00	1.46	1.38
6	D	359	PHE	CG-CD1	6.00	1.47	1.38
6	D	295	ARG	CD-NE	5.99	1.56	1.46
5	A	534	TYR	CG-CD1	5.97	1.47	1.39
5	C	286	ARG	CD-NE	5.97	1.56	1.46
1	b	67	ARG	NE-CZ	5.96	1.40	1.33
5	E	123	TYR	CZ-OH	5.96	1.48	1.37
5	E	487	GLU	CB-CG	5.96	1.63	1.52
7	Q	341	TYR	CG-CD1	5.94	1.46	1.39
11	a	11	PHE	CB-CG	5.93	1.61	1.51
5	E	123	TYR	CE1-CZ	5.92	1.46	1.38
11	Z	88	PHE	CD1-CE1	5.91	1.51	1.39
4	N	5	ARG	CD-NE	5.91	1.56	1.46
5	A	409	SER	CA-CB	5.90	1.61	1.52
1	b	186	TYR	CG-CD2	5.90	1.46	1.39
7	Q	92	ARG	NE-CZ	5.89	1.40	1.33
5	A	28	TYR	CD1-CE1	5.88	1.48	1.39
5	A	135	ARG	CD-NE	5.88	1.56	1.46
1	b	186	TYR	CG-CD1	5.88	1.46	1.39
5	E	280	TYR	CB-CG	5.88	1.60	1.51
3	M	168	ARG	CZ-NH1	5.88	1.40	1.33
8	J	27	TYR	CG-CD1	5.88	1.46	1.39
11	Z	120	SER	CA-CB	5.88	1.61	1.52
11	T	142	TYR	N-CA	-5.88	1.34	1.46
1	b	261	TYR	CG-CD1	5.88	1.46	1.39
11	S	100	SER	C-N	5.88	1.43	1.33
9	G	158	ARG	CZ-NH1	5.85	1.40	1.33
3	M	30	SER	CA-CB	5.85	1.61	1.52
5	E	221	ARG	CZ-NH2	5.84	1.40	1.33
1	b	359	ARG	CG-CD	5.84	1.66	1.51
9	K	160	TYR	CG-CD2	5.84	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	G	25	ARG	CZ-NH1	5.84	1.40	1.33
5	A	493	GLU	CG-CD	5.83	1.60	1.51
11	W	153	ARG	NE-CZ	5.83	1.40	1.33
7	Q	181	ARG	NE-CZ	5.83	1.40	1.33
5	A	301	TYR	CB-CG	-5.83	1.43	1.51
5	A	119	SER	CB-OG	5.82	1.49	1.42
5	E	605	SER	CA-CB	5.81	1.61	1.52
6	F	466	ARG	CZ-NH2	5.80	1.40	1.33
5	C	179	ARG	CD-NE	5.80	1.56	1.46
4	N	40	TYR	CZ-OH	5.79	1.47	1.37
6	D	325	ARG	CD-NE	5.79	1.56	1.46
10	P	396	ARG	NE-CZ	5.79	1.40	1.33
5	C	126	ARG	CZ-NH2	5.78	1.40	1.33
3	M	91	ARG	CZ-NH2	5.78	1.40	1.33
6	B	304	TYR	CZ-OH	5.78	1.47	1.37
11	W	48	ASP	CA-CB	5.76	1.66	1.53
2	O	53	PHE	CB-CG	-5.76	1.41	1.51
5	E	28	TYR	CD1-CE1	5.76	1.48	1.39
6	F	297	GLU	CG-CD	5.76	1.60	1.51
5	A	523	GLU	CD-OE1	5.76	1.31	1.25
6	F	71	ARG	CZ-NH1	5.76	1.40	1.33
1	b	332	ARG	NE-CZ	5.75	1.40	1.33
11	X	17	CYS	CB-SG	5.74	1.92	1.82
5	C	33	PRO	N-CD	-5.74	1.39	1.47
11	W	46	ARG	CD-NE	5.74	1.56	1.46
2	O	312	TYR	CZ-OH	5.73	1.47	1.37
5	C	187	PRO	N-CD	-5.73	1.39	1.47
6	F	252	ARG	CZ-NH1	5.73	1.40	1.33
11	X	87	GLY	CA-C	-5.73	1.42	1.51
6	F	272	ARG	CD-NE	5.72	1.56	1.46
9	K	52	ARG	CZ-NH2	5.72	1.40	1.33
5	E	471	TYR	CB-CG	-5.71	1.43	1.51
5	A	158	TYR	CG-CD2	5.71	1.46	1.39
2	O	114	PHE	CG-CD2	5.71	1.47	1.38
9	I	160	TYR	CB-CG	-5.71	1.43	1.51
11	U	117	ARG	CZ-NH1	5.70	1.40	1.33
6	B	393	ARG	NE-CZ	5.70	1.40	1.33
6	B	252	ARG	CD-NE	5.70	1.56	1.46
1	b	359	ARG	CD-NE	5.69	1.56	1.46
10	P	219	GLN	CA-CB	5.69	1.66	1.53
1	b	20	TYR	CG-CD2	5.68	1.46	1.39
7	Q	343	SER	CB-OG	5.67	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	58	GLY	CA-C	-5.66	1.42	1.51
1	b	315	ARG	CZ-NH1	5.66	1.40	1.33
6	D	111	ARG	NE-CZ	5.66	1.40	1.33
6	D	190	GLN	CG-CD	5.66	1.64	1.51
4	N	34	GLU	CD-OE2	-5.65	1.19	1.25
5	E	107	GLY	CA-C	-5.65	1.42	1.51
9	I	25	ARG	CD-NE	5.65	1.56	1.46
6	F	237	ARG	NE-CZ	5.64	1.40	1.33
3	M	140	SER	CA-C	-5.64	1.38	1.52
5	A	334	TYR	CG-CD2	5.64	1.46	1.39
5	E	27	ILE	CA-CB	-5.63	1.41	1.54
6	B	189	ARG	CD-NE	5.62	1.56	1.46
6	B	466	ARG	CZ-NH2	5.62	1.40	1.33
6	B	362	ARG	CZ-NH2	5.62	1.40	1.33
5	C	359	ARG	CZ-NH2	5.62	1.40	1.33
11	a	117	ARG	NE-CZ	5.62	1.40	1.33
8	L	46	TYR	CE1-CZ	5.61	1.45	1.38
10	P	144	PHE	CB-CG	-5.61	1.41	1.51
11	Z	152	SER	CA-CB	5.61	1.61	1.52
6	B	388	GLY	CA-C	-5.60	1.42	1.51
11	R	91	LEU	C-N	5.60	1.43	1.33
11	X	36	GLY	CA-C	-5.59	1.43	1.51
6	F	268	TYR	CE1-CZ	5.58	1.45	1.38
2	O	319	TYR	CE1-CZ	5.57	1.45	1.38
5	E	261	GLY	CA-C	-5.57	1.43	1.51
6	D	189	ARG	CZ-NH1	5.57	1.40	1.33
5	C	62	ARG	CZ-NH2	5.57	1.40	1.33
10	P	336	ARG	CZ-NH2	5.57	1.40	1.33
5	E	165	SER	CA-CB	5.56	1.61	1.52
11	W	130	ILE	C-N	5.55	1.46	1.34
7	Q	219	ARG	CZ-NH2	5.55	1.40	1.33
5	A	484	ARG	CD-NE	5.55	1.55	1.46
8	J	42	GLU	CG-CD	5.55	1.60	1.51
1	b	320	PHE	CG-CD1	5.54	1.47	1.38
9	G	43	TYR	CA-CB	5.54	1.66	1.53
6	F	324	GLY	CA-C	-5.54	1.43	1.51
8	H	14	GLU	CD-OE2	5.53	1.31	1.25
2	O	6	TYR	CZ-OH	5.53	1.47	1.37
5	A	33	PRO	N-CD	-5.53	1.40	1.47
5	C	507	LEU	C-N	5.53	1.46	1.34
7	Q	118	ARG	CZ-NH2	5.52	1.40	1.33
4	N	80	ARG	CD-NE	5.52	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	J	5	ASN	N-CA	-5.52	1.35	1.46
6	B	443	PHE	CG-CD1	5.51	1.47	1.38
11	Y	11	PHE	CG-CD1	5.51	1.47	1.38
5	A	296	GLU	CD-OE1	5.51	1.31	1.25
6	B	95	PHE	CB-CG	-5.51	1.42	1.51
5	C	238	ARG	CD-NE	5.51	1.55	1.46
7	Q	94	PHE	CE1-CZ	5.51	1.47	1.37
11	T	137	GLU	CD-OE1	5.51	1.31	1.25
5	A	38	GLU	CG-CD	5.51	1.60	1.51
6	B	171	PRO	N-CD	-5.50	1.40	1.47
11	a	96	SER	CA-CB	5.49	1.61	1.52
5	E	189	GLY	N-CA	-5.49	1.37	1.46
5	E	221	ARG	CD-NE	5.48	1.55	1.46
5	E	314	ARG	CZ-NH2	5.47	1.40	1.33
9	I	90	SER	CA-CB	5.47	1.61	1.52
9	G	223	TYR	CZ-OH	5.47	1.47	1.37
6	F	267	ALA	N-CA	-5.47	1.35	1.46
10	P	54	LYS	CA-CB	5.47	1.66	1.53
9	K	93	GLU	CD-OE1	5.46	1.31	1.25
11	V	56	PRO	N-CA	-5.46	1.38	1.47
5	C	609	GLU	CD-OE2	5.46	1.31	1.25
6	B	212	PHE	CB-CG	-5.46	1.42	1.51
5	C	365	ARG	CD-NE	5.46	1.55	1.46
10	P	331	SER	CA-CB	5.45	1.61	1.52
11	T	152	SER	CA-CB	5.45	1.61	1.52
5	E	407	THR	C-N	5.45	1.42	1.33
6	D	318	ARG	CZ-NH1	5.45	1.40	1.33
5	A	286	ARG	CZ-NH1	5.45	1.40	1.33
6	D	452	ARG	NE-CZ	5.45	1.40	1.33
11	Z	76	TYR	CB-CG	-5.44	1.43	1.51
6	D	307	TYR	CZ-OH	5.44	1.47	1.37
9	G	212	GLU	CD-OE2	5.44	1.31	1.25
5	A	591	ARG	CZ-NH1	5.43	1.40	1.33
10	P	188	ARG	NE-CZ	5.43	1.40	1.33
6	B	435	PHE	CG-CD1	5.42	1.46	1.38
6	B	224	PHE	CB-CG	5.42	1.60	1.51
5	E	74	GLU	CD-OE2	5.41	1.31	1.25
5	C	275	SER	CA-CB	5.41	1.61	1.52
5	C	314	ARG	CZ-NH1	5.41	1.40	1.33
7	Q	80	PHE	CG-CD1	5.41	1.46	1.38
6	B	189	ARG	NE-CZ	5.41	1.40	1.33
11	Z	142	TYR	C-N	5.40	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	A	555	ASP	CA-CB	5.40	1.65	1.53
7	Q	294	GLU	CG-CD	5.40	1.60	1.51
5	E	534	TYR	N-CA	-5.39	1.35	1.46
9	G	162	GLU	CG-CD	5.39	1.60	1.51
7	Q	297	ARG	CD-NE	5.39	1.55	1.46
6	F	407	TYR	CE2-CZ	5.38	1.45	1.38
6	D	422	GLU	CG-CD	5.37	1.60	1.51
5	E	182	ILE	N-CA	-5.37	1.35	1.46
2	O	93	SER	CA-CB	5.36	1.60	1.52
6	F	475	ARG	CZ-NH2	5.36	1.40	1.33
5	E	392	TYR	CD2-CE2	5.36	1.47	1.39
8	H	14	GLU	CD-OE1	5.36	1.31	1.25
6	B	452	ARG	CD-NE	5.36	1.55	1.46
11	S	30	TYR	CG-CD2	5.35	1.46	1.39
5	A	370	ARG	CZ-NH2	5.35	1.40	1.33
5	E	158	TYR	CG-CD2	5.34	1.46	1.39
2	O	39	ILE	C-N	5.34	1.42	1.33
6	D	48	ARG	NE-CZ	5.34	1.40	1.33
10	P	125	GLU	CG-CD	5.34	1.59	1.51
11	Y	117	ARG	CD-NE	5.34	1.55	1.46
11	V	117	ARG	CZ-NH2	5.34	1.40	1.33
6	B	318	ARG	CZ-NH2	5.34	1.40	1.33
5	C	87	ARG	NE-CZ	5.33	1.40	1.33
5	A	231	TYR	C-O	-5.33	1.13	1.23
7	Q	249	TYR	CE2-CZ	5.33	1.45	1.38
1	b	132	GLU	CB-CG	5.33	1.62	1.52
5	C	95	GLU	CB-CG	5.33	1.62	1.52
5	C	613	GLU	CD-OE2	5.32	1.31	1.25
11	U	40	CYS	CB-SG	-5.32	1.73	1.81
3	M	17	LEU	N-CA	-5.32	1.35	1.46
7	Q	84	ARG	NE-CZ	5.32	1.40	1.33
5	A	212	TYR	CB-CG	5.31	1.59	1.51
5	A	475	TYR	CG-CD1	5.31	1.46	1.39
1	b	310	PHE	CG-CD1	5.31	1.46	1.38
6	B	63	ARG	NE-CZ	5.31	1.40	1.33
10	P	215	PHE	CE2-CZ	5.31	1.47	1.37
10	P	392	TYR	CZ-OH	5.31	1.46	1.37
5	C	460	TYR	CZ-OH	5.30	1.46	1.37
11	a	116	VAL	CB-CG2	5.30	1.64	1.52
3	M	97	ARG	CD-NE	5.30	1.55	1.46
6	B	42	GLU	CD-OE2	5.29	1.31	1.25
5	A	87	ARG	CZ-NH2	5.29	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	F	188	CYS	N-CA	-5.29	1.35	1.46
5	C	599	GLU	CD-OE2	-5.29	1.19	1.25
6	F	95	PHE	CG-CD2	5.28	1.46	1.38
7	Q	21	ARG	CZ-NH1	5.28	1.40	1.33
8	H	16	GLU	CB-CG	5.28	1.62	1.52
1	b	193	ARG	CZ-NH1	5.27	1.40	1.33
5	A	448	ARG	CD-NE	5.27	1.55	1.46
1	b	141	TYR	CE2-CZ	5.27	1.45	1.38
11	a	106	PHE	CG-CD1	5.27	1.46	1.38
5	E	301	TYR	CE2-CZ	5.26	1.45	1.38
5	E	537	PHE	CB-CG	-5.26	1.42	1.51
8	H	67	GLU	CB-CG	5.26	1.62	1.52
5	A	403	SER	CA-CB	5.26	1.60	1.52
8	H	27	TYR	CD1-CE1	5.26	1.47	1.39
5	E	62	ARG	CZ-NH2	5.25	1.39	1.33
11	X	35	SER	C-N	5.25	1.42	1.33
6	D	225	PHE	CG-CD2	5.25	1.46	1.38
11	W	117	ARG	NE-CZ	5.25	1.39	1.33
7	Q	190	GLU	CG-CD	5.24	1.59	1.51
11	W	153	ARG	CD-NE	5.24	1.55	1.46
8	L	19	GLU	CD-OE1	5.24	1.31	1.25
3	M	15	LEU	C-N	5.23	1.42	1.33
7	Q	126	ARG	NE-CZ	5.23	1.39	1.33
5	E	301	TYR	CE1-CZ	5.23	1.45	1.38
11	T	76	TYR	CD2-CE2	5.23	1.47	1.39
6	F	223	ARG	CZ-NH2	5.22	1.39	1.33
2	O	110	TYR	CE1-CZ	5.22	1.45	1.38
5	A	158	TYR	CE2-CZ	5.22	1.45	1.38
4	N	80	ARG	CZ-NH2	5.22	1.39	1.33
5	C	591	ARG	CD-NE	5.22	1.55	1.46
7	Q	97	TYR	CE1-CZ	5.21	1.45	1.38
3	M	58	GLY	CA-C	-5.21	1.43	1.51
3	M	44	ARG	CZ-NH1	5.21	1.39	1.33
5	E	159	GLY	CA-C	-5.21	1.43	1.51
5	E	590	SER	CA-CB	5.21	1.60	1.52
5	A	593	GLU	CB-CG	5.21	1.62	1.52
11	X	46	ARG	N-CA	-5.20	1.35	1.46
6	D	355	GLU	CG-CD	5.20	1.59	1.51
5	E	184	TRP	CZ2-CH2	5.20	1.47	1.37
6	B	301	ARG	CD-NE	5.19	1.55	1.46
11	U	124	ARG	CZ-NH2	5.19	1.39	1.33
11	V	85	TYR	CE1-CZ	5.19	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	C	74	GLU	CG-CD	5.19	1.59	1.51
7	Q	67	LEU	N-CA	-5.18	1.35	1.46
7	Q	218	ARG	CZ-NH2	5.18	1.39	1.33
8	J	46	TYR	CA-CB	5.18	1.65	1.53
10	P	210	PHE	CG-CD1	5.18	1.46	1.38
6	B	109	LEU	C-N	5.18	1.42	1.33
10	P	144	PHE	CG-CD2	5.17	1.46	1.38
10	P	276	LYS	N-CA	-5.15	1.36	1.46
3	M	123	THR	C-N	5.14	1.42	1.33
5	C	448	ARG	CZ-NH1	5.14	1.39	1.33
8	J	28	ARG	CZ-NH1	5.14	1.39	1.33
2	O	388	TYR	CG-CD1	5.14	1.45	1.39
5	E	548	ARG	CD-NE	5.13	1.55	1.46
11	a	73	LEU	CA-CB	5.13	1.65	1.53
5	A	463	TYR	CE2-CZ	5.13	1.45	1.38
11	X	27	GLY	CA-C	5.13	1.60	1.51
11	U	51	PHE	CG-CD2	5.13	1.46	1.38
6	D	389	GLU	C-N	5.12	1.42	1.33
5	E	292	GLU	CB-CG	5.12	1.61	1.52
5	E	610	ARG	CZ-NH1	5.12	1.39	1.33
5	E	600	PHE	CG-CD1	5.12	1.46	1.38
9	G	150	GLU	CB-CG	5.12	1.61	1.52
5	E	305	SER	CA-CB	5.12	1.60	1.52
6	B	313	SER	CB-OG	5.12	1.49	1.42
5	C	334	TYR	CZ-OH	5.12	1.46	1.37
10	P	23	ARG	CZ-NH1	5.12	1.39	1.33
5	C	168	SER	CA-CB	5.12	1.60	1.52
2	O	184	PHE	CE2-CZ	5.11	1.47	1.37
11	U	26	LEU	CA-CB	5.11	1.65	1.53
5	E	62	ARG	CD-NE	5.11	1.55	1.46
5	C	215	TRP	CZ2-CH2	5.11	1.47	1.37
2	O	309	LEU	N-CA	-5.11	1.36	1.46
6	B	178	LEU	N-CA	-5.10	1.36	1.46
5	C	184	TRP	CB-CG	5.10	1.59	1.50
5	E	31	SER	C-N	5.09	1.42	1.33
5	E	221	ARG	NE-CZ	5.09	1.39	1.33
11	R	139	LEU	C-N	5.09	1.42	1.33
5	C	329	ARG	C-N	5.09	1.45	1.34
7	Q	217	ASP	N-CA	-5.09	1.36	1.46
6	B	265	TYR	CZ-OH	5.09	1.46	1.37
1	b	352	ARG	CZ-NH2	5.08	1.39	1.33
2	O	97	TYR	CG-CD1	5.08	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	O	98	ARG	NE-CZ	5.08	1.39	1.33
5	E	366	GLU	CD-OE1	5.08	1.31	1.25
5	E	460	TYR	CG-CD2	5.08	1.45	1.39
5	C	484	ARG	CZ-NH2	5.08	1.39	1.33
9	G	97	ASP	CB-CG	5.08	1.62	1.51
5	E	484	ARG	NE-CZ	5.07	1.39	1.33
1	b	296	GLU	CB-CG	5.07	1.61	1.52
5	A	576	ASP	CB-CG	5.07	1.62	1.51
6	F	462	TRP	CA-C	-5.07	1.39	1.52
5	C	356	SER	CA-CB	5.07	1.60	1.52
9	I	205	GLU	CG-CD	5.07	1.59	1.51
11	S	155	THR	CB-OG1	5.06	1.53	1.43
2	O	251	ARG	CD-NE	5.05	1.55	1.46
5	C	360	TRP	CD2-CE2	-5.05	1.35	1.41
7	Q	157	PRO	N-CD	-5.05	1.40	1.47
10	P	220	ARG	CD-NE	5.05	1.55	1.46
6	B	229	PHE	CG-CD1	5.05	1.46	1.38
10	P	475	TYR	CE2-CZ	5.05	1.45	1.38
6	D	381	ARG	CZ-NH1	5.04	1.39	1.33
5	E	392	TYR	CE2-CZ	5.04	1.45	1.38
2	O	177	ASP	C-N	5.04	1.45	1.34
6	F	82	GLY	N-CA	-5.04	1.38	1.46
6	F	231	GLU	CB-CG	5.03	1.61	1.52
6	B	301	ARG	NE-CZ	5.03	1.39	1.33
5	E	281	VAL	CB-CG1	5.03	1.63	1.52
11	V	117	ARG	CD-NE	5.02	1.54	1.46
1	b	193	ARG	CD-NE	5.02	1.54	1.46
6	B	111	ARG	CZ-NH1	5.02	1.39	1.33
2	O	173	ARG	CZ-NH2	5.02	1.39	1.33
3	M	91	ARG	CD-NE	5.02	1.54	1.46
5	E	613	GLU	CG-CD	5.02	1.59	1.51
6	F	452	ARG	CZ-NH1	5.02	1.39	1.33
5	E	415	ALA	N-CA	-5.01	1.36	1.46
5	A	487	GLU	CA-CB	5.01	1.65	1.53
2	O	343	GLU	CB-CG	5.01	1.61	1.52
6	B	381	ARG	CZ-NH2	5.01	1.39	1.33
5	A	191	TYR	CG-CD2	5.00	1.45	1.39
3	M	42	ARG	CD-NE	5.00	1.54	1.46
5	A	365	ARG	CZ-NH1	5.00	1.39	1.33
6	B	301	ARG	CZ-NH1	5.00	1.39	1.33
9	G	144	ARG	CZ-NH2	5.00	1.39	1.33
11	Z	25	SER	CB-OG	-5.00	1.35	1.42

All (1320) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	62	ARG	NE-CZ-NH1	19.24	129.92	120.30
11	U	12	PHE	CB-CG-CD1	18.18	133.52	120.80
1	b	285	TYR	CB-CG-CD1	16.96	131.18	121.00
6	D	325	ARG	NE-CZ-NH2	-16.76	111.92	120.30
1	b	285	TYR	CB-CG-CD2	-16.54	111.07	121.00
11	T	135	PHE	CB-CG-CD1	16.45	132.32	120.80
1	b	248	ARG	NE-CZ-NH1	15.72	128.16	120.30
6	B	352	TYR	CB-CG-CD2	-15.56	111.66	121.00
11	a	157	ASP	CB-CG-OD2	-15.29	104.53	118.30
11	T	135	PHE	CB-CG-CD2	-15.01	110.29	120.80
1	b	112	ARG	NE-CZ-NH1	15.00	127.80	120.30
5	E	221	ARG	NE-CZ-NH2	-14.96	112.82	120.30
5	E	394	ARG	NE-CZ-NH2	14.63	127.61	120.30
8	L	27	TYR	CB-CG-CD1	-14.57	112.26	121.00
9	G	160	TYR	CB-CG-CD2	-14.49	112.31	121.00
11	U	117	ARG	NE-CZ-NH2	-14.24	113.18	120.30
11	R	46	ARG	NE-CZ-NH1	14.21	127.40	120.30
6	B	49	TYR	CB-CG-CD2	-14.07	112.56	121.00
9	K	219	ARG	NE-CZ-NH2	13.96	127.28	120.30
5	E	448	ARG	NE-CZ-NH1	-13.93	113.34	120.30
6	B	289	ARG	NE-CZ-NH2	-13.76	113.42	120.30
11	a	142	TYR	CB-CG-CD1	-13.70	112.78	121.00
5	A	343	PHE	CB-CG-CD2	-13.63	111.26	120.80
7	Q	77	TYR	CB-CG-CD2	-13.32	113.01	121.00
11	U	12	PHE	CB-CG-CD2	-13.21	111.55	120.80
11	R	124	ARG	NE-CZ-NH2	-13.19	113.70	120.30
2	O	119	ARG	NE-CZ-NH2	-13.18	113.71	120.30
11	W	142	TYR	CB-CG-CD2	-13.14	113.11	121.00
6	B	265	TYR	CB-CG-CD2	-13.09	113.15	121.00
5	A	383	TYR	CB-CG-CD1	-13.08	113.15	121.00
11	R	76	TYR	CB-CG-CD1	13.00	128.80	121.00
5	C	62	ARG	NE-CZ-NH2	-12.98	113.81	120.30
10	P	184	TYR	CB-CG-CD2	-12.95	113.23	121.00
4	N	80	ARG	NE-CZ-NH1	12.92	126.76	120.30
7	Q	77	TYR	CB-CG-CD1	12.85	128.71	121.00
11	X	46	ARG	NE-CZ-NH2	12.76	126.68	120.30
11	U	30	TYR	CB-CG-CD2	-12.74	113.35	121.00
5	A	484	ARG	NE-CZ-NH2	-12.65	113.98	120.30
2	O	258	ARG	NE-CZ-NH2	-12.58	114.01	120.30
6	B	142	TYR	CB-CG-CD2	-12.46	113.52	121.00
6	B	118	ARG	NE-CZ-NH1	12.24	126.42	120.30
11	a	157	ASP	CB-CG-OD1	12.18	129.26	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	49	TYR	CB-CG-CD1	12.11	128.27	121.00
2	O	119	ARG	NE-CZ-NH1	12.05	126.33	120.30
11	R	46	ARG	NE-CZ-NH2	-12.04	114.28	120.30
9	K	166	ARG	NE-CZ-NH2	12.04	126.32	120.30
11	U	11	PHE	CB-CG-CD2	-12.03	112.38	120.80
5	E	334	TYR	CB-CG-CD2	-11.99	113.81	121.00
5	A	343	PHE	CB-CG-CD1	11.95	129.16	120.80
5	E	406	ARG	NE-CZ-NH2	-11.93	114.33	120.30
6	F	257	ARG	NE-CZ-NH2	-11.87	114.37	120.30
5	A	126	ARG	NE-CZ-NH2	-11.77	114.41	120.30
1	b	110	TYR	CB-CG-CD1	11.76	128.06	121.00
5	E	394	ARG	NE-CZ-NH1	-11.72	114.44	120.30
4	N	78	ARG	NE-CZ-NH1	11.66	126.13	120.30
5	C	301	TYR	CB-CG-CD2	-11.65	114.01	121.00
6	D	71	ARG	NE-CZ-NH2	-11.63	114.48	120.30
2	O	275	ASP	CB-CG-OD2	-11.58	107.88	118.30
11	R	85	TYR	CB-CG-CD1	11.57	127.94	121.00
1	b	112	ARG	NE-CZ-NH2	-11.55	114.52	120.30
11	X	76	TYR	CB-CG-CD2	-11.53	114.08	121.00
9	G	144	ARG	NE-CZ-NH2	-11.49	114.55	120.30
6	D	223	ARG	NE-CZ-NH1	11.48	126.04	120.30
5	C	534	TYR	CB-CG-CD2	-11.43	114.14	121.00
5	E	406	ARG	NE-CZ-NH1	11.39	126.00	120.30
1	b	69	TYR	CB-CG-CD1	11.37	127.82	121.00
2	O	374	TYR	CB-CG-CD2	11.32	127.79	121.00
11	V	117	ARG	NE-CZ-NH1	11.23	125.92	120.30
11	Y	85	TYR	CB-CG-CD2	-11.20	114.28	121.00
11	R	11	PHE	CB-CG-CD1	11.18	128.63	120.80
11	X	126	PHE	CB-CG-CD2	-11.17	112.98	120.80
5	E	359	ARG	NE-CZ-NH1	11.15	125.87	120.30
6	B	63	ARG	NE-CZ-NH2	11.13	125.87	120.30
6	B	46	PHE	CB-CG-CD1	11.09	128.56	120.80
11	W	11	PHE	CB-CG-CD1	11.06	128.54	120.80
9	K	117	TYR	CB-CG-CD1	-10.99	114.41	121.00
9	I	52	ARG	NE-CZ-NH1	10.90	125.75	120.30
5	E	531	TYR	CB-CG-CD2	-10.88	114.47	121.00
6	D	95	PHE	CB-CG-CD2	-10.87	113.19	120.80
11	T	76	TYR	CB-CG-CD1	10.86	127.51	121.00
11	X	76	TYR	CB-CG-CD1	10.85	127.51	121.00
11	R	76	TYR	CB-CG-CD2	-10.83	114.50	121.00
6	D	398	ASP	CB-CG-OD1	10.80	128.02	118.30
11	Z	85	TYR	CB-CG-CD2	-10.74	114.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	258	ARG	NE-CZ-NH1	10.71	125.65	120.30
3	M	187	TYR	CB-CG-CD2	-10.68	114.59	121.00
11	Y	76	TYR	CB-CG-CD2	-10.64	114.62	121.00
11	Z	142	TYR	CB-CG-CD2	-10.63	114.62	121.00
6	D	301	ARG	NE-CZ-NH1	-10.59	115.00	120.30
5	A	297	PHE	CB-CG-CD1	10.58	128.21	120.80
11	a	76	TYR	CB-CG-CD2	-10.54	114.67	121.00
11	W	85	TYR	CB-CG-CD2	-10.51	114.69	121.00
11	T	12	PHE	CB-CG-CD1	10.48	128.14	120.80
2	O	385	PHE	CB-CG-CD2	-10.46	113.48	120.80
2	O	206	PHE	CB-CG-CD2	10.41	128.09	120.80
10	P	199	TYR	CB-CG-CD1	10.41	127.24	121.00
11	R	11	PHE	CB-CG-CD2	-10.38	113.53	120.80
5	C	534	TYR	CB-CG-CD1	10.36	127.22	121.00
6	D	237	ARG	NE-CZ-NH2	-10.36	115.12	120.30
5	A	238	ARG	NE-CZ-NH2	-10.33	115.14	120.30
6	D	74	ARG	NE-CZ-NH1	10.31	125.45	120.30
5	A	531	TYR	CB-CG-CD2	-10.17	114.90	121.00
11	U	46	ARG	NE-CZ-NH2	-10.16	115.22	120.30
5	C	392	TYR	CB-CG-CD2	-10.14	114.91	121.00
3	M	141	ARG	NE-CZ-NH2	-10.12	115.24	120.30
5	E	334	TYR	CB-CG-CD1	10.06	127.04	121.00
6	D	223	ARG	NE-CZ-NH2	-10.04	115.28	120.30
9	I	85	ARG	NE-CZ-NH1	10.02	125.31	120.30
6	F	63	ARG	NE-CZ-NH2	-10.01	115.30	120.30
6	B	449	TYR	CB-CG-CD1	10.01	127.01	121.00
5	A	482	ARG	NE-CZ-NH1	10.00	125.30	120.30
5	A	258	PHE	CB-CG-CD1	-9.99	113.81	120.80
10	P	136	PHE	CB-CG-CD2	-9.99	113.81	120.80
6	B	468	TYR	CB-CG-CD1	-9.98	115.01	121.00
11	a	124	ARG	NE-CZ-NH2	-9.97	115.32	120.30
5	C	146	PHE	CB-CG-CD1	-9.91	113.86	120.80
6	F	284	TYR	CB-CG-CD1	-9.90	115.06	121.00
5	C	231	TYR	CB-CG-CD2	9.89	126.93	121.00
11	V	51	PHE	CB-CG-CD2	-9.85	113.91	120.80
6	D	404	TYR	CB-CG-CD1	-9.84	115.10	121.00
1	b	205	ARG	NE-CZ-NH1	9.82	125.21	120.30
7	Q	249	TYR	CB-CG-CD1	-9.82	115.11	121.00
5	E	342	TYR	CB-CG-CD2	-9.80	115.12	121.00
5	C	611	PHE	CB-CG-CD2	-9.78	113.96	120.80
1	b	69	TYR	CB-CG-CD2	-9.76	115.14	121.00
1	b	205	ARG	NE-CZ-NH2	-9.73	115.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	193	TYR	CB-CG-CD2	-9.72	115.17	121.00
11	W	23	PHE	CB-CG-CD2	9.71	127.60	120.80
6	B	189	ARG	NE-CZ-NH2	-9.71	115.45	120.30
6	B	381	ARG	NE-CZ-NH2	9.65	125.13	120.30
5	C	258	PHE	CB-CG-CD1	-9.59	114.08	120.80
10	P	244	TYR	CB-CG-CD2	9.54	126.72	121.00
1	b	31	TYR	CB-CG-CD2	9.50	126.70	121.00
7	Q	297	ARG	NE-CZ-NH1	9.50	125.05	120.30
11	V	30	TYR	CB-CG-CD2	-9.47	115.32	121.00
6	F	301	ARG	NE-CZ-NH2	-9.44	115.58	120.30
5	C	272	TYR	CB-CG-CD1	-9.43	115.34	121.00
11	a	46	ARG	NE-CZ-NH1	-9.43	115.58	120.30
11	W	11	PHE	CB-CG-CD2	-9.41	114.21	120.80
2	O	374	TYR	CB-CG-CD1	-9.40	115.36	121.00
11	Y	124	ARG	NE-CZ-NH2	9.39	125.00	120.30
5	E	359	ARG	NE-CZ-NH2	-9.39	115.61	120.30
6	D	127	PHE	CB-CG-CD1	9.37	127.36	120.80
5	C	470	PHE	CB-CG-CD2	-9.37	114.24	120.80
11	U	46	ARG	NE-CZ-NH1	9.34	124.97	120.30
5	E	135	ARG	NE-CZ-NH2	9.34	124.97	120.30
9	I	206	ARG	NE-CZ-NH1	-9.33	115.63	120.30
2	O	285	ARG	NE-CZ-NH2	-9.32	115.64	120.30
11	W	12	PHE	CB-CG-CD2	-9.28	114.30	120.80
6	B	80	PHE	CB-CG-CD1	9.24	127.27	120.80
6	B	352	TYR	CB-CG-CD1	9.23	126.53	121.00
5	C	332	SER	N-CA-CB	9.20	124.29	110.50
11	U	11	PHE	CB-CG-CD1	9.19	127.23	120.80
5	E	297	PHE	CB-CG-CD1	9.16	127.22	120.80
6	F	485	TYR	CB-CG-CD1	9.14	126.48	121.00
2	O	42	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	b	20	TYR	CB-CG-CD2	-9.07	115.56	121.00
6	B	257	ARG	NE-CZ-NH2	-9.07	115.77	120.30
11	W	117	ARG	NE-CZ-NH2	-9.05	115.77	120.30
5	A	544	PHE	CB-CG-CD1	9.05	127.13	120.80
6	B	449	TYR	CB-CG-CD2	-9.04	115.58	121.00
11	T	85	TYR	CB-CG-CD1	9.04	126.42	121.00
9	G	43	TYR	CB-CG-CD2	9.03	126.42	121.00
3	M	73	TYR	CB-CG-CD1	9.02	126.41	121.00
6	F	48	ARG	NE-CZ-NH1	9.01	124.80	120.30
3	M	42	ARG	NE-CZ-NH2	-8.94	115.83	120.30
5	E	110	ARG	NE-CZ-NH2	-8.94	115.83	120.30
11	V	11	PHE	CB-CG-CD1	8.93	127.05	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	X	124	ARG	NE-CZ-NH1	8.93	124.76	120.30
5	A	423	PHE	CB-CG-CD2	-8.90	114.57	120.80
11	S	142	TYR	CB-CG-CD1	-8.90	115.66	121.00
5	E	383	TYR	CB-CG-CD2	-8.89	115.67	121.00
1	b	72	PHE	CB-CG-CD1	8.88	127.02	120.80
11	a	76	TYR	CB-CG-CD1	8.88	126.33	121.00
1	b	41	PHE	CB-CG-CD2	-8.88	114.58	120.80
5	A	244	PHE	CB-CG-CD2	-8.88	114.58	120.80
2	O	296	TYR	CB-CG-CD1	8.87	126.32	121.00
5	E	392	TYR	CB-CG-CD2	-8.86	115.68	121.00
6	D	95	PHE	CB-CG-CD1	8.86	127.00	120.80
6	F	289	ARG	NE-CZ-NH1	-8.84	115.88	120.30
5	E	286	ARG	NE-CZ-NH2	-8.77	115.92	120.30
5	E	380	PHE	CB-CG-CD1	8.74	126.92	120.80
5	C	123	TYR	CB-CG-CD1	8.73	126.24	121.00
5	C	258	PHE	CB-CG-CD2	8.73	126.91	120.80
5	A	544	PHE	CB-CG-CD2	-8.71	114.70	120.80
5	A	105	TYR	CG-CD2-CE2	-8.71	114.33	121.30
10	P	28	ASP	CB-CG-OD2	-8.70	110.47	118.30
9	I	37	LEU	CB-CG-CD1	8.69	125.77	111.00
5	A	355	ASP	CB-CG-OD2	8.65	126.09	118.30
5	A	244	PHE	CB-CG-CD1	8.64	126.85	120.80
6	D	146	TYR	CB-CG-CD2	-8.63	115.82	121.00
7	Q	133	PHE	CB-CG-CD1	8.61	126.83	120.80
6	D	484	PHE	CB-CG-CD2	-8.60	114.78	120.80
11	W	23	PHE	CB-CG-CD1	-8.59	114.78	120.80
5	E	460	TYR	CB-CG-CD1	8.58	126.15	121.00
6	F	113	PHE	CB-CG-CD2	8.58	126.81	120.80
11	X	51	PHE	CB-CG-CD2	-8.58	114.79	120.80
6	B	101	ARG	NE-CZ-NH2	-8.56	116.02	120.30
5	C	48	LEU	CB-CG-CD2	-8.56	96.45	111.00
2	O	382	TYR	CG-CD2-CE2	-8.53	114.47	121.30
6	F	485	TYR	CB-CG-CD2	-8.53	115.89	121.00
6	D	295	ARG	NE-CZ-NH1	8.53	124.56	120.30
10	P	184	TYR	CB-CG-CD1	8.51	126.11	121.00
11	Z	142	TYR	CB-CG-CD1	8.51	126.11	121.00
5	E	280	TYR	CB-CG-CD2	8.50	126.10	121.00
6	F	224	PHE	CB-CG-CD1	8.49	126.75	120.80
9	G	206	ARG	NE-CZ-NH2	8.49	124.55	120.30
8	H	46	TYR	CB-CG-CD2	-8.48	115.91	121.00
5	A	470	PHE	CB-CG-CD1	-8.48	114.87	120.80
6	B	391	MET	CG-SD-CE	-8.48	86.64	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	129	ASP	CB-CG-OD1	8.46	125.92	118.30
5	C	295	MET	CG-SD-CE	-8.45	86.68	100.20
11	X	117	ARG	NE-CZ-NH1	-8.45	116.08	120.30
5	C	422	ASP	CB-CG-OD1	8.44	125.90	118.30
2	O	382	TYR	CZ-CE2-CD2	8.44	127.39	119.80
5	C	565	ALA	N-CA-CB	8.43	121.90	110.10
6	B	265	TYR	CB-CG-CD1	8.41	126.05	121.00
10	P	391	ASN	CB-CA-C	8.40	127.19	110.40
6	D	286	ASP	CB-CG-OD2	8.39	125.86	118.30
6	D	468	TYR	CB-CG-CD1	8.38	126.03	121.00
11	Z	30	TYR	CB-CG-CD2	-8.37	115.98	121.00
9	K	158	ARG	NE-CZ-NH1	8.36	124.48	120.30
9	K	43	TYR	CB-CG-CD2	-8.36	115.99	121.00
11	Y	135	PHE	CB-CG-CD1	-8.34	114.96	120.80
11	R	85	TYR	CB-CG-CD2	-8.32	116.01	121.00
5	A	451	PHE	CB-CG-CD2	-8.31	114.98	120.80
2	O	318	ARG	NE-CZ-NH1	8.29	124.45	120.30
6	B	404	TYR	CB-CG-CD1	8.29	125.98	121.00
5	E	597	HIS	CA-CB-CG	8.29	127.69	113.60
11	W	51	PHE	CB-CG-CD2	-8.29	115.00	120.80
5	A	134	ASP	CB-CG-OD1	8.24	125.72	118.30
7	Q	50	ASP	CB-CG-OD1	8.23	125.71	118.30
11	a	104	ALA	N-CA-CB	8.23	121.62	110.10
11	T	88	PHE	CB-CG-CD2	-8.22	115.05	120.80
3	M	202	ARG	NE-CZ-NH2	-8.18	116.21	120.30
5	C	611	PHE	CB-CG-CD1	8.17	126.52	120.80
5	A	272	TYR	CB-CG-CD1	8.17	125.90	121.00
10	P	259	PHE	CB-CG-CD2	-8.16	115.09	120.80
7	Q	236	ASP	CB-CG-OD1	8.14	125.63	118.30
5	C	141	PHE	CB-CG-CD2	-8.13	115.11	120.80
5	A	534	TYR	CB-CG-CD1	8.13	125.88	121.00
6	F	393	ARG	NE-CZ-NH2	8.13	124.36	120.30
2	O	300	PHE	CB-CG-CD2	8.11	126.48	120.80
7	Q	161	TYR	CB-CG-CD1	8.11	125.87	121.00
5	E	106	ASP	CB-CG-OD1	8.10	125.59	118.30
5	C	484	ARG	NE-CZ-NH2	-8.10	116.25	120.30
11	W	97	VAL	CG1-CB-CG2	8.09	123.85	110.90
3	M	95	ARG	NE-CZ-NH2	8.08	124.34	120.30
5	A	484	ARG	NE-CZ-NH1	8.08	124.34	120.30
5	E	591	ARG	NE-CZ-NH1	8.07	124.33	120.30
6	F	359	PHE	CB-CG-CD2	-8.06	115.15	120.80
2	O	167	THR	N-CA-CB	8.06	125.61	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	285	ARG	NE-CZ-NH1	8.04	124.32	120.30
5	C	525	PHE	CB-CG-CD1	8.04	126.43	120.80
5	C	475	TYR	CB-CG-CD1	-8.03	116.18	121.00
9	I	223	TYR	CB-CG-CD1	-8.02	116.19	121.00
8	H	25	ARG	NE-CZ-NH1	-8.01	116.29	120.30
6	F	318	ARG	NE-CZ-NH2	-8.01	116.29	120.30
5	E	212	TYR	CB-CG-CD1	8.00	125.80	121.00
5	E	257	ALA	N-CA-CB	8.00	121.29	110.10
6	B	404	TYR	CB-CG-CD2	-7.98	116.21	121.00
11	a	135	PHE	CB-CG-CD1	7.97	126.38	120.80
1	b	141	TYR	CB-CG-CD2	-7.96	116.22	121.00
5	C	46	TYR	CB-CG-CD1	-7.95	116.23	121.00
7	Q	102	TYR	CD1-CE1-CZ	7.92	126.93	119.80
2	O	239	PHE	CB-CG-CD1	7.91	126.34	120.80
6	D	71	ARG	NE-CZ-NH1	7.90	124.25	120.30
7	Q	20	TYR	CB-CG-CD2	7.90	125.74	121.00
7	Q	82	TYR	CB-CG-CD2	-7.89	116.27	121.00
9	K	195	ASP	CB-CG-OD1	7.89	125.40	118.30
5	E	66	ASP	CB-CG-OD2	-7.86	111.22	118.30
5	E	54	ASP	CB-CG-OD2	-7.86	111.23	118.30
9	G	23	PHE	CB-CG-CD2	-7.86	115.30	120.80
6	B	173	PHE	CB-CG-CD2	-7.85	115.31	120.80
6	F	449	TYR	CB-CG-CD2	-7.84	116.30	121.00
1	b	99	TYR	CB-CG-CD2	-7.83	116.30	121.00
5	C	344	ARG	NE-CZ-NH2	-7.82	116.39	120.30
10	P	200	ARG	NE-CZ-NH2	-7.82	116.39	120.30
11	Y	60	ALA	CB-CA-C	-7.82	98.38	110.10
10	P	288	ARG	NE-CZ-NH2	-7.81	116.40	120.30
5	E	28	TYR	CG-CD2-CE2	-7.80	115.06	121.30
7	Q	38	THR	CA-CB-CG2	-7.79	101.49	112.40
5	C	76	THR	CA-CB-CG2	-7.79	101.49	112.40
5	E	377	ASP	CB-CG-OD2	-7.79	111.29	118.30
7	Q	192	PHE	CB-CG-CD2	-7.79	115.35	120.80
4	N	37	PHE	CB-CG-CD1	-7.78	115.35	120.80
6	F	131	TYR	CB-CG-CD2	-7.78	116.33	121.00
5	A	258	PHE	CB-CG-CD2	7.77	126.24	120.80
11	Z	85	TYR	CB-CG-CD1	7.75	125.65	121.00
4	N	101	TYR	CB-CG-CD2	-7.74	116.36	121.00
7	Q	188	TYR	CB-CG-CD2	-7.74	116.36	121.00
6	F	229	PHE	CB-CG-CD1	-7.74	115.39	120.80
1	b	332	ARG	NE-CZ-NH2	-7.73	116.44	120.30
5	C	463	TYR	CG-CD1-CE1	-7.73	115.11	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	Y	142	TYR	CB-CG-CD1	7.73	125.64	121.00
5	A	534	TYR	CB-CG-CD2	-7.72	116.37	121.00
2	O	251	ARG	NE-CZ-NH1	-7.71	116.45	120.30
1	b	63	ASP	CB-CG-OD1	7.70	125.23	118.30
1	b	344	ASP	CB-CG-OD2	-7.68	111.39	118.30
5	A	87	ARG	NE-CZ-NH1	7.68	124.14	120.30
11	R	135	PHE	CB-CG-CD2	7.68	126.17	120.80
11	Z	153	ARG	NE-CZ-NH1	7.68	124.14	120.30
6	F	466	ARG	NE-CZ-NH1	7.68	124.14	120.30
6	D	131	TYR	CB-CG-CD1	-7.66	116.41	121.00
5	C	409	SER	N-CA-CB	7.65	121.98	110.50
6	F	359	PHE	CB-CG-CD1	7.64	126.15	120.80
10	P	475	TYR	CG-CD2-CE2	7.63	127.41	121.30
10	P	259	PHE	CB-CG-CD1	7.62	126.13	120.80
10	P	220	ARG	NE-CZ-NH2	-7.61	116.49	120.30
10	P	267	TYR	CD1-CE1-CZ	-7.60	112.96	119.80
6	F	225	PHE	CB-CG-CD1	-7.59	115.49	120.80
5	A	344	ARG	NE-CZ-NH1	-7.58	116.51	120.30
5	C	406	ARG	NE-CZ-NH1	7.58	124.09	120.30
6	D	395	ASP	CB-CG-OD1	7.58	125.12	118.30
6	B	249	THR	CA-CB-CG2	-7.56	101.82	112.40
5	C	394	ARG	NE-CZ-NH2	-7.56	116.52	120.30
5	C	135	ARG	NE-CZ-NH1	7.55	124.07	120.30
6	F	468	TYR	CB-CG-CD2	-7.51	116.49	121.00
1	b	343	ARG	NE-CZ-NH1	7.50	124.05	120.30
3	M	139	TYR	CB-CG-CD1	7.49	125.49	121.00
10	P	136	PHE	CB-CG-CD1	7.48	126.04	120.80
3	M	187	TYR	CB-CG-CD1	7.47	125.48	121.00
5	E	380	PHE	CB-CG-CD2	-7.47	115.57	120.80
6	B	321	ARG	NE-CZ-NH2	-7.47	116.57	120.30
5	E	62	ARG	NE-CZ-NH1	7.46	124.03	120.30
7	Q	161	TYR	CB-CG-CD2	-7.44	116.54	121.00
1	b	328	TYR	CB-CG-CD2	-7.44	116.54	121.00
6	D	415	ALA	N-CA-CB	7.44	120.51	110.10
10	P	144	PHE	CB-CG-CD1	-7.43	115.60	120.80
11	Y	51	PHE	CB-CG-CD2	7.43	126.00	120.80
11	X	51	PHE	CB-CG-CD1	7.42	126.00	120.80
5	E	534	TYR	CB-CG-CD2	-7.42	116.55	121.00
6	F	304	TYR	CG-CD2-CE2	-7.42	115.36	121.30
10	P	468	ALA	N-CA-CB	7.40	120.46	110.10
6	B	407	TYR	CB-CG-CD2	-7.39	116.57	121.00
5	A	158	TYR	CB-CG-CD2	-7.38	116.57	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	565	ALA	N-CA-CB	7.36	120.41	110.10
11	U	104	ALA	CB-CA-C	-7.35	99.07	110.10
6	D	265	TYR	CG-CD2-CE2	7.35	127.18	121.30
7	Q	273	TYR	CB-CG-CD1	-7.33	116.60	121.00
5	C	334	TYR	CB-CG-CD1	-7.33	116.60	121.00
3	M	42	ARG	NE-CZ-NH1	7.32	123.96	120.30
11	Z	129	MET	CG-SD-CE	-7.32	88.50	100.20
1	b	320	PHE	CB-CG-CD2	-7.31	115.68	120.80
5	E	553	TYR	CB-CG-CD1	-7.31	116.61	121.00
9	K	115	ASP	CB-CG-OD1	-7.31	111.72	118.30
5	E	28	TYR	CZ-CE2-CD2	7.31	126.38	119.80
9	I	86	LEU	CB-CG-CD2	7.31	123.42	111.00
6	B	128	ALA	N-CA-CB	7.29	120.31	110.10
9	K	128	ALA	N-CA-CB	7.29	120.31	110.10
11	Y	124	ARG	NE-CZ-NH1	-7.28	116.66	120.30
6	D	101	ARG	NE-CZ-NH2	7.28	123.94	120.30
6	F	435	PHE	CB-CG-CD2	-7.27	115.71	120.80
11	V	30	TYR	CD1-CE1-CZ	7.27	126.35	119.80
9	G	23	PHE	CB-CG-CD1	7.27	125.89	120.80
2	O	382	TYR	CB-CG-CD2	-7.26	116.64	121.00
6	F	223	ARG	NE-CZ-NH1	7.26	123.93	120.30
10	P	476	THR	CA-CB-CG2	-7.25	102.25	112.40
3	M	121	ARG	NE-CZ-NH1	7.25	123.92	120.30
1	b	72	PHE	CB-CG-CD2	-7.24	115.74	120.80
1	b	315	ARG	NE-CZ-NH1	7.23	123.92	120.30
7	Q	82	TYR	CB-CG-CD1	7.23	125.34	121.00
11	a	142	TYR	CG-CD2-CE2	-7.23	115.52	121.30
6	B	46	PHE	CB-CG-CD2	-7.22	115.75	120.80
5	A	399	VAL	CA-CB-CG2	7.21	121.72	110.90
8	L	57	PHE	CB-CG-CD1	-7.20	115.76	120.80
9	K	111	ALA	N-CA-CB	7.20	120.18	110.10
5	C	126	ARG	NE-CZ-NH2	-7.20	116.70	120.30
5	A	525	PHE	CB-CG-CD2	-7.19	115.77	120.80
9	G	137	ALA	N-CA-CB	7.19	120.16	110.10
6	F	150	MET	CA-CB-CG	7.18	125.51	113.30
5	A	297	PHE	CB-CG-CD2	-7.18	115.77	120.80
6	B	74	ARG	NE-CZ-NH1	-7.18	116.71	120.30
6	B	48	ARG	NE-CZ-NH1	7.17	123.88	120.30
6	B	252	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	b	71	TYR	CA-CB-CG	7.16	127.01	113.40
7	Q	276	ARG	NE-CZ-NH2	-7.16	116.72	120.30
5	A	134	ASP	CB-CG-OD2	-7.16	111.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	W	79	GLY	N-CA-C	-7.15	95.22	113.10
5	A	448	ARG	NE-CZ-NH1	7.14	123.87	120.30
6	D	144	ARG	NE-CZ-NH2	-7.13	116.73	120.30
6	F	95	PHE	CB-CG-CD2	7.12	125.78	120.80
11	T	51	PHE	CB-CG-CD1	-7.11	115.82	120.80
6	D	88	VAL	CA-CB-CG2	-7.10	100.24	110.90
11	T	85	TYR	CB-CG-CD2	-7.10	116.74	121.00
5	E	295	MET	CA-CB-CG	7.10	125.36	113.30
8	H	101	THR	CA-CB-CG2	-7.08	102.49	112.40
1	b	194	ASP	CB-CG-OD1	7.08	124.67	118.30
1	b	309	TRP	CG-CD2-CE3	-7.08	127.53	133.90
6	D	74	ARG	NE-CZ-NH2	-7.06	116.77	120.30
5	E	405	ASP	CB-CG-OD2	-7.05	111.95	118.30
6	D	127	PHE	CB-CG-CD2	-7.05	115.86	120.80
11	U	30	TYR	CB-CG-CD1	7.05	125.23	121.00
11	T	76	TYR	CB-CG-CD2	-7.05	116.77	121.00
9	I	92	ARG	NE-CZ-NH1	-7.04	116.78	120.30
7	Q	30	TYR	CZ-CE2-CD2	-7.04	113.46	119.80
9	G	178	TYR	CB-CG-CD1	-7.04	116.78	121.00
11	W	124	ARG	NE-CZ-NH2	-7.03	116.78	120.30
11	T	12	PHE	CB-CG-CD2	-7.02	115.89	120.80
2	O	172	VAL	CA-CB-CG2	7.01	121.41	110.90
6	D	195	ARG	NE-CZ-NH1	-7.01	116.80	120.30
11	a	153	ARG	NE-CZ-NH1	7.01	123.80	120.30
6	F	224	PHE	CB-CG-CD2	-7.00	115.90	120.80
5	A	26	ALA	N-CA-CB	7.00	119.90	110.10
5	E	221	ARG	NE-CZ-NH1	6.99	123.80	120.30
5	A	272	TYR	CB-CG-CD2	-6.99	116.81	121.00
6	D	404	TYR	CD1-CE1-CZ	6.99	126.09	119.80
5	A	203	ASP	CB-CG-OD2	6.98	124.58	118.30
8	L	27	TYR	CB-CG-CD2	6.98	125.19	121.00
10	P	17	ARG	NE-CZ-NH1	6.98	123.79	120.30
11	Z	124	ARG	NE-CZ-NH1	6.98	123.79	120.30
11	W	85	TYR	CG-CD1-CE1	-6.96	115.73	121.30
6	F	46	PHE	CB-CG-CD2	-6.94	115.94	120.80
7	Q	239	SER	CB-CA-C	-6.94	96.91	110.10
6	B	104	VAL	CG1-CB-CG2	6.94	122.01	110.90
11	T	129	MET	CG-SD-CE	-6.94	89.10	100.20
6	D	452	ARG	NE-CZ-NH1	-6.93	116.83	120.30
11	X	158	VAL	CG1-CB-CG2	-6.93	99.81	110.90
6	B	225	PHE	CB-CG-CD2	-6.93	115.95	120.80
6	B	407	TYR	CB-CG-CD1	6.93	125.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	319	TYR	CZ-CE2-CD2	6.93	126.04	119.80
9	K	219	ARG	NE-CZ-NH1	-6.93	116.84	120.30
9	K	206	ARG	NE-CZ-NH2	-6.92	116.84	120.30
6	D	173	PHE	CB-CG-CD1	6.92	125.65	120.80
5	E	150	ASP	CB-CG-OD2	-6.92	112.07	118.30
5	A	423	PHE	CB-CG-CD1	6.90	125.63	120.80
3	M	81	TYR	CB-CG-CD1	6.88	125.13	121.00
5	C	280	TYR	CB-CG-CD1	-6.88	116.87	121.00
11	S	157	ASP	CB-CG-OD2	-6.88	112.11	118.30
7	Q	51	TYR	CB-CG-CD1	-6.88	116.87	121.00
5	E	548	ARG	CD-NE-CZ	-6.88	113.97	123.60
11	X	126	PHE	CG-CD2-CE2	-6.88	113.24	120.80
2	O	275	ASP	CB-CG-OD1	6.87	124.49	118.30
9	K	40	ASP	CB-CG-OD2	-6.87	112.11	118.30
5	E	121	SER	CB-CA-C	-6.87	97.04	110.10
6	F	343	THR	CA-CB-CG2	-6.87	102.78	112.40
5	E	531	TYR	CG-CD2-CE2	-6.86	115.81	121.30
11	U	85	TYR	CG-CD1-CE1	6.86	126.79	121.30
6	B	95	PHE	CB-CG-CD1	-6.85	116.00	120.80
7	Q	322	ASN	N-CA-CB	6.85	122.93	110.60
7	Q	249	TYR	CG-CD1-CE1	-6.84	115.83	121.30
2	O	173	ARG	NE-CZ-NH2	-6.84	116.88	120.30
6	B	113	PHE	CB-CG-CD2	-6.84	116.01	120.80
10	P	322	VAL	CA-CB-CG2	-6.83	100.65	110.90
11	W	42	THR	CA-CB-CG2	-6.83	102.84	112.40
6	D	252	ARG	NE-CZ-NH2	-6.83	116.89	120.30
11	R	23	PHE	CB-CG-CD1	-6.83	116.02	120.80
5	C	40	MET	CG-SD-CE	-6.82	89.28	100.20
5	E	158	TYR	CB-CG-CD1	-6.82	116.91	121.00
7	Q	188	TYR	CB-CG-CD1	6.82	125.09	121.00
5	C	463	TYR	CB-CG-CD1	-6.80	116.92	121.00
9	G	115	ASP	CB-CG-OD1	6.80	124.42	118.30
5	A	391	PHE	CB-CG-CD1	6.80	125.56	120.80
10	P	165	LEU	CB-CG-CD1	6.79	122.55	111.00
9	G	25	ARG	NE-CZ-NH2	6.79	123.70	120.30
6	B	340	ASP	CB-CG-OD2	-6.79	112.19	118.30
9	G	224	GLY	N-CA-C	-6.78	96.14	113.10
5	A	238	ARG	NE-CZ-NH1	6.78	123.69	120.30
7	Q	50	ASP	CB-CG-OD2	-6.78	112.20	118.30
6	D	111	ARG	NE-CZ-NH2	-6.78	116.91	120.30
1	b	33	LEU	C-N-CA	6.77	136.53	122.30
2	O	366	LYS	O-C-N	-6.77	111.87	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	179	ALA	CB-CA-C	-6.77	99.95	110.10
7	Q	173	ASP	CB-CG-OD2	-6.77	112.21	118.30
6	B	173	PHE	CB-CG-CD1	6.76	125.53	120.80
6	F	213	ALA	N-CA-CB	6.75	119.55	110.10
5	A	359	ARG	NE-CZ-NH2	-6.75	116.93	120.30
5	E	327	ALA	CB-CA-C	-6.74	99.99	110.10
9	I	117	TYR	CB-CG-CD2	6.74	125.04	121.00
9	K	76	THR	CA-CB-CG2	-6.73	102.98	112.40
11	V	11	PHE	CB-CG-CD2	-6.73	116.09	120.80
11	Y	117	ARG	NE-CZ-NH2	6.73	123.66	120.30
7	Q	102	TYR	CG-CD1-CE1	-6.72	115.92	121.30
8	J	51	ASP	CB-CG-OD1	-6.72	112.25	118.30
9	K	178	TYR	CZ-CE2-CD2	-6.71	113.76	119.80
5	E	352	MET	CG-SD-CE	-6.71	89.46	100.20
5	E	29	SER	N-CA-CB	6.71	120.57	110.50
6	D	307	TYR	CB-CG-CD1	6.71	125.03	121.00
11	Z	117	ARG	NE-CZ-NH2	-6.71	116.94	120.30
5	C	123	TYR	CB-CG-CD2	-6.71	116.98	121.00
6	D	63	ARG	NE-CZ-NH2	-6.70	116.95	120.30
5	C	356	SER	N-CA-CB	6.69	120.54	110.50
1	b	208	ARG	NE-CZ-NH1	6.69	123.65	120.30
5	E	158	TYR	CB-CG-CD2	6.69	125.01	121.00
5	E	548	ARG	NE-CZ-NH2	-6.69	116.96	120.30
9	I	76	THR	CA-CB-CG2	-6.68	103.05	112.40
1	b	352	ARG	N-CA-CB	6.68	122.62	110.60
9	G	43	TYR	CG-CD1-CE1	6.67	126.64	121.30
6	D	149	GLU	N-CA-CB	6.67	122.61	110.60
2	O	210	TYR	CB-CG-CD2	-6.67	117.00	121.00
5	A	266	SER	N-CA-CB	6.67	120.50	110.50
11	V	55	VAL	CA-CB-CG2	-6.66	100.91	110.90
6	D	142	TYR	CB-CG-CD1	-6.66	117.01	121.00
2	O	350	PHE	CB-CG-CD2	-6.65	116.14	120.80
11	R	30	TYR	CB-CG-CD1	-6.65	117.01	121.00
11	X	46	ARG	NH1-CZ-NH2	-6.65	112.09	119.40
5	C	141	PHE	CB-CG-CD1	6.65	125.45	120.80
11	W	153	ARG	NE-CZ-NH1	-6.64	116.98	120.30
6	F	46	PHE	CB-CG-CD1	6.64	125.44	120.80
10	P	395	PHE	CB-CG-CD2	6.63	125.44	120.80
5	C	485	MET	CG-SD-CE	-6.63	89.60	100.20
7	Q	143	THR	CA-CB-CG2	-6.63	103.12	112.40
6	B	73	ASP	CB-CG-OD1	-6.62	112.34	118.30
10	P	181	ASP	CB-CG-OD2	-6.61	112.36	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	273	ASP	CB-CG-OD2	-6.61	112.36	118.30
1	b	63	ASP	CB-CG-OD2	-6.60	112.36	118.30
9	G	116	GLU	CB-CA-C	-6.60	97.20	110.40
5	A	64	ASP	CB-CG-OD1	6.60	124.24	118.30
9	I	113	ASN	N-CA-C	-6.60	93.18	111.00
6	F	289	ARG	NE-CZ-NH2	6.58	123.59	120.30
5	C	156	ASP	CB-CG-OD2	-6.58	112.38	118.30
1	b	149	ASP	CB-CG-OD2	-6.58	112.38	118.30
5	A	324	MET	CG-SD-CE	6.58	110.73	100.20
6	F	407	TYR	CB-CG-CD2	-6.58	117.05	121.00
9	I	9	THR	N-CA-CB	6.58	122.80	110.30
10	P	275	LEU	CB-CG-CD2	6.58	122.18	111.00
9	I	9	THR	CA-CB-CG2	-6.56	103.21	112.40
5	A	73	TYR	CB-CG-CD2	-6.56	117.06	121.00
6	F	449	TYR	CB-CG-CD1	6.56	124.93	121.00
9	K	117	TYR	CB-CG-CD2	6.56	124.93	121.00
3	M	74	ALA	CB-CA-C	-6.55	100.27	110.10
5	E	535	ASP	CB-CG-OD1	-6.55	112.40	118.30
5	E	44	ALA	CB-CA-C	-6.53	100.30	110.10
5	C	616	ASP	CB-CG-OD2	-6.53	112.42	118.30
11	S	153	ARG	NE-CZ-NH1	-6.53	117.04	120.30
6	D	325	ARG	NE-CZ-NH1	6.51	123.56	120.30
5	C	24	TYR	CZ-CE2-CD2	-6.51	113.94	119.80
5	C	68	ALA	CB-CA-C	-6.51	100.34	110.10
4	N	101	TYR	CG-CD1-CE1	-6.50	116.10	121.30
3	M	120	PHE	CB-CG-CD1	6.50	125.35	120.80
6	B	281	MET	CG-SD-CE	-6.50	89.81	100.20
6	D	53	VAL	CA-CB-CG1	6.50	120.65	110.90
3	M	36	SER	N-CA-CB	6.50	120.24	110.50
10	P	21	ARG	NE-CZ-NH1	6.50	123.55	120.30
11	T	153	ARG	NE-CZ-NH1	-6.49	117.05	120.30
4	N	51	THR	CA-CB-CG2	-6.49	103.31	112.40
5	A	281	VAL	CG1-CB-CG2	-6.49	100.52	110.90
2	O	78	SER	CB-CA-C	-6.48	97.78	110.10
6	B	225	PHE	CB-CG-CD1	6.48	125.34	120.80
9	G	207	LEU	CB-CG-CD1	6.48	122.01	111.00
5	C	422	ASP	CB-CG-OD2	-6.48	112.47	118.30
1	b	358	ALA	N-CA-CB	6.47	119.17	110.10
3	M	97	ARG	NE-CZ-NH2	-6.47	117.06	120.30
5	E	212	TYR	CB-CG-CD2	-6.47	117.12	121.00
5	E	587	PHE	CB-CG-CD2	-6.47	116.27	120.80
11	R	124	ARG	NE-CZ-NH1	6.46	123.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	545	ASP	CB-CG-OD2	-6.46	112.48	118.30
5	C	217	VAL	CA-CB-CG2	6.46	120.59	110.90
8	H	28	ARG	NE-CZ-NH2	-6.46	117.07	120.30
3	M	121	ARG	NE-CZ-NH2	-6.45	117.07	120.30
6	B	420	VAL	CA-CB-CG2	6.45	120.57	110.90
5	C	460	TYR	CG-CD2-CE2	-6.45	116.14	121.30
1	b	248	ARG	NE-CZ-NH2	-6.44	117.08	120.30
9	I	158	ARG	NE-CZ-NH1	6.43	123.52	120.30
11	R	51	PHE	CB-CG-CD2	6.43	125.30	120.80
10	P	368	LEU	N-CA-CB	6.42	123.25	110.40
5	C	581	VAL	CA-CB-CG1	-6.42	101.27	110.90
5	C	383	TYR	CB-CG-CD1	-6.42	117.15	121.00
9	I	115	ASP	CB-CG-OD2	6.41	124.07	118.30
5	E	572	ASP	CB-CG-OD2	-6.41	112.53	118.30
6	D	381	ARG	NE-CZ-NH2	6.40	123.50	120.30
11	R	142	TYR	CB-CG-CD1	6.40	124.84	121.00
6	B	468	TYR	CB-CG-CD2	6.39	124.84	121.00
10	P	218	LEU	CB-CG-CD1	-6.39	100.13	111.00
5	A	438	PHE	CB-CG-CD1	6.39	125.27	120.80
6	B	340	ASP	CB-CG-OD1	6.38	124.05	118.30
7	Q	289	TYR	CG-CD2-CE2	6.38	126.41	121.30
7	Q	65	THR	CA-CB-CG2	-6.38	103.46	112.40
5	E	179	ARG	NE-CZ-NH2	-6.38	117.11	120.30
6	B	393	ARG	NE-CZ-NH2	-6.37	117.12	120.30
11	V	117	ARG	NE-CZ-NH2	-6.37	117.12	120.30
9	I	52	ARG	NE-CZ-NH2	-6.36	117.12	120.30
9	G	180	ASN	CB-CA-C	-6.36	97.68	110.40
6	F	146	TYR	CG-CD2-CE2	-6.36	116.21	121.30
7	Q	219	ARG	NE-CZ-NH2	6.36	123.48	120.30
11	X	99	LEU	N-CA-CB	6.36	123.12	110.40
5	C	334	TYR	CB-CG-CD2	6.36	124.81	121.00
5	E	342	TYR	CB-CG-CD1	6.36	124.81	121.00
11	T	88	PHE	CG-CD1-CE1	-6.35	113.82	120.80
6	B	295	ARG	NE-CZ-NH2	-6.35	117.13	120.30
5	C	220	PRO	N-CD-CG	6.34	112.72	103.20
1	b	116	TYR	CB-CG-CD2	6.34	124.80	121.00
5	C	548	ARG	NE-CZ-NH1	6.34	123.47	120.30
9	G	177	ASP	CB-CG-OD2	6.34	124.00	118.30
5	A	449	LYS	N-CA-CB	6.33	122.00	110.60
5	A	286	ARG	NE-CZ-NH1	-6.33	117.13	120.30
6	D	404	TYR	CG-CD1-CE1	-6.33	116.24	121.30
11	Z	153	ARG	NE-CZ-NH2	-6.33	117.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	a	138	VAL	C-N-CA	6.33	137.52	121.70
3	M	187	TYR	CG-CD2-CE2	-6.31	116.25	121.30
7	Q	102	TYR	CG-CD2-CE2	-6.31	116.25	121.30
11	V	25	SER	N-CA-CB	6.31	119.96	110.50
5	C	191	TYR	CB-CG-CD1	-6.30	117.22	121.00
11	R	153	ARG	NE-CZ-NH1	6.30	123.45	120.30
5	A	135	ARG	NE-CZ-NH2	-6.29	117.16	120.30
5	E	448	ARG	NH1-CZ-NH2	6.28	126.31	119.40
11	R	76	TYR	CG-CD1-CE1	6.28	126.33	121.30
8	L	2	SER	N-CA-CB	6.28	119.92	110.50
6	D	114	ASP	CB-CG-OD2	-6.27	112.66	118.30
11	S	133	LEU	CB-CA-C	-6.27	98.29	110.20
6	F	466	ARG	NE-CZ-NH2	-6.26	117.17	120.30
6	F	321	ARG	NE-CZ-NH2	-6.25	117.17	120.30
7	Q	117	ASP	N-CA-CB	6.25	121.86	110.60
3	M	44	ARG	CD-NE-CZ	6.25	132.35	123.60
4	N	113	ARG	NE-CZ-NH2	6.25	123.42	120.30
11	S	142	TYR	CB-CG-CD2	6.24	124.75	121.00
5	E	405	ASP	CB-CG-OD1	6.24	123.92	118.30
6	D	341	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	b	193	ARG	NE-CZ-NH1	6.24	123.42	120.30
4	N	111	ARG	NE-CZ-NH1	6.24	123.42	120.30
6	D	307	TYR	CB-CG-CD2	-6.24	117.26	121.00
5	E	120	GLN	N-CA-CB	6.23	121.82	110.60
5	A	129	ASP	CB-CG-OD2	6.23	123.91	118.30
6	F	284	TYR	CB-CG-CD2	6.22	124.73	121.00
1	b	71	TYR	CB-CG-CD2	-6.22	117.27	121.00
6	B	451	ASP	CB-CG-OD1	-6.21	112.71	118.30
7	Q	267	ALA	N-CA-CB	6.21	118.80	110.10
7	Q	266	ARG	CD-NE-CZ	6.21	132.29	123.60
6	F	475	ARG	NE-CZ-NH2	-6.21	117.19	120.30
3	M	51	ASP	CB-CG-OD1	6.21	123.89	118.30
6	F	450	GLU	N-CA-C	-6.21	94.24	111.00
6	D	131	TYR	CG-CD2-CE2	-6.21	116.33	121.30
5	C	24	TYR	CG-CD2-CE2	6.21	126.27	121.30
10	P	288	ARG	NE-CZ-NH1	6.21	123.40	120.30
6	F	416	MET	CG-SD-CE	-6.19	90.29	100.20
10	P	32	ARG	NE-CZ-NH1	6.19	123.39	120.30
5	A	610	ARG	NE-CZ-NH1	6.17	123.39	120.30
11	R	51	PHE	CB-CG-CD1	-6.17	116.48	120.80
11	V	30	TYR	CG-CD1-CE1	-6.17	116.36	121.30
1	b	110	TYR	CB-CG-CD2	-6.17	117.30	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	155	ASP	CB-CG-OD1	-6.17	112.75	118.30
6	F	396	HIS	CA-CB-CG	6.17	124.08	113.60
6	D	304	TYR	CG-CD1-CE1	-6.17	116.37	121.30
3	M	63	THR	N-CA-CB	6.16	122.01	110.30
5	E	475	TYR	CB-CG-CD2	-6.16	117.30	121.00
5	E	438	PHE	CB-CG-CD2	6.15	125.11	120.80
2	O	366	LYS	CA-C-O	6.15	133.01	120.10
7	Q	319	GLU	N-CA-CB	6.15	121.67	110.60
1	b	186	TYR	CG-CD2-CE2	-6.14	116.39	121.30
11	a	111	VAL	CA-CB-CG1	-6.14	101.69	110.90
6	F	121	ASP	CB-CG-OD1	-6.13	112.78	118.30
5	C	453	SER	CB-CA-C	-6.13	98.46	110.10
5	C	365	ARG	NE-CZ-NH2	6.13	123.36	120.30
11	R	20	ALA	N-CA-CB	6.13	118.68	110.10
5	C	293	VAL	CG1-CB-CG2	6.12	120.69	110.90
11	S	86	THR	CA-CB-CG2	-6.12	103.83	112.40
6	D	321	ARG	NE-CZ-NH1	-6.12	117.24	120.30
7	Q	181	ARG	NE-CZ-NH2	-6.12	117.24	120.30
9	I	223	TYR	CG-CD1-CE1	-6.11	116.41	121.30
6	B	278	LEU	CB-CG-CD1	-6.11	100.62	111.00
6	F	308	MET	CG-SD-CE	-6.11	90.43	100.20
11	Y	76	TYR	CB-CG-CD1	6.10	124.66	121.00
5	E	238	ARG	NE-CZ-NH1	6.09	123.35	120.30
5	E	191	TYR	CG-CD2-CE2	-6.09	116.43	121.30
7	Q	216	ALA	N-CA-CB	-6.09	101.57	110.10
5	E	184	TRP	CA-CB-CG	6.09	125.27	113.70
5	A	438	PHE	CB-CG-CD2	-6.09	116.54	120.80
5	A	406	ARG	NE-CZ-NH1	-6.09	117.26	120.30
5	A	463	TYR	CB-CG-CD1	6.08	124.65	121.00
1	b	31	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	b	20	TYR	CB-CG-CD1	6.08	124.65	121.00
5	A	227	LEU	CB-CG-CD2	6.07	121.33	111.00
11	T	35	SER	N-CA-CB	6.07	119.61	110.50
9	I	25	ARG	NE-CZ-NH2	6.06	123.33	120.30
6	F	121	ASP	CB-CG-OD2	6.06	123.76	118.30
11	S	126	PHE	CB-CG-CD1	6.06	125.04	120.80
11	T	119	SER	N-CA-CB	6.06	119.59	110.50
11	X	88	PHE	CG-CD1-CE1	6.05	127.46	120.80
9	G	198	GLU	CB-CA-C	-6.05	98.30	110.40
6	F	247	ASP	N-CA-CB	6.04	121.48	110.60
5	E	318	VAL	N-CA-C	-6.03	94.72	111.00
5	A	123	TYR	CG-CD2-CE2	-6.03	116.48	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	124	ARG	NE-CZ-NH2	-6.03	117.28	120.30
1	b	71	TYR	CG-CD1-CE1	-6.03	116.48	121.30
10	P	332	ASP	N-CA-CB	6.02	121.44	110.60
11	Y	88	PHE	CZ-CE2-CD2	6.02	127.33	120.10
6	B	150	MET	CA-CB-CG	6.02	123.53	113.30
9	K	160	TYR	CG-CD1-CE1	-6.02	116.49	121.30
10	P	242	LEU	CB-CG-CD1	6.01	121.22	111.00
5	E	301	TYR	CB-CG-CD2	-6.01	117.40	121.00
11	Y	33	ALA	N-CA-CB	6.00	118.51	110.10
3	M	59	ARG	CG-CD-NE	-6.00	99.19	111.80
7	Q	286	ASP	CB-CG-OD2	6.00	123.70	118.30
6	D	30	THR	CA-CB-CG2	-6.00	104.00	112.40
8	J	39	ALA	CB-CA-C	-6.00	101.10	110.10
5	E	400	ALA	N-CA-CB	-5.99	101.71	110.10
6	D	400	SER	N-CA-CB	5.99	119.49	110.50
11	a	126	PHE	CB-CG-CD1	-5.99	116.61	120.80
8	J	51	ASP	CB-CG-OD2	5.98	123.68	118.30
6	F	202	ASP	CB-CG-OD2	5.97	123.67	118.30
11	R	142	TYR	CB-CG-CD2	-5.97	117.42	121.00
8	L	27	TYR	CG-CD2-CE2	-5.97	116.53	121.30
11	S	30	TYR	CB-CG-CD1	-5.97	117.42	121.00
11	S	48	ASP	CB-CG-OD1	-5.97	112.93	118.30
6	B	439	PHE	CB-CG-CD1	5.96	124.98	120.80
5	C	344	ARG	NE-CZ-NH1	5.96	123.28	120.30
6	D	142	TYR	C-N-CA	5.96	136.60	121.70
6	F	159	ASP	O-C-N	-5.96	113.17	122.70
10	P	338	ASP	CB-CG-OD2	5.96	123.66	118.30
11	X	114	ALA	CB-CA-C	5.96	119.03	110.10
5	E	276	ASP	CB-CG-OD1	5.95	123.66	118.30
6	D	439	PHE	CB-CG-CD2	5.95	124.97	120.80
11	R	155	THR	CA-CB-CG2	-5.95	104.06	112.40
8	L	62	ALA	CB-CA-C	-5.95	101.17	110.10
1	b	351	ALA	O-C-N	5.95	132.22	122.70
5	A	334	TYR	CB-CG-CD2	-5.94	117.44	121.00
5	A	390	SER	N-CA-CB	5.94	119.41	110.50
10	P	131	SER	N-CA-CB	5.94	119.41	110.50
2	O	290	ARG	NE-CZ-NH2	-5.93	117.33	120.30
7	Q	174	ASP	CB-CG-OD2	-5.93	112.97	118.30
11	U	157	ASP	CB-CG-OD2	5.93	123.64	118.30
11	S	125	LEU	CB-CG-CD1	-5.93	100.92	111.00
6	B	444	ILE	CA-CB-CG2	5.92	122.75	110.90
11	T	88	PHE	CD1-CE1-CZ	5.92	127.21	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	113	ASP	CB-CG-OD1	5.92	123.63	118.30
6	D	173	PHE	CB-CA-C	-5.92	98.56	110.40
3	M	34	ARG	NE-CZ-NH1	5.92	123.26	120.30
10	P	332	ASP	CB-CG-OD1	-5.92	112.98	118.30
6	D	443	PHE	CB-CG-CD2	5.91	124.94	120.80
5	E	46	TYR	CB-CG-CD2	-5.90	117.46	121.00
9	G	24	ILE	O-C-N	5.90	132.14	122.70
5	A	191	TYR	CA-CB-CG	-5.90	102.19	113.40
5	C	560	ALA	CB-CA-C	-5.90	101.25	110.10
9	K	79	THR	CA-CB-CG2	-5.90	104.14	112.40
5	C	207	SER	N-CA-CB	5.90	119.34	110.50
7	Q	34	THR	CA-CB-CG2	-5.89	104.16	112.40
11	a	51	PHE	CB-CG-CD1	-5.88	116.68	120.80
2	O	2	ALA	N-CA-CB	5.88	118.34	110.10
6	D	302	ARG	NE-CZ-NH1	-5.88	117.36	120.30
5	E	308	LYS	N-CA-CB	5.88	121.18	110.60
5	C	83	ASP	CB-CG-OD1	5.88	123.59	118.30
2	O	319	TYR	CB-CG-CD2	5.87	124.52	121.00
6	D	38	LEU	CB-CG-CD2	5.87	120.98	111.00
5	E	212	TYR	CG-CD1-CE1	5.87	126.00	121.30
6	B	127	PHE	CB-CG-CD1	5.87	124.91	120.80
5	C	301	TYR	CB-CG-CD1	5.87	124.52	121.00
6	D	395	ASP	CB-CA-C	-5.87	98.66	110.40
11	Z	117	ARG	NE-CZ-NH1	5.87	123.23	120.30
5	E	460	TYR	CD1-CE1-CZ	5.87	125.08	119.80
1	b	261	TYR	CB-CG-CD1	-5.86	117.48	121.00
6	B	101	ARG	CD-NE-CZ	-5.86	115.40	123.60
8	H	57	PHE	CB-CG-CD2	-5.86	116.70	120.80
5	A	126	ARG	NE-CZ-NH1	5.86	123.23	120.30
3	M	156	PHE	CB-CG-CD1	5.85	124.90	120.80
5	C	392	TYR	CG-CD2-CE2	-5.85	116.62	121.30
6	D	208	PHE	CB-CG-CD2	5.85	124.89	120.80
5	C	230	ASP	CB-CG-OD1	5.84	123.56	118.30
5	E	28	TYR	CD1-CE1-CZ	-5.84	114.55	119.80
10	P	128	PHE	CB-CG-CD2	5.84	124.89	120.80
9	K	206	ARG	NE-CZ-NH1	5.84	123.22	120.30
11	S	158	VAL	CB-CA-C	-5.83	100.32	111.40
6	F	166	ARG	N-CA-CB	5.83	121.09	110.60
2	O	33	TRP	CG-CD2-CE3	-5.83	128.66	133.90
3	M	139	TYR	CG-CD1-CE1	5.83	125.96	121.30
5	A	160	SER	CB-CA-C	-5.83	99.03	110.10
10	P	242	LEU	CB-CG-CD2	-5.82	101.10	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	B	451	ASP	CB-CG-OD2	5.82	123.54	118.30
6	D	166	ARG	NE-CZ-NH1	5.82	123.21	120.30
11	a	142	TYR	CA-CB-CG	5.82	124.45	113.40
5	C	438	PHE	CB-CG-CD1	5.82	124.87	120.80
11	Z	106	PHE	CB-CG-CD2	-5.82	116.73	120.80
5	E	343	PHE	CB-CG-CD2	-5.81	116.73	120.80
6	B	455	PHE	CB-CG-CD2	-5.81	116.73	120.80
6	B	151	ILE	N-CA-C	-5.81	95.32	111.00
6	D	118	ARG	N-CA-CB	5.81	121.05	110.60
6	F	127	PHE	CB-CG-CD1	-5.80	116.74	120.80
2	O	197	ALA	N-CA-CB	5.80	118.22	110.10
8	H	46	TYR	CB-CG-CD1	5.80	124.48	121.00
6	D	188	CYS	CB-CA-C	-5.79	98.81	110.40
9	I	198	GLU	OE1-CD-OE2	-5.79	116.35	123.30
11	W	124	ARG	CD-NE-CZ	-5.79	115.50	123.60
6	F	42	GLU	CB-CA-C	-5.79	98.83	110.40
6	F	396	HIS	CB-CA-C	-5.78	98.83	110.40
11	U	127	VAL	CA-CB-CG1	-5.78	102.22	110.90
3	M	95	ARG	NE-CZ-NH1	-5.78	117.41	120.30
11	X	126	PHE	CD1-CG-CD2	5.78	125.82	118.30
5	E	297	PHE	CB-CG-CD2	-5.78	116.75	120.80
9	I	151	SER	O-C-N	-5.78	113.45	122.70
11	R	113	ASP	CB-CG-OD2	5.78	123.50	118.30
5	E	439	TRP	CE2-CD2-CE3	5.78	125.63	118.70
7	Q	77	TYR	CG-CD1-CE1	-5.77	116.68	121.30
3	M	65	ALA	N-CA-CB	5.77	118.17	110.10
6	D	253	ILE	N-CA-CB	5.77	124.07	110.80
10	P	106	SER	N-CA-CB	5.77	119.15	110.50
5	E	513	ILE	CA-CB-CG1	-5.76	100.06	111.00
6	F	229	PHE	CB-CG-CD2	5.76	124.83	120.80
6	B	335	LEU	CB-CG-CD1	5.76	120.80	111.00
6	B	289	ARG	NH1-CZ-NH2	5.76	125.73	119.40
5	E	547	MET	CG-SD-CE	-5.76	90.99	100.20
7	Q	259	ALA	N-CA-CB	5.76	118.16	110.10
11	W	113	ASP	CB-CG-OD2	5.75	123.48	118.30
6	B	265	TYR	CG-CD2-CE2	-5.75	116.70	121.30
10	P	271	PHE	CB-CG-CD1	5.75	124.83	120.80
3	M	112	TYR	CG-CD1-CE1	-5.75	116.70	121.30
1	b	323	LEU	CB-CG-CD1	5.75	120.77	111.00
6	F	189	ARG	NE-CZ-NH1	5.75	123.17	120.30
9	I	23	PHE	CB-CG-CD2	5.75	124.82	120.80
9	G	132	LEU	CB-CG-CD1	5.75	120.77	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	b	217	GLU	N-CA-CB	5.75	120.94	110.60
5	A	324	MET	N-CA-CB	5.75	120.94	110.60
10	P	17	ARG	N-CA-CB	5.75	120.94	110.60
11	U	126	PHE	CB-CG-CD1	-5.74	116.78	120.80
6	F	482	ASP	N-CA-CB	5.74	120.93	110.60
9	I	76	THR	N-CA-CB	5.74	121.20	110.30
9	G	87	LYS	O-C-N	-5.74	113.52	122.70
11	U	23	PHE	CB-CG-CD2	5.74	124.82	120.80
6	F	429	ASP	CB-CG-OD2	5.74	123.46	118.30
6	B	393	ARG	NE-CZ-NH1	5.74	123.17	120.30
2	O	175	LEU	CB-CG-CD2	5.73	120.74	111.00
7	Q	80	PHE	CB-CG-CD1	5.73	124.81	120.80
5	C	54	ASP	CB-CG-OD2	5.72	123.45	118.30
10	P	244	TYR	CA-CB-CG	5.72	124.28	113.40
4	N	78	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
6	B	439	PHE	CB-CG-CD2	-5.72	116.80	120.80
5	C	203	ASP	CB-CG-OD1	5.72	123.45	118.30
6	F	127	PHE	N-CA-CB	5.72	120.89	110.60
9	I	222	LEU	CB-CA-C	-5.71	99.35	110.20
6	F	304	TYR	CB-CG-CD2	-5.71	117.57	121.00
3	M	83	VAL	CA-CB-CG2	-5.71	102.34	110.90
4	N	20	LEU	CB-CG-CD2	5.71	120.70	111.00
11	Z	124	ARG	NE-CZ-NH2	-5.71	117.45	120.30
5	E	553	TYR	CZ-CE2-CD2	5.70	124.93	119.80
7	Q	114	THR	CA-CB-CG2	-5.70	104.42	112.40
5	C	492	ALA	N-CA-CB	5.70	118.08	110.10
11	a	30	TYR	CD1-CE1-CZ	-5.69	114.67	119.80
11	Y	113	ASP	CB-CG-OD1	-5.69	113.18	118.30
8	J	36	LYS	N-CA-CB	5.69	120.83	110.60
9	G	197	ILE	N-CA-C	-5.68	95.65	111.00
6	B	370	TYR	CB-CG-CD2	-5.68	117.59	121.00
11	V	59	MET	CG-SD-CE	-5.68	91.11	100.20
1	b	78	LYS	CB-CA-C	-5.68	99.04	110.40
9	I	160	TYR	CB-CG-CD1	-5.68	117.59	121.00
5	C	434	ILE	C-N-CA	5.68	135.89	121.70
11	U	83	ALA	CB-CA-C	-5.68	101.58	110.10
6	B	308	MET	CG-SD-CE	-5.67	91.12	100.20
5	E	98	PRO	N-CA-CB	5.67	110.11	103.30
5	E	235	THR	CA-CB-CG2	-5.67	104.46	112.40
6	D	118	ARG	NE-CZ-NH2	5.67	123.14	120.30
7	Q	118	ARG	O-C-N	-5.67	113.62	122.70
7	Q	240	ASP	O-C-N	5.67	131.77	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	T	131	LEU	O-C-N	5.67	131.77	122.70
1	b	315	ARG	CD-NE-CZ	-5.66	115.67	123.60
1	b	340	TRP	CG-CD2-CE3	-5.66	128.80	133.90
9	I	43	TYR	CB-CG-CD2	5.66	124.40	121.00
11	W	12	PHE	CB-CG-CD1	5.66	124.76	120.80
6	D	462	TRP	CH2-CZ2-CE2	-5.66	111.74	117.40
10	P	413	ALA	N-CA-CB	5.66	118.02	110.10
5	A	460	TYR	CZ-CE2-CD2	5.65	124.88	119.80
5	A	460	TYR	CG-CD2-CE2	-5.65	116.78	121.30
5	E	246	CYS	N-CA-CB	5.64	120.76	110.60
5	C	460	TYR	CB-CG-CD1	-5.64	117.61	121.00
9	K	59	ASP	CB-CG-OD1	-5.64	113.22	118.30
3	M	134	ARG	NE-CZ-NH1	-5.64	117.48	120.30
6	B	280	ASP	CB-CG-OD1	-5.64	113.22	118.30
10	P	202	VAL	CA-CB-CG1	-5.64	102.44	110.90
10	P	305	HIS	CA-CB-CG	5.64	123.19	113.60
1	b	345	GLU	CG-CD-OE2	5.64	129.57	118.30
6	F	173	PHE	CZ-CE2-CD2	5.64	126.86	120.10
11	T	107	ALA	CB-CA-C	-5.63	101.65	110.10
10	P	117	PHE	CB-CG-CD2	5.63	124.74	120.80
5	E	577	VAL	CA-CB-CG2	5.63	119.34	110.90
11	W	74	VAL	O-C-N	-5.63	113.69	122.70
5	A	39	ASN	CB-CA-C	5.62	121.65	110.40
2	O	150	ALA	CB-CA-C	5.62	118.54	110.10
6	B	142	TYR	CG-CD1-CE1	-5.62	116.80	121.30
10	P	181	ASP	CB-CG-OD1	5.62	123.36	118.30
6	B	104	VAL	CA-CB-CG1	-5.62	102.47	110.90
1	b	73	TYR	CB-CG-CD1	-5.62	117.63	121.00
5	C	24	TYR	CG-CD1-CE1	-5.62	116.81	121.30
2	O	328	LYS	N-CA-CB	5.62	120.71	110.60
8	J	92	ASP	CB-CA-C	-5.62	99.17	110.40
5	A	272	TYR	CG-CD2-CE2	5.61	125.79	121.30
8	H	61	ASN	N-CA-CB	5.61	120.70	110.60
7	Q	279	LEU	CB-CG-CD1	5.61	120.53	111.00
11	V	156	GLN	N-CA-C	-5.61	95.86	111.00
7	Q	88	SER	N-CA-CB	5.61	118.91	110.50
8	J	102	VAL	CA-CB-CG2	-5.61	102.49	110.90
10	P	264	VAL	CG1-CB-CG2	-5.61	101.93	110.90
7	Q	336	GLU	N-CA-CB	5.60	120.68	110.60
5	A	43	CYS	CA-CB-SG	5.60	124.08	114.00
6	B	224	PHE	CB-CG-CD2	-5.60	116.88	120.80
2	O	97	TYR	N-CA-CB	5.59	120.67	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	D	257	ARG	NE-CZ-NH1	5.59	123.10	120.30
7	Q	160	PRO	N-CD-CG	5.59	111.59	103.20
11	Y	46	ARG	NE-CZ-NH1	5.59	123.10	120.30
5	E	83	ASP	CB-CG-OD1	5.59	123.33	118.30
5	A	470	PHE	CD1-CG-CD2	5.59	125.57	118.30
1	b	261	TYR	CG-CD1-CE1	-5.59	116.83	121.30
6	F	131	TYR	CB-CG-CD1	5.59	124.35	121.00
5	C	231	TYR	CG-CD2-CE2	5.59	125.77	121.30
5	C	470	PHE	CB-CG-CD1	5.59	124.71	120.80
7	Q	20	TYR	N-CA-CB	5.59	120.66	110.60
11	T	14	ALA	N-CA-CB	5.58	117.92	110.10
6	F	435	PHE	CG-CD2-CE2	-5.58	114.66	120.80
5	A	208	ASP	CB-CG-OD2	-5.58	113.28	118.30
9	I	91	ALA	CB-CA-C	-5.58	101.73	110.10
11	T	146	VAL	CA-CB-CG1	5.58	119.27	110.90
7	Q	65	THR	CA-CB-OG1	5.58	120.72	109.00
6	F	211	VAL	CG1-CB-CG2	-5.58	101.98	110.90
11	Y	59	MET	CG-SD-CE	-5.58	91.28	100.20
10	P	384	ILE	CA-CB-CG1	5.57	121.59	111.00
6	B	137	SER	O-C-N	-5.57	110.52	121.10
11	Y	63	ILE	C-N-CA	5.57	135.62	121.70
6	F	113	PHE	CB-CG-CD1	-5.57	116.90	120.80
6	B	51	GLU	N-CA-CB	5.57	120.62	110.60
5	C	156	ASP	CB-CG-OD1	5.57	123.31	118.30
9	K	117	TYR	CD1-CE1-CZ	-5.57	114.79	119.80
11	Z	78	LEU	CB-CG-CD2	5.57	120.46	111.00
5	A	460	TYR	CA-CB-CG	5.57	123.97	113.40
6	B	143	ALA	C-N-CA	5.57	135.61	121.70
11	S	153	ARG	NE-CZ-NH2	5.57	123.08	120.30
3	M	187	TYR	CD1-CE1-CZ	-5.56	114.80	119.80
5	E	383	TYR	CB-CG-CD1	5.56	124.34	121.00
9	K	155	ASP	CB-CG-OD1	-5.56	113.30	118.30
11	R	30	TYR	CD1-CE1-CZ	-5.56	114.80	119.80
1	b	42	ARG	NE-CZ-NH2	-5.55	117.52	120.30
6	F	404	TYR	CB-CG-CD2	-5.55	117.67	121.00
5	A	158	TYR	CG-CD2-CE2	-5.55	116.86	121.30
2	O	231	TYR	CB-CG-CD2	5.55	124.33	121.00
2	O	231	TYR	CB-CG-CD1	-5.55	117.67	121.00
5	E	312	MET	CG-SD-CE	-5.55	91.32	100.20
5	A	471	TYR	CB-CG-CD2	5.55	124.33	121.00
11	X	157	ASP	N-CA-CB	5.54	120.58	110.60
10	P	458	ASP	N-CA-CB	5.54	120.57	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	R	23	PHE	CB-CG-CD2	5.54	124.68	120.80
5	A	302	THR	CA-CB-CG2	-5.54	104.64	112.40
11	X	23	PHE	N-CA-CB	5.54	120.57	110.60
9	G	76	THR	CA-CB-CG2	-5.54	104.65	112.40
5	A	471	TYR	CB-CG-CD1	-5.53	117.68	121.00
1	b	272	GLN	N-CA-CB	5.52	120.54	110.60
6	B	127	PHE	CB-CG-CD2	-5.52	116.94	120.80
5	C	405	ASP	N-CA-CB	5.52	120.54	110.60
5	E	499	VAL	CG1-CB-CG2	-5.52	102.07	110.90
9	K	200	ASN	CB-CG-OD1	-5.52	110.56	121.60
11	a	142	TYR	CB-CG-CD2	5.52	124.31	121.00
11	U	20	ALA	CB-CA-C	-5.52	101.82	110.10
5	C	458	VAL	CA-CB-CG2	-5.52	102.62	110.90
9	G	108	SER	CA-C-N	5.51	127.23	116.20
11	W	46	ARG	N-CA-CB	5.51	120.53	110.60
6	F	159	ASP	CB-CG-OD1	5.51	123.26	118.30
6	F	62	VAL	CA-CB-CG2	-5.51	102.63	110.90
6	B	95	PHE	CB-CG-CD2	5.51	124.66	120.80
7	Q	306	ILE	CA-CB-CG1	5.51	121.47	111.00
9	K	195	ASP	CB-CG-OD2	-5.51	113.34	118.30
4	N	106	ASP	CB-CG-OD1	-5.51	113.34	118.30
6	B	195	ARG	NE-CZ-NH2	-5.51	117.55	120.30
6	D	237	ARG	NE-CZ-NH1	5.50	123.05	120.30
6	D	484	PHE	CB-CG-CD1	5.50	124.65	120.80
11	X	153	ARG	NE-CZ-NH1	5.49	123.05	120.30
6	B	46	PHE	CA-C-N	5.49	132.47	117.10
9	G	178	TYR	CG-CD2-CE2	-5.49	116.91	121.30
3	M	139	TYR	CD1-CE1-CZ	-5.49	114.86	119.80
5	A	404	PRO	N-CD-CG	5.48	111.42	103.20
7	Q	200	ILE	CA-C-O	-5.48	108.59	120.10
1	b	362	ILE	N-CA-C	-5.48	96.20	111.00
5	E	292	GLU	O-C-N	-5.48	113.93	122.70
3	M	8	VAL	CB-CA-C	5.48	121.81	111.40
5	E	550	PHE	O-C-N	5.48	131.46	122.70
11	Y	44	VAL	N-CA-CB	5.48	123.55	111.50
5	A	591	ARG	NE-CZ-NH2	5.47	123.04	120.30
11	U	77	SER	O-C-N	5.47	131.45	122.70
9	K	195	ASP	N-CA-CB	5.47	120.44	110.60
2	O	247	THR	CA-CB-CG2	-5.46	104.75	112.40
2	O	237	HIS	O-C-N	-5.46	113.96	122.70
3	M	169	ARG	CD-NE-CZ	-5.46	115.96	123.60
5	E	538	CYS	N-CA-CB	5.46	120.43	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	Q	337	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	b	47	LYS	N-CA-CB	5.46	120.43	110.60
1	b	90	LYS	N-CA-CB	5.46	120.43	110.60
5	C	399	VAL	CA-CB-CG2	-5.46	102.71	110.90
5	C	426	PRO	N-CA-CB	5.46	109.85	103.30
2	O	316	VAL	CA-CB-CG2	5.45	119.08	110.90
5	A	475	TYR	CB-CG-CD2	5.45	124.27	121.00
5	E	264	VAL	CG1-CB-CG2	5.45	119.62	110.90
11	V	135	PHE	CG-CD1-CE1	-5.45	114.80	120.80
1	b	320	PHE	CG-CD1-CE1	-5.45	114.80	120.80
8	H	76	VAL	CA-CB-CG2	5.45	119.07	110.90
3	M	181	THR	CA-CB-CG2	5.44	120.02	112.40
5	C	448	ARG	NE-CZ-NH1	5.44	123.02	120.30
7	Q	119	ASP	CB-CG-OD2	5.44	123.20	118.30
6	D	104	VAL	O-C-N	-5.44	114.00	122.70
5	E	470	PHE	CB-CG-CD1	-5.44	116.99	120.80
2	O	152	TYR	CB-CG-CD1	-5.43	117.74	121.00
5	C	567	TRP	CE3-CZ3-CH2	-5.43	115.23	121.20
5	C	95	GLU	OE1-CD-OE2	5.42	129.81	123.30
11	S	106	PHE	CB-CG-CD1	5.42	124.60	120.80
1	b	291	THR	CA-CB-CG2	-5.42	104.81	112.40
8	J	82	GLU	CA-CB-CG	5.42	125.33	113.40
4	N	92	LEU	N-CA-C	-5.42	96.37	111.00
5	C	354	ALA	N-CA-C	-5.42	96.37	111.00
6	F	96	THR	CA-CB-CG2	-5.42	104.81	112.40
8	L	17	ALA	CB-CA-C	-5.42	101.97	110.10
11	Z	43	CYS	CB-CA-C	-5.42	99.57	110.40
6	B	204	HIS	N-CA-CB	5.42	120.35	110.60
6	D	388	GLY	N-CA-C	-5.41	99.58	113.10
11	W	51	PHE	CD1-CG-CD2	5.41	125.33	118.30
5	E	410	VAL	CA-CB-CG1	5.41	119.01	110.90
11	Y	85	TYR	CB-CG-CD1	5.41	124.24	121.00
11	Y	97	VAL	C-N-CA	5.41	133.65	122.30
11	R	51	PHE	O-C-N	5.41	131.35	122.70
11	W	154	ALA	CB-CA-C	-5.41	101.99	110.10
11	W	35	SER	C-N-CA	5.40	133.64	122.30
9	G	81	ALA	N-CA-CB	5.40	117.66	110.10
8	J	25	ARG	NE-CZ-NH1	5.40	123.00	120.30
6	D	420	VAL	CA-CB-CG2	5.39	118.99	110.90
11	a	126	PHE	CB-CG-CD2	5.39	124.58	120.80
5	A	383	TYR	CB-CG-CD2	5.39	124.23	121.00
5	A	292	GLU	OE1-CD-OE2	5.39	129.77	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	461	SER	N-CA-CB	5.39	118.58	110.50
6	F	443	PHE	CB-CG-CD1	-5.38	117.03	120.80
6	B	294	ALA	N-CA-CB	5.38	117.64	110.10
10	P	116	PHE	CB-CG-CD1	-5.38	117.03	120.80
6	D	152	SER	N-CA-C	-5.38	96.47	111.00
9	G	160	TYR	CB-CG-CD1	5.38	124.23	121.00
5	C	461	SER	N-CA-C	-5.38	96.48	111.00
7	Q	193	TYR	CG-CD1-CE1	-5.38	117.00	121.30
10	P	175	GLN	N-CA-CB	5.38	120.28	110.60
5	C	83	ASP	CB-CG-OD2	-5.38	113.46	118.30
11	U	106	PHE	CB-CG-CD1	5.37	124.56	120.80
5	E	463	TYR	CG-CD1-CE1	-5.37	117.00	121.30
1	b	287	VAL	CA-CB-CG1	5.37	118.95	110.90
1	b	80	ASP	O-C-N	-5.37	114.12	122.70
11	Y	106	PHE	CB-CG-CD2	-5.37	117.04	120.80
11	S	157	ASP	CB-CG-OD1	5.37	123.13	118.30
5	E	300	LEU	CB-CG-CD2	5.36	120.12	111.00
2	O	371	LEU	CB-CA-C	-5.36	100.01	110.20
6	D	215	MET	CA-CB-CG	5.36	122.42	113.30
7	Q	148	LEU	CB-CA-C	-5.36	100.02	110.20
5	A	350	VAL	CA-CB-CG2	-5.36	102.86	110.90
8	L	92	ASP	CB-CG-OD1	-5.36	113.48	118.30
8	L	94	VAL	CG1-CB-CG2	-5.35	102.34	110.90
10	P	426	ASP	CB-CG-OD2	-5.35	113.48	118.30
11	S	124	ARG	NE-CZ-NH1	-5.35	117.62	120.30
11	R	88	PHE	CB-CG-CD1	-5.35	117.06	120.80
5	E	110	ARG	N-CA-C	-5.35	96.56	111.00
9	I	166	ARG	NE-CZ-NH1	5.35	122.97	120.30
5	E	83	ASP	CB-CG-OD2	-5.35	113.49	118.30
6	F	393	ARG	NH1-CZ-NH2	-5.34	113.52	119.40
6	B	340	ASP	N-CA-CB	5.34	120.22	110.60
5	E	233	LEU	CB-CG-CD2	5.34	120.08	111.00
1	b	217	GLU	OE1-CD-OE2	5.34	129.71	123.30
5	A	531	TYR	N-CA-CB	5.34	120.21	110.60
10	P	28	ASP	CB-CG-OD1	5.34	123.11	118.30
5	C	223	VAL	CG1-CB-CG2	5.34	119.44	110.90
5	A	53	HIS	CA-CB-CG	5.34	122.67	113.60
1	b	71	TYR	CZ-CE2-CD2	5.33	124.60	119.80
1	b	143	PHE	CB-CG-CD1	-5.33	117.06	120.80
4	N	41	GLN	N-CA-C	-5.33	96.60	111.00
6	D	464	LEU	C-N-CA	5.33	135.03	121.70
6	D	464	LEU	CB-CG-CD2	5.33	120.07	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	A	417	SER	N-CA-C	-5.33	96.61	111.00
5	C	382	ALA	CB-CA-C	-5.33	102.10	110.10
5	A	123	TYR	CB-CG-CD1	-5.33	117.80	121.00
5	A	470	PHE	CG-CD1-CE1	-5.33	114.94	120.80
5	E	72	VAL	CB-CA-C	5.33	121.52	111.40
6	F	455	PHE	CG-CD1-CE1	5.32	126.66	120.80
5	A	553	TYR	CB-CG-CD2	-5.32	117.81	121.00
5	C	278	ILE	N-CA-C	-5.32	96.63	111.00
6	D	197	THR	CA-CB-CG2	-5.32	104.95	112.40
1	b	64	ASN	CB-CA-C	-5.32	99.76	110.40
1	b	307	ASP	CB-CG-OD2	-5.32	113.51	118.30
6	F	103	PRO	O-C-N	-5.32	114.19	122.70
2	O	218	VAL	CG1-CB-CG2	-5.32	102.39	110.90
11	Y	78	LEU	CB-CA-C	-5.32	100.10	110.20
7	Q	174	ASP	N-CA-CB	5.32	120.17	110.60
7	Q	244	ASN	N-CA-C	-5.32	96.65	111.00
11	V	51	PHE	CB-CG-CD1	5.32	124.52	120.80
5	A	123	TYR	CG-CD1-CE1	-5.31	117.05	121.30
1	b	87	ASP	CB-CG-OD1	-5.31	113.52	118.30
6	F	249	THR	CA-CB-CG2	-5.31	104.97	112.40
5	A	355	ASP	CB-CG-OD1	-5.31	113.52	118.30
10	P	192	GLU	N-CA-CB	5.31	120.16	110.60
5	E	470	PHE	CG-CD2-CE2	-5.30	114.97	120.80
9	I	178	TYR	CB-CG-CD1	5.30	124.18	121.00
8	H	51	ASP	N-CA-CB	5.30	120.14	110.60
11	U	126	PHE	CB-CG-CD2	5.30	124.51	120.80
6	B	43	LYS	CA-CB-CG	5.29	125.05	113.40
2	O	295	ALA	CB-CA-C	-5.29	102.16	110.10
5	C	66	ASP	CB-CG-OD1	-5.29	113.54	118.30
8	L	72	ALA	N-CA-CB	5.29	117.51	110.10
1	b	50	ALA	CB-CA-C	-5.29	102.17	110.10
5	C	432	LEU	CB-CG-CD2	-5.29	102.02	111.00
10	P	357	ASP	CB-CG-OD1	-5.28	113.55	118.30
5	E	93	SER	N-CA-CB	5.28	118.42	110.50
6	F	343	THR	N-CA-CB	5.28	120.33	110.30
10	P	190	LEU	CB-CG-CD2	5.28	119.97	111.00
1	b	71	TYR	CG-CD2-CE2	-5.28	117.08	121.30
5	A	374	MET	CG-SD-CE	-5.28	91.76	100.20
7	Q	218	ARG	O-C-N	-5.28	114.25	122.70
5	C	483	ASP	CB-CG-OD1	-5.28	113.55	118.30
11	a	79	GLY	N-CA-C	-5.28	99.91	113.10
11	S	21	ILE	O-C-N	-5.28	114.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	C	383	TYR	CB-CA-C	-5.27	99.85	110.40
2	O	254	LYS	N-CA-CB	5.27	120.08	110.60
1	b	309	TRP	NE1-CE2-CZ2	5.27	136.19	130.40
10	P	144	PHE	CB-CG-CD2	5.27	124.49	120.80
10	P	292	SER	CB-CA-C	5.27	120.11	110.10
6	D	173	PHE	CB-CG-CD2	-5.26	117.12	120.80
11	W	120	SER	CB-CA-C	-5.26	100.11	110.10
1	b	243	ASP	CB-CG-OD1	5.25	123.03	118.30
6	B	121	ASP	CB-CG-OD2	5.25	123.03	118.30
6	B	133	ASP	CB-CG-OD2	-5.25	113.57	118.30
11	V	104	ALA	CB-CA-C	-5.25	102.22	110.10
3	M	157	ILE	O-C-N	-5.25	114.30	122.70
5	A	360	TRP	CD1-NE1-CE2	-5.25	104.27	109.00
6	B	143	ALA	N-CA-CB	5.25	117.45	110.10
1	b	56	VAL	CA-CB-CG2	5.25	118.77	110.90
2	O	206	PHE	CB-CG-CD1	-5.25	117.13	120.80
5	E	54	ASP	N-CA-CB	5.25	120.05	110.60
10	P	336	ARG	NE-CZ-NH1	-5.25	117.68	120.30
1	b	69	TYR	CD1-CE1-CZ	5.25	124.52	119.80
7	Q	51	TYR	CD1-CG-CD2	5.24	123.67	117.90
10	P	379	PHE	CB-CG-CD2	-5.24	117.13	120.80
11	Y	93	ALA	N-CA-CB	5.24	117.44	110.10
3	M	82	GLN	N-CA-CB	5.24	120.04	110.60
3	M	29	TYR	CB-CG-CD1	-5.24	117.86	121.00
6	B	137	SER	CA-C-N	5.24	131.78	117.10
9	K	214	ALA	N-CA-CB	5.24	117.43	110.10
11	Y	96	SER	N-CA-CB	5.24	118.36	110.50
9	G	23	PHE	N-CA-CB	5.24	120.03	110.60
6	F	298	VAL	CA-CB-CG2	5.23	118.75	110.90
5	C	98	PRO	N-CA-CB	5.23	109.58	103.30
6	D	268	TYR	CB-CG-CD2	-5.23	117.86	121.00
7	Q	192	PHE	CB-CG-CD1	5.23	124.46	120.80
3	M	31	LEU	CB-CG-CD1	-5.23	102.11	111.00
6	F	251	GLU	N-CA-CB	5.23	120.01	110.60
5	A	329	ARG	CB-CA-C	-5.23	99.94	110.40
10	P	3	ALA	N-CA-CB	5.23	117.42	110.10
5	E	202	PHE	N-CA-C	-5.23	96.89	111.00
7	Q	174	ASP	CB-CG-OD1	5.23	123.00	118.30
4	N	102	ASP	N-CA-C	-5.22	96.89	111.00
5	E	276	ASP	CB-CG-OD2	-5.22	113.60	118.30
1	b	85	GLU	N-CA-C	-5.22	96.90	111.00
5	E	458	VAL	CA-CB-CG2	5.22	118.73	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	G	171	GLU	OE1-CD-OE2	5.22	129.57	123.30
5	E	468	ASN	N-CA-CB	5.22	120.00	110.60
6	B	63	ARG	NE-CZ-NH1	-5.22	117.69	120.30
2	O	126	SER	N-CA-CB	5.22	118.33	110.50
3	M	61	MET	CG-SD-CE	-5.22	91.86	100.20
5	E	600	PHE	CB-CG-CD2	5.22	124.45	120.80
5	E	129	ASP	N-CA-CB	5.21	119.99	110.60
3	M	53	ALA	N-CA-CB	5.21	117.40	110.10
5	E	451	PHE	CG-CD2-CE2	-5.21	115.06	120.80
5	A	546	MET	CG-SD-CE	5.21	108.54	100.20
5	E	103	THR	CA-CB-CG2	-5.21	105.10	112.40
8	L	38	ASP	CB-CG-OD1	-5.21	113.61	118.30
6	D	276	THR	N-CA-CB	5.21	120.20	110.30
2	O	4	ALA	N-CA-CB	5.21	117.39	110.10
5	A	257	ALA	CB-CA-C	-5.21	102.29	110.10
11	a	157	ASP	N-CA-CB	5.21	119.97	110.60
6	D	154	GLY	O-C-N	-5.20	114.37	122.70
10	P	331	SER	N-CA-CB	5.20	118.30	110.50
11	Y	87	GLY	CA-C-O	5.20	129.96	120.60
6	F	252	ARG	NE-CZ-NH1	5.20	122.90	120.30
5	A	524	ASP	CB-CG-OD1	-5.20	113.62	118.30
2	O	294	THR	CA-CB-CG2	-5.20	105.12	112.40
3	M	17	LEU	C-N-CA	5.20	134.69	121.70
10	P	155	LEU	CB-CG-CD2	5.20	119.83	111.00
10	P	215	PHE	CG-CD1-CE1	5.19	126.51	120.80
6	F	298	VAL	CG1-CB-CG2	-5.19	102.60	110.90
8	L	49	GLN	N-CA-CB	5.19	119.94	110.60
11	U	159	VAL	CA-CB-CG2	5.19	118.68	110.90
7	Q	275	TYR	CB-CG-CD1	-5.19	117.89	121.00
5	E	603	LEU	CB-CG-CD1	5.19	119.82	111.00
11	R	60	ALA	N-CA-CB	-5.19	102.84	110.10
11	W	157	ASP	N-CA-CB	5.19	119.94	110.60
11	a	48	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	b	55	PHE	N-CA-CB	5.18	119.93	110.60
1	b	129	ASP	CB-CA-C	-5.18	100.03	110.40
7	Q	173	ASP	CB-CA-C	-5.18	100.03	110.40
8	H	38	ASP	CB-CG-OD1	-5.18	113.63	118.30
9	K	160	TYR	CB-CG-CD2	-5.18	117.89	121.00
5	C	273	SER	N-CA-CB	5.18	118.27	110.50
11	Y	51	PHE	CB-CG-CD1	-5.18	117.17	120.80
6	F	35	ASN	N-CA-CB	5.18	119.92	110.60
6	B	72	GLY	C-N-CA	5.17	134.64	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	P	244	TYR	CG-CD2-CE2	5.17	125.44	121.30
11	R	68	LEU	CB-CA-C	-5.17	100.37	110.20
10	P	96	VAL	CA-CB-CG2	-5.17	103.14	110.90
6	B	39	VAL	C-N-CA	5.17	134.63	121.70
2	O	316	VAL	CG1-CB-CG2	-5.17	102.63	110.90
6	D	398	ASP	CB-CG-OD2	-5.17	113.65	118.30
5	C	416	VAL	CA-CB-CG1	-5.17	103.15	110.90
9	I	158	ARG	NE-CZ-NH2	-5.17	117.72	120.30
10	P	164	LEU	N-CA-CB	-5.17	100.06	110.40
11	S	29	ALA	CB-CA-C	5.17	117.85	110.10
9	G	215	LEU	CA-C-O	-5.17	109.25	120.10
2	O	177	ASP	CB-CG-OD1	-5.16	113.65	118.30
5	E	125	PRO	N-CA-C	-5.16	98.69	112.10
10	P	51	LEU	CB-CG-CD1	5.16	119.77	111.00
5	A	474	ASN	CB-CA-C	-5.16	100.08	110.40
6	D	118	ARG	CB-CA-C	-5.16	100.08	110.40
10	P	6	ILE	CA-CB-CG2	-5.16	100.58	110.90
5	C	437	VAL	CG1-CB-CG2	5.16	119.15	110.90
11	U	21	ILE	CB-CA-C	-5.15	101.30	111.60
11	T	30	TYR	CZ-CE2-CD2	-5.15	115.16	119.80
11	R	117	ARG	N-CA-CB	5.15	119.87	110.60
5	C	475	TYR	CB-CG-CD2	5.14	124.09	121.00
5	E	391	PHE	CG-CD1-CE1	-5.14	115.14	120.80
11	W	152	SER	O-C-N	-5.14	114.47	122.70
2	O	148	THR	CA-CB-CG2	-5.14	105.20	112.40
5	C	405	ASP	CB-CG-OD1	-5.14	113.67	118.30
6	F	211	VAL	N-CA-CB	5.14	122.80	111.50
5	A	37	ALA	C-N-CA	5.14	134.54	121.70
9	G	71	LEU	CB-CG-CD1	5.14	119.73	111.00
9	G	9	THR	CA-CB-CG2	-5.13	105.21	112.40
11	X	85	TYR	CB-CG-CD1	-5.13	117.92	121.00
11	S	135	PHE	CB-CG-CD2	5.13	124.39	120.80
5	C	483	ASP	CB-CG-OD2	5.13	122.92	118.30
9	G	160	TYR	CA-CB-CG	-5.13	103.66	113.40
2	O	152	TYR	CB-CG-CD2	5.13	124.08	121.00
3	M	169	ARG	NE-CZ-NH2	-5.13	117.74	120.30
5	A	329	ARG	NE-CZ-NH1	-5.12	117.74	120.30
5	C	407	THR	N-CA-C	-5.12	97.17	111.00
2	O	171	SER	N-CA-CB	5.12	118.18	110.50
6	D	278	LEU	N-CA-C	-5.12	97.18	111.00
11	W	75	CYS	O-C-N	-5.12	114.51	122.70
6	B	268	TYR	CA-CB-CG	5.12	123.12	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	125	PRO	N-CA-CB	5.12	109.44	103.30
7	Q	299	ALA	CB-CA-C	-5.12	102.43	110.10
5	C	471	TYR	CG-CD2-CE2	5.11	125.39	121.30
6	F	101	ARG	NE-CZ-NH2	5.11	122.86	120.30
10	P	353	LEU	N-CA-CB	5.11	120.62	110.40
5	C	596	VAL	N-CA-C	-5.11	97.21	111.00
6	F	69	GLU	CB-CA-C	-5.11	100.19	110.40
7	Q	166	PHE	CB-CG-CD2	-5.10	117.23	120.80
6	F	208	PHE	CB-CG-CD2	-5.10	117.23	120.80
6	F	279	THR	O-C-N	-5.10	114.54	122.70
5	A	203	ASP	CB-CG-OD1	-5.10	113.71	118.30
10	P	19	ILE	CA-CB-CG1	5.10	120.69	111.00
6	F	272	ARG	NE-CZ-NH2	-5.10	117.75	120.30
6	D	376	LEU	CB-CG-CD2	5.10	119.67	111.00
5	E	475	TYR	CG-CD2-CE2	-5.10	117.22	121.30
6	F	212	PHE	O-C-N	5.09	130.85	122.70
5	A	462	LYS	CB-CA-C	-5.09	100.21	110.40
6	F	452	ARG	NE-CZ-NH1	-5.09	117.75	120.30
6	D	322	VAL	C-N-CA	5.09	134.43	121.70
6	F	354	THR	CA-CB-OG1	5.09	119.68	109.00
2	O	164	ARG	NE-CZ-NH1	5.09	122.84	120.30
6	F	424	ALA	CB-CA-C	-5.09	102.47	110.10
6	F	268	TYR	CG-CD1-CE1	-5.08	117.23	121.30
7	Q	303	GLN	N-CA-CB	5.08	119.75	110.60
6	B	412	ASP	N-CA-CB	5.08	119.75	110.60
6	D	321	ARG	NE-CZ-NH2	-5.08	117.76	120.30
6	D	448	ALA	CB-CA-C	-5.08	102.48	110.10
6	D	321	ARG	NH1-CZ-NH2	5.08	124.98	119.40
7	Q	187	ALA	N-CA-CB	5.08	117.21	110.10
5	A	444	LYS	CB-CG-CD	5.07	124.79	111.60
7	Q	97	TYR	CB-CG-CD1	-5.07	117.96	121.00
11	a	30	TYR	CB-CG-CD2	5.07	124.05	121.00
7	Q	278	PHE	CB-CG-CD2	-5.07	117.25	120.80
5	C	567	TRP	CD1-CG-CD2	-5.07	102.25	106.30
11	W	76	TYR	CB-CG-CD2	5.07	124.04	121.00
2	O	303	TRP	CG-CD2-CE3	-5.07	129.34	133.90
5	C	88	THR	CA-CB-CG2	-5.07	105.31	112.40
11	X	125	LEU	CB-CG-CD2	5.07	119.61	111.00
2	O	276	SER	CB-CA-C	-5.06	100.48	110.10
6	D	291	VAL	CA-CB-CG1	-5.06	103.30	110.90
11	X	68	LEU	CB-CG-CD2	-5.06	102.39	111.00
8	L	39	ALA	CB-CA-C	-5.06	102.51	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	K	166	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
1	b	211	LEU	CB-CG-CD1	-5.06	102.40	111.00
6	B	237	ARG	NE-CZ-NH1	-5.06	117.77	120.30
11	W	137	GLU	CB-CA-C	-5.06	100.28	110.40
7	Q	237	LEU	CB-CG-CD2	-5.06	102.40	111.00
7	Q	289	TYR	CZ-CE2-CD2	-5.05	115.25	119.80
9	I	173	VAL	O-C-N	5.05	130.79	122.70
10	P	269	SER	N-CA-CB	5.05	118.08	110.50
5	E	494	GLU	CA-CB-CG	5.05	124.52	113.40
1	b	346	LEU	C-N-CA	5.05	134.33	121.70
2	O	107	VAL	CA-C-N	5.05	131.25	117.10
2	O	313	VAL	CA-CB-CG2	-5.05	103.32	110.90
5	E	135	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
5	E	442	ASP	CA-CB-CG	-5.05	102.28	113.40
6	F	173	PHE	CG-CD2-CE2	-5.05	115.24	120.80
5	E	541	TRP	CB-CG-CD1	5.05	133.56	127.00
11	Z	53	ASN	CB-CG-OD1	5.05	131.70	121.60
9	G	78	SER	N-CA-CB	5.05	118.07	110.50
11	Z	128	GLY	O-C-N	5.05	130.78	122.70
5	A	139	TRP	CG-CD2-CE3	-5.05	129.36	133.90
11	Y	126	PHE	CZ-CE2-CD2	-5.05	114.04	120.10
11	W	126	PHE	CB-CG-CD2	5.04	124.33	120.80
6	B	259	ALA	CB-CA-C	-5.04	102.53	110.10
11	U	135	PHE	CB-CG-CD2	-5.04	117.27	120.80
11	Z	48	ASP	CB-CA-C	-5.04	100.31	110.40
5	E	391	PHE	CA-C-O	-5.04	109.51	120.10
5	E	586	PHE	CB-CG-CD2	-5.04	117.27	120.80
9	I	24	ILE	C-N-CA	5.04	134.30	121.70
9	K	45	ILE	CA-CB-CG1	5.04	120.57	111.00
9	K	223	TYR	CG-CD1-CE1	5.04	125.33	121.30
1	b	61	ARG	NE-CZ-NH2	-5.04	117.78	120.30
7	Q	95	MET	CG-SD-CE	-5.04	92.14	100.20
1	b	37	GLY	CA-C-O	-5.03	111.54	120.60
5	A	93	SER	O-C-N	5.03	130.75	122.70
8	J	28	ARG	NE-CZ-NH2	-5.03	117.78	120.30
5	E	531	TYR	CB-CG-CD1	5.03	124.02	121.00
11	T	14	ALA	CB-CA-C	-5.03	102.56	110.10
6	F	310	THR	CA-CB-CG2	-5.03	105.36	112.40
6	D	144	ARG	NE-CZ-NH1	5.02	122.81	120.30
5	A	123	TYR	CD1-CG-CD2	5.02	123.42	117.90
5	E	355	ASP	N-CA-CB	5.02	119.64	110.60
5	C	209	PHE	CB-CG-CD2	5.02	124.31	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	V	158	VAL	N-CA-CB	5.02	122.54	111.50
11	V	142	TYR	CG-CD1-CE1	5.02	125.31	121.30
11	R	68	LEU	CB-CG-CD1	5.01	119.52	111.00
11	a	114	ALA	C-N-CA	5.01	132.83	122.30
1	b	187	VAL	N-CA-C	-5.01	97.47	111.00
3	M	132	VAL	CA-CB-CG2	-5.01	103.38	110.90
11	X	30	TYR	CB-CG-CD1	-5.01	117.99	121.00
11	T	147	ALA	N-CA-CB	-5.01	103.08	110.10
1	b	20	TYR	CG-CD2-CE2	-5.01	117.29	121.30
11	S	46	ARG	NE-CZ-NH2	-5.01	117.80	120.30
5	E	475	TYR	CD1-CE1-CZ	5.01	124.31	119.80
5	A	449	LYS	CB-CG-CD	5.01	124.62	111.60
11	Y	159	VAL	N-CA-CB	5.01	122.51	111.50
6	B	370	TYR	CA-C-O	-5.00	109.59	120.10
5	C	297	PHE	CB-CG-CD1	-5.00	117.30	120.80
5	A	339	LEU	CB-CA-C	-5.00	100.69	110.20
10	P	460	ARG	NE-CZ-NH1	5.00	122.80	120.30
5	E	264	VAL	CA-CB-CG2	-5.00	103.40	110.90

There are no chirality outliers.

All (167) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
5	A	105	TYR	Sidechain
5	A	110	ARG	Sidechain
5	A	123	TYR	Sidechain
5	A	126	ARG	Sidechain
5	A	135	ARG	Sidechain
5	A	158	TYR	Sidechain
5	A	212	TYR	Sidechain
5	A	28	TYR	Sidechain
5	A	344	ARG	Sidechain
5	A	383	TYR	Sidechain
5	A	46	TYR	Sidechain
5	A	460	TYR	Sidechain
5	A	475	TYR	Sidechain
5	A	610	ARG	Sidechain
6	B	101	ARG	Sidechain
6	B	111	ARG	Sidechain
6	B	131	TYR	Sidechain
6	B	142	TYR	Sidechain
6	B	147	PRO	Peptide

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Mol	Chain	Res	Type	Group
6	B	166	ARG	Sidechain
6	B	229	PHE	Sidechain
6	B	237	ARG	Sidechain
6	B	257	ARG	Sidechain
6	B	265	TYR	Sidechain
6	B	268	TYR	Sidechain
6	B	272	ARG	Sidechain
6	B	284	TYR	Sidechain
6	B	301	ARG	Sidechain
6	B	307	TYR	Sidechain
6	B	316	TYR	Sidechain
6	B	352	TYR	Sidechain
6	B	404	TYR	Sidechain
6	B	485	TYR	Sidechain
6	B	49	TYR	Sidechain
5	C	105	TYR	Sidechain
5	C	123	TYR	Sidechain
5	C	126	ARG	Sidechain
5	C	231	TYR	Sidechain
5	C	238	ARG	Sidechain
5	C	28	TYR	Sidechain
5	C	334	TYR	Sidechain
5	C	342	TYR	Sidechain
5	C	344	ARG	Sidechain
5	C	383	TYR	Sidechain
5	C	448	ARG	Sidechain
5	C	463	TYR	Sidechain
5	C	471	TYR	Sidechain
5	C	482	ARG	Sidechain
5	C	531	TYR	Sidechain
5	C	579	HIS	Sidechain
5	C	73	TYR	Sidechain
6	D	142	TYR	Sidechain
6	D	166	ARG	Sidechain
6	D	223	ARG	Sidechain
6	D	265	TYR	Sidechain
6	D	301	ARG	Sidechain
6	D	325	ARG	Sidechain
6	D	352	TYR	Sidechain
6	D	49	TYR	Sidechain
5	E	126	ARG	Sidechain
5	E	212	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	E	218	ARG	Sidechain
5	E	244	PHE	Sidechain
5	E	272	TYR	Sidechain
5	E	359	ARG	Sidechain
5	E	383	TYR	Sidechain
5	E	46	TYR	Sidechain
5	E	470	PHE	Sidechain
5	E	471	TYR	Sidechain
5	E	482	ARG	Sidechain
5	E	531	TYR	Sidechain
5	E	534	TYR	Sidechain
5	E	548	ARG	Sidechain
5	E	553	TYR	Sidechain
5	E	587	PHE	Sidechain
5	E	591	ARG	Sidechain
5	E	62	ARG	Sidechain
5	E	73	TYR	Sidechain
6	F	127	PHE	Sidechain
6	F	142	TYR	Sidechain
6	F	223	ARG	Sidechain
6	F	225	PHE	Sidechain
6	F	257	ARG	Sidechain
6	F	268	TYR	Sidechain
6	F	302	ARG	Sidechain
6	F	352	TYR	Sidechain
6	F	370	TYR	Sidechain
6	F	404	TYR	Sidechain
6	F	485	TYR	Sidechain
9	G	114	ARG	Sidechain
9	G	206	ARG	Sidechain
9	G	219	ARG	Sidechain
9	G	52	ARG	Sidechain
9	I	117	TYR	Sidechain
9	I	160	TYR	Sidechain
9	I	223	TYR	Sidechain
8	J	28	ARG	Sidechain
8	J	46	TYR	Sidechain
9	K	114	ARG	Sidechain
9	K	117	TYR	Sidechain
9	K	160	TYR	Sidechain
9	K	178	TYR	Sidechain
8	L	27	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	M	139	TYR	Sidechain
3	M	201	TYR	Sidechain
3	M	29	TYR	Sidechain
3	M	42	ARG	Sidechain
2	O	11	PHE	Sidechain
2	O	110	TYR	Sidechain
2	O	210	TYR	Sidechain
2	O	251	ARG	Sidechain
2	O	258	ARG	Sidechain
2	O	285	ARG	Sidechain
2	O	356	PHE	Sidechain
2	O	44	PHE	Sidechain
2	O	53	PHE	Sidechain
2	O	6	TYR	Sidechain
10	P	188	ARG	Sidechain
10	P	206	HIS	Sidechain
10	P	220	ARG	Sidechain
10	P	305	HIS	Sidechain
10	P	32	ARG	Sidechain
10	P	328	ARG	Sidechain
10	P	330	TYR	Sidechain
10	P	463	TYR	Sidechain
10	P	475	TYR	Sidechain
7	Q	126	ARG	Sidechain
7	Q	181	ARG	Sidechain
7	Q	218	ARG	Sidechain
7	Q	266	ARG	Sidechain
7	Q	51	TYR	Sidechain
7	Q	77	TYR	Sidechain
11	R	124	ARG	Sidechain
11	R	153	ARG	Sidechain
11	R	85	TYR	Sidechain
11	S	76	TYR	Sidechain
11	T	85	TYR	Sidechain
11	U	126	PHE	Sidechain
11	U	30	TYR	Sidechain
11	U	76	TYR	Sidechain
11	W	142	TYR	Sidechain
11	X	117	ARG	Sidechain
11	X	124	ARG	Sidechain
11	X	126	PHE	Sidechain
11	X	142	TYR	Sidechain

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Mol	Chain	Res	Type	Group
11	X	153	ARG	Sidechain
11	X	46	ARG	Sidechain
11	X	76	TYR	Sidechain
11	Y	106	PHE	Sidechain
11	Y	23	PHE	Sidechain
11	Y	30	TYR	Sidechain
11	Z	11	PHE	Sidechain
11	Z	124	ARG	Sidechain
11	a	142	TYR	Sidechain
11	a	30	TYR	Sidechain
11	a	85	TYR	Sidechain
1	b	116	TYR	Sidechain
1	b	186	TYR	Sidechain
1	b	193	ARG	Sidechain
1	b	212	PHE	Sidechain
1	b	268	GLU	Peptide
1	b	352	ARG	Sidechain
1	b	61	ARG	Sidechain
1	b	69	TYR	Sidechain
1	b	73	TYR	Sidechain
1	b	86	GLY	Peptide
1	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	b	2540	0	2537	0	0
2	O	3122	0	3155	6	0
3	M	1691	0	1740	7	0
4	N	928	0	926	1	0
5	A	4578	0	4519	15	0
5	C	4578	0	4519	23	0
5	E	4578	0	4519	20	0
6	B	3585	0	3567	11	0
6	D	3585	0	3567	14	0
6	F	3585	0	3567	14	0
7	Q	2802	0	2689	11	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	824	0	877	1	0
8	J	824	0	877	0	0
8	L	824	0	877	0	0
9	G	1731	0	1797	2	0
9	I	1731	0	1797	6	0
9	K	1731	0	1797	2	0
10	P	3712	0	3829	13	0
11	R	1071	0	1141	5	0
11	S	1071	0	1141	4	0
11	T	1071	0	1141	8	0
11	U	1071	0	1141	0	0
11	V	1071	0	1141	2	0
11	W	1071	0	1141	8	0
11	X	1071	0	1141	7	0
11	Y	1071	0	1141	2	0
11	Z	1071	0	1141	7	0
11	a	1071	0	1141	0	0
All	All	57659	0	58566	169	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 (169) 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:S:66:TYR:HB3	11:S:144:LEU:HD22	1.32	1.07
11:T:66:TYR:HB3	11:T:144:LEU:HD22	1.36	1.06
11:X:66:TYR:HB3	11:X:144:LEU:HD22	1.38	1.02
11:R:66:TYR:HB3	11:R:144:LEU:HD22	1.45	0.97
11:X:66:TYR:CB	11:X:144:LEU:HD22	2.05	0.86
11:X:66:TYR:HB3	11:X:144:LEU:CD2	2.13	0.77
11:T:66:TYR:CB	11:T:144:LEU:HD22	2.13	0.75
11:T:66:TYR:HB3	11:T:144:LEU:CD2	2.16	0.74
11:R:66:TYR:HB3	11:R:144:LEU:CD2	2.20	0.72
11:X:66:TYR:CG	11:X:144:LEU:HD22	2.25	0.71
11:W:66:TYR:HB3	11:W:144:LEU:HD22	1.78	0.66
5:C:148:VAL:HG13	5:C:185:ILE:HG22	1.79	0.65
6:F:254:ILE:HG12	6:F:257:ARG:HH21	1.63	0.64
5:C:198:LEU:HD23	5:C:209:PHE:HB2	1.79	0.63
6:F:250:ILE:HD13	6:F:250:ILE:H	1.64	0.62
2:O:170:LEU:HD23	2:O:173:ARG:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:66:TYR:HB3	11:V:144:LEU:HD22	1.82	0.61
11:Z:66:TYR:HB3	11:Z:144:LEU:HD22	1.83	0.60
9:K:37:LEU:HD21	10:P:252:LEU:HD21	1.82	0.60
5:C:481:LEU:HD23	5:C:484:ARG:HH21	1.68	0.58
5:E:47:GLU:HG2	5:E:87:ARG:HE	1.69	0.58
5:C:259:GLY:H	6:D:381:ARG:HH21	1.51	0.57
11:R:66:TYR:CB	11:R:144:LEU:HD22	2.26	0.57
5:E:482:ARG:HH22	5:E:544:PHE:HA	1.69	0.57
4:N:40:TYR:CE1	4:N:50:ILE:HD11	2.40	0.56
11:S:66:TYR:CB	11:S:144:LEU:HD22	2.21	0.56
11:S:80:GLN:H	11:S:158:VAL:HG13	1.69	0.56
7:Q:237:LEU:N	7:Q:237:LEU:HD12	2.21	0.55
6:F:402:GLN:HE22	6:F:475:ARG:HB2	1.72	0.55
11:X:66:TYR:CG	11:X:144:LEU:CD2	2.90	0.55
5:E:406:ARG:HE	5:E:406:ARG:H	1.53	0.55
5:C:81:VAL:HG21	6:D:70:ILE:HG21	1.89	0.55
3:M:121:ARG:HH12	7:Q:238:LYS:HZ2	1.55	0.54
3:M:66:PHE:HB2	7:Q:337:ARG:HH22	1.72	0.54
3:M:30:SER:HB3	3:M:34:ARG:HH12	1.72	0.54
5:A:333:ILE:HD13	5:A:360:TRP:CD1	2.41	0.54
11:W:47:PRO:HA	11:V:125:LEU:HD11	1.90	0.54
6:B:43:LYS:HD2	6:B:93:VAL:HG21	1.90	0.54
5:E:104:ILE:HG23	5:E:112:LEU:HB2	1.90	0.54
11:W:113:ASP:O	11:W:116:VAL:HG22	2.08	0.53
5:A:592:GLY:HA3	5:A:598:GLY:H	1.74	0.53
5:C:548:ARG:HH21	5:C:551:ILE:HG23	1.72	0.53
11:T:66:TYR:CG	11:T:144:LEU:HD22	2.44	0.52
5:C:61:ILE:HG13	5:C:71:GLN:HE21	1.74	0.52
6:B:359:PHE:CD2	6:B:377:PRO:HG2	2.44	0.52
9:I:222:LEU:HB2	9:I:223:TYR:CD2	2.46	0.50
7:Q:109:LEU:HG	7:Q:181:ARG:HE	1.75	0.50
11:W:66:TYR:CG	11:W:144:LEU:HD22	2.46	0.50
9:I:222:LEU:HB2	9:I:223:TYR:CE2	2.47	0.49
11:Y:66:TYR:CG	11:Y:144:LEU:HD22	2.47	0.49
5:C:122:ILE:HD12	6:D:144:ARG:HG3	1.94	0.49
6:B:102:ILE:HG23	6:B:104:VAL:HG13	1.94	0.49
6:F:290:GLU:O	6:F:291:VAL:HG13	2.11	0.49
5:C:599:GLU:O	5:C:603:LEU:HD23	2.12	0.49
7:Q:26:SER:H	7:Q:29:GLN:HB3	1.78	0.49
11:W:66:TYR:HB3	11:W:144:LEU:HD13	1.94	0.49
6:D:403:LEU:HD21	6:D:461:ALA:HB1	1.93	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:238:ARG:HG2	5:C:543:THR:HG23	1.95	0.49
11:Z:27:GLY:HA3	11:Z:102:LEU:HA	1.93	0.49
6:D:257:ARG:HA	6:D:260:LEU:HD12	1.95	0.48
6:F:195:ARG:HE	6:F:207:ASN:HA	1.76	0.48
11:T:108:ILE:HG23	11:T:133:LEU:HD22	1.95	0.48
6:D:319:ALA:HA	6:D:329:ILE:HG23	1.95	0.48
6:B:403:LEU:O	6:B:407:TYR:HB2	2.13	0.48
5:A:44:ALA:H	5:A:47:GLU:HG3	1.77	0.48
10:P:241:GLN:O	10:P:245:HIS:CD2	2.66	0.48
6:F:192:GLY:H	6:F:194:VAL:HG22	1.79	0.48
6:D:339:ASN:HD22	6:D:344:HIS:CD2	2.33	0.47
5:C:56:LEU:HD21	5:C:126:ARG:HE	1.79	0.47
5:A:333:ILE:HG12	5:A:360:TRP:CG	2.49	0.47
5:A:185:ILE:O	5:A:185:ILE:HG23	2.15	0.47
2:O:165:LYS:HD3	2:O:270:LEU:HD22	1.97	0.47
11:R:46:ARG:HH21	11:R:49:LEU:HD21	1.80	0.47
5:C:326:VAL:HG11	5:C:370:ARG:HH22	1.79	0.47
8:H:35:ALA:HB2	9:G:43:TYR:HA	1.97	0.46
11:Z:70:VAL:O	11:Z:74:VAL:HG23	2.16	0.46
6:D:305:PRO:HB3	6:D:307:TYR:CE1	2.51	0.46
11:Z:32:THR:HG23	11:Z:57:VAL:HG13	1.98	0.46
11:R:126:PHE:CE1	11:R:127:VAL:HG13	2.50	0.46
9:I:121:LEU:HD11	9:I:188:VAL:HG13	1.97	0.46
5:E:272:TYR:CD1	5:E:536:ALA:HB1	2.50	0.45
11:T:97:VAL:HG22	11:T:144:LEU:HA	1.99	0.45
5:E:112:LEU:HA	5:E:115:ILE:HG12	1.98	0.45
10:P:284:GLU:H	10:P:284:GLU:CD	2.20	0.45
11:T:139:LEU:H	11:T:139:LEU:HD23	1.81	0.45
6:F:357:GLN:HE22	6:F:359:PHE:HB2	1.81	0.45
5:A:81:VAL:HG13	6:B:70:ILE:HD12	1.99	0.45
5:E:192:THR:HG22	5:E:193:LEU:N	2.32	0.45
10:P:368:LEU:HB3	10:P:422:VAL:HG11	1.98	0.45
6:D:71:ARG:HB2	6:D:74:ARG:HG3	1.98	0.45
11:Y:66:TYR:HB3	11:Y:144:LEU:HD13	1.99	0.45
5:C:73:TYR:CD1	5:C:326:VAL:HB	2.52	0.44
6:B:127:PHE:CZ	9:I:92:ARG:HD2	2.51	0.44
7:Q:304:PHE:HB2	11:Z:117:ARG:HH22	1.83	0.44
5:E:365:ARG:HH12	6:F:301:ARG:HH21	1.64	0.44
7:Q:110:MET:SD	7:Q:123:ILE:HD12	2.58	0.44
9:I:126:VAL:HG23	9:I:156:ILE:HG23	1.99	0.44
11:W:66:TYR:CB	11:W:144:LEU:HD22	2.46	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:162:PHE:HA	5:C:168:SER:HA	2.00	0.43
5:A:243:LEU:HD12	5:A:243:LEU:HA	1.89	0.43
10:P:14:ASN:ND2	10:P:17:ARG:HH21	2.15	0.43
11:X:63:ILE:HG21	11:X:101:GLY:HA2	1.99	0.43
10:P:47:LEU:HA	10:P:50:ILE:HG12	1.99	0.43
5:A:323:ASN:HD22	6:B:313:SER:HB3	1.82	0.43
6:D:137:SER:HA	6:D:138:PRO:HD3	1.83	0.43
10:P:380:TRP:CD1	10:P:429:HIS:HB3	2.53	0.43
2:O:162:ALA:HB1	2:O:274:HIS:HA	2.01	0.43
10:P:281:THR:HB	10:P:283:LYS:H	1.83	0.43
10:P:228:THR:HG22	10:P:230:ILE:H	1.84	0.43
5:C:522:LYS:HA	5:C:526:LEU:HD13	2.01	0.43
6:F:346:ILE:H	6:F:346:ILE:HD12	1.84	0.43
5:C:364:LEU:HD13	5:C:364:LEU:HA	1.93	0.42
5:E:73:TYR:CG	5:E:327:ALA:HB2	2.54	0.42
5:E:450:HIS:HB3	5:E:526:LEU:HG	2.00	0.42
7:Q:106:ASN:HD21	7:Q:126:ARG:HD3	1.84	0.42
2:O:97:TYR:H	2:O:100:LEU:HB2	1.85	0.42
5:E:227:LEU:HD11	5:E:399:VAL:HG13	2.00	0.42
6:D:395:ASP:O	6:D:399:VAL:HG23	2.19	0.42
5:C:294:LEU:HD22	6:D:144:ARG:HH11	1.83	0.42
10:P:248:LEU:HA	10:P:248:LEU:HD23	1.90	0.42
3:M:107:SER:H	3:M:158:ILE:HD12	1.85	0.42
5:A:597:HIS:CE1	5:A:599:GLU:OE2	2.73	0.42
5:A:496:GLU:O	5:A:500:GLN:HG3	2.19	0.42
9:G:142:LEU:O	9:G:146:VAL:HG13	2.19	0.42
5:C:61:ILE:HG21	5:C:371:LEU:HD11	2.02	0.42
6:D:362:ARG:H	6:D:362:ARG:HD2	1.84	0.42
5:A:247:VAL:HG21	5:A:463:TYR:CD2	2.55	0.42
11:X:89:ILE:HG23	11:X:150:LEU:HD22	2.02	0.42
6:B:192:GLY:H	6:B:194:VAL:HG22	1.85	0.42
5:E:192:THR:HG22	5:E:193:LEU:H	1.85	0.42
5:E:175:PRO:HG2	5:E:209:PHE:CE1	2.55	0.42
11:S:74:VAL:HG12	11:S:78:LEU:HD21	2.02	0.42
6:F:393:ARG:HH21	6:F:458:LEU:HB3	1.85	0.42
5:C:218:ARG:HH22	5:C:330:GLU:HG3	1.85	0.41
6:F:142:TYR:CE2	6:F:318:ARG:HA	2.54	0.41
6:B:402:GLN:HE21	6:B:473:LEU:HD22	1.86	0.41
5:E:44:ALA:HB1	6:D:85:GLY:HA2	2.02	0.41
5:E:112:LEU:HD22	5:E:122:ILE:O	2.20	0.41
5:E:233:LEU:HD22	5:E:235:THR:HG23	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:C:300:LEU:HD23	5:C:300:LEU:HA	1.86	0.41
3:M:158:ILE:O	3:M:162:VAL:HG23	2.19	0.41
11:W:52:LYS:HB3	11:W:126:PHE:CZ	2.56	0.41
6:F:366:ASN:HD21	5:A:457:SER:HA	1.86	0.41
10:P:275:LEU:HB3	10:P:321:THR:HG21	2.02	0.41
10:P:47:LEU:HD22	10:P:80:LEU:HD11	2.03	0.41
5:A:171:LYS:H	5:A:346:GLN:CD	2.24	0.41
9:I:38:LYS:O	9:I:42:GLU:HG3	2.20	0.41
5:E:280:TYR:HA	5:E:353:ILE:HG23	2.02	0.41
5:A:249:GLY:H	5:A:411:SER:HB2	1.85	0.41
5:C:513:ILE:HG22	5:C:554:HIS:CE1	2.56	0.41
11:Z:141:LEU:O	11:Z:144:LEU:HB3	2.21	0.41
5:E:545:ASP:HB3	5:E:600:PHE:CG	2.56	0.41
11:Z:135:PHE:O	11:Z:138:VAL:HG22	2.20	0.41
3:M:18:MET:HE1	3:M:180:ARG:HH12	1.86	0.41
2:O:86:LEU:HD13	2:O:97:TYR:CZ	2.56	0.40
3:M:57:MET:SD	3:M:146:LEU:HG	2.61	0.40
11:T:141:LEU:HD23	11:T:141:LEU:HA	1.89	0.40
5:E:261:GLY:HA3	5:E:441:LEU:HD11	2.03	0.40
6:B:86:ILE:HB	5:C:44:ALA:HA	2.03	0.40
5:C:135:ARG:HA	5:C:193:LEU:HD23	2.03	0.40
9:K:41:GLN:HG3	10:P:255:PHE:CE2	2.56	0.40
5:E:116:LYS:HE3	6:F:325:ARG:HH21	1.86	0.40
5:A:323:ASN:HA	6:B:313:SER:HB3	2.04	0.40
6:F:312:LEU:O	6:F:316:TYR:CD2	2.74	0.40
2:O:48:PHE:CE2	2:O:308:ALA:HB2	2.56	0.40
7:Q:109:LEU:HD23	7:Q:181:ARG:HH21	1.87	0.40
7:Q:84:ARG:HG2	7:Q:95:MET:SD	2.62	0.40
7:Q:186:LYS:HE3	7:Q:241:LEU:H	1.86	0.40
11:W:50:LEU:O	11:W:54:ILE:HG13	2.21	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	b	306/840 (36%)	283 (92%)	16 (5%)	7 (2%)	8	48
2	O	390/392 (100%)	359 (92%)	19 (5%)	12 (3%)	5	42
3	M	208/256 (81%)	201 (97%)	6 (3%)	1 (0%)	34	77
4	N	113/118 (96%)	103 (91%)	8 (7%)	2 (2%)	11	53
5	A	591/616 (96%)	543 (92%)	34 (6%)	14 (2%)	7	47
5	C	591/616 (96%)	540 (91%)	35 (6%)	16 (3%)	6	45
5	E	591/616 (96%)	536 (91%)	43 (7%)	12 (2%)	9	51
6	B	455/517 (88%)	415 (91%)	32 (7%)	8 (2%)	11	53
6	D	455/517 (88%)	406 (89%)	34 (8%)	15 (3%)	5	40
6	F	455/517 (88%)	405 (89%)	39 (9%)	11 (2%)	7	47
7	Q	343/345 (99%)	312 (91%)	24 (7%)	7 (2%)	9	51
8	H	103/114 (90%)	101 (98%)	0	2 (2%)	10	52
8	J	103/114 (90%)	99 (96%)	2 (2%)	2 (2%)	10	52
8	L	103/114 (90%)	99 (96%)	2 (2%)	2 (2%)	10	52
9	G	215/233 (92%)	205 (95%)	8 (4%)	2 (1%)	21	67
9	I	215/233 (92%)	209 (97%)	6 (3%)	0	100	100
9	K	215/233 (92%)	207 (96%)	5 (2%)	3 (1%)	14	58
10	P	457/478 (96%)	429 (94%)	19 (4%)	9 (2%)	9	51
11	R	148/160 (92%)	138 (93%)	6 (4%)	4 (3%)	6	45
11	S	148/160 (92%)	139 (94%)	7 (5%)	2 (1%)	14	58
11	T	148/160 (92%)	137 (93%)	7 (5%)	4 (3%)	6	45
11	U	148/160 (92%)	135 (91%)	10 (7%)	3 (2%)	9	51
11	V	148/160 (92%)	139 (94%)	7 (5%)	2 (1%)	14	58
11	W	148/160 (92%)	143 (97%)	4 (3%)	1 (1%)	26	71
11	X	148/160 (92%)	138 (93%)	6 (4%)	4 (3%)	6	45
11	Y	148/160 (92%)	140 (95%)	5 (3%)	3 (2%)	9	51
11	Z	148/160 (92%)	138 (93%)	6 (4%)	4 (3%)	6	45
11	a	148/160 (92%)	136 (92%)	8 (5%)	4 (3%)	6	45
All	All	7389/8469 (87%)	6835 (92%)	398 (5%)	156 (2%)	13	50

All (156) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	O	167	THR
2	O	172	VAL
5	E	475	TYR
6	F	125	LYS
6	F	207	ASN
6	F	293	ALA
5	A	475	TYR
5	C	475	TYR
5	C	565	ALA
6	D	143	ALA
6	D	319	ALA
7	Q	126	ARG
7	Q	174	ASP
9	K	144	ARG
10	P	389	LYS
11	Y	159	VAL
11	Z	48	ASP
11	a	158	VAL
11	a	159	VAL
2	O	39	ILE
2	O	97	TYR
2	O	116	TRP
2	O	176	HIS
5	E	120	GLN
5	E	456	THR
5	E	575	GLY
5	E	593	GLU
6	F	340	ASP
5	A	177	ARG
5	A	234	LEU
5	A	449	LYS
5	A	450	HIS
5	A	565	ALA
5	A	575	GLY
6	B	163	SER
6	B	294	ALA
5	C	75	GLU
5	C	125	PRO
5	C	575	GLY
6	D	88	VAL
6	D	323	GLU
6	D	377	PRO
6	D	467	ILE

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Mol	Chain	Res	Type
7	Q	230	SER
7	Q	245	ILE
8	J	77	GLN
10	P	391	ASN
10	P	392	TYR
8	H	77	GLN
11	X	157	ASP
11	Y	156	GLN
11	W	157	ASP
11	V	158	VAL
11	a	47	PRO
11	T	156	GLN
11	T	159	VAL
1	b	47	LYS
1	b	89	ASP
1	b	178	ALA
4	N	4	LYS
5	E	308	LYS
5	E	529	ASN
6	F	135	ASN
5	A	305	SER
5	A	405	ASP
5	A	441	LEU
6	B	83	THR
6	B	293	ALA
5	C	325	PRO
6	D	141	PRO
6	D	203	GLY
7	Q	121	GLY
7	Q	171	GLU
8	L	63	GLY
9	K	192	ASN
10	P	234	ASN
10	P	332	ASP
11	U	155	THR
11	X	156	GLN
11	Y	158	VAL
11	Z	47	PRO
11	a	157	ASP
11	S	47	PRO
1	b	86	GLY
2	O	2	ALA

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Mol	Chain	Res	Type
2	O	229	ALA
2	O	360	LYS
2	O	375	ALA
4	N	115	LEU
5	E	207	SER
6	F	202	ASP
6	F	296	GLU
5	A	257	ALA
6	B	121	ASP
6	B	391	MET
5	C	230	ASP
5	C	405	ASP
5	C	449	LYS
6	D	179	PRO
10	P	34	GLU
10	P	232	ALA
10	P	458	ASP
9	G	195	ASP
11	R	123	PRO
11	R	155	THR
11	Z	159	VAL
11	V	159	VAL
1	b	80	ASP
1	b	87	ASP
1	b	355	GLU
2	O	254	LYS
5	E	449	LYS
5	E	476	PRO
6	F	372	PRO
5	A	594	LYS
5	C	126	ARG
5	C	207	SER
5	C	528	GLN
6	D	125	LYS
6	D	138	PRO
6	D	391	MET
7	Q	260	GLN
8	L	62	ALA
9	K	195	ASP
9	G	133	LEU
11	R	158	VAL
11	X	159	VAL

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Mol	Chain	Res	Type
11	Z	157	ASP
11	S	159	VAL
11	T	157	ASP
11	T	158	VAL
6	F	124	PRO
5	A	78	GLY
6	D	202	ASP
8	J	105	PRO
10	P	54	LYS
8	H	105	PRO
11	U	156	GLN
5	A	284	GLY
6	B	372	PRO
5	C	310	PRO
5	C	403	SER
11	U	158	VAL
5	E	284	GLY
11	R	159	VAL
11	X	47	PRO
2	O	384	PRO
3	M	115	PRO
6	F	137	SER
6	F	179	PRO
5	C	375	PRO
5	E	310	PRO
6	B	126	VAL
6	D	248	PRO
5	C	589	PRO
6	D	375	VAL

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	b	275/728 (38%)	261 (95%)	14 (5%)	29	66
2	O	348/348 (100%)	345 (99%)	3 (1%)	84	93

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	M	183/221 (83%)	177 (97%)	6 (3%)	45	76
4	N	102/104 (98%)	100 (98%)	2 (2%)	63	85
5	A	497/515 (96%)	480 (97%)	17 (3%)	44	75
5	C	497/515 (96%)	477 (96%)	20 (4%)	38	71
5	E	497/515 (96%)	473 (95%)	24 (5%)	31	67
6	B	391/444 (88%)	374 (96%)	17 (4%)	35	70
6	D	391/444 (88%)	377 (96%)	14 (4%)	42	74
6	F	391/444 (88%)	373 (95%)	18 (5%)	33	68
7	Q	309/309 (100%)	302 (98%)	7 (2%)	58	83
8	H	87/94 (93%)	86 (99%)	1 (1%)	80	91
8	J	87/94 (93%)	83 (95%)	4 (5%)	33	68
8	L	87/94 (93%)	85 (98%)	2 (2%)	58	83
9	G	194/208 (93%)	191 (98%)	3 (2%)	72	88
9	I	194/208 (93%)	193 (100%)	1 (0%)	92	96
9	K	194/208 (93%)	192 (99%)	2 (1%)	82	92
10	P	426/439 (97%)	413 (97%)	13 (3%)	47	77
11	R	110/119 (92%)	107 (97%)	3 (3%)	52	79
11	S	110/119 (92%)	102 (93%)	8 (7%)	17	54
11	T	110/119 (92%)	106 (96%)	4 (4%)	42	74
11	U	110/119 (92%)	104 (94%)	6 (6%)	27	63
11	V	110/119 (92%)	107 (97%)	3 (3%)	52	79
11	W	110/119 (92%)	104 (94%)	6 (6%)	27	63
11	X	110/119 (92%)	107 (97%)	3 (3%)	52	79
11	Y	110/119 (92%)	110 (100%)	0	100	100
11	Z	110/119 (92%)	107 (97%)	3 (3%)	52	79
11	a	110/119 (92%)	109 (99%)	1 (1%)	84	93
All	All	6250/7122 (88%)	6045 (97%)	205 (3%)	49	76

All (205) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	b	17	VAL
1	b	20	TYR

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Mol	Chain	Res	Type
1	b	69	TYR
1	b	82	LYS
1	b	90	LYS
1	b	103	SER
1	b	137	ASP
1	b	186	TYR
1	b	193	ARG
1	b	247	LYS
1	b	250	ARG
1	b	329	ASP
1	b	330	THR
1	b	357	ILE
2	O	7	THR
2	O	98	ARG
2	O	164	ARG
3	M	13	MET
3	M	42	ARG
3	M	60	VAL
3	M	115	PRO
3	M	139	TYR
3	M	180	ARG
4	N	10	VAL
4	N	41	GLN
5	E	54	ASP
5	E	67	LYS
5	E	103	THR
5	E	124	ILE
5	E	161	VAL
5	E	169	SER
5	E	197	ILE
5	E	203	ASP
5	E	233	LEU
5	E	262	LYS
5	E	263	THR
5	E	286	ARG
5	E	295	MET
5	E	325	PRO
5	E	359	ARG
5	E	383	TYR
5	E	406	ARG
5	E	435	THR
5	E	468	ASN

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Mol	Chain	Res	Type
5	E	476	PRO
5	E	482	ARG
5	E	483	ASP
5	E	504	LYS
5	E	570	LEU
6	F	67	VAL
6	F	119	PRO
6	F	132	LEU
6	F	133	ASP
6	F	140	ASN
6	F	155	VAL
6	F	206	GLU
6	F	220	GLU
6	F	246	ASN
6	F	250	ILE
6	F	296	GLU
6	F	307	TYR
6	F	329	ILE
6	F	346	ILE
6	F	357	GLN
6	F	374	ASN
6	F	389	GLU
6	F	474	ASN
5	A	49	VAL
5	A	60	VAL
5	A	90	LYS
5	A	96	LEU
5	A	193	LEU
5	A	230	ASP
5	A	239	VAL
5	A	246	CYS
5	A	279	ILE
5	A	286	ARG
5	A	356	SER
5	A	406	ARG
5	A	456	THR
5	A	466	VAL
5	A	545	ASP
5	A	596	VAL
5	A	603	LEU
6	B	44	VAL
6	B	86	ILE

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Mol	Chain	Res	Type
6	B	122	ASN
6	B	178	LEU
6	B	215	MET
6	B	232	ASN
6	B	248	PRO
6	B	250	ILE
6	B	298	VAL
6	B	302	ARG
6	B	329	ILE
6	B	340	ASP
6	B	353	ILE
6	B	357	GLN
6	B	392	THR
6	B	432	SER
6	B	467	ILE
5	C	87	ARG
5	C	90	LYS
5	C	171	LYS
5	C	175	PRO
5	C	196	LYS
5	C	225	GLU
5	C	232	PRO
5	C	286	ARG
5	C	352	MET
5	C	364	LEU
5	C	406	ARG
5	C	435	THR
5	C	465	ASN
5	C	476	PRO
5	C	478	PHE
5	C	482	ARG
5	C	527	GLN
5	C	529	ASN
5	C	593	GLU
5	C	603	LEU
6	D	34	VAL
6	D	44	VAL
6	D	47	PRO
6	D	180	HIS
6	D	206	GLU
6	D	232	ASN
6	D	243	ASN

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Mol	Chain	Res	Type
6	D	279	THR
6	D	357	GLN
6	D	362	ARG
6	D	391	MET
6	D	428	GLU
6	D	475	ARG
6	D	479	LYS
7	Q	4	VAL
7	Q	128	HIS
7	Q	145	LEU
7	Q	188	TYR
7	Q	208	MET
7	Q	219	ARG
7	Q	304	PHE
8	J	38	ASP
8	J	52	LYS
8	J	82	GLU
8	J	105	PRO
9	I	191	SER
8	L	50	LYS
8	L	79	GLU
9	K	76	THR
9	K	147	ASP
10	P	36	LEU
10	P	79	PRO
10	P	87	SER
10	P	173	ILE
10	P	231	VAL
10	P	238	LEU
10	P	249	LEU
10	P	284	GLU
10	P	285	LYS
10	P	303	LYS
10	P	363	LEU
10	P	384	ILE
10	P	460	ARG
8	H	79	GLU
9	G	61	ASN
9	G	89	LEU
9	G	165	GLN
11	R	54	ILE
11	R	56	PRO

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Mol	Chain	Res	Type
11	R	124	ARG
11	U	21	ILE
11	U	51	PHE
11	U	56	PRO
11	U	85	TYR
11	U	97	VAL
11	U	120	SER
11	X	47	PRO
11	X	121	GLN
11	X	137	GLU
11	W	11	PHE
11	W	54	ILE
11	W	56	PRO
11	W	81	LYS
11	W	123	PRO
11	W	129	MET
11	Z	51	PHE
11	Z	56	PRO
11	Z	139	LEU
11	V	17	CYS
11	V	124	ARG
11	V	134	ILE
11	a	138	VAL
11	S	21	ILE
11	S	48	ASP
11	S	70	VAL
11	S	113	ASP
11	S	123	PRO
11	S	134	ILE
11	S	148	LEU
11	S	158	VAL
11	T	15	ILE
11	T	70	VAL
11	T	116	VAL
11	T	139	LEU

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	b	35	GLN
1	b	146	GLN
1	b	278	ASN

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Mol	Chain	Res	Type
2	O	115	GLN
2	O	336	ASN
3	M	130	GLN
3	M	171	ASN
5	E	491	ASN
6	F	35	ASN
6	F	180	HIS
6	F	201	HIS
6	F	227	GLN
6	F	357	GLN
6	F	365	HIS
6	F	374	ASN
6	F	396	HIS
6	F	402	GLN
5	A	109	GLN
5	A	323	ASN
5	A	436	GLN
5	A	455	ASN
5	A	597	HIS
6	B	140	ASN
6	B	204	HIS
6	B	273	HIS
6	B	396	HIS
6	B	402	GLN
6	B	446	GLN
5	C	71	GLN
5	C	109	GLN
5	C	151	HIS
5	C	274	ASN
5	C	447	GLN
5	C	491	ASN
5	C	554	HIS
6	D	190	GLN
6	D	339	ASN
6	D	396	HIS
7	Q	222	ASN
7	Q	226	ASN
7	Q	260	GLN
7	Q	318	GLN
9	K	12	GLN
9	K	36	GLN
9	K	56	ASN

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Mol	Chain	Res	Type
10	P	14	ASN
10	P	245	HIS
10	P	265	GLN
10	P	296	GLN
10	P	317	ASN
10	P	348	ASN
10	P	374	HIS
8	H	5	ASN
9	G	122	GLN
11	U	90	GLN
11	Y	151	ASN
11	W	151	ASN
11	W	156	GLN
11	V	151	ASN
11	a	151	ASN
11	S	151	ASN

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 ⓘ

There are no chain breaks in this entry.