



Full wwPDB/EMDatabank EM Map/Model Validation Report ⓘ

Mar 2, 2017 – 11:28 am GMT

PDB ID : 3J1B
EMDB ID: : EMD-5391
Title : Cryo-EM structure of 8-fold symmetric rATcpn-alpha in apo state
Authors : Zhang, K.; Wang, L.; Liu, Y.X.; Wang, X.; Gao, B.; Hu, Z.J.; Ji, G.; Chan, K.Y.; Schulten, K.; Dong, Z.Y.; Sun, F.
Deposited on : 2012-02-06
Resolution : 4.90 Å(reported)
Based on PDB ID : 3KO1

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

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

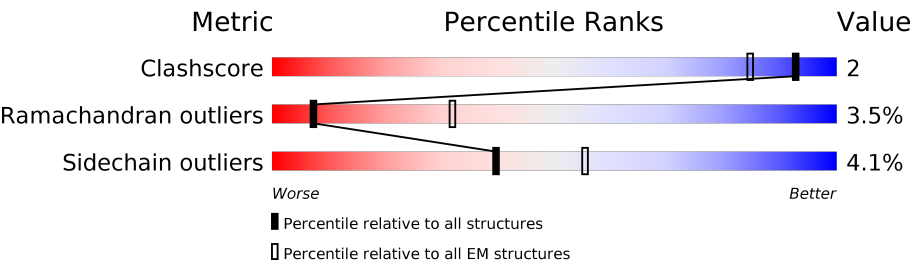
MolProbity : 4.02b-467
Percentile statistics : 20161228.v01 (using entries in the PDB archive December 28th 2016)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP) : recalc29047

1 Overall quality at a glance i

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

The reported resolution of this entry is 4.90 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	125131	1336
Ramachandran outliers	121729	1120
Sidechain outliers	121581	1026

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

Mol	Chain	Length	Quality of chain
1	A	563	68% 20% . . 8%
1	B	563	70% 18% . . 8%
1	C	563	70% 17% . . 8%
1	D	563	66% 22% . . 8%
1	E	563	68% 19% . . 8%
1	F	563	71% 18% . . 8%
1	G	563	65% 22% . 8%
1	H	563	69% 19% . . 8%
1	I	563	70% 18% . . 8%

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Mol	Chain	Length	Quality of chain
1	J	563	<div><div></div><div>67%</div><div>20%</div><div>5%</div><div>8%</div></div>
1	K	563	<div><div></div><div>67%</div><div>21%</div><div></div><div>8%</div></div>
1	L	563	<div><div></div><div>68%</div><div>20%</div><div></div><div>8%</div></div>
1	M	563	<div><div></div><div>67%</div><div>20%</div><div>5%</div><div>8%</div></div>
1	N	563	<div><div></div><div>68%</div><div>19%</div><div></div><div>8%</div></div>
1	O	563	<div><div></div><div>69%</div><div>17%</div><div>5%</div><div>8%</div></div>
1	P	563	<div><div></div><div>69%</div><div>20%</div><div></div><div>8%</div></div>

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 62992 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.

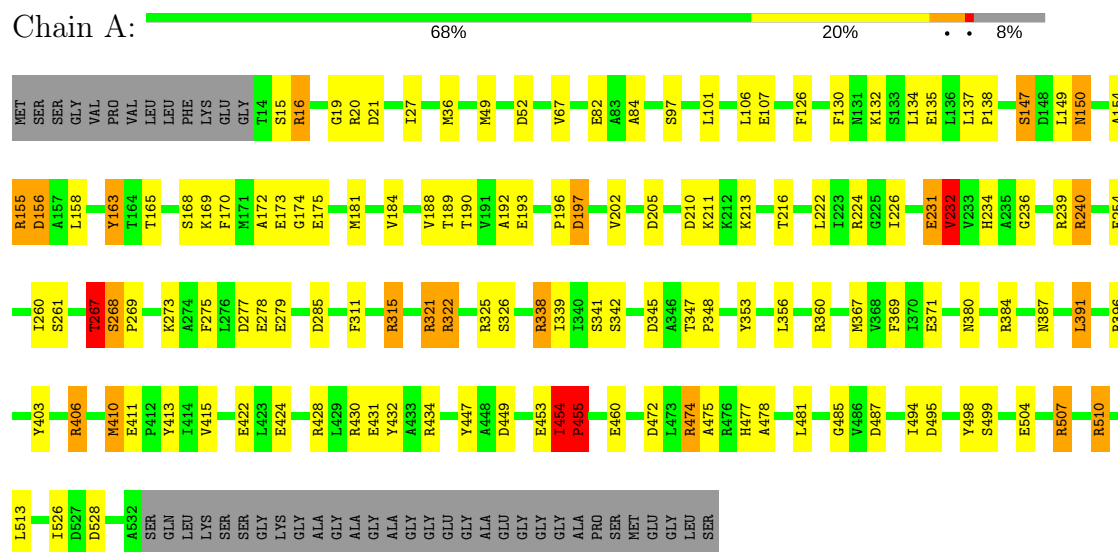
- Molecule 1 is a protein called Chaperonin alpha subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	B	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	C	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	D	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	E	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	F	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	G	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	H	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	I	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	J	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	K	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	L	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	M	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	N	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	O	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		
1	P	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		

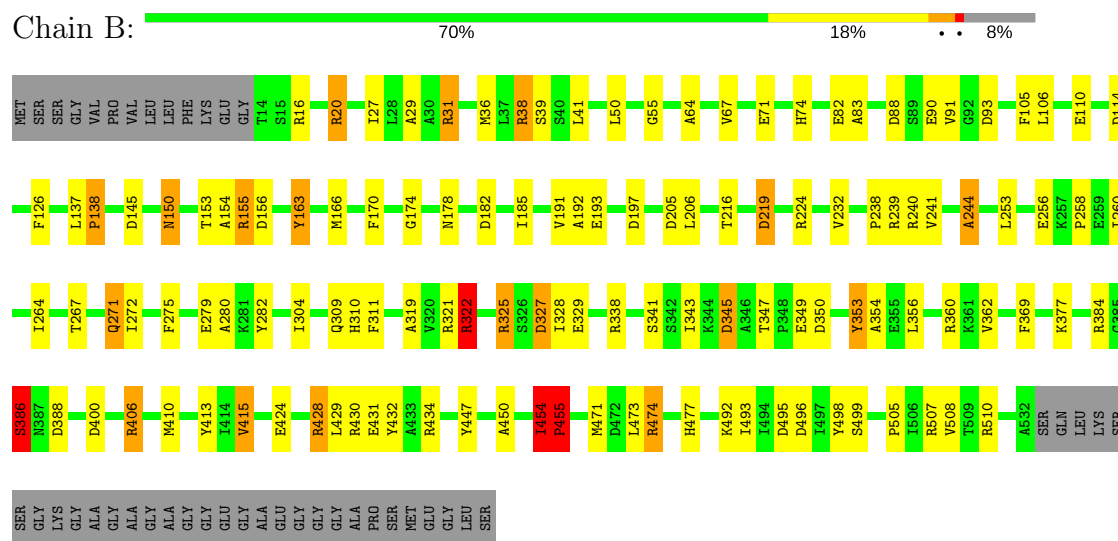
3 Residue-property plots

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

• Molecule 1: Chaperonin alpha subunit



• Molecule 1: Chaperonin alpha subunit



• Molecule 1: Chaperonin alpha subunit

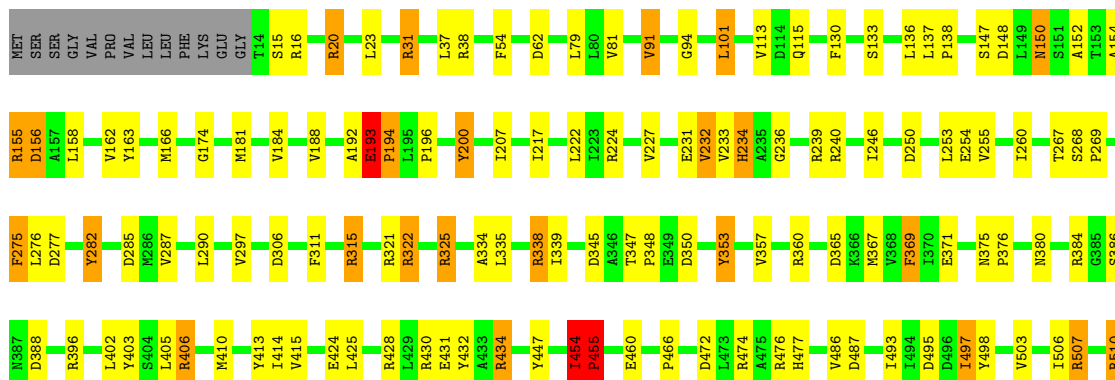


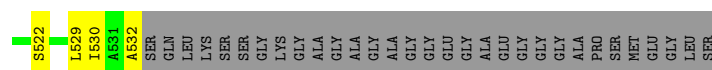
- Molecule 1: Chaperonin alpha subunit

Chain D: 66% 22% . . 8%

- Molecule 1: Chaperonin alpha subunit

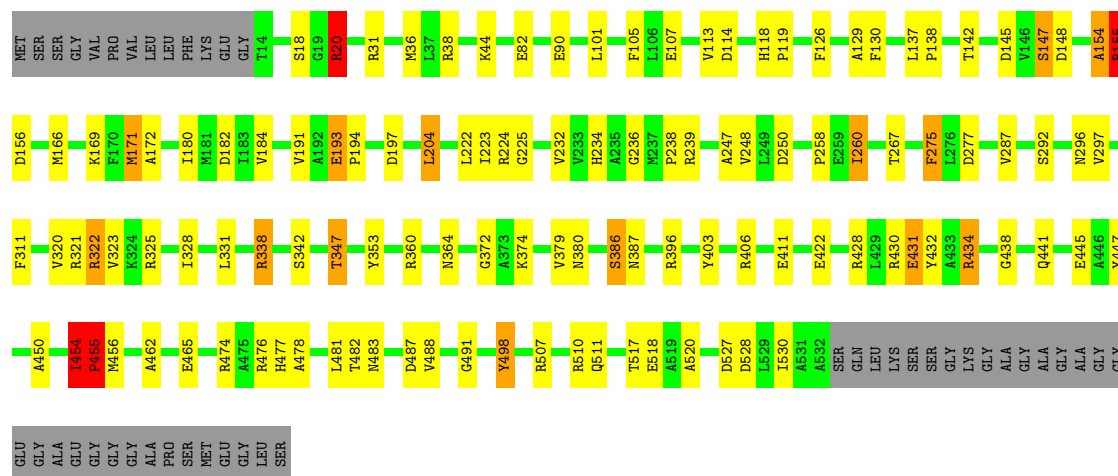
Chain E:  68% 19% . . 8%





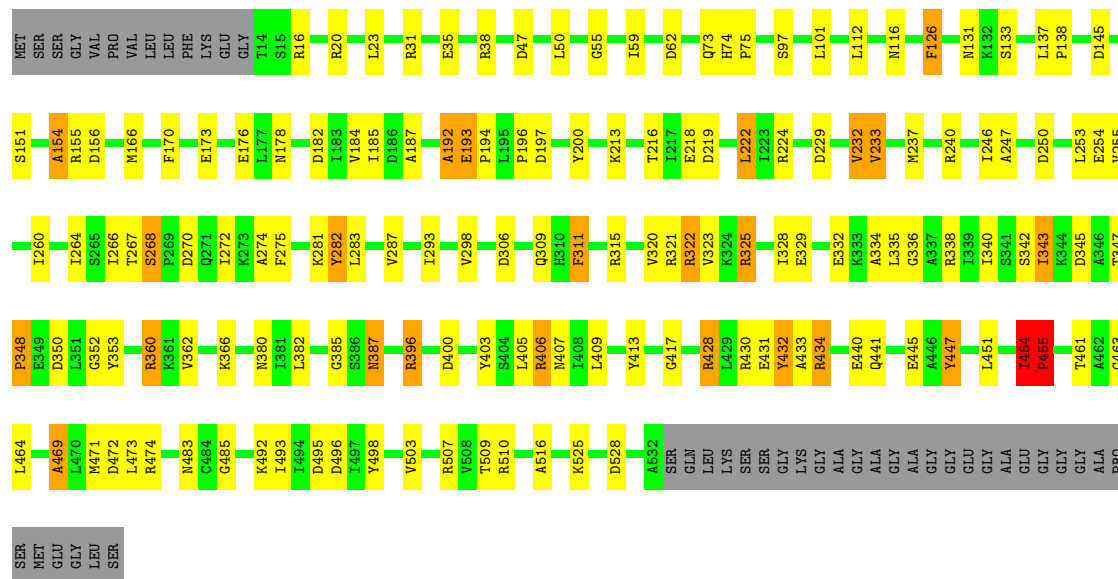
• Molecule 1: Chaperonin alpha subunit

Chain F: 71% 18% 8%



• Molecule 1: Chaperonin alpha subunit

Chain G: 65% 22% 8%

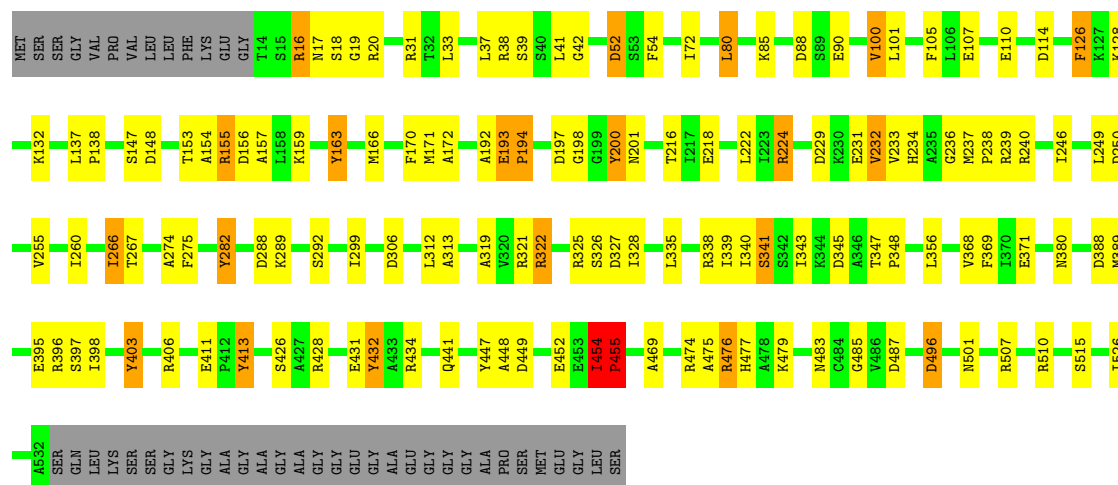


• Molecule 1: Chaperonin alpha subunit

Chain H: 69% 19% 8%

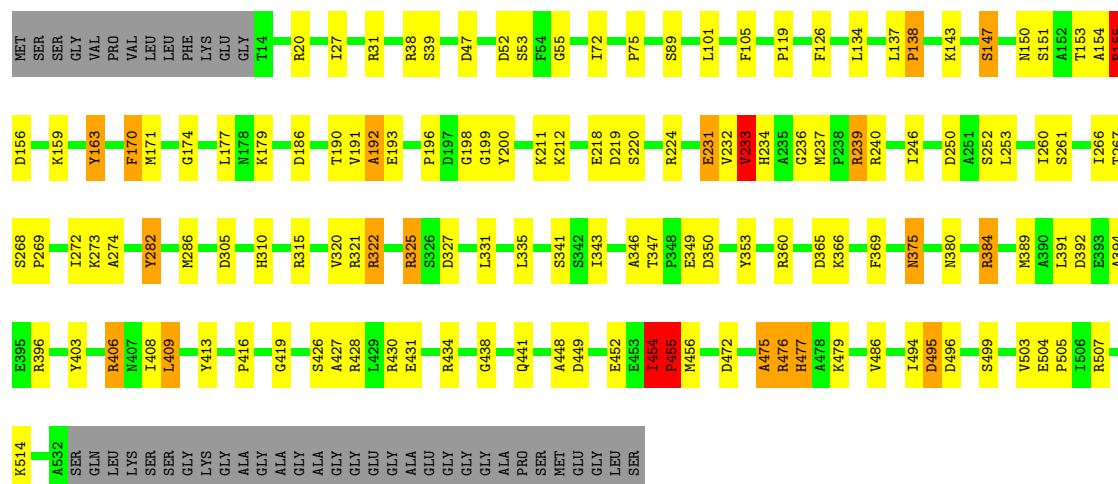


Chain K: 



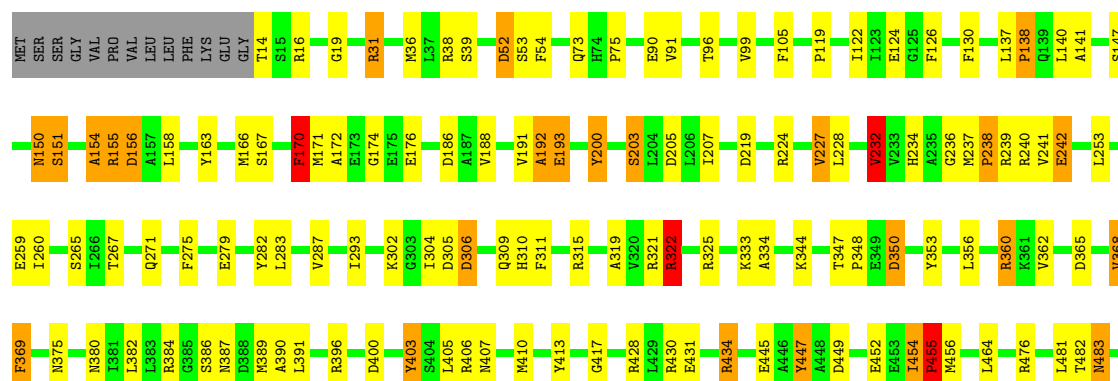
• Molecule 1: Chaperonin alpha subunit

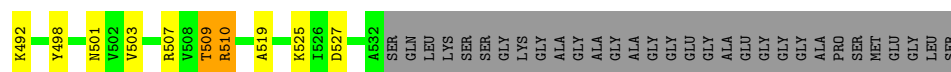
Chain L: 



• Molecule 1: Chaperonin alpha subunit

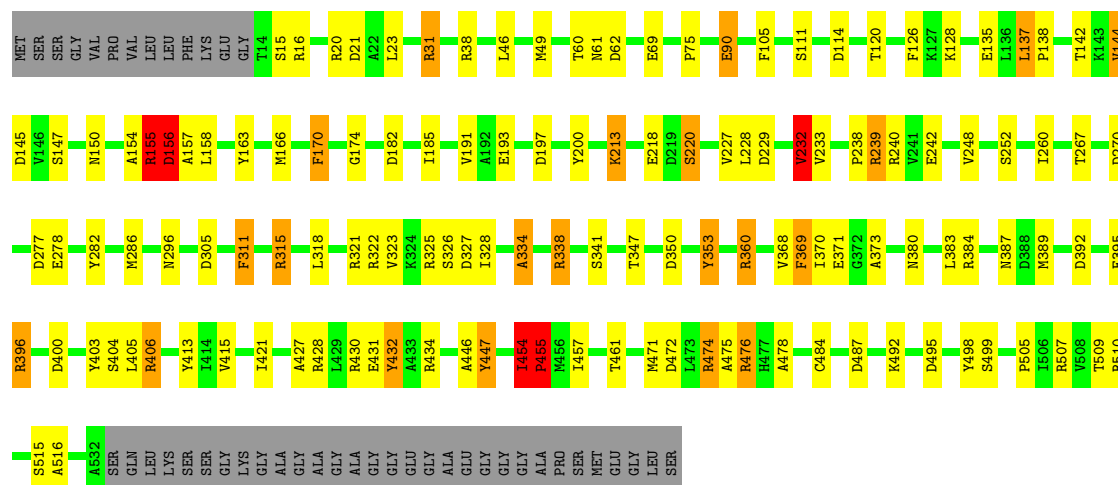
Chain M: 





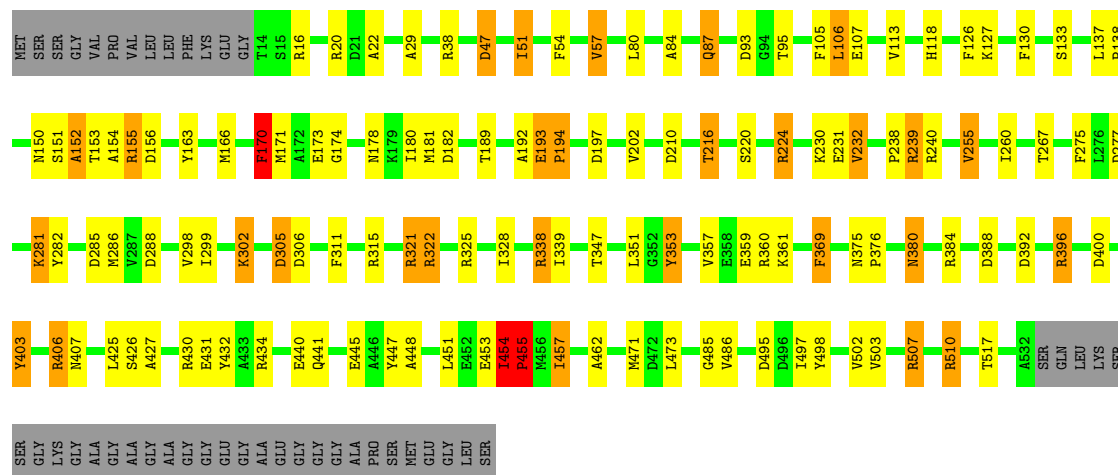
• Molecule 1: Chaperonin alpha subunit

Chain N: 68% 19% 8%



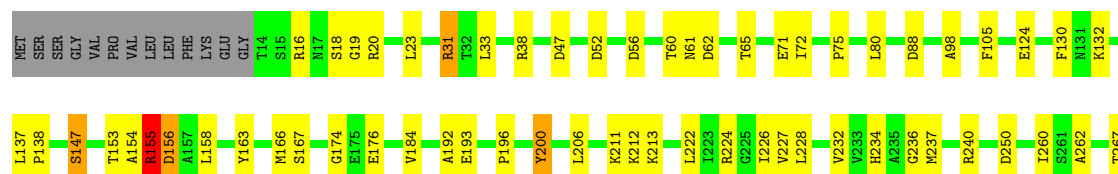
• Molecule 1: Chaperonin alpha subunit

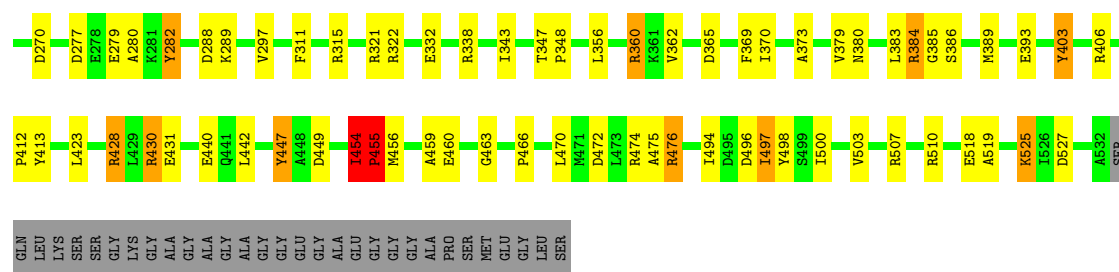
Chain O: 69% 17% 5% 8%



• Molecule 1: Chaperonin alpha subunit

Chain P: 69% 20% 8%





4 Experimental information

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of particles used	55460	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	The whole micrograph	Depositor
Microscope	FEI Titan Krios	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	20	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	96000	Depositor
Image detector	Gatan Ultrascan 4000 Model 895	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >2	RMSZ	# Z >2
1	A	1.60	20/3974 (0.5%)	1.93	83/5360 (1.5%)
1	B	1.59	17/3974 (0.4%)	1.98	94/5360 (1.8%)
1	C	1.55	16/3974 (0.4%)	1.93	90/5360 (1.7%)
1	D	1.57	21/3974 (0.5%)	2.00	116/5360 (2.2%)
1	E	1.53	12/3974 (0.3%)	2.05	103/5360 (1.9%)
1	F	1.57	17/3974 (0.4%)	1.99	95/5360 (1.8%)
1	G	1.57	20/3974 (0.5%)	2.01	101/5360 (1.9%)
1	H	1.58	19/3974 (0.5%)	1.97	95/5360 (1.8%)
1	I	1.56	22/3974 (0.6%)	1.94	80/5360 (1.5%)
1	J	1.58	21/3974 (0.5%)	2.00	112/5360 (2.1%)
1	K	1.56	23/3974 (0.6%)	1.95	84/5360 (1.6%)
1	L	1.53	19/3974 (0.5%)	1.99	99/5360 (1.8%)
1	M	1.56	20/3974 (0.5%)	2.01	120/5360 (2.2%)
1	N	1.59	20/3974 (0.5%)	1.97	101/5360 (1.9%)
1	O	1.58	13/3974 (0.3%)	2.01	116/5360 (2.2%)
1	P	1.60	26/3974 (0.7%)	1.97	92/5360 (1.7%)
All	All	1.57	306/63584 (0.5%)	1.98	1581/85760 (1.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	20
1	B	0	21
1	C	0	21
1	D	0	19
1	E	0	24
1	F	0	15
1	G	0	25
1	H	0	19
1	I	0	23

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	J	0	23
1	K	0	20
1	L	0	17
1	M	0	17
1	N	0	26
1	O	0	19
1	P	0	20
All	All	0	329

All (306) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	N	447	TYR	CE1-CZ	9.27	1.50	1.38
1	O	353	TYR	CG-CD1	8.65	1.50	1.39
1	D	326	SER	CA-CB	8.46	1.65	1.52
1	B	386	SER	CA-CB	8.39	1.65	1.52
1	F	491	GLY	CA-C	-8.08	1.39	1.51
1	A	371	GLU	CD-OE1	8.07	1.34	1.25
1	B	256	GLU	CB-CG	8.07	1.67	1.52
1	B	275	PHE	CG-CD2	7.74	1.50	1.38
1	M	417	GLY	N-CA	-7.69	1.34	1.46
1	A	499	SER	CA-CB	7.59	1.64	1.52
1	C	39	SER	CA-CB	7.49	1.64	1.52
1	P	498	TYR	CB-CG	-7.38	1.40	1.51
1	J	403	TYR	CZ-OH	7.33	1.50	1.37
1	I	491	GLY	CA-C	-7.29	1.40	1.51
1	G	432	TYR	CG-CD1	7.23	1.48	1.39
1	L	55	GLY	CA-C	-7.21	1.40	1.51
1	N	220	SER	CA-CB	7.20	1.63	1.52
1	P	176	GLU	CB-CG	7.14	1.65	1.52
1	F	507	ARG	CD-NE	7.13	1.58	1.46
1	H	198	GLY	CA-C	-7.12	1.40	1.51
1	M	265	SER	CA-CB	7.10	1.63	1.52
1	I	40	SER	CA-CB	7.04	1.63	1.52
1	I	485	GLY	CA-C	7.00	1.63	1.51
1	L	89	SER	CA-CB	6.94	1.63	1.52
1	F	498	TYR	CB-CG	-6.92	1.41	1.51
1	J	163	TYR	CG-CD2	6.92	1.48	1.39
1	D	476	ARG	CD-NE	6.89	1.58	1.46
1	E	369	PHE	CG-CD2	6.89	1.49	1.38
1	J	360	ARG	CD-NE	6.87	1.58	1.46
1	J	435	SER	CA-CB	6.80	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	397	SER	CA-CB	6.76	1.63	1.52
1	N	404	SER	CA-CB	6.73	1.63	1.52
1	A	311	PHE	CG-CD2	6.70	1.48	1.38
1	C	441	GLN	CA-CB	6.68	1.68	1.53
1	K	411	GLU	CD-OE1	-6.58	1.18	1.25
1	I	268	SER	CA-CB	6.56	1.62	1.52
1	K	282	TYR	CZ-OH	6.51	1.49	1.37
1	H	170	PHE	CG-CD2	6.50	1.48	1.38
1	D	453	GLU	CD-OE1	-6.50	1.18	1.25
1	H	413	TYR	CE1-CZ	6.49	1.47	1.38
1	O	133	SER	CA-CB	6.47	1.62	1.52
1	L	72	ILE	CA-CB	-6.47	1.40	1.54
1	P	19	GLY	N-CA	6.46	1.55	1.46
1	B	362	VAL	CA-CB	-6.44	1.41	1.54
1	A	460	GLU	CB-CG	6.41	1.64	1.52
1	F	292	SER	CB-OG	6.39	1.50	1.42
1	P	385	GLY	CA-C	-6.39	1.41	1.51
1	P	518	GLU	CG-CD	6.37	1.61	1.51
1	K	107	GLU	CB-CG	6.34	1.64	1.52
1	K	292	SER	CA-CB	6.34	1.62	1.52
1	M	413	TYR	CG-CD2	6.34	1.47	1.39
1	O	445	GLU	CD-OE1	6.34	1.32	1.25
1	O	298	VAL	CA-CB	-6.33	1.41	1.54
1	C	240	ARG	CD-NE	6.33	1.57	1.46
1	M	151	SER	CA-CB	6.30	1.62	1.52
1	P	147	SER	CA-CB	6.26	1.62	1.52
1	L	240	ARG	CD-NE	6.23	1.57	1.46
1	B	71	GLU	CD-OE1	6.23	1.32	1.25
1	H	369	PHE	CG-CD2	6.20	1.48	1.38
1	F	498	TYR	CG-CD2	6.19	1.47	1.39
1	E	54	PHE	CG-CD2	6.19	1.48	1.38
1	J	431	GLU	CD-OE2	-6.18	1.18	1.25
1	C	242	GLU	CD-OE1	6.18	1.32	1.25
1	M	53	SER	CA-CB	6.16	1.62	1.52
1	I	406	ARG	CD-NE	6.15	1.56	1.46
1	M	224	ARG	CD-NE	6.15	1.56	1.46
1	I	282	TYR	CB-CG	6.14	1.60	1.51
1	O	231	GLU	CB-CG	6.14	1.63	1.52
1	L	499	SER	CB-OG	6.14	1.50	1.42
1	M	279	GLU	CD-OE2	6.12	1.32	1.25
1	D	315	ARG	CD-NE	6.11	1.56	1.46
1	K	515	SER	N-CA	6.10	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	15	SER	CA-CB	6.09	1.62	1.52
1	A	268	SER	CA-CB	6.09	1.62	1.52
1	H	522	SER	CA-CB	6.09	1.62	1.52
1	H	41	LEU	C-N	6.08	1.44	1.33
1	I	31	ARG	CD-NE	6.07	1.56	1.46
1	D	460	GLU	CD-OE1	6.06	1.32	1.25
1	I	453	GLU	CB-CG	6.06	1.63	1.52
1	J	92	GLY	N-CA	6.05	1.55	1.46
1	H	453	GLU	CD-OE2	6.04	1.32	1.25
1	B	163	TYR	CG-CD2	6.03	1.47	1.39
1	A	147	SER	CA-CB	6.02	1.61	1.52
1	K	163	TYR	CE2-CZ	6.02	1.46	1.38
1	F	403	TYR	CZ-OH	6.00	1.48	1.37
1	E	367	MET	N-CA	-6.00	1.34	1.46
1	J	20	ARG	NE-CZ	5.98	1.40	1.33
1	J	163	TYR	CZ-OH	5.98	1.48	1.37
1	L	426	SER	CA-CB	5.94	1.61	1.52
1	G	55	GLY	CA-C	-5.92	1.42	1.51
1	G	353	TYR	CG-CD1	5.92	1.46	1.39
1	E	447	TYR	CE1-CZ	5.92	1.46	1.38
1	D	69	GLU	CB-CG	5.92	1.63	1.52
1	P	440	GLU	N-CA	-5.92	1.34	1.46
1	I	90	GLU	CD-OE2	5.91	1.32	1.25
1	G	133	SER	CB-OG	5.89	1.50	1.42
1	E	15	SER	CA-CB	5.89	1.61	1.52
1	M	242	GLU	CG-CD	-5.88	1.43	1.51
1	M	19	GLY	CA-C	5.86	1.61	1.51
1	P	240	ARG	NE-CZ	5.85	1.40	1.33
1	O	151	SER	CA-CB	5.85	1.61	1.52
1	D	463	GLY	CA-C	-5.84	1.42	1.51
1	N	395	GLU	CB-CG	5.84	1.63	1.52
1	N	499	SER	CA-C	-5.83	1.37	1.52
1	O	163	TYR	CE2-CZ	5.83	1.46	1.38
1	K	447	TYR	CG-CD1	5.83	1.46	1.39
1	M	90	GLU	CB-CG	5.83	1.63	1.52
1	I	403	TYR	CB-CG	5.82	1.60	1.51
1	F	474	ARG	CD-NE	5.81	1.56	1.46
1	G	268	SER	C-N	5.81	1.45	1.34
1	G	329	GLU	CG-CD	-5.80	1.43	1.51
1	P	124	GLU	CD-OE2	5.80	1.32	1.25
1	E	269	PRO	N-CD	5.80	1.55	1.47
1	P	510	ARG	CD-NE	5.80	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	329	GLU	CD-OE2	5.79	1.32	1.25
1	I	356	LEU	CA-CB	5.79	1.67	1.53
1	L	147	SER	CA-CB	5.78	1.61	1.52
1	K	526	ILE	CA-CB	-5.77	1.41	1.54
1	D	151	SER	CB-OG	5.77	1.49	1.42
1	L	220	SER	CA-CB	5.76	1.61	1.52
1	F	406	ARG	CD-NE	5.75	1.56	1.46
1	L	199	GLY	CA-C	-5.75	1.42	1.51
1	P	279	GLU	CD-OE1	5.75	1.31	1.25
1	N	90	GLU	CD-OE1	-5.73	1.19	1.25
1	K	479	LYS	N-CA	-5.73	1.34	1.46
1	M	434	ARG	CD-NE	5.73	1.56	1.46
1	N	200	TYR	CG-CD1	5.72	1.46	1.39
1	O	361	LYS	CD-CE	5.72	1.65	1.51
1	G	311	PHE	CG-CD2	5.71	1.47	1.38
1	G	332	GLU	CG-CD	5.71	1.60	1.51
1	J	224	ARG	CD-NE	5.71	1.56	1.46
1	K	105	PHE	CG-CD1	5.70	1.47	1.38
1	N	505	PRO	N-CD	-5.69	1.39	1.47
1	D	311	PHE	CG-CD1	5.69	1.47	1.38
1	G	352	GLY	CA-C	-5.68	1.42	1.51
1	C	220	SER	CB-OG	5.67	1.49	1.42
1	H	419	GLY	CA-C	-5.66	1.42	1.51
1	J	460	GLU	CB-CG	5.65	1.62	1.52
1	G	485	GLY	N-CA	-5.62	1.37	1.46
1	M	445	GLU	CD-OE2	5.62	1.31	1.25
1	C	231	GLU	CD-OE2	5.61	1.31	1.25
1	C	35	GLU	CB-CG	5.61	1.62	1.52
1	I	262	ALA	CA-CB	5.60	1.64	1.52
1	A	428	ARG	CD-NE	5.60	1.55	1.46
1	B	279	GLU	CB-CG	5.60	1.62	1.52
1	L	39	SER	CA-CB	5.60	1.61	1.52
1	A	175	GLU	CD-OE2	5.59	1.31	1.25
1	B	325	ARG	CD-NE	5.58	1.55	1.46
1	G	218	GLU	CG-CD	5.58	1.60	1.51
1	H	413	TYR	CG-CD2	5.57	1.46	1.39
1	H	261	SER	CA-CB	5.56	1.61	1.52
1	A	485	GLY	N-CA	-5.56	1.37	1.46
1	I	318	LEU	CA-CB	5.55	1.66	1.53
1	E	38	ARG	CD-NE	5.54	1.55	1.46
1	K	369	PHE	CG-CD2	5.53	1.47	1.38
1	F	403	TYR	CG-CD2	5.52	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	229	ASP	CA-CB	5.52	1.66	1.53
1	J	465	GLU	CD-OE2	5.52	1.31	1.25
1	H	43	PRO	N-CD	-5.51	1.40	1.47
1	M	271	GLN	CA-CB	5.51	1.66	1.53
1	G	417	GLY	CA-C	5.50	1.60	1.51
1	C	279	GLU	CB-CG	5.50	1.62	1.52
1	P	447	TYR	CG-CD2	5.49	1.46	1.39
1	P	31	ARG	CD-NE	5.48	1.55	1.46
1	F	353	TYR	CG-CD2	5.48	1.46	1.39
1	L	315	ARG	C-N	5.48	1.43	1.33
1	N	498	TYR	CB-CG	-5.48	1.43	1.51
1	I	282	TYR	CG-CD2	5.47	1.46	1.39
1	K	485	GLY	CA-C	-5.47	1.43	1.51
1	P	167	SER	CB-OG	5.47	1.49	1.42
1	D	38	ARG	CD-NE	5.46	1.55	1.46
1	L	282	TYR	CZ-OH	5.46	1.47	1.37
1	H	270	ASP	CA-CB	5.46	1.66	1.53
1	N	135	GLU	CG-CD	5.45	1.60	1.51
1	P	498	TYR	CE2-CZ	5.45	1.45	1.38
1	F	18	SER	CA-CB	5.45	1.61	1.52
1	O	486	VAL	CA-CB	-5.45	1.43	1.54
1	A	422	GLU	CD-OE1	-5.45	1.19	1.25
1	K	31	ARG	CD-NE	5.44	1.55	1.46
1	A	19	GLY	N-CA	5.44	1.54	1.46
1	I	238	PRO	N-CD	-5.44	1.40	1.47
1	P	262	ALA	CA-CB	5.43	1.63	1.52
1	P	338	ARG	CB-CG	5.43	1.67	1.52
1	D	338	ARG	NE-CZ	5.43	1.40	1.33
1	L	138	PRO	CA-C	-5.42	1.42	1.52
1	P	20	ARG	CA-CB	5.41	1.65	1.53
1	M	447	TYR	CB-CG	5.41	1.59	1.51
1	E	254	GLU	CB-CG	5.40	1.62	1.52
1	K	85	LYS	N-CA	-5.39	1.35	1.46
1	A	278	GLU	CD-OE1	5.39	1.31	1.25
1	I	261	SER	CA-CB	5.39	1.61	1.52
1	D	133	SER	CB-OG	5.39	1.49	1.42
1	J	297	VAL	N-CA	-5.39	1.35	1.46
1	H	212	LYS	CA-CB	5.39	1.65	1.53
1	B	41	LEU	CA-CB	5.38	1.66	1.53
1	H	174	GLY	N-CA	5.37	1.54	1.46
1	H	353	TYR	CG-CD2	5.37	1.46	1.39
1	N	499	SER	CA-CB	5.37	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	282	TYR	CD2-CE2	5.36	1.47	1.39
1	I	353	TYR	CZ-OH	5.35	1.47	1.37
1	N	145	ASP	CA-CB	-5.35	1.42	1.53
1	D	406	ARG	CZ-NH1	5.35	1.40	1.33
1	G	385	GLY	CA-C	-5.35	1.43	1.51
1	M	241	VAL	CA-C	-5.34	1.39	1.52
1	K	426	SER	CA-CB	5.33	1.60	1.52
1	B	349	GLU	CD-OE2	5.33	1.31	1.25
1	L	151	SER	CA-CB	5.33	1.60	1.52
1	L	159	LYS	CD-CE	5.33	1.64	1.51
1	A	173	GLU	CD-OE1	-5.32	1.19	1.25
1	C	382	LEU	N-CA	-5.32	1.35	1.46
1	E	200	TYR	CG-CD2	5.31	1.46	1.39
1	G	447	TYR	CG-CD1	5.31	1.46	1.39
1	N	252	SER	CB-OG	5.31	1.49	1.42
1	M	333	LYS	CA-CB	5.30	1.65	1.53
1	K	110	GLU	CD-OE1	5.30	1.31	1.25
1	P	18	SER	CA-CB	5.30	1.60	1.52
1	D	152	ALA	CA-CB	5.30	1.63	1.52
1	M	498	TYR	CE2-CZ	5.29	1.45	1.38
1	F	82	GLU	CD-OE2	-5.28	1.19	1.25
1	J	175	GLU	CD-OE1	5.27	1.31	1.25
1	M	14	THR	N-CA	5.27	1.56	1.46
1	E	532	ALA	CA-C	5.26	1.66	1.52
1	E	474	ARG	NE-CZ	-5.26	1.26	1.33
1	F	20	ARG	CD-NE	5.26	1.55	1.46
1	O	375	ASN	C-N	-5.26	1.24	1.34
1	L	53	SER	CA-CB	5.26	1.60	1.52
1	O	180	ILE	N-CA	-5.25	1.35	1.46
1	C	200	TYR	CG-CD2	5.25	1.46	1.39
1	H	91	VAL	C-N	5.25	1.42	1.33
1	J	498	TYR	CG-CD1	5.24	1.46	1.39
1	K	388	ASP	N-CA	-5.24	1.35	1.46
1	F	321	ARG	CD-NE	5.23	1.55	1.46
1	G	320	VAL	CB-CG1	5.23	1.63	1.52
1	L	448	ALA	N-CA	-5.22	1.35	1.46
1	B	311	PHE	CG-CD2	5.21	1.46	1.38
1	F	403	TYR	CB-CG	5.21	1.59	1.51
1	I	413	TYR	CE1-CZ	5.21	1.45	1.38
1	B	36	MET	N-CA	-5.20	1.35	1.46
1	L	310	HIS	CB-CG	-5.20	1.40	1.50
1	K	274	ALA	N-CA	-5.19	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	B	454	ILE	C-N	5.19	1.44	1.34
1	N	163	TYR	CG-CD2	5.18	1.45	1.39
1	I	54	PHE	C-N	5.18	1.42	1.33
1	K	100	VAL	CB-CG2	5.17	1.63	1.52
1	G	366	LYS	CD-CE	5.17	1.64	1.51
1	B	360	ARG	CD-NE	5.17	1.55	1.46
1	C	124	GLU	CD-OE2	5.16	1.31	1.25
1	G	200	TYR	CB-CG	5.16	1.59	1.51
1	P	60	THR	N-CA	5.16	1.56	1.46
1	G	321	ARG	CD-NE	5.15	1.55	1.46
1	P	440	GLU	CB-CG	5.15	1.61	1.52
1	C	265	SER	CB-OG	5.15	1.49	1.42
1	J	287	VAL	CA-CB	-5.14	1.44	1.54
1	D	147	SER	CA-CB	5.14	1.60	1.52
1	N	406	ARG	NE-CZ	5.13	1.39	1.33
1	G	336	GLY	N-CA	5.13	1.53	1.46
1	H	38	ARG	NE-CZ	5.13	1.39	1.33
1	J	384	ARG	CD-NE	5.13	1.55	1.46
1	A	342	SER	CA-CB	5.12	1.60	1.52
1	D	424	GLU	CG-CD	-5.12	1.44	1.51
1	P	184	VAL	CB-CG2	5.12	1.63	1.52
1	P	412	PRO	N-CD	-5.12	1.40	1.47
1	M	396	ARG	CD-NE	5.12	1.55	1.46
1	H	447	TYR	CB-CG	5.12	1.59	1.51
1	A	254	GLU	CB-CG	5.11	1.61	1.52
1	E	466	PRO	N-CD	-5.11	1.40	1.47
1	F	372	GLY	CA-C	-5.11	1.43	1.51
1	H	107	GLU	CD-OE1	-5.11	1.20	1.25
1	I	38	ARG	CZ-NH2	5.11	1.39	1.33
1	C	174	GLY	N-CA	-5.10	1.38	1.46
1	D	137	LEU	CA-CB	5.10	1.65	1.53
1	A	413	TYR	CB-CG	-5.09	1.44	1.51
1	L	231	GLU	CB-CG	5.09	1.61	1.52
1	M	163	TYR	CZ-OH	5.09	1.46	1.37
1	D	31	ARG	CD-NE	5.08	1.55	1.46
1	N	105	PHE	CA-CB	5.08	1.65	1.53
1	N	326	SER	CA-CB	5.08	1.60	1.52
1	O	38	ARG	CD-NE	5.08	1.55	1.46
1	D	225	GLY	CA-C	5.08	1.59	1.51
1	J	91	VAL	C-N	5.08	1.42	1.33
1	D	365	ASP	N-CA	5.08	1.56	1.46
1	N	15	SER	CA-CB	5.08	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	82	GLU	CD-OE1	5.07	1.31	1.25
1	J	484	CYS	CB-SG	-5.07	1.73	1.81
1	B	473	LEU	C-N	5.07	1.45	1.34
1	F	465	GLU	CD-OE1	-5.07	1.20	1.25
1	I	167	SER	CA-CB	5.07	1.60	1.52
1	K	434	ARG	NE-CZ	5.07	1.39	1.33
1	A	168	SER	CA-CB	5.06	1.60	1.52
1	O	173	GLU	CD-OE2	5.06	1.31	1.25
1	P	454	ILE	C-N	5.05	1.43	1.34
1	P	373	ALA	N-CA	5.05	1.56	1.46
1	C	349	GLU	CB-CG	5.04	1.61	1.52
1	D	55	GLY	N-CA	5.04	1.53	1.46
1	G	433	ALA	N-CA	-5.03	1.36	1.46
1	J	413	TYR	CE1-CZ	5.03	1.45	1.38
1	J	437	GLY	CA-C	-5.03	1.43	1.51
1	A	326	SER	CA-CB	5.03	1.60	1.52
1	P	393	GLU	CG-CD	-5.02	1.44	1.51
1	N	156	ASP	CA-CB	5.02	1.65	1.53
1	C	242	GLU	CG-CD	5.02	1.59	1.51
1	B	510	ARG	CD-NE	5.01	1.54	1.46
1	K	371	GLU	CG-CD	5.01	1.59	1.51
1	C	125	GLY	CA-C	5.01	1.59	1.51
1	N	403	TYR	CE1-CZ	5.00	1.45	1.38
1	J	278	GLU	CB-CG	5.00	1.61	1.52

All (1581) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	406	ARG	NE-CZ-NH1	-19.65	110.47	120.30
1	I	507	ARG	NE-CZ-NH2	19.50	130.05	120.30
1	L	430	ARG	NE-CZ-NH2	18.88	129.74	120.30
1	I	507	ARG	NE-CZ-NH1	-17.58	111.51	120.30
1	J	240	ARG	NE-CZ-NH2	17.26	128.93	120.30
1	E	430	ARG	NE-CZ-NH2	17.03	128.82	120.30
1	F	360	ARG	NE-CZ-NH1	-16.88	111.86	120.30
1	D	224	ARG	NE-CZ-NH1	-16.87	111.87	120.30
1	B	360	ARG	NE-CZ-NH1	-16.77	111.92	120.30
1	G	474	ARG	NE-CZ-NH1	-16.57	112.02	120.30
1	G	430	ARG	NE-CZ-NH2	16.52	128.56	120.30
1	P	428	ARG	NE-CZ-NH1	-16.45	112.07	120.30
1	G	16	ARG	NE-CZ-NH2	16.32	128.46	120.30
1	P	338	ARG	NE-CZ-NH1	-15.98	112.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	474	ARG	NE-CZ-NH2	15.97	128.28	120.30
1	E	510	ARG	NE-CZ-NH2	15.93	128.27	120.30
1	L	403	TYR	CB-CG-CD1	-15.53	111.68	121.00
1	K	428	ARG	NE-CZ-NH2	15.51	128.06	120.30
1	E	474	ARG	NE-CZ-NH2	15.37	127.99	120.30
1	L	155	ARG	NE-CZ-NH1	-15.33	112.63	120.30
1	F	321	ARG	NE-CZ-NH2	15.26	127.93	120.30
1	N	430	ARG	NE-CZ-NH1	-14.97	112.81	120.30
1	H	474	ARG	NE-CZ-NH1	-14.87	112.86	120.30
1	D	384	ARG	NE-CZ-NH2	14.64	127.62	120.30
1	E	360	ARG	NE-CZ-NH1	-14.63	112.98	120.30
1	E	434	ARG	NE-CZ-NH1	-14.47	113.06	120.30
1	P	510	ARG	NE-CZ-NH1	-14.43	113.08	120.30
1	D	507	ARG	NE-CZ-NH2	14.35	127.48	120.30
1	H	360	ARG	NE-CZ-NH1	14.31	127.45	120.30
1	N	430	ARG	NE-CZ-NH2	14.28	127.44	120.30
1	C	338	ARG	NE-CZ-NH1	-14.18	113.21	120.30
1	H	434	ARG	NE-CZ-NH2	14.13	127.36	120.30
1	F	322	ARG	NE-CZ-NH1	-14.05	113.27	120.30
1	F	322	ARG	NE-CZ-NH2	14.02	127.31	120.30
1	E	240	ARG	NE-CZ-NH2	13.97	127.29	120.30
1	O	434	ARG	NE-CZ-NH1	-13.90	113.35	120.30
1	D	498	TYR	CB-CG-CD2	-13.89	112.66	121.00
1	J	224	ARG	NE-CZ-NH2	13.83	127.21	120.30
1	C	474	ARG	NE-CZ-NH2	13.64	127.12	120.30
1	B	432	TYR	CB-CG-CD1	13.64	129.18	121.00
1	A	403	TYR	CB-CG-CD1	-13.62	112.83	121.00
1	J	507	ARG	NE-CZ-NH2	13.58	127.09	120.30
1	E	338	ARG	NE-CZ-NH2	13.56	127.08	120.30
1	F	474	ARG	NE-CZ-NH1	-13.51	113.54	120.30
1	O	16	ARG	NE-CZ-NH2	13.48	127.04	120.30
1	A	239	ARG	NE-CZ-NH2	13.47	127.03	120.30
1	L	430	ARG	NE-CZ-NH1	-13.33	113.63	120.30
1	N	240	ARG	NE-CZ-NH2	13.31	126.96	120.30
1	J	155	ARG	NE-CZ-NH2	13.27	126.94	120.30
1	E	315	ARG	NE-CZ-NH1	-13.25	113.68	120.30
1	G	432	TYR	CB-CG-CD2	-13.19	113.08	121.00
1	K	396	ARG	NE-CZ-NH2	13.07	126.83	120.30
1	E	321	ARG	NE-CZ-NH1	-12.99	113.81	120.30
1	L	315	ARG	NE-CZ-NH2	12.93	126.77	120.30
1	C	384	ARG	NE-CZ-NH2	12.88	126.74	120.30
1	A	338	ARG	NE-CZ-NH2	12.86	126.73	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	403	TYR	CB-CG-CD2	12.86	128.72	121.00
1	I	510	ARG	NE-CZ-NH2	12.84	126.72	120.30
1	E	315	ARG	NE-CZ-NH2	12.80	126.70	120.30
1	P	474	ARG	NE-CZ-NH1	-12.75	113.93	120.30
1	L	360	ARG	NE-CZ-NH2	12.74	126.67	120.30
1	B	406	ARG	NE-CZ-NH1	-12.67	113.96	120.30
1	B	432	TYR	CB-CG-CD2	-12.65	113.41	121.00
1	M	321	ARG	NE-CZ-NH2	12.64	126.62	120.30
1	I	315	ARG	NE-CZ-NH2	12.61	126.60	120.30
1	F	476	ARG	NE-CZ-NH1	12.57	126.59	120.30
1	H	322	ARG	NE-CZ-NH1	12.56	126.58	120.30
1	C	16	ARG	NE-CZ-NH1	-12.52	114.04	120.30
1	D	498	TYR	CB-CG-CD1	12.51	128.51	121.00
1	A	322	ARG	NE-CZ-NH2	12.39	126.50	120.30
1	E	239	ARG	NE-CZ-NH1	-12.39	114.11	120.30
1	D	360	ARG	NE-CZ-NH1	-12.38	114.11	120.30
1	N	315	ARG	NE-CZ-NH1	-12.38	114.11	120.30
1	M	360	ARG	NE-CZ-NH2	12.30	126.45	120.30
1	O	510	ARG	NE-CZ-NH1	-12.30	114.15	120.30
1	G	432	TYR	CB-CG-CD1	12.18	128.31	121.00
1	B	16	ARG	NE-CZ-NH1	-12.12	114.24	120.30
1	N	476	ARG	NE-CZ-NH2	12.02	126.31	120.30
1	D	224	ARG	NE-CZ-NH2	12.01	126.30	120.30
1	P	20	ARG	NE-CZ-NH2	11.98	126.29	120.30
1	K	507	ARG	NE-CZ-NH1	-11.95	114.33	120.30
1	H	406	ARG	NE-CZ-NH1	-11.88	114.36	120.30
1	F	455	PRO	CA-N-CD	-11.87	94.88	111.50
1	M	455	PRO	CA-N-CD	-11.83	94.94	111.50
1	N	353	TYR	CB-CG-CD2	-11.81	113.91	121.00
1	H	428	ARG	NE-CZ-NH2	11.78	126.19	120.30
1	O	311	PHE	CB-CG-CD2	11.78	129.04	120.80
1	P	428	ARG	NE-CZ-NH2	11.76	126.18	120.30
1	L	396	ARG	NE-CZ-NH2	11.74	126.17	120.30
1	D	455	PRO	CA-N-CD	-11.74	95.07	111.50
1	H	321	ARG	NE-CZ-NH1	-11.70	114.45	120.30
1	M	498	TYR	CB-CG-CD1	-11.66	114.01	121.00
1	N	325	ARG	NE-CZ-NH2	11.66	126.13	120.30
1	B	430	ARG	NE-CZ-NH2	11.61	126.11	120.30
1	B	430	ARG	NE-CZ-NH1	-11.61	114.50	120.30
1	D	384	ARG	NE-CZ-NH1	-11.61	114.50	120.30
1	B	455	PRO	CA-N-CD	-11.61	95.25	111.50
1	B	321	ARG	NE-CZ-NH1	-11.50	114.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	474	ARG	NE-CZ-NH2	11.49	126.04	120.30
1	O	360	ARG	NE-CZ-NH2	11.47	126.03	120.30
1	O	321	ARG	NE-CZ-NH2	11.46	126.03	120.30
1	J	224	ARG	NE-CZ-NH1	-11.44	114.58	120.30
1	G	406	ARG	NE-CZ-NH2	11.37	125.98	120.30
1	P	476	ARG	NE-CZ-NH1	-11.33	114.64	120.30
1	F	476	ARG	NE-CZ-NH2	-11.33	114.64	120.30
1	A	432	TYR	CB-CG-CD2	-11.30	114.22	121.00
1	C	31	ARG	NE-CZ-NH2	11.29	125.94	120.30
1	O	325	ARG	NE-CZ-NH2	11.29	125.94	120.30
1	O	311	PHE	CB-CG-CD1	-11.26	112.92	120.80
1	O	224	ARG	NE-CZ-NH2	11.24	125.92	120.30
1	P	200	TYR	CB-CG-CD2	-11.22	114.27	121.00
1	P	16	ARG	NE-CZ-NH1	-11.20	114.70	120.30
1	H	396	ARG	NE-CZ-NH2	11.19	125.89	120.30
1	H	474	ARG	NE-CZ-NH2	11.18	125.89	120.30
1	K	369	PHE	CB-CG-CD1	11.18	128.62	120.80
1	D	239	ARG	NE-CZ-NH2	11.14	125.87	120.30
1	H	311	PHE	CB-CG-CD1	-11.09	113.04	120.80
1	L	163	TYR	CB-CG-CD1	-11.07	114.36	121.00
1	C	455	PRO	CA-N-CD	-11.06	96.02	111.50
1	E	155	ARG	NE-CZ-NH2	11.04	125.82	120.30
1	G	396	ARG	NE-CZ-NH1	-11.03	114.78	120.30
1	K	20	ARG	NE-CZ-NH2	11.03	125.81	120.30
1	J	455	PRO	CA-N-CD	-11.01	96.09	111.50
1	I	311	PHE	CB-CG-CD1	10.96	128.47	120.80
1	L	38	ARG	NE-CZ-NH1	10.94	125.77	120.30
1	L	455	PRO	CA-N-CD	-10.94	96.18	111.50
1	O	171	MET	CG-SD-CE	-10.92	82.72	100.20
1	I	155	ARG	NE-CZ-NH2	10.86	125.73	120.30
1	F	507	ARG	NE-CZ-NH2	10.85	125.72	120.30
1	D	396	ARG	NE-CZ-NH2	10.80	125.70	120.30
1	E	434	ARG	NE-CZ-NH2	10.72	125.66	120.30
1	D	360	ARG	NE-CZ-NH2	10.65	125.63	120.30
1	C	476	ARG	NE-CZ-NH2	10.65	125.62	120.30
1	P	455	PRO	CA-N-CD	-10.63	96.61	111.50
1	J	432	TYR	CB-CG-CD2	-10.62	114.62	121.00
1	N	315	ARG	NE-CZ-NH2	10.60	125.60	120.30
1	C	200	TYR	CB-CG-CD2	10.60	127.36	121.00
1	K	31	ARG	NE-CZ-NH2	10.57	125.59	120.30
1	H	350	ASP	CB-CG-OD1	10.55	127.79	118.30
1	I	528	ASP	CB-CG-OD1	10.51	127.76	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	428	ARG	NE-CZ-NH1	-10.51	115.05	120.30
1	E	325	ARG	NE-CZ-NH2	10.51	125.55	120.30
1	D	338	ARG	NE-CZ-NH1	-10.49	115.06	120.30
1	N	428	ARG	NE-CZ-NH1	10.49	125.54	120.30
1	L	434	ARG	NE-CZ-NH1	-10.48	115.06	120.30
1	M	430	ARG	NE-CZ-NH2	10.48	125.54	120.30
1	E	403	TYR	CB-CG-CD1	-10.44	114.74	121.00
1	M	170	PHE	CB-CG-CD1	-10.44	113.50	120.80
1	L	507	ARG	NE-CZ-NH2	10.43	125.52	120.30
1	F	353	TYR	CB-CG-CD2	-10.43	114.74	121.00
1	L	239	ARG	NE-CZ-NH2	10.40	125.50	120.30
1	H	455	PRO	CA-N-CD	-10.36	97.00	111.50
1	G	507	ARG	NE-CZ-NH2	10.35	125.48	120.30
1	L	224	ARG	NE-CZ-NH2	10.32	125.46	120.30
1	I	322	ARG	NE-CZ-NH1	-10.31	115.15	120.30
1	O	38	ARG	NE-CZ-NH1	-10.29	115.16	120.30
1	E	360	ARG	NE-CZ-NH2	10.28	125.44	120.30
1	G	474	ARG	NE-CZ-NH2	10.28	125.44	120.30
1	H	432	TYR	CB-CG-CD1	-10.27	114.84	121.00
1	L	384	ARG	NE-CZ-NH2	10.26	125.43	120.30
1	L	126	PHE	CB-CG-CD2	-10.20	113.66	120.80
1	O	275	PHE	CB-CG-CD1	-10.16	113.69	120.80
1	K	54	PHE	CB-CG-CD2	10.15	127.90	120.80
1	N	474	ARG	NE-CZ-NH1	-10.14	115.23	120.30
1	I	396	ARG	NE-CZ-NH1	-10.13	115.23	120.30
1	E	507	ARG	NE-CZ-NH1	-10.12	115.24	120.30
1	J	38	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	B	275	PHE	CB-CG-CD1	10.10	127.87	120.80
1	G	240	ARG	NE-CZ-NH2	10.03	125.31	120.30
1	K	54	PHE	CB-CG-CD1	-10.01	113.79	120.80
1	J	507	ARG	NE-CZ-NH1	-10.01	115.30	120.30
1	M	369	PHE	CB-CG-CD2	10.00	127.80	120.80
1	D	240	ARG	NE-CZ-NH1	-9.98	115.31	120.30
1	N	360	ARG	NE-CZ-NH2	9.96	125.28	120.30
1	H	430	ARG	NE-CZ-NH2	9.94	125.27	120.30
1	I	315	ARG	NE-CZ-NH1	-9.92	115.34	120.30
1	A	275	PHE	CB-CG-CD1	9.92	127.74	120.80
1	J	56	ASP	CB-CG-OD2	-9.89	109.40	118.30
1	C	224	ARG	NE-CZ-NH2	9.88	125.24	120.30
1	L	315	ARG	NE-CZ-NH1	-9.88	115.36	120.30
1	M	428	ARG	NE-CZ-NH2	9.88	125.24	120.30
1	E	507	ARG	NE-CZ-NH2	9.88	125.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	321	ARG	NE-CZ-NH1	-9.86	115.37	120.30
1	M	384	ARG	NE-CZ-NH2	9.84	125.22	120.30
1	F	155	ARG	NE-CZ-NH2	9.84	125.22	120.30
1	F	527	ASP	CB-CG-OD2	9.83	127.15	118.30
1	G	338	ARG	NE-CZ-NH1	-9.82	115.39	120.30
1	L	507	ARG	NE-CZ-NH1	-9.81	115.39	120.30
1	E	150	ASN	N-CA-CB	9.80	128.24	110.60
1	B	38	ARG	NE-CZ-NH2	9.75	125.18	120.30
1	M	413	TYR	CB-CG-CD1	9.73	126.84	121.00
1	D	474	ARG	NE-CZ-NH2	9.72	125.16	120.30
1	I	434	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	J	311	PHE	CB-CG-CD2	9.69	127.58	120.80
1	N	476	ARG	NE-CZ-NH1	-9.66	115.47	120.30
1	M	239	ARG	NE-CZ-NH2	9.65	125.12	120.30
1	K	455	PRO	CA-N-CD	-9.64	98.00	111.50
1	N	240	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	D	16	ARG	NE-CZ-NH2	9.61	125.11	120.30
1	B	327	ASP	CB-CG-OD2	9.59	126.93	118.30
1	N	155	ARG	NE-CZ-NH1	9.59	125.09	120.30
1	E	224	ARG	NE-CZ-NH2	9.58	125.09	120.30
1	K	38	ARG	NE-CZ-NH2	9.58	125.09	120.30
1	P	510	ARG	NE-CZ-NH2	9.56	125.08	120.30
1	O	384	ARG	NE-CZ-NH2	9.56	125.08	120.30
1	B	20	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	K	38	ARG	NE-CZ-NH1	-9.48	115.56	120.30
1	A	322	ARG	NE-CZ-NH1	-9.47	115.56	120.30
1	B	105	PHE	CB-CG-CD1	-9.46	114.18	120.80
1	P	282	TYR	CG-CD2-CE2	-9.45	113.74	121.30
1	F	171	MET	CG-SD-CE	-9.43	85.11	100.20
1	J	31	ARG	NE-CZ-NH1	-9.43	115.59	120.30
1	J	325	ARG	NE-CZ-NH2	9.39	125.00	120.30
1	E	455	PRO	CA-N-CD	-9.36	98.39	111.50
1	J	321	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	J	315	ARG	NE-CZ-NH2	9.36	124.98	120.30
1	B	471	MET	CG-SD-CE	-9.35	85.25	100.20
1	G	498	TYR	CZ-CE2-CD2	9.34	128.21	119.80
1	J	447	TYR	CB-CG-CD2	-9.34	115.40	121.00
1	O	38	ARG	NE-CZ-NH2	9.32	124.96	120.30
1	O	430	ARG	NE-CZ-NH2	9.28	124.94	120.30
1	P	105	PHE	CB-CG-CD2	-9.25	114.33	120.80
1	J	434	ARG	NE-CZ-NH2	9.23	124.92	120.30
1	F	487	ASP	CB-CG-OD1	9.23	126.61	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	434	ARG	NE-CZ-NH2	9.20	124.90	120.30
1	J	31	ARG	NE-CZ-NH2	9.20	124.90	120.30
1	B	447	TYR	CB-CG-CD1	-9.19	115.49	121.00
1	F	277	ASP	CB-CG-OD1	9.17	126.56	118.30
1	O	282	TYR	CG-CD1-CE1	-9.17	113.96	121.30
1	E	476	ARG	NE-CZ-NH2	9.16	124.88	120.30
1	K	413	TYR	CB-CG-CD1	-9.16	115.50	121.00
1	J	432	TYR	CB-CG-CD1	9.15	126.49	121.00
1	H	288	ASP	CB-CG-OD1	9.14	126.53	118.30
1	M	325	ARG	NE-CZ-NH2	9.11	124.86	120.30
1	O	338	ARG	NE-CZ-NH2	-9.09	115.75	120.30
1	M	400	ASP	CB-CG-OD2	9.08	126.47	118.30
1	J	396	ARG	NE-CZ-NH2	9.02	124.81	120.30
1	D	507	ARG	NE-CZ-NH1	-9.01	115.80	120.30
1	L	224	ARG	NE-CZ-NH1	-9.00	115.80	120.30
1	K	126	PHE	CB-CG-CD2	-8.99	114.50	120.80
1	L	325	ARG	NE-CZ-NH2	8.97	124.79	120.30
1	B	322	ARG	NE-CZ-NH1	-8.97	115.81	120.30
1	G	455	PRO	CA-N-CD	-8.97	98.94	111.50
1	M	510	ARG	NE-CZ-NH1	-8.97	115.82	120.30
1	I	474	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	B	105	PHE	CB-CG-CD2	8.96	127.07	120.80
1	A	170	PHE	CB-CG-CD2	-8.96	114.53	120.80
1	P	224	ARG	NE-CZ-NH2	8.95	124.77	120.30
1	N	455	PRO	CA-N-CD	-8.94	98.98	111.50
1	C	325	ARG	NE-CZ-NH2	8.94	124.77	120.30
1	M	126	PHE	CB-CG-CD2	8.93	127.05	120.80
1	C	306	ASP	CB-CG-OD2	8.91	126.32	118.30
1	A	455	PRO	CA-N-CD	-8.91	99.03	111.50
1	D	105	PHE	CB-CG-CD2	8.87	127.01	120.80
1	I	455	PRO	CA-N-CD	-8.87	99.09	111.50
1	H	428	ARG	NH1-CZ-NH2	-8.86	109.66	119.40
1	M	192	ALA	N-CA-CB	8.85	122.49	110.10
1	L	428	ARG	NE-CZ-NH1	-8.84	115.88	120.30
1	A	510	ARG	NE-CZ-NH2	8.83	124.72	120.30
1	D	406	ARG	NE-CZ-NH2	8.83	124.71	120.30
1	B	126	PHE	CB-CG-CD2	-8.82	114.62	120.80
1	M	105	PHE	CB-CG-CD1	8.82	126.97	120.80
1	O	455	PRO	CA-N-CD	-8.81	99.16	111.50
1	A	434	ARG	NE-CZ-NH2	8.81	124.71	120.30
1	J	56	ASP	CB-CG-OD1	8.81	126.23	118.30
1	K	345	ASP	CB-CG-OD2	8.79	126.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	428	ARG	NE-CZ-NH1	-8.79	115.91	120.30
1	F	224	ARG	NE-CZ-NH1	-8.79	115.91	120.30
1	C	396	ARG	NE-CZ-NH1	-8.78	115.91	120.30
1	I	406	ARG	NE-CZ-NH2	8.78	124.69	120.30
1	C	510	ARG	NE-CZ-NH2	-8.78	115.91	120.30
1	G	447	TYR	CB-CG-CD1	-8.76	115.74	121.00
1	M	155	ARG	NE-CZ-NH1	8.75	124.67	120.30
1	P	163	TYR	CB-CG-CD2	-8.74	115.76	121.00
1	O	315	ARG	NE-CZ-NH2	8.73	124.66	120.30
1	B	360	ARG	NE-CZ-NH2	8.70	124.65	120.30
1	E	472	ASP	CB-CG-OD1	8.70	126.13	118.30
1	N	510	ARG	NE-CZ-NH1	-8.65	115.97	120.30
1	C	200	TYR	CB-CG-CD1	-8.65	115.81	121.00
1	I	282	TYR	CB-CG-CD2	8.64	126.19	121.00
1	A	240	ARG	NE-CZ-NH2	8.64	124.62	120.30
1	M	282	TYR	CB-CG-CD2	8.63	126.18	121.00
1	G	219	ASP	CB-CG-OD1	-8.63	110.53	118.30
1	A	507	ARG	NE-CZ-NH2	8.59	124.60	120.30
1	M	353	TYR	CB-CG-CD1	-8.58	115.85	121.00
1	E	166	MET	CG-SD-CE	-8.57	86.49	100.20
1	I	38	ARG	NE-CZ-NH1	-8.56	116.02	120.30
1	J	191	VAL	CA-CB-CG1	-8.56	98.06	110.90
1	M	447	TYR	CB-CG-CD2	8.55	126.13	121.00
1	F	114	ASP	CB-CG-OD1	8.50	125.95	118.30
1	P	406	ARG	NE-CZ-NH2	8.49	124.55	120.30
1	F	105	PHE	CB-CG-CD2	-8.49	114.86	120.80
1	D	496	ASP	CB-CG-OD2	8.47	125.92	118.30
1	I	38	ARG	NE-CZ-NH2	8.47	124.53	120.30
1	O	338	ARG	NE-CZ-NH1	8.46	124.53	120.30
1	D	22	ALA	N-CA-CB	-8.45	98.27	110.10
1	B	38	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	M	126	PHE	CB-CG-CD1	-8.44	114.89	120.80
1	M	527	ASP	CB-CG-OD1	8.43	125.89	118.30
1	M	105	PHE	CB-CG-CD2	-8.43	114.90	120.80
1	J	200	TYR	CB-CG-CD1	-8.43	115.94	121.00
1	E	403	TYR	CG-CD1-CE1	-8.42	114.56	121.30
1	P	507	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	O	388	ASP	CB-CG-OD2	8.41	125.87	118.30
1	D	89	SER	N-CA-CB	8.40	123.09	110.50
1	M	200	TYR	CB-CG-CD2	-8.39	115.97	121.00
1	K	396	ARG	NH1-CZ-NH2	-8.37	110.19	119.40
1	C	130	PHE	CB-CG-CD1	8.37	126.66	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	L	239	ARG	NH1-CZ-NH2	-8.33	110.24	119.40
1	K	282	TYR	CB-CG-CD1	8.31	125.99	121.00
1	M	311	PHE	CB-CG-CD1	-8.31	114.98	120.80
1	L	496	ASP	CB-CG-OD1	8.31	125.78	118.30
1	D	428	ARG	NE-CZ-NH1	-8.30	116.15	120.30
1	P	56	ASP	CB-CG-OD2	8.29	125.76	118.30
1	D	400	ASP	CB-CG-OD1	8.29	125.76	118.30
1	J	306	ASP	CB-CG-OD2	-8.28	110.85	118.30
1	F	197	ASP	CB-CG-OD2	-8.24	110.88	118.30
1	H	315	ARG	NE-CZ-NH2	8.23	124.42	120.30
1	G	315	ARG	NE-CZ-NH2	8.23	124.41	120.30
1	K	194	PRO	N-CA-CB	8.22	113.17	103.30
1	O	181	MET	CG-SD-CE	-8.22	87.04	100.20
1	A	353	TYR	CB-CG-CD1	-8.22	116.07	121.00
1	D	528	ASP	CB-CG-OD2	8.19	125.67	118.30
1	H	237	MET	CG-SD-CE	-8.18	87.11	100.20
1	J	170	PHE	CB-CG-CD2	-8.18	115.07	120.80
1	A	432	TYR	CG-CD2-CE2	-8.18	114.76	121.30
1	O	353	TYR	CB-CG-CD2	8.17	125.91	121.00
1	A	498	TYR	CB-CG-CD2	-8.17	116.10	121.00
1	K	432	TYR	CB-CG-CD1	-8.16	116.10	121.00
1	K	476	ARG	NE-CZ-NH1	8.15	124.38	120.30
1	L	31	ARG	NE-CZ-NH1	-8.14	116.23	120.30
1	H	472	ASP	CB-CG-OD2	8.12	125.61	118.30
1	M	311	PHE	CB-CG-CD2	8.12	126.48	120.80
1	M	428	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	O	434	ARG	NE-CZ-NH2	8.10	124.35	120.30
1	I	396	ARG	NE-CZ-NH2	8.09	124.34	120.30
1	E	239	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	J	126	PHE	CB-CG-CD1	8.08	126.45	120.80
1	D	148	ASP	CB-CG-OD2	-8.07	111.03	118.30
1	J	322	ARG	NE-CZ-NH2	8.07	124.34	120.30
1	L	31	ARG	NE-CZ-NH2	-8.07	116.27	120.30
1	B	138	PRO	O-C-N	-8.04	109.83	122.70
1	K	239	ARG	NE-CZ-NH1	-8.04	116.28	120.30
1	E	474	ARG	NH1-CZ-NH2	-8.03	110.56	119.40
1	F	105	PHE	CB-CG-CD1	8.03	126.42	120.80
1	J	413	TYR	CB-CG-CD2	-8.02	116.19	121.00
1	B	384	ARG	NE-CZ-NH2	-8.02	116.29	120.30
1	E	321	ARG	NE-CZ-NH2	7.99	124.30	120.30
1	N	323	VAL	CG1-CB-CG2	-7.99	98.12	110.90
1	P	454	ILE	CB-CA-C	7.99	127.57	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	469	ALA	N-CA-CB	7.98	121.28	110.10
1	G	430	ARG	NE-CZ-NH1	-7.98	116.31	120.30
1	J	130	PHE	CB-CG-CD2	7.97	126.38	120.80
1	K	239	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	E	510	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	P	130	PHE	CB-CG-CD1	7.95	126.36	120.80
1	C	126	PHE	CB-CG-CD1	7.95	126.36	120.80
1	L	52	ASP	CB-CG-OD2	-7.95	111.15	118.30
1	H	31	ARG	NE-CZ-NH2	7.93	124.27	120.30
1	F	126	PHE	CB-CG-CD1	7.92	126.35	120.80
1	A	403	TYR	CB-CG-CD2	7.91	125.75	121.00
1	M	158	LEU	CB-CG-CD1	-7.90	97.57	111.00
1	A	495	ASP	CB-CG-OD2	-7.89	111.19	118.30
1	G	97	SER	N-CA-CB	7.89	122.34	110.50
1	G	447	TYR	CB-CG-CD2	7.88	125.73	121.00
1	H	171	MET	CG-SD-CE	-7.88	87.60	100.20
1	M	38	ARG	NE-CZ-NH1	7.87	124.24	120.30
1	C	338	ARG	NE-CZ-NH2	7.87	124.23	120.30
1	E	430	ARG	NH1-CZ-NH2	-7.87	110.75	119.40
1	O	392	ASP	CB-CG-OD1	7.86	125.38	118.30
1	L	239	ARG	NE-CZ-NH1	7.86	124.23	120.30
1	E	20	ARG	NE-CZ-NH1	-7.86	116.37	120.30
1	J	510	ARG	NE-CZ-NH2	7.82	124.21	120.30
1	C	31	ARG	NE-CZ-NH1	-7.81	116.39	120.30
1	I	413	TYR	CB-CG-CD1	-7.79	116.32	121.00
1	M	403	TYR	CB-CG-CD2	-7.79	116.33	121.00
1	K	306	ASP	CB-CG-OD2	7.78	125.30	118.30
1	D	455	PRO	CB-CA-C	7.77	131.41	112.00
1	D	510	ARG	NE-CZ-NH2	7.75	124.18	120.30
1	G	275	PHE	CB-CG-CD2	-7.75	115.37	120.80
1	O	384	ARG	NE-CZ-NH1	-7.73	116.44	120.30
1	E	20	ARG	NE-CZ-NH2	7.73	124.16	120.30
1	J	93	ASP	CB-CG-OD2	7.72	125.25	118.30
1	J	153	THR	CA-CB-CG2	-7.72	101.58	112.40
1	E	322	ARG	NE-CZ-NH1	-7.72	116.44	120.30
1	F	20	ARG	NE-CZ-NH1	7.72	124.16	120.30
1	P	156	ASP	CB-CG-OD1	-7.71	111.36	118.30
1	E	353	TYR	CB-CG-CD2	-7.70	116.38	121.00
1	A	155	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	B	510	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	N	403	TYR	CB-CG-CD1	-7.70	116.38	121.00
1	B	170	PHE	CB-CG-CD1	-7.69	115.41	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	471	MET	CG-SD-CE	-7.67	87.92	100.20
1	P	155	ARG	NE-CZ-NH2	7.67	124.13	120.30
1	M	365	ASP	CB-CG-OD2	7.66	125.20	118.30
1	C	428	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	C	189	THR	CA-CB-CG2	-7.66	101.67	112.40
1	G	311	PHE	CB-CG-CD2	-7.66	115.44	120.80
1	A	21	ASP	CB-CG-OD2	7.65	125.18	118.30
1	F	454	ILE	CB-CA-C	7.62	126.85	111.60
1	M	434	ARG	NE-CZ-NH2	7.62	124.11	120.30
1	N	455	PRO	CB-CA-C	7.62	131.05	112.00
1	M	350	ASP	CB-CG-OD1	7.62	125.16	118.30
1	F	434	ARG	NE-CZ-NH2	-7.61	116.49	120.30
1	C	210	ASP	CB-CG-OD2	7.61	125.15	118.30
1	L	200	TYR	CB-CG-CD2	7.61	125.56	121.00
1	F	454	ILE	C-N-CD	-7.60	103.88	120.60
1	L	219	ASP	CB-CG-OD2	7.59	125.13	118.30
1	G	345	ASP	CB-CG-OD1	7.59	125.13	118.30
1	L	163	TYR	CB-CG-CD2	7.59	125.55	121.00
1	F	353	TYR	CB-CG-CD1	7.58	125.55	121.00
1	I	338	ARG	NE-CZ-NH1	-7.57	116.52	120.30
1	O	107	GLU	OE1-CD-OE2	-7.57	114.22	123.30
1	B	31	ARG	NE-CZ-NH2	-7.56	116.52	120.30
1	G	16	ARG	NE-CZ-NH1	-7.56	116.52	120.30
1	G	396	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	M	455	PRO	CB-CA-C	7.56	130.90	112.00
1	L	305	ASP	CB-CG-OD2	7.56	125.10	118.30
1	K	449	ASP	CB-CG-OD1	7.55	125.09	118.30
1	E	410	MET	CG-SD-CE	-7.55	88.13	100.20
1	E	224	ARG	NE-CZ-NH1	-7.54	116.53	120.30
1	O	447	TYR	CB-CG-CD1	7.54	125.52	121.00
1	K	126	PHE	CB-CG-CD1	7.52	126.07	120.80
1	C	71	GLU	OE1-CD-OE2	-7.52	114.27	123.30
1	B	153	THR	CA-CB-CG2	-7.52	101.87	112.40
1	D	413	TYR	CD1-CE1-CZ	-7.52	113.03	119.80
1	E	16	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	P	311	PHE	CB-CG-CD2	7.52	126.06	120.80
1	H	128	LYS	O-C-N	-7.51	110.68	122.70
1	N	325	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	H	130	PHE	CB-CG-CD2	-7.51	115.55	120.80
1	M	353	TYR	CG-CD2-CE2	-7.50	115.30	121.30
1	L	438	GLY	O-C-N	-7.48	110.73	122.70
1	M	413	TYR	CB-CG-CD2	-7.48	116.51	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	360	ARG	NE-CZ-NH1	-7.47	116.56	120.30
1	B	434	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	H	472	ASP	CB-CG-OD1	-7.46	111.58	118.30
1	I	154	ALA	CB-CA-C	7.45	121.27	110.10
1	O	16	ARG	NE-CZ-NH1	-7.45	116.58	120.30
1	G	35	GLU	OE1-CD-OE2	-7.44	114.37	123.30
1	M	170	PHE	CB-CG-CD2	7.43	126.00	120.80
1	H	498	TYR	CB-CG-CD2	-7.42	116.55	121.00
1	P	315	ARG	NE-CZ-NH1	7.42	124.01	120.30
1	C	237	MET	CG-SD-CE	-7.40	88.36	100.20
1	O	403	TYR	CB-CG-CD2	-7.37	116.58	121.00
1	C	375	ASN	CA-C-O	-7.36	104.64	120.10
1	G	282	TYR	CB-CG-CD2	-7.36	116.58	121.00
1	P	389	MET	CG-SD-CE	-7.36	88.42	100.20
1	J	496	ASP	CB-CG-OD1	7.36	124.92	118.30
1	J	455	PRO	CB-CA-C	7.34	130.35	112.00
1	G	403	TYR	CB-CG-CD1	7.34	125.40	121.00
1	N	197	ASP	CB-CG-OD2	7.34	124.90	118.30
1	J	447	TYR	CG-CD1-CE1	-7.33	115.44	121.30
1	O	57	VAL	CA-CB-CG1	7.33	121.90	110.90
1	B	197	ASP	CB-CG-OD1	7.32	124.89	118.30
1	A	325	ARG	NE-CZ-NH1	-7.32	116.64	120.30
1	A	406	ARG	NE-CZ-NH1	-7.31	116.64	120.30
1	H	428	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	O	240	ARG	NE-CZ-NH2	-7.29	116.66	120.30
1	J	275	PHE	CB-CG-CD1	7.29	125.90	120.80
1	D	126	PHE	CB-CG-CD2	-7.28	115.70	120.80
1	E	155	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	F	396	ARG	NE-CZ-NH1	7.28	123.94	120.30
1	O	403	TYR	CB-CG-CD1	7.28	125.37	121.00
1	K	455	PRO	CB-CA-C	7.28	130.19	112.00
1	P	31	ARG	NE-CZ-NH2	7.27	123.93	120.30
1	H	359	GLU	OE1-CD-OE2	-7.26	114.59	123.30
1	L	428	ARG	NE-CZ-NH2	7.26	123.93	120.30
1	D	270	ASP	CB-CG-OD1	7.26	124.83	118.30
1	N	428	ARG	NE-CZ-NH2	-7.26	116.67	120.30
1	F	432	TYR	CG-CD1-CE1	-7.25	115.50	121.30
1	L	233	VAL	CA-CB-CG2	-7.25	100.03	110.90
1	I	434	ARG	NE-CZ-NH2	7.25	123.92	120.30
1	G	360	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	J	286	MET	CG-SD-CE	-7.22	88.64	100.20
1	F	297	VAL	CA-CB-CG1	7.22	121.73	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	288	ASP	CB-CG-OD2	-7.22	111.80	118.30
1	D	54	PHE	CB-CG-CD1	-7.21	115.75	120.80
1	I	447	TYR	CB-CG-CD1	-7.20	116.68	121.00
1	L	31	ARG	NH1-CZ-NH2	7.20	127.31	119.40
1	K	327	ASP	CB-CG-OD1	7.19	124.77	118.30
1	G	38	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	I	456	MET	CG-SD-CE	-7.18	88.72	100.20
1	K	406	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	E	405	LEU	N-CA-CB	-7.16	96.09	110.40
1	E	322	ARG	NE-CZ-NH2	7.15	123.88	120.30
1	B	360	ARG	N-CA-CB	7.15	123.47	110.60
1	H	340	ILE	O-C-N	-7.15	111.26	122.70
1	I	373	ALA	CB-CA-C	7.14	120.81	110.10
1	D	126	PHE	CB-CG-CD1	7.14	125.80	120.80
1	K	229	ASP	CB-CG-OD2	-7.13	111.88	118.30
1	J	482	THR	CA-CB-CG2	7.13	122.38	112.40
1	E	454	ILE	C-N-CD	-7.12	104.93	120.60
1	H	31	ARG	NE-CZ-NH1	-7.12	116.74	120.30
1	O	153	THR	CA-CB-CG2	-7.11	102.44	112.40
1	G	471	MET	CG-SD-CE	-7.10	88.83	100.20
1	C	474	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	G	166	MET	CG-SD-CE	-7.10	88.85	100.20
1	I	311	PHE	CB-CG-CD2	-7.09	115.84	120.80
1	G	428	ARG	NE-CZ-NH1	-7.08	116.76	120.30
1	O	432	TYR	CG-CD2-CE2	-7.07	115.64	121.30
1	P	282	TYR	CG-CD1-CE1	-7.06	115.65	121.30
1	P	282	TYR	CB-CG-CD1	-7.05	116.77	121.00
1	O	170	PHE	CB-CG-CD2	7.05	125.73	120.80
1	D	392	ASP	CB-CG-OD1	7.04	124.64	118.30
1	F	130	PHE	CB-CG-CD1	7.04	125.73	120.80
1	K	474	ARG	NE-CZ-NH1	-7.04	116.78	120.30
1	K	80	LEU	CB-CG-CD1	7.04	122.96	111.00
1	G	233	VAL	CA-CB-CG2	7.03	121.45	110.90
1	M	481	LEU	CB-CG-CD1	-7.03	99.05	111.00
1	E	455	PRO	N-CA-CB	7.03	111.73	103.30
1	M	322	ARG	NE-CZ-NH2	7.02	123.81	120.30
1	J	313	ALA	N-CA-CB	7.01	119.91	110.10
1	M	130	PHE	CB-CG-CD1	7.01	125.70	120.80
1	K	322	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	I	288	ASP	CB-CG-OD2	7.00	124.60	118.30
1	G	237	MET	CG-SD-CE	-7.00	89.00	100.20
1	E	200	TYR	CB-CG-CD1	7.00	125.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	224	ARG	NE-CZ-NH2	6.99	123.80	120.30
1	I	432	TYR	CB-CG-CD2	6.99	125.19	121.00
1	L	286	MET	CG-SD-CE	-6.99	89.02	100.20
1	B	16	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	D	369	PHE	CB-CG-CD2	-6.98	115.91	120.80
1	G	176	GLU	OE1-CD-OE2	-6.98	114.92	123.30
1	O	282	TYR	CB-CG-CD1	-6.98	116.81	121.00
1	G	498	TYR	CG-CD2-CE2	-6.97	115.72	121.30
1	M	447	TYR	CB-CG-CD1	-6.97	116.82	121.00
1	F	406	ARG	NE-CZ-NH1	6.97	123.78	120.30
1	L	392	ASP	CB-CG-OD1	6.96	124.57	118.30
1	M	527	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	B	321	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	L	170	PHE	CB-CG-CD2	6.95	125.67	120.80
1	L	455	PRO	CB-CA-C	6.95	129.38	112.00
1	P	71	GLU	O-C-N	-6.95	111.59	122.70
1	H	360	ARG	NH1-CZ-NH2	-6.91	111.80	119.40
1	B	88	ASP	CB-CG-OD1	6.91	124.52	118.30
1	F	38	ARG	NE-CZ-NH1	6.91	123.75	120.30
1	C	400	ASP	CB-CG-OD2	-6.91	112.08	118.30
1	O	322	ARG	NE-CZ-NH1	-6.91	116.85	120.30
1	O	510	ARG	NE-CZ-NH2	6.91	123.75	120.30
1	P	472	ASP	CB-CG-OD1	6.90	124.51	118.30
1	G	62	ASP	CB-CG-OD1	6.89	124.50	118.30
1	L	476	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	I	499	SER	CB-CA-C	-6.89	97.01	110.10
1	L	475	ALA	N-CA-CB	6.88	119.74	110.10
1	B	498	TYR	CB-CG-CD2	-6.88	116.87	121.00
1	P	475	ALA	N-CA-CB	-6.88	100.47	110.10
1	N	472	ASP	CB-CG-OD2	6.87	124.48	118.30
1	G	403	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	A	410	MET	CG-SD-CE	-6.87	89.21	100.20
1	N	229	ASP	CB-CG-OD1	6.86	124.48	118.30
1	P	369	PHE	CB-CG-CD2	-6.86	116.00	120.80
1	D	449	ASP	CB-CG-OD1	6.86	124.47	118.30
1	J	155	ARG	NE-CZ-NH1	-6.86	116.87	120.30
1	N	360	ARG	NE-CZ-NH1	-6.85	116.87	120.30
1	A	275	PHE	CB-CG-CD2	-6.85	116.00	120.80
1	P	332	GLU	OE1-CD-OE2	-6.85	115.08	123.30
1	H	311	PHE	CB-CG-CD2	6.85	125.59	120.80
1	O	285	ASP	CB-CG-OD2	6.85	124.47	118.30
1	K	403	TYR	CB-CG-CD1	-6.84	116.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	O	502	VAL	CA-CB-CG2	-6.84	100.65	110.90
1	M	176	GLU	OE1-CD-OE2	-6.83	115.10	123.30
1	L	375	ASN	CA-C-N	6.83	136.22	117.10
1	I	428	ARG	NE-CZ-NH1	-6.83	116.89	120.30
1	M	54	PHE	CB-CG-CD1	6.82	125.58	120.80
1	A	449	ASP	CB-CG-OD1	-6.82	112.17	118.30
1	F	147	SER	CB-CA-C	-6.82	97.15	110.10
1	D	200	TYR	CB-CG-CD2	-6.80	116.92	121.00
1	B	93	ASP	CB-CG-OD2	6.80	124.42	118.30
1	H	498	TYR	CG-CD2-CE2	-6.79	115.87	121.30
1	J	130	PHE	CB-CG-CD1	-6.78	116.06	120.80
1	H	455	PRO	CB-CA-C	6.76	128.91	112.00
1	M	306	ASP	CB-CG-OD2	-6.76	112.21	118.30
1	H	20	ARG	CD-NE-CZ	6.75	133.06	123.60
1	G	455	PRO	CA-CB-CG	-6.75	91.17	104.00
1	C	353	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	M	167	SER	CB-CA-C	-6.75	97.28	110.10
1	O	448	ALA	N-CA-CB	-6.74	100.66	110.10
1	M	509	THR	CA-CB-CG2	-6.74	102.97	112.40
1	O	202	VAL	CB-CA-C	-6.73	98.61	111.40
1	O	47	ASP	CB-CG-OD1	6.73	124.36	118.30
1	B	341	SER	N-CA-CB	6.73	120.59	110.50
1	F	396	ARG	NE-CZ-NH2	-6.72	116.94	120.30
1	B	386	SER	O-C-N	-6.72	111.95	122.70
1	A	413	TYR	CB-CG-CD2	-6.72	116.97	121.00
1	F	360	ARG	NE-CZ-NH2	6.71	123.66	120.30
1	G	455	PRO	CB-CA-C	6.71	128.78	112.00
1	G	321	ARG	C-N-CA	6.71	138.47	121.70
1	L	170	PHE	CB-CG-CD1	-6.71	116.11	120.80
1	C	275	PHE	CB-CG-CD2	-6.70	116.11	120.80
1	H	396	ARG	NH1-CZ-NH2	-6.70	112.03	119.40
1	D	428	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	B	20	ARG	NH1-CZ-NH2	-6.69	112.04	119.40
1	M	186	ASP	CB-CG-OD1	6.69	124.32	118.30
1	L	153	THR	CA-CB-CG2	-6.68	103.04	112.40
1	O	360	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	O	471	MET	CG-SD-CE	-6.67	89.53	100.20
1	G	498	TYR	CB-CG-CD1	-6.66	117.00	121.00
1	I	498	TYR	CB-CG-CD2	-6.66	117.00	121.00
1	O	155	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	I	447	TYR	CG-CD2-CE2	-6.65	115.98	121.30
1	J	250	ASP	CB-CG-OD2	-6.65	112.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	360	ARG	NE-CZ-NH1	-6.65	116.98	120.30
1	I	338	ARG	N-CA-CB	6.64	122.56	110.60
1	F	447	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	M	203	SER	N-CA-CB	6.64	120.46	110.50
1	H	516	ALA	CB-CA-C	-6.63	100.15	110.10
1	J	88	ASP	CB-CG-OD1	6.63	124.27	118.30
1	M	275	PHE	CB-CG-CD2	6.63	125.44	120.80
1	D	474	ARG	NH1-CZ-NH2	-6.62	112.11	119.40
1	K	237	MET	CG-SD-CE	-6.62	89.61	100.20
1	I	400	ASP	CB-CG-OD2	6.62	124.26	118.30
1	P	379	VAL	CA-CB-CG1	-6.62	100.98	110.90
1	B	280	ALA	N-CA-CB	-6.61	100.84	110.10
1	B	353	TYR	CG-CD1-CE1	-6.61	116.01	121.30
1	G	496	ASP	CB-CG-OD1	6.61	124.25	118.30
1	I	210	ASP	CB-CG-OD1	-6.61	112.35	118.30
1	G	400	ASP	CB-CG-OD2	-6.60	112.36	118.30
1	K	487	ASP	CB-CG-OD1	6.58	124.22	118.30
1	N	434	ARG	NE-CZ-NH1	-6.58	117.01	120.30
1	D	238	PRO	N-CA-C	6.56	129.15	112.10
1	I	130	PHE	CB-CG-CD2	-6.56	116.21	120.80
1	O	403	TYR	CZ-CE2-CD2	6.56	125.70	119.80
1	J	102	ALA	N-CA-CB	-6.55	100.92	110.10
1	K	250	ASP	CB-CG-OD2	6.55	124.20	118.30
1	M	219	ASP	CB-CG-OD2	6.55	124.20	118.30
1	B	455	PRO	CB-CA-C	6.55	128.37	112.00
1	E	254	GLU	N-CA-CB	-6.54	98.83	110.60
1	K	16	ARG	CD-NE-CZ	6.54	132.76	123.60
1	E	476	ARG	NE-CZ-NH1	-6.53	117.03	120.30
1	A	315	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	I	496	ASP	CB-CG-OD1	6.53	124.17	118.30
1	B	415	VAL	CB-CA-C	-6.52	99.01	111.40
1	G	498	TYR	CD1-CE1-CZ	6.52	125.67	119.80
1	N	311	PHE	CB-CG-CD1	-6.52	116.24	120.80
1	O	210	ASP	CB-CG-OD1	6.52	124.17	118.30
1	M	282	TYR	CB-CG-CD1	-6.51	117.09	121.00
1	K	510	ARG	NE-CZ-NH1	-6.51	117.05	120.30
1	E	306	ASP	CB-CG-OD2	6.51	124.16	118.30
1	E	338	ARG	NH1-CZ-NH2	-6.51	112.24	119.40
1	K	31	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	B	126	PHE	CB-CG-CD1	6.50	125.35	120.80
1	N	321	ARG	NE-CZ-NH2	-6.50	117.05	120.30
1	N	457	ILE	CA-CB-CG1	6.50	123.35	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	150	ASN	N-CA-CB	6.50	122.29	110.60
1	F	247	ALA	CB-CA-C	-6.49	100.36	110.10
1	E	276	LEU	CB-CG-CD1	6.49	122.03	111.00
1	L	375	ASN	CA-C-O	-6.49	106.48	120.10
1	E	367	MET	CG-SD-CE	-6.48	89.83	100.20
1	E	31	ARG	CG-CD-NE	-6.48	98.20	111.80
1	J	528	ASP	CB-CG-OD2	6.48	124.13	118.30
1	K	413	TYR	CG-CD1-CE1	-6.48	116.12	121.30
1	J	306	ASP	CB-CG-OD1	6.47	124.13	118.30
1	K	348	PRO	N-CA-CB	6.47	111.07	103.30
1	E	62	ASP	CB-CG-OD2	6.47	124.12	118.30
1	G	387	ASN	CB-CA-C	6.47	123.34	110.40
1	B	507	ARG	NE-CZ-NH1	-6.47	117.06	120.30
1	O	396	ARG	NE-CZ-NH1	6.47	123.53	120.30
1	G	287	VAL	CA-CB-CG2	-6.46	101.20	110.90
1	D	148	ASP	CB-CG-OD1	6.46	124.11	118.30
1	J	428	ARG	NE-CZ-NH1	-6.46	117.07	120.30
1	P	442	LEU	CB-CG-CD2	6.46	121.97	111.00
1	B	429	LEU	O-C-N	-6.45	112.39	122.70
1	P	321	ARG	NE-CZ-NH1	-6.44	117.08	120.30
1	O	427	ALA	CB-CA-C	-6.44	100.44	110.10
1	D	496	ASP	CB-CG-OD1	-6.43	112.51	118.30
1	I	286	MET	CG-SD-CE	-6.43	89.92	100.20
1	K	282	TYR	CB-CG-CD2	-6.43	117.14	121.00
1	B	495	ASP	CB-CG-OD1	6.42	124.08	118.30
1	L	475	ALA	CB-CA-C	-6.42	100.47	110.10
1	N	239	ARG	NE-CZ-NH1	-6.41	117.09	120.30
1	A	126	PHE	CB-CG-CD2	-6.41	116.31	120.80
1	P	455	PRO	CB-CA-C	6.41	128.02	112.00
1	F	474	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	K	90	GLU	OE1-CD-OE2	-6.41	115.61	123.30
1	P	384	ARG	NE-CZ-NH2	6.41	123.50	120.30
1	D	47	ASP	CB-CG-OD1	6.40	124.06	118.30
1	G	503	VAL	CA-CB-CG2	6.39	120.49	110.90
1	N	111	SER	O-C-N	-6.39	112.48	122.70
1	P	288	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	E	345	ASP	CB-CG-OD1	6.39	124.05	118.30
1	O	166	MET	CA-CB-CG	-6.38	102.45	113.30
1	N	396	ARG	CG-CD-NE	-6.38	98.40	111.80
1	C	507	ARG	CD-NE-CZ	6.38	132.53	123.60
1	K	224	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	O	357	VAL	CG1-CB-CG2	-6.37	100.70	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	38	ARG	NE-CZ-NH2	6.37	123.49	120.30
1	C	287	VAL	CA-CB-CG2	-6.37	101.35	110.90
1	D	186	ASP	CB-CG-OD1	6.36	124.02	118.30
1	M	124	GLU	CB-CA-C	-6.36	97.68	110.40
1	P	88	ASP	N-CA-CB	-6.35	99.16	110.60
1	G	23	LEU	O-C-N	-6.35	112.54	122.70
1	D	406	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	O	454	ILE	C-N-CD	-6.33	106.67	120.60
1	P	282	TYR	CD1-CG-CD2	6.33	124.86	117.90
1	J	460	GLU	N-CA-CB	-6.33	99.21	110.60
1	A	498	TYR	CG-CD2-CE2	-6.33	116.24	121.30
1	L	449	ASP	CB-CG-OD2	6.33	124.00	118.30
1	M	283	LEU	CB-CG-CD2	6.32	121.75	111.00
1	D	399	ASN	O-C-N	-6.32	112.59	122.70
1	F	38	ARG	O-C-N	-6.32	112.59	122.70
1	B	454	ILE	C-N-CD	-6.32	106.71	120.60
1	D	34	ALA	N-CA-CB	-6.31	101.26	110.10
1	B	205	ASP	O-C-N	-6.31	112.60	122.70
1	K	289	LYS	N-CA-CB	6.31	121.96	110.60
1	P	360	ARG	NE-CZ-NH1	-6.31	117.14	120.30
1	N	454	ILE	C-N-CD	-6.31	106.72	120.60
1	C	62	ASP	CB-CG-OD1	6.31	123.98	118.30
1	B	454	ILE	CB-CA-C	6.30	124.21	111.60
1	E	282	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	I	250	ASP	CB-CG-OD1	6.30	123.97	118.30
1	F	224	ARG	NH1-CZ-NH2	6.30	126.33	119.40
1	N	282	TYR	CB-CG-CD2	6.30	124.78	121.00
1	O	197	ASP	CB-CG-OD2	6.30	123.97	118.30
1	O	224	ARG	NE-CZ-NH1	-6.30	117.15	120.30
1	G	20	ARG	NE-CZ-NH1	-6.29	117.15	120.30
1	K	16	ARG	NE-CZ-NH1	-6.29	117.15	120.30
1	D	311	PHE	CB-CG-CD2	6.29	125.20	120.80
1	D	325	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	M	287	VAL	CA-CB-CG1	6.28	120.32	110.90
1	E	428	ARG	NE-CZ-NH2	6.28	123.44	120.30
1	A	135	GLU	CB-CA-C	-6.27	97.85	110.40
1	D	499	SER	CB-CA-C	-6.27	98.19	110.10
1	A	197	ASP	CB-CG-OD2	6.26	123.94	118.30
1	J	462	ALA	N-CA-CB	-6.25	101.35	110.10
1	L	406	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	N	62	ASP	CB-CG-OD2	6.24	123.92	118.30
1	A	190	THR	N-CA-CB	6.24	122.16	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	487	ASP	CB-CG-OD2	-6.24	112.69	118.30
1	L	27	ILE	O-C-N	-6.23	112.73	122.70
1	O	130	PHE	CB-CG-CD1	6.23	125.16	120.80
1	P	460	GLU	OE1-CD-OE2	-6.23	115.82	123.30
1	C	251	ALA	CB-CA-C	-6.23	100.75	110.10
1	G	469	ALA	O-C-N	-6.23	112.73	122.70
1	I	321	ARG	C-N-CA	6.23	137.27	121.70
1	E	287	VAL	CA-CB-CG2	-6.22	101.56	110.90
1	G	192	ALA	CB-CA-C	6.22	119.44	110.10
1	C	262	ALA	CB-CA-C	6.22	119.43	110.10
1	A	360	ARG	NE-CZ-NH2	6.22	123.41	120.30
1	P	130	PHE	CB-CG-CD2	-6.22	116.45	120.80
1	C	150	ASN	CB-CA-C	6.21	122.83	110.40
1	D	413	TYR	CG-CD1-CE1	6.21	126.27	121.30
1	B	496	ASP	N-CA-CB	-6.21	99.43	110.60
1	E	447	TYR	CB-CG-CD2	-6.20	117.28	121.00
1	H	16	ARG	NE-CZ-NH2	6.20	123.40	120.30
1	K	200	TYR	CG-CD2-CE2	-6.20	116.34	121.30
1	F	432	TYR	CD1-CG-CD2	6.17	124.69	117.90
1	G	528	ASP	CB-CG-OD1	-6.17	112.74	118.30
1	K	193	GLU	OE1-CD-OE2	-6.17	115.89	123.30
1	M	140	LEU	CB-CG-CD2	6.17	121.49	111.00
1	E	275	PHE	CG-CD2-CE2	-6.17	114.01	120.80
1	G	270	ASP	CB-CG-OD1	6.17	123.85	118.30
1	H	70	MET	CG-SD-CE	-6.16	90.34	100.20
1	P	277	ASP	CB-CG-OD2	6.16	123.84	118.30
1	I	365	ASP	CB-CG-OD1	6.16	123.84	118.30
1	L	322	ARG	NE-CZ-NH1	-6.16	117.22	120.30
1	I	455	PRO	CB-CA-C	6.16	127.39	112.00
1	A	432	TYR	CD1-CG-CD2	6.15	124.67	117.90
1	P	155	ARG	NE-CZ-NH1	-6.15	117.22	120.30
1	P	250	ASP	CB-CG-OD2	6.15	123.84	118.30
1	M	38	ARG	NE-CZ-NH2	-6.15	117.22	120.30
1	C	182	ASP	CB-CG-OD1	6.15	123.83	118.30
1	D	413	TYR	CG-CD2-CE2	-6.15	116.38	121.30
1	I	496	ASP	CB-CG-OD2	-6.15	112.77	118.30
1	K	496	ASP	N-CA-CB	-6.15	99.53	110.60
1	N	31	ARG	NE-CZ-NH2	6.15	123.37	120.30
1	P	228	LEU	CB-CG-CD2	6.15	121.45	111.00
1	C	454	ILE	C-N-CD	-6.14	107.09	120.60
1	H	403	TYR	CD1-CE1-CZ	-6.14	114.27	119.80
1	F	126	PHE	CB-CG-CD2	-6.13	116.51	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	H	130	PHE	CD1-CG-CD2	6.13	126.28	118.30
1	L	20	ARG	NE-CZ-NH2	6.13	123.37	120.30
1	N	170	PHE	CB-CG-CD2	6.13	125.09	120.80
1	O	105	PHE	CB-CG-CD1	6.13	125.09	120.80
1	D	209	ILE	O-C-N	-6.13	112.89	122.70
1	H	325	ARG	NE-CZ-NH2	6.13	123.36	120.30
1	I	232	VAL	CA-CB-CG1	6.13	120.09	110.90
1	L	171	MET	CG-SD-CE	-6.13	90.40	100.20
1	I	148	ASP	N-CA-CB	-6.12	99.58	110.60
1	M	16	ARG	NE-CZ-NH1	6.12	123.36	120.30
1	I	154	ALA	C-N-CA	6.12	137.00	121.70
1	F	277	ASP	CB-CG-OD2	-6.12	112.80	118.30
1	N	487	ASP	CB-CG-OD2	6.11	123.80	118.30
1	A	369	PHE	CB-CG-CD2	-6.11	116.52	120.80
1	J	481	LEU	C-N-CA	6.11	136.97	121.70
1	I	454	ILE	C-N-CD	-6.11	107.17	120.60
1	H	235	ALA	CB-CA-C	-6.10	100.94	110.10
1	B	406	ARG	NE-CZ-NH2	6.10	123.35	120.30
1	G	250	ASP	CB-CG-OD2	6.09	123.78	118.30
1	D	297	VAL	CA-CB-CG1	6.08	120.03	110.90
1	E	472	ASP	CB-CG-OD2	-6.08	112.83	118.30
1	J	327	ASP	CB-CG-OD2	6.08	123.77	118.30
1	M	449	ASP	CB-CG-OD1	6.08	123.78	118.30
1	F	148	ASP	CB-CG-OD1	6.08	123.77	118.30
1	M	403	TYR	CA-CB-CG	6.08	124.95	113.40
1	J	169	LYS	N-CA-CB	-6.08	99.66	110.60
1	N	484	CYS	O-C-N	-6.08	112.87	123.20
1	H	38	ARG	NE-CZ-NH2	6.08	123.34	120.30
1	D	239	ARG	NH1-CZ-NH2	-6.06	112.73	119.40
1	O	430	ARG	NE-CZ-NH1	-6.06	117.27	120.30
1	J	36	MET	CG-SD-CE	-6.06	90.51	100.20
1	F	224	ARG	NE-CZ-NH2	-6.05	117.27	120.30
1	F	197	ASP	CB-CG-OD1	6.05	123.75	118.30
1	A	367	MET	O-C-N	-6.05	113.02	122.70
1	F	260	ILE	O-C-N	-6.05	113.02	122.70
1	C	445	GLU	OE1-CD-OE2	6.05	130.56	123.30
1	E	130	PHE	CB-CG-CD2	-6.05	116.56	120.80
1	J	387	ASN	N-CA-CB	6.05	121.49	110.60
1	J	240	ARG	NH1-CZ-NH2	-6.05	112.75	119.40
1	O	282	TYR	CD1-CG-CD2	6.04	124.55	117.90
1	C	149	LEU	CB-CA-C	6.03	121.67	110.20
1	I	256	GLU	OE1-CD-OE2	-6.03	116.06	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	21	ASP	N-CA-CB	-6.03	99.74	110.60
1	F	428	ARG	CD-NE-CZ	6.03	132.04	123.60
1	D	325	ARG	O-C-N	-6.03	113.05	122.70
1	I	224	ARG	NE-CZ-NH1	6.03	123.32	120.30
1	J	461	THR	CA-CB-CG2	-6.03	103.96	112.40
1	O	166	MET	CG-SD-CE	-6.03	90.55	100.20
1	F	431	GLU	N-CA-CB	6.03	121.45	110.60
1	P	362	VAL	N-CA-C	-6.02	94.74	111.00
1	A	150	ASN	N-CA-CB	6.02	121.44	110.60
1	D	323	VAL	CA-CB-CG2	-6.02	101.87	110.90
1	F	432	TYR	CB-CG-CD2	-6.02	117.39	121.00
1	G	154	ALA	C-N-CA	6.02	136.74	121.70
1	C	65	THR	O-C-N	-6.01	113.08	122.70
1	D	41	LEU	CB-CG-CD1	6.01	121.22	111.00
1	F	275	PHE	CB-CG-CD2	6.01	125.01	120.80
1	H	275	PHE	CB-CG-CD2	6.01	125.00	120.80
1	L	126	PHE	CB-CG-CD1	6.01	125.00	120.80
1	L	239	ARG	CD-NE-CZ	-6.01	115.19	123.60
1	J	16	ARG	CG-CD-NE	-6.00	99.19	111.80
1	L	353	TYR	CB-CG-CD2	-6.00	117.40	121.00
1	P	459	ALA	CB-CA-C	-6.00	101.10	110.10
1	P	61	ASN	N-CA-CB	-6.00	99.80	110.60
1	M	368	VAL	CA-CB-CG2	-6.00	101.91	110.90
1	F	36	MET	CA-CB-CG	5.99	123.48	113.30
1	L	394	ALA	CB-CA-C	5.99	119.09	110.10
1	P	470	LEU	O-C-N	-5.99	113.11	122.70
1	G	516	ALA	N-CA-CB	-5.99	101.72	110.10
1	J	487	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	N	20	ARG	NE-CZ-NH1	-5.99	117.31	120.30
1	C	454	ILE	O-C-N	-5.98	109.73	121.10
1	I	477	HIS	CA-CB-CG	5.98	123.77	113.60
1	G	38	ARG	NE-CZ-NH1	-5.98	117.31	120.30
1	L	237	MET	CG-SD-CE	-5.98	90.63	100.20
1	M	31	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	B	240	ARG	NE-CZ-NH1	-5.97	117.31	120.30
1	B	338	ARG	NE-CZ-NH1	5.97	123.28	120.30
1	J	102	ALA	CB-CA-C	5.96	119.05	110.10
1	P	297	VAL	CA-CB-CG1	5.96	119.85	110.90
1	O	126	PHE	CB-CG-CD2	5.96	124.97	120.80
1	P	503	VAL	CA-CB-CG1	-5.96	101.96	110.90
1	C	58	THR	N-CA-CB	5.95	121.61	110.30
1	H	413	TYR	CB-CG-CD1	-5.95	117.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	38	ARG	NE-CZ-NH1	-5.95	117.33	120.30
1	B	400	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	P	454	ILE	CA-CB-CG1	5.95	122.30	111.00
1	H	388	ASP	CB-CG-OD2	5.94	123.65	118.30
1	E	350	ASP	C-N-CA	5.94	136.56	121.70
1	J	186	ASP	O-C-N	-5.94	113.19	122.70
1	O	275	PHE	CB-CG-CD2	5.94	124.96	120.80
1	H	67	VAL	O-C-N	-5.94	113.20	122.70
1	O	54	PHE	CZ-CE2-CD2	5.94	127.23	120.10
1	C	447	TYR	CB-CG-CD2	-5.93	117.44	121.00
1	I	498	TYR	CG-CD2-CE2	-5.93	116.55	121.30
1	K	39	SER	CB-CA-C	-5.93	98.83	110.10
1	P	270	ASP	CB-CG-OD2	5.93	123.64	118.30
1	N	434	ARG	NE-CZ-NH2	5.93	123.26	120.30
1	N	478	ALA	CB-CA-C	-5.93	101.21	110.10
1	N	495	ASP	CB-CG-OD2	5.92	123.63	118.30
1	O	455	PRO	CB-CA-C	5.92	126.80	112.00
1	C	224	ARG	NE-CZ-NH1	-5.92	117.34	120.30
1	F	456	MET	O-C-N	-5.92	113.23	122.70
1	K	17	ASN	CB-CA-C	-5.92	98.56	110.40
1	A	84	ALA	CB-CA-C	5.92	118.97	110.10
1	N	400	ASP	CB-CG-OD1	5.91	123.62	118.30
1	D	468	SER	N-CA-CB	5.91	119.36	110.50
1	C	112	LEU	O-C-N	-5.91	113.25	122.70
1	D	454	ILE	CA-C-O	-5.91	107.69	120.10
1	O	407	ASN	O-C-N	-5.91	113.25	122.70
1	C	105	PHE	CB-CG-CD2	-5.91	116.67	120.80
1	P	338	ARG	NE-CZ-NH2	5.90	123.25	120.30
1	B	309	GLN	CG-CD-OE1	-5.90	109.81	121.60
1	A	163	TYR	CB-CG-CD1	-5.89	117.46	121.00
1	K	88	ASP	CB-CG-OD2	5.89	123.60	118.30
1	B	450	ALA	N-CA-CB	-5.89	101.85	110.10
1	G	126	PHE	CB-CG-CD2	-5.89	116.68	120.80
1	H	529	LEU	CB-CG-CD2	5.89	121.02	111.00
1	A	49	MET	O-C-N	-5.89	113.28	122.70
1	P	413	TYR	CZ-CE2-CD2	-5.89	114.50	119.80
1	A	474	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	C	20	ARG	NE-CZ-NH2	5.88	123.24	120.30
1	E	285	ASP	CB-CG-OD1	5.88	123.59	118.30
1	M	130	PHE	CB-CG-CD2	-5.87	116.69	120.80
1	O	473	LEU	CB-CG-CD2	5.87	120.98	111.00
1	F	113	VAL	CG1-CB-CG2	-5.87	101.51	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	27	ILE	O-C-N	5.87	132.09	122.70
1	H	461	THR	N-CA-CB	5.86	121.44	110.30
1	I	413	TYR	CD1-CG-CD2	5.86	124.35	117.90
1	K	476	ARG	NH1-CZ-NH2	-5.86	112.95	119.40
1	C	31	ARG	CG-CD-NE	-5.86	99.50	111.80
1	A	360	ARG	NE-CZ-NH1	-5.86	117.37	120.30
1	M	362	VAL	CA-CB-CG1	-5.85	102.12	110.90
1	D	472	ASP	CB-CG-OD1	-5.84	113.04	118.30
1	N	454	ILE	CA-C-N	5.84	133.45	117.10
1	E	460	GLU	O-C-N	-5.84	113.36	122.70
1	E	529	LEU	CB-CG-CD1	5.84	120.93	111.00
1	E	530	ILE	O-C-N	-5.84	113.36	122.70
1	P	476	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	E	325	ARG	NH1-CZ-NH2	-5.83	112.98	119.40
1	F	406	ARG	NH1-CZ-NH2	-5.83	112.98	119.40
1	L	346	ALA	N-CA-CB	-5.83	101.93	110.10
1	O	20	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	O	369	PHE	CB-CG-CD2	-5.83	116.72	120.80
1	O	95	THR	OG1-CB-CG2	-5.83	96.59	110.00
1	C	181	MET	CG-SD-CE	-5.83	90.88	100.20
1	A	210	ASP	CB-CG-OD1	5.82	123.54	118.30
1	E	148	ASP	CB-CG-OD2	5.82	123.54	118.30
1	L	315	ARG	CD-NE-CZ	5.82	131.75	123.60
1	N	128	LYS	O-C-N	-5.82	113.39	122.70
1	B	182	ASP	N-CA-CB	-5.82	100.13	110.60
1	D	259	GLU	CG-CD-OE1	5.82	129.94	118.30
1	I	232	VAL	CG1-CB-CG2	-5.82	101.59	110.90
1	N	516	ALA	N-CA-CB	-5.81	101.96	110.10
1	P	496	ASP	CB-CG-OD2	5.81	123.53	118.30
1	K	288	ASP	CB-CG-OD1	5.81	123.53	118.30
1	A	20	ARG	NE-CZ-NH1	-5.81	117.39	120.30
1	F	338	ARG	CD-NE-CZ	5.81	131.74	123.60
1	O	426	SER	CB-CA-C	-5.81	99.06	110.10
1	F	325	ARG	NE-CZ-NH2	5.80	123.20	120.30
1	N	126	PHE	CB-CG-CD1	5.80	124.86	120.80
1	H	450	ALA	CB-CA-C	-5.80	101.40	110.10
1	E	454	ILE	CB-CA-C	5.80	123.20	111.60
1	H	130	PHE	CG-CD1-CE1	-5.80	114.42	120.80
1	H	471	MET	CA-CB-CG	5.80	123.16	113.30
1	K	428	ARG	CD-NE-CZ	5.80	131.72	123.60
1	G	342	SER	N-CA-CB	5.80	119.19	110.50
1	H	357	VAL	CA-CB-CG1	-5.79	102.21	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	163	TYR	CB-CG-CD1	5.79	124.47	121.00
1	N	457	ILE	CA-CB-CG2	-5.79	99.32	110.90
1	L	38	ARG	CD-NE-CZ	5.79	131.70	123.60
1	O	239	ARG	NE-CZ-NH1	-5.79	117.41	120.30
1	E	487	ASP	CB-CG-OD1	5.79	123.51	118.30
1	M	452	GLU	CG-CD-OE1	5.79	129.87	118.30
1	B	197	ASP	CB-CG-OD2	-5.78	113.09	118.30
1	A	169	LYS	N-CA-CB	-5.78	100.20	110.60
1	C	188	VAL	CG1-CB-CG2	-5.78	101.65	110.90
1	D	219	ASP	CB-CG-OD2	5.78	123.50	118.30
1	N	454	ILE	O-C-N	-5.78	110.12	121.10
1	E	231	GLU	N-CA-CB	-5.78	100.20	110.60
1	J	62	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	C	322	ARG	O-C-N	-5.77	113.47	122.70
1	D	472	ASP	CB-CG-OD2	5.77	123.49	118.30
1	F	347	THR	CA-CB-CG2	-5.77	104.33	112.40
1	O	220	SER	O-C-N	-5.77	113.47	122.70
1	G	473	LEU	CB-CG-CD2	-5.76	101.20	111.00
1	D	16	ARG	NE-CZ-NH1	-5.76	117.42	120.30
1	C	396	ARG	NE-CZ-NH2	5.76	123.18	120.30
1	D	69	GLU	CG-CD-OE1	5.76	129.81	118.30
1	F	445	GLU	O-C-N	-5.76	113.49	122.70
1	J	111	SER	O-C-N	-5.76	113.49	122.70
1	N	353	TYR	CG-CD1-CE1	-5.75	116.70	121.30
1	O	84	ALA	N-CA-CB	-5.75	102.05	110.10
1	P	282	TYR	CZ-CE2-CD2	5.75	124.97	119.80
1	E	240	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	J	288	ASP	CB-CG-OD1	5.75	123.47	118.30
1	E	250	ASP	N-CA-CB	-5.75	100.26	110.60
1	N	396	ARG	NE-CZ-NH1	-5.75	117.43	120.30
1	G	173	GLU	C-N-CA	5.75	134.36	122.30
1	I	498	TYR	CB-CA-C	-5.74	98.91	110.40
1	M	476	ARG	NE-CZ-NH2	5.74	123.17	120.30
1	J	467	ILE	O-C-N	-5.74	113.52	122.70
1	A	224	ARG	NE-CZ-NH1	-5.74	117.43	120.30
1	I	197	ASP	O-C-N	-5.74	113.45	123.20
1	K	240	ARG	NE-CZ-NH2	5.73	123.17	120.30
1	D	479	LYS	N-CA-CB	-5.73	100.29	110.60
1	N	403	TYR	CG-CD1-CE1	-5.73	116.72	121.30
1	M	36	MET	CG-SD-CE	-5.73	91.03	100.20
1	I	130	PHE	CB-CG-CD1	5.72	124.81	120.80
1	B	388	ASP	O-C-N	-5.72	113.55	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	142	THR	CA-CB-CG2	5.72	120.41	112.40
1	A	279	GLU	CG-CD-OE1	5.72	129.74	118.30
1	H	338	ARG	CD-NE-CZ	5.72	131.61	123.60
1	J	405	LEU	CB-CG-CD2	-5.72	101.27	111.00
1	B	206	LEU	CB-CG-CD2	5.72	120.72	111.00
1	E	388	ASP	CB-CA-C	-5.72	98.96	110.40
1	N	286	MET	CG-SD-CE	-5.72	91.05	100.20
1	K	255	VAL	CA-CB-CG2	-5.72	102.33	110.90
1	O	29	ALA	N-CA-CB	-5.72	102.10	110.10
1	O	406	ARG	NE-CZ-NH2	5.72	123.16	120.30
1	E	369	PHE	CD1-CE1-CZ	5.71	126.96	120.10
1	N	392	ASP	CB-CG-OD1	5.71	123.44	118.30
1	H	403	TYR	CB-CG-CD2	-5.71	117.57	121.00
1	J	378	ALA	CB-CA-C	-5.71	101.53	110.10
1	O	150	ASN	N-CA-CB	5.71	120.88	110.60
1	P	519	ALA	N-CA-CB	-5.71	102.11	110.10
1	F	250	ASP	CA-C-O	5.71	132.09	120.10
1	L	456	MET	CG-SD-CE	-5.71	91.07	100.20
1	O	380	ASN	N-CA-CB	-5.71	100.33	110.60
1	K	148	ASP	N-CA-CB	-5.70	100.33	110.60
1	M	305	ASP	CB-CG-OD1	5.70	123.43	118.30
1	N	270	ASP	CB-CG-OD2	5.70	123.43	118.30
1	G	264	ILE	O-C-N	-5.70	113.58	122.70
1	L	408	ILE	O-C-N	-5.70	113.58	122.70
1	G	182	ASP	CB-CG-OD1	5.70	123.43	118.30
1	N	145	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	E	81	VAL	CA-CB-CG1	5.69	119.44	110.90
1	O	182	ASP	CB-CG-OD1	5.69	123.42	118.30
1	D	141	ALA	C-N-CA	5.69	135.93	121.70
1	G	309	GLN	N-CA-CB	-5.69	100.35	110.60
1	C	487	ASP	CB-CA-C	5.69	121.78	110.40
1	G	396	ARG	CD-NE-CZ	-5.69	115.63	123.60
1	L	454	ILE	O-C-N	-5.69	110.29	121.10
1	M	237	MET	CG-SD-CE	-5.68	91.10	100.20
1	B	163	TYR	CB-CG-CD1	5.68	124.41	121.00
1	P	365	ASP	CB-CG-OD2	5.68	123.42	118.30
1	J	126	PHE	CB-CG-CD2	-5.68	116.83	120.80
1	J	395	GLU	OE1-CD-OE2	-5.68	116.49	123.30
1	J	96	THR	N-CA-CB	5.67	121.08	110.30
1	H	152	ALA	CB-CA-C	5.67	118.60	110.10
1	J	319	ALA	N-CA-CB	-5.66	102.17	110.10
1	N	144	VAL	CA-CB-CG2	-5.66	102.41	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	334	ALA	N-CA-CB	-5.66	102.18	110.10
1	N	166	MET	CG-SD-CE	-5.66	91.15	100.20
1	D	379	VAL	CA-CB-CG1	-5.65	102.42	110.90
1	D	450	ALA	CB-CA-C	-5.65	101.62	110.10
1	D	384	ARG	CG-CD-NE	-5.65	99.94	111.80
1	A	277	ASP	CB-CG-OD1	5.65	123.38	118.30
1	M	390	ALA	CB-CA-C	-5.64	101.63	110.10
1	M	315	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	D	155	ARG	N-CA-C	5.64	126.22	111.00
1	L	250	ASP	CB-CG-OD1	5.64	123.38	118.30
1	N	155	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	C	496	ASP	CB-CG-OD2	5.64	123.37	118.30
1	O	286	MET	CG-SD-CE	-5.64	91.18	100.20
1	C	322	ARG	N-CA-CB	-5.63	100.46	110.60
1	E	522	SER	N-CA-CB	5.63	118.94	110.50
1	F	31	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	C	375	ASN	CA-C-N	5.63	132.85	117.10
1	J	454	ILE	C-N-CD	-5.62	108.22	120.60
1	C	211	LYS	C-N-CA	5.62	135.76	121.70
1	D	70	MET	CG-SD-CE	-5.62	91.21	100.20
1	H	224	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	J	20	ARG	N-CA-CB	5.62	120.71	110.60
1	N	278	GLU	O-C-N	-5.62	113.71	122.70
1	E	384	ARG	NE-CZ-NH1	5.62	123.11	120.30
1	D	505	PRO	N-CA-CB	5.62	110.04	103.30
1	P	163	TYR	CG-CD1-CE1	-5.62	116.81	121.30
1	H	521	THR	OG1-CB-CG2	-5.61	97.09	110.00
1	I	101	LEU	CB-CG-CD2	5.61	120.54	111.00
1	J	62	ASP	CB-CG-OD1	5.61	123.35	118.30
1	J	504	GLU	OE1-CD-OE2	-5.61	116.56	123.30
1	D	171	MET	CG-SD-CE	-5.61	91.22	100.20
1	G	400	ASP	CB-CG-OD1	5.61	123.35	118.30
1	L	496	ASP	CB-CG-OD2	-5.61	113.25	118.30
1	B	354	ALA	N-CA-CB	5.61	117.95	110.10
1	M	154	ALA	N-CA-CB	-5.61	102.25	110.10
1	B	114	ASP	CB-CG-OD2	5.61	123.35	118.30
1	I	170	PHE	CA-CB-CG	5.61	127.35	113.90
1	P	62	ASP	CB-CG-OD1	5.61	123.35	118.30
1	D	454	ILE	CA-C-N	5.60	132.79	117.10
1	D	456	MET	CG-SD-CE	-5.60	91.24	100.20
1	H	38	ARG	CD-NE-CZ	5.60	131.44	123.60
1	E	403	TYR	CD1-CE1-CZ	5.60	124.84	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	P	406	ARG	NE-CZ-NH1	-5.60	117.50	120.30
1	G	498	TYR	CG-CD1-CE1	-5.60	116.82	121.30
1	M	227	VAL	CA-CB-CG2	-5.60	102.50	110.90
1	M	315	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	K	200	TYR	CD1-CE1-CZ	-5.59	114.77	119.80
1	E	79	LEU	CB-CG-CD2	-5.59	101.50	111.00
1	O	306	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	P	20	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	O	163	TYR	CB-CG-CD2	-5.58	117.65	121.00
1	N	510	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	D	24	LYS	N-CA-CB	-5.58	100.56	110.60
1	D	31	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	F	323	VAL	CG1-CB-CG2	-5.58	101.98	110.90
1	I	344	LYS	CB-CA-C	5.58	121.55	110.40
1	C	282	TYR	CB-CG-CD1	-5.57	117.66	121.00
1	C	484	CYS	O-C-N	-5.57	113.73	123.20
1	E	156	ASP	CB-CG-OD2	-5.57	113.28	118.30
1	F	450	ALA	N-CA-CB	-5.57	102.30	110.10
1	L	389	MET	N-CA-CB	-5.57	100.57	110.60
1	N	369	PHE	CB-CG-CD1	-5.57	116.90	120.80
1	F	182	ASP	N-CA-CB	-5.57	100.58	110.60
1	N	239	ARG	NE-CZ-NH2	5.57	123.08	120.30
1	L	360	ARG	O-C-N	-5.57	113.80	122.70
1	L	476	ARG	CG-CD-NE	-5.57	100.11	111.80
1	B	83	ALA	CB-CA-C	5.56	118.44	110.10
1	N	432	TYR	CG-CD1-CE1	-5.56	116.85	121.30
1	L	179	LYS	CB-CA-C	-5.56	99.29	110.40
1	K	452	GLU	OE1-CD-OE2	-5.55	116.63	123.30
1	N	446	ALA	N-CA-CB	-5.55	102.32	110.10
1	O	507	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	J	434	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	J	449	ASP	CB-CG-OD2	5.55	123.30	118.30
1	A	261	SER	N-CA-CB	5.55	118.82	110.50
1	J	369	PHE	CB-CG-CD2	5.55	124.68	120.80
1	I	126	PHE	CB-CG-CD2	-5.54	116.92	120.80
1	B	353	TYR	CD1-CE1-CZ	5.54	124.79	119.80
1	C	189	THR	CA-CB-OG1	5.54	120.64	109.00
1	M	400	ASP	CB-CG-OD1	-5.54	113.31	118.30
1	K	449	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	L	396	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
1	F	107	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	A	325	ARG	NE-CZ-NH2	5.53	123.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	387	ASN	CB-CG-OD1	5.53	132.65	121.60
1	K	282	TYR	CZ-CE2-CD2	-5.52	114.83	119.80
1	J	81	VAL	CG1-CB-CG2	-5.52	102.07	110.90
1	A	453	GLU	OE1-CD-OE2	-5.52	116.68	123.30
1	M	350	ASP	CB-CG-OD2	-5.52	113.33	118.30
1	L	253	LEU	CB-CA-C	5.51	120.68	110.20
1	L	369	PHE	CB-CG-CD1	5.51	124.66	120.80
1	M	507	ARG	CD-NE-CZ	5.51	131.32	123.60
1	D	250	ASP	CB-CG-OD1	-5.51	113.34	118.30
1	G	353	TYR	CB-CG-CD1	5.51	124.31	121.00
1	A	478	ALA	CB-CA-C	-5.51	101.83	110.10
1	C	369	PHE	CG-CD2-CE2	5.51	126.86	120.80
1	F	430	ARG	CD-NE-CZ	5.51	131.31	123.60
1	N	228	LEU	O-C-N	-5.51	113.89	122.70
1	N	338	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	N	461	THR	O-C-N	-5.50	113.89	122.70
1	O	432	TYR	CD1-CE1-CZ	-5.50	114.85	119.80
1	D	197	ASP	CB-CG-OD2	5.50	123.25	118.30
1	K	469	ALA	N-CA-CB	-5.50	102.40	110.10
1	E	357	VAL	N-CA-C	-5.50	96.15	111.00
1	B	428	ARG	NE-CZ-NH1	5.50	123.05	120.30
1	H	177	LEU	CB-CG-CD2	5.50	120.35	111.00
1	H	413	TYR	CG-CD2-CE2	-5.50	116.90	121.30
1	H	436	VAL	CA-CB-CG1	5.50	119.14	110.90
1	H	356	LEU	CB-CG-CD2	5.49	120.34	111.00
1	H	410	MET	O-C-N	-5.49	113.91	122.70
1	G	454	ILE	CA-C-N	5.49	132.48	117.10
1	C	510	ARG	NE-CZ-NH1	5.49	123.04	120.30
1	L	89	SER	N-CA-CB	5.49	118.73	110.50
1	N	16	ARG	CD-NE-CZ	5.49	131.28	123.60
1	P	23	LEU	O-C-N	-5.49	113.92	122.70
1	M	130	PHE	CD1-CE1-CZ	5.49	126.69	120.10
1	M	391	LEU	CB-CG-CD1	5.49	120.33	111.00
1	D	31	ARG	NE-CZ-NH2	5.49	123.04	120.30
1	F	517	THR	O-C-N	-5.49	113.92	122.70
1	C	454	ILE	CA-C-N	5.48	132.46	117.10
1	L	274	ALA	N-CA-CB	5.48	117.77	110.10
1	I	488	VAL	CA-CB-CG2	-5.48	102.68	110.90
1	D	120	THR	CA-CB-CG2	-5.48	104.73	112.40
1	G	281	LYS	O-C-N	-5.47	113.94	122.70
1	O	288	ASP	CB-CG-OD2	5.47	123.23	118.30
1	O	325	ARG	NH1-CZ-NH2	-5.47	113.38	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	155	ARG	NH1-CZ-NH2	-5.47	113.38	119.40
1	F	518	GLU	O-C-N	-5.47	113.95	122.70
1	B	50	LEU	CB-CG-CD1	5.47	120.29	111.00
1	D	287	VAL	CA-CB-CG2	-5.46	102.70	110.90
1	G	274	ALA	O-C-N	-5.46	113.96	122.70
1	J	216	THR	CA-CB-CG2	-5.46	104.75	112.40
1	D	500	ILE	C-N-CA	5.46	135.35	121.70
1	P	105	PHE	CG-CD1-CE1	-5.46	114.79	120.80
1	F	432	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	D	130	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	D	510	ARG	NH1-CZ-NH2	-5.46	113.40	119.40
1	L	321	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	M	389	MET	CG-SD-CE	-5.46	91.47	100.20
1	O	80	LEU	CB-CG-CD2	5.46	120.28	111.00
1	L	321	ARG	NE-CZ-NH2	5.45	123.03	120.30
1	H	359	GLU	CG-CD-OE1	5.45	129.20	118.30
1	H	400	ASP	CB-CG-OD2	5.45	123.21	118.30
1	J	149	LEU	C-N-CA	5.45	135.32	121.70
1	M	36	MET	CA-CB-CG	5.45	122.56	113.30
1	M	207	ILE	CA-CB-CG1	5.45	121.35	111.00
1	E	162	VAL	O-C-N	-5.45	113.98	122.70
1	M	403	TYR	CD1-CE1-CZ	-5.45	114.90	119.80
1	M	52	ASP	CB-CG-OD2	-5.45	113.40	118.30
1	A	205	ASP	CB-CG-OD2	5.44	123.20	118.30
1	L	89	SER	CB-CA-C	-5.44	99.76	110.10
1	F	520	ALA	CB-CA-C	-5.44	101.94	110.10
1	P	497	ILE	CA-CB-CG2	-5.44	100.03	110.90
1	I	224	ARG	NE-CZ-NH2	5.43	123.02	120.30
1	L	514	LYS	O-C-N	-5.43	114.01	122.70
1	J	527	ASP	CB-CG-OD2	5.43	123.19	118.30
1	A	341	SER	O-C-N	-5.43	114.02	122.70
1	F	353	TYR	CZ-CE2-CD2	-5.43	114.92	119.80
1	I	71	GLU	OE1-CD-OE2	5.43	129.81	123.30
1	G	472	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	J	315	ARG	CD-NE-CZ	5.42	131.19	123.60
1	C	62	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	D	219	ASP	CA-C-O	5.42	131.48	120.10
1	N	427	ALA	O-C-N	-5.42	114.03	122.70
1	N	60	THR	O-C-N	-5.42	114.03	122.70
1	B	90	GLU	N-CA-C	5.41	125.62	111.00
1	P	525	LYS	N-CA-CB	-5.41	100.86	110.60
1	B	310	HIS	CB-CA-C	-5.41	99.58	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	323	VAL	CA-CB-CG2	-5.41	102.78	110.90
1	L	406	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	L	327	ASP	CB-CG-OD2	5.40	123.16	118.30
1	M	382	LEU	O-C-N	5.40	131.34	122.70
1	F	114	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	H	269	PRO	N-CA-CB	5.40	109.78	103.30
1	H	275	PHE	CB-CG-CD1	-5.40	117.02	120.80
1	E	255	VAL	CB-CA-C	-5.40	101.14	111.40
1	G	229	ASP	C-N-CA	5.40	135.19	121.70
1	J	348	PRO	O-C-N	-5.40	114.06	122.70
1	O	282	TYR	CD1-CE1-CZ	5.40	124.66	119.80
1	B	191	VAL	C-N-CA	5.40	135.19	121.70
1	G	73	GLN	CB-CA-C	-5.40	99.61	110.40
1	E	136	LEU	CB-CG-CD2	-5.39	101.83	111.00
1	N	46	LEU	CB-CG-CD2	5.39	120.17	111.00
1	O	170	PHE	CZ-CE2-CD2	-5.39	113.63	120.10
1	C	176	GLU	O-C-N	-5.39	114.08	122.70
1	A	384	ARG	O-C-N	-5.39	114.04	123.20
1	H	338	ARG	NE-CZ-NH2	5.39	122.99	120.30
1	A	454	ILE	CB-CA-C	5.39	122.37	111.60
1	A	156	ASP	CB-CA-C	5.38	121.17	110.40
1	I	288	ASP	O-C-N	-5.38	114.08	122.70
1	K	216	THR	CA-CB-CG2	-5.38	104.86	112.40
1	C	476	ARG	NH1-CZ-NH2	-5.38	113.48	119.40
1	K	18	SER	CB-CA-C	-5.38	99.87	110.10
1	B	271	GLN	N-CA-CB	-5.38	100.91	110.60
1	H	505	PRO	N-CA-CB	5.38	109.76	103.30
1	K	88	ASP	CB-CG-OD1	-5.38	113.46	118.30
1	F	247	ALA	N-CA-CB	5.38	117.63	110.10
1	J	519	ALA	CB-CA-C	-5.38	102.03	110.10
1	A	475	ALA	CA-C-O	5.38	131.39	120.10
1	K	229	ASP	CB-CG-OD1	5.38	123.14	118.30
1	L	384	ARG	NE-CZ-NH1	-5.37	117.61	120.30
1	E	255	VAL	CA-CB-CG2	5.37	118.96	110.90
1	O	155	ARG	N-CA-C	5.37	125.50	111.00
1	L	105	PHE	CB-CG-CD1	5.37	124.56	120.80
1	L	171	MET	CA-CB-CG	5.37	122.42	113.30
1	G	407	ASN	CA-C-N	5.37	129.00	117.20
1	J	388	ASP	CB-CG-OD1	5.37	123.13	118.30
1	J	403	TYR	CB-CG-CD1	-5.37	117.78	121.00
1	M	498	TYR	CB-CG-CD2	5.37	124.22	121.00
1	N	182	ASP	N-CA-CB	-5.37	100.94	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	223	ILE	O-C-N	-5.36	114.12	122.70
1	J	309	GLN	O-C-N	-5.36	114.12	122.70
1	L	261	SER	C-N-CA	5.36	135.11	121.70
1	I	29	ALA	CB-CA-C	5.36	118.14	110.10
1	A	239	ARG	NH1-CZ-NH2	-5.36	113.50	119.40
1	F	129	ALA	N-CA-CB	-5.36	102.60	110.10
1	G	184	VAL	O-C-N	-5.36	114.12	122.70
1	I	515	SER	N-CA-CB	-5.36	102.46	110.50
1	L	186	ASP	N-CA-CB	-5.36	100.95	110.60
1	J	182	ASP	CB-CG-OD1	-5.36	113.48	118.30
1	J	371	GLU	C-N-CA	5.36	133.55	122.30
1	O	454	ILE	CA-C-N	5.36	132.10	117.10
1	C	192	ALA	CB-CA-C	5.35	118.13	110.10
1	I	275	PHE	CB-CG-CD2	-5.35	117.05	120.80
1	J	202	VAL	CG1-CB-CG2	-5.35	102.34	110.90
1	B	455	PRO	CA-CB-CG	-5.35	93.84	104.00
1	E	277	ASP	O-C-N	-5.35	114.14	122.70
1	M	519	ALA	O-C-N	-5.35	114.14	122.70
1	D	105	PHE	CB-CG-CD1	-5.35	117.06	120.80
1	N	114	ASP	CB-CG-OD1	-5.35	113.49	118.30
1	G	197	ASP	CB-CG-OD1	5.34	123.11	118.30
1	I	457	ILE	CA-CB-CG2	-5.34	100.21	110.90
1	C	126	PHE	CB-CG-CD2	-5.34	117.06	120.80
1	N	323	VAL	C-N-CA	5.34	135.05	121.70
1	P	527	ASP	CB-CG-OD1	-5.34	113.49	118.30
1	P	237	MET	CG-SD-CE	-5.34	91.66	100.20
1	D	440	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	P	206	LEU	CB-CG-CD1	-5.33	101.93	111.00
1	N	475	ALA	N-CA-CB	-5.33	102.63	110.10
1	B	219	ASP	CB-CG-OD1	5.33	123.10	118.30
1	E	148	ASP	CB-CG-OD1	-5.33	113.50	118.30
1	H	62	ASP	CB-CG-OD2	5.33	123.10	118.30
1	I	200	TYR	CB-CG-CD2	-5.33	117.80	121.00
1	A	384	ARG	NE-CZ-NH1	5.33	122.96	120.30
1	F	325	ARG	CG-CD-NE	-5.33	100.61	111.80
1	D	250	ASP	CB-CG-OD2	5.33	123.09	118.30
1	F	411	GLU	OE1-CD-OE2	-5.33	116.91	123.30
1	H	110	GLU	N-CA-CB	-5.33	101.02	110.60
1	B	31	ARG	CD-NE-CZ	5.32	131.05	123.60
1	B	496	ASP	CB-CG-OD1	-5.32	113.51	118.30
1	G	451	LEU	CB-CG-CD1	-5.32	101.95	111.00
1	H	56	ASP	CB-CG-OD2	-5.32	113.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	184	VAL	CG1-CB-CG2	-5.32	102.39	110.90
1	A	16	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	A	273	LYS	O-C-N	-5.32	114.19	122.70
1	B	110	GLU	CG-CD-OE2	5.32	128.94	118.30
1	E	432	TYR	CB-CG-CD1	5.32	124.19	121.00
1	B	328	ILE	CB-CA-C	-5.32	100.97	111.60
1	D	357	VAL	N-CA-C	-5.31	96.65	111.00
1	O	457	ILE	CA-CB-CG1	5.31	121.10	111.00
1	F	224	ARG	CG-CD-NE	-5.31	100.64	111.80
1	G	440	GLU	O-C-N	-5.31	114.20	122.70
1	I	151	SER	O-C-N	-5.31	114.20	122.70
1	D	149	LEU	CB-CA-C	5.31	120.29	110.20
1	H	502	VAL	CA-CB-CG1	5.31	118.86	110.90
1	A	165	THR	CA-CB-CG2	-5.31	104.97	112.40
1	F	166	MET	CG-SD-CE	-5.31	91.71	100.20
1	L	20	ARG	O-C-N	-5.30	114.21	122.70
1	A	474	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	I	224	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
1	A	311	PHE	CB-CG-CD1	-5.30	117.09	120.80
1	O	302	LYS	O-C-N	-5.30	114.20	123.20
1	K	52	ASP	O-C-N	-5.29	114.23	122.70
1	A	526	ILE	CA-CB-CG1	-5.29	100.95	111.00
1	H	54	PHE	CB-CG-CD2	-5.29	117.10	120.80
1	P	297	VAL	CG1-CB-CG2	-5.29	102.43	110.90
1	J	30	ALA	N-CA-CB	-5.29	102.69	110.10
1	C	154	ALA	N-CA-CB	5.29	117.50	110.10
1	O	93	ASP	CB-CG-OD2	-5.29	113.54	118.30
1	J	428	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	D	322	ARG	N-CA-C	5.28	125.26	111.00
1	D	323	VAL	CG1-CB-CG2	-5.28	102.45	110.90
1	E	91	VAL	CA-CB-CG2	5.28	118.82	110.90
1	M	171	MET	N-CA-CB	5.28	120.11	110.60
1	D	210	ASP	CB-CG-OD1	5.28	123.05	118.30
1	D	499	SER	N-CA-CB	5.28	118.42	110.50
1	H	317	ILE	O-C-N	-5.28	114.25	122.70
1	L	409	LEU	CB-CG-CD2	5.28	119.98	111.00
1	O	517	THR	CA-CB-CG2	-5.28	105.01	112.40
1	A	285	ASP	N-CA-CB	-5.28	101.11	110.60
1	J	54	PHE	CB-CG-CD2	-5.28	117.11	120.80
1	N	120	THR	OG1-CB-CG2	-5.28	97.87	110.00
1	G	322	ARG	CG-CD-NE	-5.27	100.73	111.80
1	D	235	ALA	N-CA-CB	-5.27	102.72	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	342	SER	N-CA-CB	5.27	118.41	110.50
1	K	19	GLY	C-N-CA	5.27	134.87	121.70
1	M	405	LEU	CB-CG-CD2	-5.27	102.04	111.00
1	J	341	SER	N-CA-CB	5.27	118.40	110.50
1	B	275	PHE	CG-CD1-CE1	5.26	126.59	120.80
1	G	403	TYR	CG-CD2-CE2	5.26	125.51	121.30
1	G	131	ASN	N-CA-CB	-5.26	101.13	110.60
1	P	403	TYR	CB-CG-CD1	5.26	124.16	121.00
1	D	496	ASP	N-CA-CB	-5.26	101.13	110.60
1	M	360	ARG	N-CA-C	-5.26	96.80	111.00
1	K	313	ALA	N-CA-CB	-5.26	102.74	110.10
1	M	39	SER	N-CA-CB	5.26	118.39	110.50
1	C	454	ILE	CB-CA-C	5.25	122.10	111.60
1	C	379	VAL	CA-CB-CG1	-5.25	103.03	110.90
1	M	259	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	H	41	LEU	CB-CG-CD2	5.25	119.92	111.00
1	M	193	GLU	CG-CD-OE2	5.25	128.79	118.30
1	C	186	ASP	O-C-N	-5.25	114.31	122.70
1	N	370	ILE	CA-CB-CG1	5.25	120.97	111.00
1	E	290	LEU	CB-CG-CD1	-5.24	102.09	111.00
1	M	238	PRO	N-CA-C	5.24	125.73	112.10
1	O	113	VAL	CG1-CB-CG2	-5.24	102.51	110.90
1	J	485	GLY	O-C-N	-5.24	114.32	122.70
1	F	182	ASP	CB-CG-OD1	5.24	123.02	118.30
1	J	208	LYS	CA-CB-CG	5.24	124.93	113.40
1	C	338	ARG	N-CA-C	-5.24	96.86	111.00
1	E	275	PHE	CD1-CG-CD2	5.23	125.10	118.30
1	N	137	LEU	N-CA-C	5.23	125.13	111.00
1	H	498	TYR	O-C-N	-5.23	114.34	122.70
1	G	193	GLU	CA-C-N	5.23	131.73	117.10
1	D	163	TYR	O-C-N	-5.22	114.34	122.70
1	J	150	ASN	CB-CA-C	5.22	120.85	110.40
1	O	447	TYR	CG-CD1-CE1	5.22	125.48	121.30
1	D	456	MET	CA-CB-CG	5.22	122.18	113.30
1	K	114	ASP	CB-CG-OD1	5.22	123.00	118.30
1	N	213	LYS	N-CA-CB	5.22	120.00	110.60
1	N	282	TYR	CG-CD2-CE2	5.22	125.48	121.30
1	A	434	ARG	CD-NE-CZ	5.22	130.91	123.60
1	I	208	LYS	O-C-N	-5.22	114.35	122.70
1	K	153	THR	OG1-CB-CG2	-5.22	97.99	110.00
1	L	349	GLU	OE1-CD-OE2	-5.22	117.03	123.30
1	N	277	ASP	O-C-N	-5.22	114.35	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	N	498	TYR	CB-CG-CD2	-5.22	117.87	121.00
1	H	197	ASP	O-C-N	-5.22	114.33	123.20
1	B	166	MET	CG-SD-CE	-5.21	91.86	100.20
1	B	496	ASP	CB-CG-OD2	5.21	122.99	118.30
1	M	407	ASN	CA-C-N	5.21	128.67	117.20
1	N	334	ALA	CB-CA-C	-5.21	102.28	110.10
1	O	106	LEU	CB-CA-C	-5.21	100.30	110.20
1	O	306	ASP	CB-CG-OD1	5.21	122.99	118.30
1	P	406	ARG	CD-NE-CZ	5.21	130.90	123.60
1	H	403	TYR	CG-CD1-CE1	5.21	125.47	121.30
1	K	321	ARG	NE-CZ-NH2	5.21	122.91	120.30
1	L	331	LEU	CB-CG-CD1	-5.21	102.14	111.00
1	O	353	TYR	CZ-CE2-CD2	5.21	124.49	119.80
1	K	448	ALA	N-CA-CB	-5.21	102.81	110.10
1	A	67	VAL	CA-CB-CG2	-5.21	103.09	110.90
1	A	455	PRO	CB-CA-C	5.21	125.02	112.00
1	P	153	THR	N-CA-C	-5.21	96.94	111.00
1	O	400	ASP	CB-CG-OD1	5.21	122.99	118.30
1	P	16	ARG	NE-CZ-NH2	5.21	122.90	120.30
1	A	430	ARG	C-N-CA	5.20	134.70	121.70
1	C	282	TYR	CB-CG-CD2	-5.20	117.88	121.00
1	D	286	MET	CG-SD-CE	-5.20	91.88	100.20
1	F	148	ASP	N-CA-CB	-5.20	101.24	110.60
1	F	422	GLU	O-C-N	-5.20	114.38	122.70
1	M	73	GLN	O-C-N	-5.20	114.38	122.70
1	C	403	TYR	CG-CD1-CE1	-5.20	117.14	121.30
1	J	288	ASP	CB-CG-OD2	-5.20	113.62	118.30
1	L	365	ASP	CB-CG-OD1	5.20	122.98	118.30
1	L	486	VAL	O-C-N	-5.20	114.39	122.70
1	H	277	ASP	O-C-N	-5.19	114.39	122.70
1	P	38	ARG	N-CA-CB	-5.19	101.25	110.60
1	M	91	VAL	O-C-N	-5.19	114.37	123.20
1	H	454	ILE	CB-CA-C	5.19	121.98	111.60
1	K	475	ALA	O-C-N	-5.19	114.39	122.70
1	M	503	VAL	CA-CB-CG1	-5.19	103.12	110.90
1	A	432	TYR	CA-CB-CG	-5.19	103.54	113.40
1	P	277	ASP	CB-CG-OD1	-5.19	113.63	118.30
1	A	507	ARG	NE-CZ-NH1	-5.19	117.71	120.30
1	C	455	PRO	CB-CA-C	5.19	124.97	112.00
1	B	55	GLY	O-C-N	-5.18	114.41	122.70
1	K	395	GLU	OE1-CD-OE2	-5.18	117.08	123.30
1	B	311	PHE	O-C-N	-5.18	114.41	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	322	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
1	M	353	TYR	CB-CA-C	-5.18	100.05	110.40
1	E	163	TYR	CG-CD2-CE2	-5.17	117.16	121.30
1	I	125	GLY	O-C-N	-5.17	114.42	122.70
1	M	344	LYS	C-N-CA	5.17	134.63	121.70
1	P	280	ALA	N-CA-CB	-5.17	102.86	110.10
1	H	145	ASP	CB-CG-OD1	-5.17	113.64	118.30
1	O	127	LYS	O-C-N	-5.17	114.43	122.70
1	A	356	LEU	CB-CG-CD1	5.17	119.78	111.00
1	B	138	PRO	N-CD-CG	5.17	110.95	103.20
1	C	351	LEU	O-C-N	-5.17	114.42	123.20
1	M	507	ARG	NE-CZ-NH1	5.17	122.88	120.30
1	B	163	TYR	N-CA-CB	-5.17	101.30	110.60
1	O	440	GLU	O-C-N	-5.17	114.44	122.70
1	N	455	PRO	CA-CB-CG	-5.17	94.19	104.00
1	G	219	ASP	CB-CG-OD2	5.16	122.95	118.30
1	M	239	ARG	CD-NE-CZ	5.16	130.83	123.60
1	A	189	THR	CA-CB-OG1	5.16	119.84	109.00
1	G	224	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	O	454	ILE	CB-CA-C	5.16	121.92	111.60
1	A	345	ASP	CB-CG-OD1	5.16	122.94	118.30
1	C	108	LYS	CB-CG-CD	5.16	125.01	111.60
1	E	396	ARG	CD-NE-CZ	5.16	130.82	123.60
1	G	145	ASP	O-C-N	-5.16	114.45	122.70
1	M	369	PHE	CB-CG-CD1	-5.16	117.19	120.80
1	A	36	MET	CG-SD-CE	-5.16	91.95	100.20
1	B	82	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	L	105	PHE	CG-CD1-CE1	5.16	126.47	120.80
1	N	61	ASN	O-C-N	-5.16	114.45	122.70
1	O	255	VAL	CA-CB-CG2	-5.16	103.17	110.90
1	K	171	MET	CG-SD-CE	-5.15	91.95	100.20
1	K	222	LEU	CB-CG-CD1	5.15	119.76	111.00
1	N	389	MET	CG-SD-CE	-5.15	91.95	100.20
1	J	170	PHE	CB-CG-CD1	5.15	124.41	120.80
1	O	406	ARG	N-CA-CB	-5.15	101.33	110.60
1	I	454	ILE	CB-CA-C	5.15	121.90	111.60
1	L	134	LEU	O-C-N	-5.15	114.46	122.70
1	O	166	MET	O-C-N	-5.15	114.46	122.70
1	J	396	ARG	NE-CZ-NH1	-5.15	117.73	120.30
1	G	311	PHE	O-C-N	-5.15	114.47	122.70
1	H	432	TYR	CG-CD1-CE1	-5.15	117.18	121.30
1	N	242	GLU	OE1-CD-OE2	-5.15	117.12	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	461	THR	OG1-CB-CG2	-5.14	98.17	110.00
1	D	329	GLU	OE1-CD-OE2	-5.14	117.13	123.30
1	L	350	ASP	CB-CG-OD1	5.14	122.93	118.30
1	C	73	GLN	O-C-N	-5.14	114.47	122.70
1	P	430	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	C	346	ALA	N-CA-CB	-5.14	102.90	110.10
1	E	297	VAL	CA-CB-CG1	5.14	118.61	110.90
1	J	391	LEU	CB-CA-C	5.14	119.97	110.20
1	N	350	ASP	CB-CG-OD2	5.14	122.93	118.30
1	D	433	ALA	CB-CA-C	-5.14	102.39	110.10
1	K	339	ILE	C-N-CA	5.13	134.53	121.70
1	M	360	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	D	262	ALA	CB-CA-C	5.13	117.79	110.10
1	K	157	ALA	N-CA-CB	-5.13	102.92	110.10
1	O	453	GLU	N-CA-CB	-5.13	101.37	110.60
1	L	186	ASP	CB-CG-OD1	5.13	122.92	118.30
1	M	141	ALA	C-N-CA	5.13	134.52	121.70
1	F	478	ALA	CB-CA-C	5.12	117.78	110.10
1	H	39	SER	CB-CA-C	-5.12	100.37	110.10
1	H	461	THR	CA-CB-CG2	-5.12	105.23	112.40
1	N	157	ALA	O-C-N	-5.12	114.51	122.70
1	O	216	THR	C-N-CA	5.12	134.50	121.70
1	A	321	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	494	ILE	CB-CA-C	5.12	121.83	111.60
1	B	413	TYR	CD1-CE1-CZ	-5.12	115.19	119.80
1	H	381	ILE	O-C-N	-5.12	114.52	122.70
1	G	461	THR	CA-CB-OG1	5.11	119.74	109.00
1	G	325	ARG	NE-CZ-NH2	5.11	122.86	120.30
1	B	345	ASP	CB-CG-OD1	5.11	122.90	118.30
1	O	285	ASP	CB-CG-OD1	-5.11	113.70	118.30
1	G	464	LEU	O-C-N	-5.11	114.53	122.70
1	I	186	ASP	CB-CG-OD2	5.11	122.90	118.30
1	O	503	VAL	CA-CB-CG1	-5.11	103.24	110.90
1	B	311	PHE	CB-CG-CD1	5.11	124.37	120.80
1	H	322	ARG	NH1-CZ-NH2	-5.11	113.78	119.40
1	J	325	ARG	NE-CZ-NH1	-5.11	117.75	120.30
1	M	445	GLU	CG-CD-OE1	5.10	128.51	118.30
1	P	166	MET	CG-SD-CE	-5.10	92.03	100.20
1	D	404	SER	O-C-N	-5.10	114.54	122.70
1	I	15	SER	N-CA-CB	5.10	118.15	110.50
1	L	353	TYR	CB-CG-CD1	5.10	124.06	121.00
1	G	409	LEU	CB-CG-CD2	5.10	119.66	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	138	PRO	N-CA-CB	5.09	109.41	103.30
1	H	501	ASN	CA-CB-CG	-5.09	102.19	113.40
1	M	31	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
1	J	88	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	M	73	GLN	N-CA-CB	-5.09	101.43	110.60
1	B	377	LYS	O-C-N	-5.09	114.56	122.70
1	G	528	ASP	CB-CG-OD2	5.09	122.88	118.30
1	J	191	VAL	N-CA-CB	-5.09	100.30	111.50
1	K	128	LYS	O-C-N	-5.09	114.56	122.70
1	M	171	MET	CG-SD-CE	-5.09	92.06	100.20
1	C	357	VAL	CG1-CB-CG2	-5.09	102.76	110.90
1	H	495	ASP	N-CA-CB	-5.09	101.44	110.60
1	I	148	ASP	CB-CG-OD2	5.09	122.88	118.30
1	J	285	ASP	CB-CG-OD2	-5.09	113.72	118.30
1	O	498	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	E	101	LEU	CB-CG-CD1	-5.08	102.36	111.00
1	E	371	GLU	CG-CD-OE1	5.08	128.47	118.30
1	J	453	GLU	CB-CA-C	-5.08	100.23	110.40
1	N	432	TYR	CB-CG-CD1	-5.08	117.95	121.00
1	A	487	ASP	CB-CG-OD2	5.08	122.87	118.30
1	G	509	THR	CA-CB-CG2	5.08	119.51	112.40
1	J	428	ARG	O-C-N	-5.08	114.57	122.70
1	P	65	THR	OG1-CB-CG2	-5.08	98.31	110.00
1	D	50	LEU	N-CA-CB	5.08	120.56	110.40
1	B	369	PHE	CB-CG-CD2	-5.08	117.25	120.80
1	H	87	GLN	O-C-N	-5.08	114.58	122.70
1	F	374	LYS	N-CA-CB	-5.08	101.46	110.60
1	N	69	GLU	O-C-N	-5.08	114.58	122.70
1	O	22	ALA	CB-CA-C	-5.08	102.48	110.10
1	G	112	LEU	CB-CG-CD2	5.08	119.63	111.00
1	H	201	ASN	O-C-N	-5.08	114.58	122.70
1	I	323	VAL	CA-CB-CG2	-5.08	103.29	110.90
1	O	305	ASP	CB-CG-OD1	5.07	122.86	118.30
1	F	322	ARG	N-CA-C	5.07	124.69	111.00
1	O	462	ALA	N-CA-CB	-5.07	103.00	110.10
1	B	150	ASN	N-CA-CB	5.07	119.73	110.60
1	E	113	VAL	O-C-N	-5.07	114.59	122.70
1	F	130	PHE	CB-CG-CD2	-5.07	117.25	120.80
1	G	334	ALA	N-CA-CB	-5.07	103.00	110.10
1	N	515	SER	CB-CA-C	-5.07	100.47	110.10
1	L	452	GLU	OE1-CD-OE2	-5.07	117.22	123.30
1	C	345	ASP	CB-CG-OD1	5.06	122.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	J	413	TYR	CG-CD2-CE2	-5.06	117.25	121.30
1	N	406	ARG	N-CA-CB	-5.06	101.49	110.60
1	G	59	ILE	O-C-N	-5.06	114.60	122.70
1	D	93	ASP	O-C-N	-5.06	114.60	123.20
1	D	353	TYR	CB-CG-CD2	-5.06	117.97	121.00
1	F	101	LEU	CB-CG-CD1	5.06	119.60	111.00
1	G	445	GLU	CB-CA-C	5.06	120.52	110.40
1	D	519	ALA	CB-CA-C	-5.05	102.52	110.10
1	K	341	SER	N-CA-C	5.05	124.64	111.00
1	M	405	LEU	CB-CA-C	-5.05	100.60	110.20
1	N	315	ARG	CD-NE-CZ	5.05	130.67	123.60
1	E	20	ARG	CG-CD-NE	-5.05	101.20	111.80
1	H	430	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
1	D	250	ASP	CB-CA-C	5.04	120.48	110.40
1	P	98	ALA	CB-CA-C	-5.04	102.54	110.10
1	M	482	THR	CA-CB-CG2	5.04	119.45	112.40
1	N	23	LEU	CB-CG-CD2	5.04	119.56	111.00
1	C	239	ARG	NE-CZ-NH2	5.03	122.82	120.30
1	F	462	ALA	N-CA-CB	-5.03	103.06	110.10
1	E	181	MET	CG-SD-CE	-5.03	92.15	100.20
1	F	320	VAL	O-C-N	-5.03	114.65	122.70
1	L	430	ARG	CG-CD-NE	-5.03	101.23	111.80
1	P	365	ASP	CB-CG-OD1	-5.03	113.77	118.30
1	F	169	LYS	N-CA-CB	-5.03	101.55	110.60
1	I	155	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
1	M	166	MET	CG-SD-CE	-5.03	92.16	100.20
1	P	227	VAL	CG1-CB-CG2	-5.03	102.86	110.90
1	E	23	LEU	O-C-N	-5.02	114.66	122.70
1	C	325	ARG	NE-CZ-NH1	-5.02	117.79	120.30
1	E	369	PHE	CB-CG-CD2	-5.02	117.28	120.80
1	G	170	PHE	CD1-CE1-CZ	-5.02	114.07	120.10
1	J	175	GLU	CA-CB-CG	5.02	124.45	113.40
1	P	386	SER	N-CA-C	5.02	124.56	111.00
1	C	332	GLU	O-C-N	-5.02	114.67	122.70
1	M	239	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
1	P	456	MET	CG-SD-CE	-5.02	92.17	100.20
1	M	99	VAL	CG1-CB-CG2	-5.01	102.88	110.90
1	J	495	ASP	CB-CG-OD1	5.01	122.81	118.30
1	B	244	ALA	N-CA-CB	-5.01	103.09	110.10
1	D	166	MET	CG-SD-CE	-5.01	92.19	100.20
1	D	357	VAL	N-CA-CB	5.01	122.52	111.50
1	E	365	ASP	CB-CG-OD1	-5.01	113.79	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	K	172	ALA	CB-CA-C	-5.01	102.59	110.10
1	D	156	ASP	CB-CA-C	5.01	120.42	110.40
1	K	155	ARG	NE-CZ-NH2	5.01	122.80	120.30
1	A	232	VAL	CG1-CB-CG2	-5.01	102.89	110.90
1	C	392	ASP	CB-CG-OD2	5.01	122.81	118.30
1	M	188	VAL	CG1-CB-CG2	-5.01	102.89	110.90
1	O	351	LEU	N-CA-CB	5.00	120.41	110.40
1	A	449	ASP	CB-CG-OD2	5.00	122.80	118.30
1	F	296	ASN	CB-CA-C	5.00	120.41	110.40
1	I	472	ASP	CB-CG-OD2	-5.00	113.80	118.30
1	P	289	LYS	CB-CA-C	-5.00	100.39	110.40
1	A	475	ALA	O-C-N	-5.00	114.70	122.70
1	E	282	TYR	CB-CG-CD1	5.00	124.00	121.00

There are no chirality outliers.

All (329) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	154	ALA	Peptide
1	A	16	ARG	Sidechain
1	A	163	TYR	Sidechain
1	A	193	GLU	Peptide
1	A	213	LYS	Peptide
1	A	231	GLU	Peptide
1	A	232	VAL	Peptide
1	A	240	ARG	Sidechain
1	A	260	ILE	Peptide
1	A	267	THR	Peptide
1	A	315	ARG	Sidechain
1	A	321	ARG	Sidechain
1	A	338	ARG	Mainchain
1	A	347	THR	Peptide
1	A	396	ARG	Sidechain
1	A	447	TYR	Sidechain
1	A	454	ILE	Mainchain
1	A	474	ARG	Sidechain
1	A	504	GLU	Peptide
1	A	507	ARG	Sidechain
1	B	154	ALA	Peptide
1	B	155	ARG	Sidechain
1	B	163	TYR	Sidechain
1	B	193	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	B	20	ARG	Sidechain
1	B	232	VAL	Peptide
1	B	239	ARG	Sidechain
1	B	260	ILE	Peptide
1	B	267	THR	Peptide
1	B	31	ARG	Sidechain
1	B	322	ARG	Sidechain
1	B	325	ARG	Sidechain
1	B	347	THR	Peptide
1	B	350	ASP	Mainchain
1	B	353	TYR	Sidechain
1	B	38	ARG	Sidechain
1	B	386	SER	Mainchain
1	B	428	ARG	Sidechain
1	B	454	ILE	Mainchain
1	B	474	ARG	Sidechain
1	B	492	LYS	Peptide
1	C	154	ALA	Mainchain,Peptide
1	C	193	GLU	Peptide
1	C	20	ARG	Sidechain
1	C	224	ARG	Sidechain
1	C	232	VAL	Peptide
1	C	260	ILE	Peptide
1	C	267	THR	Peptide
1	C	282	TYR	Sidechain
1	C	311	PHE	Sidechain
1	C	321	ARG	Sidechain
1	C	347	THR	Peptide
1	C	353	TYR	Sidechain
1	C	369	PHE	Sidechain
1	C	384	ARG	Sidechain
1	C	403	TYR	Sidechain
1	C	428	ARG	Sidechain
1	C	430	ARG	Sidechain
1	C	454	ILE	Mainchain
1	C	477	HIS	Sidechain
1	C	498	TYR	Sidechain
1	D	154	ALA	Peptide
1	D	163	TYR	Sidechain
1	D	193	GLU	Peptide
1	D	196	PRO	Peptide
1	D	200	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	231	GLU	Peptide
1	D	239	ARG	Sidechain
1	D	260	ILE	Peptide
1	D	267	THR	Peptide
1	D	268	SER	Peptide
1	D	282	TYR	Sidechain
1	D	347	THR	Peptide
1	D	353	TYR	Sidechain
1	D	406	ARG	Sidechain
1	D	447	TYR	Sidechain
1	D	453	GLU	Sidechain
1	D	454	ILE	Mainchain
1	D	498	TYR	Sidechain
1	D	510	ARG	Sidechain
1	E	115	GLN	Mainchain
1	E	147	SER	Peptide
1	E	154	ALA	Peptide
1	E	193	GLU	Peptide
1	E	196	PRO	Peptide
1	E	200	TYR	Sidechain
1	E	232	VAL	Peptide
1	E	234	HIS	Sidechain
1	E	260	ILE	Peptide
1	E	267	THR	Peptide
1	E	268	SER	Peptide
1	E	31	ARG	Sidechain
1	E	315	ARG	Sidechain
1	E	325	ARG	Sidechain
1	E	338	ARG	Peptide
1	E	347	THR	Peptide
1	E	353	TYR	Sidechain
1	E	386	SER	Peptide
1	E	406	ARG	Sidechain
1	E	434	ARG	Sidechain
1	E	454	ILE	Mainchain
1	E	498	TYR	Sidechain
1	E	507	ARG	Sidechain
1	E	510	ARG	Sidechain
1	F	154	ALA	Peptide
1	F	155	ARG	Sidechain
1	F	193	GLU	Peptide
1	F	20	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	F	232	VAL	Peptide
1	F	239	ARG	Sidechain
1	F	260	ILE	Peptide
1	F	267	THR	Peptide
1	F	275	PHE	Sidechain
1	F	338	ARG	Peptide
1	F	347	THR	Peptide
1	F	434	ARG	Sidechain
1	F	454	ILE	Mainchain
1	F	498	TYR	Sidechain
1	F	510	ARG	Sidechain
1	G	116	ASN	Mainchain
1	G	126	PHE	Sidechain
1	G	154	ALA	Peptide
1	G	193	GLU	Peptide
1	G	196	PRO	Peptide
1	G	213	LYS	Peptide
1	G	232	VAL	Peptide
1	G	260	ILE	Peptide
1	G	267	THR	Peptide
1	G	268	SER	Peptide
1	G	282	TYR	Sidechain
1	G	31	ARG	Sidechain
1	G	311	PHE	Sidechain
1	G	325	ARG	Sidechain
1	G	347	THR	Peptide
1	G	360	ARG	Sidechain
1	G	396	ARG	Sidechain
1	G	413	TYR	Sidechain
1	G	428	ARG	Sidechain
1	G	432	TYR	Sidechain
1	G	434	ARG	Sidechain
1	G	454	ILE	Mainchain
1	G	492	LYS	Peptide
1	G	510	ARG	Sidechain
1	G	525	LYS	Mainchain
1	H	154	ALA	Peptide
1	H	16	ARG	Sidechain
1	H	170	PHE	Sidechain
1	H	191	VAL	Peptide
1	H	193	GLU	Peptide
1	H	200	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	H	232	VAL	Peptide
1	H	260	ILE	Peptide
1	H	267	THR	Peptide
1	H	282	TYR	Sidechain
1	H	31	ARG	Sidechain
1	H	347	THR	Peptide
1	H	360	ARG	Sidechain
1	H	406	ARG	Sidechain
1	H	430	ARG	Sidechain
1	H	447	TYR	Sidechain
1	H	474	ARG	Sidechain
1	H	476	ARG	Sidechain
1	H	529	LEU	Mainchain
1	I	154	ALA	Peptide
1	I	155	ARG	Sidechain
1	I	193	GLU	Peptide
1	I	200	TYR	Sidechain
1	I	213	LYS	Peptide
1	I	232	VAL	Peptide
1	I	260	ILE	Peptide
1	I	267	THR	Peptide
1	I	282	TYR	Sidechain
1	I	302	LYS	Peptide
1	I	310	HIS	Sidechain
1	I	311	PHE	Sidechain
1	I	322	ARG	Sidechain
1	I	338	ARG	Peptide
1	I	347	THR	Peptide
1	I	353	TYR	Sidechain
1	I	360	ARG	Sidechain
1	I	396	ARG	Sidechain
1	I	406	ARG	Sidechain
1	I	432	TYR	Sidechain
1	I	454	ILE	Mainchain
1	I	465	GLU	Mainchain
1	I	476	ARG	Sidechain
1	J	126	PHE	Sidechain
1	J	130	PHE	Sidechain
1	J	154	ALA	Mainchain,Peptide
1	J	16	ARG	Sidechain
1	J	193	GLU	Peptide
1	J	200	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	J	231	GLU	Peptide
1	J	232	VAL	Peptide
1	J	260	ILE	Peptide
1	J	267	THR	Peptide
1	J	282	TYR	Sidechain
1	J	302	LYS	Peptide
1	J	338	ARG	Peptide
1	J	347	THR	Peptide
1	J	353	TYR	Sidechain
1	J	38	ARG	Sidechain
1	J	384	ARG	Sidechain
1	J	403	TYR	Sidechain
1	J	430	ARG	Sidechain
1	J	434	ARG	Sidechain
1	J	454	ILE	Mainchain
1	J	510	ARG	Sidechain
1	K	126	PHE	Sidechain
1	K	154	ALA	Peptide
1	K	163	TYR	Sidechain
1	K	193	GLU	Peptide
1	K	198	GLY	Peptide
1	K	224	ARG	Sidechain
1	K	232	VAL	Peptide
1	K	260	ILE	Peptide
1	K	267	THR	Peptide
1	K	275	PHE	Sidechain
1	K	338	ARG	Sidechain,Peptide
1	K	347	THR	Peptide
1	K	403	TYR	Sidechain
1	K	413	TYR	Sidechain
1	K	42	GLY	Peptide
1	K	432	TYR	Sidechain
1	K	454	ILE	Mainchain
1	K	476	ARG	Sidechain
1	K	72	ILE	Peptide
1	L	154	ALA	Peptide
1	L	155	ARG	Sidechain
1	L	163	TYR	Sidechain
1	L	191	VAL	Peptide
1	L	193	GLU	Peptide
1	L	196	PRO	Peptide
1	L	198	GLY	Peptide

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Mol	Chain	Res	Type	Group
1	L	231	GLU	Peptide
1	L	239	ARG	Sidechain
1	L	260	ILE	Peptide
1	L	267	THR	Mainchain,Peptide
1	L	268	SER	Peptide
1	L	347	THR	Peptide
1	L	406	ARG	Sidechain
1	L	454	ILE	Mainchain
1	L	476	ARG	Sidechain
1	M	154	ALA	Peptide
1	M	191	VAL	Peptide
1	M	193	GLU	Peptide
1	M	232	VAL	Peptide
1	M	240	ARG	Sidechain
1	M	260	ILE	Peptide
1	M	267	THR	Peptide
1	M	302	LYS	Peptide
1	M	31	ARG	Sidechain
1	M	322	ARG	Sidechain
1	M	347	THR	Peptide
1	M	350	ASP	Mainchain
1	M	360	ARG	Sidechain
1	M	403	TYR	Sidechain
1	M	454	ILE	Mainchain
1	M	510	ARG	Sidechain
1	M	525	LYS	Mainchain
1	N	154	ALA	Peptide
1	N	155	ARG	Sidechain
1	N	191	VAL	Peptide
1	N	193	GLU	Peptide
1	N	213	LYS	Peptide
1	N	232	VAL	Peptide
1	N	239	ARG	Sidechain
1	N	260	ILE	Peptide
1	N	267	THR	Peptide
1	N	31	ARG	Sidechain
1	N	311	PHE	Sidechain
1	N	315	ARG	Sidechain
1	N	338	ARG	Sidechain
1	N	347	THR	Peptide
1	N	353	TYR	Sidechain
1	N	384	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	N	396	ARG	Sidechain
1	N	406	ARG	Sidechain
1	N	413	TYR	Sidechain
1	N	432	TYR	Sidechain
1	N	447	TYR	Sidechain
1	N	454	ILE	Mainchain
1	N	474	ARG	Sidechain
1	N	476	ARG	Sidechain
1	N	492	LYS	Peptide
1	N	507	ARG	Sidechain
1	O	154	ALA	Peptide
1	O	170	PHE	Sidechain
1	O	193	GLU	Peptide
1	O	224	ARG	Sidechain
1	O	232	VAL	Peptide
1	O	239	ARG	Sidechain
1	O	260	ILE	Peptide
1	O	267	THR	Peptide
1	O	302	LYS	Peptide
1	O	321	ARG	Sidechain
1	O	338	ARG	Peptide
1	O	347	THR	Peptide
1	O	353	TYR	Sidechain
1	O	369	PHE	Sidechain
1	O	396	ARG	Sidechain
1	O	403	TYR	Sidechain
1	O	454	ILE	Mainchain
1	O	507	ARG	Sidechain
1	O	510	ARG	Sidechain
1	P	154	ALA	Peptide
1	P	155	ARG	Sidechain
1	P	196	PRO	Peptide
1	P	200	TYR	Sidechain
1	P	213	LYS	Peptide
1	P	232	VAL	Peptide
1	P	260	ILE	Peptide
1	P	267	THR	Mainchain
1	P	282	TYR	Sidechain
1	P	31	ARG	Sidechain
1	P	347	THR	Peptide
1	P	360	ARG	Sidechain
1	P	384	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	P	403	TYR	Sidechain
1	P	428	ARG	Sidechain
1	P	447	TYR	Sidechain
1	P	454	ILE	Mainchain
1	P	476	ARG	Sidechain
1	P	525	LYS	Mainchain
1	P	72	ILE	Peptide

5.2 Too-close contacts [i](#)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	3937	0	4104	12	0
1	B	3937	0	4104	14	0
1	C	3937	0	4104	12	0
1	D	3937	0	4104	8	0
1	E	3937	0	4104	18	0
1	F	3937	0	4104	13	0
1	G	3937	0	4104	20	0
1	H	3937	0	4104	11	0
1	I	3937	0	4104	8	0
1	J	3937	0	4104	13	0
1	K	3937	0	4104	14	0
1	L	3937	0	4104	15	0
1	M	3937	0	4104	15	0
1	N	3937	0	4104	13	0
1	O	3937	0	4104	15	0
1	P	3937	0	4104	10	0
All	All	62992	0	65664	207	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 (207) 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)
1:K:454:ILE:HG22	1:K:455:PRO:HD2	1.67	0.77
1:K:232:VAL:HG11	1:K:368:VAL:HG21	1.72	0.72
1:L:343:ILE:HD12	1:L:343:ILE:H	1.56	0.69
1:J:87:GLN:HE21	1:J:91:VAL:HG22	1.60	0.66
1:F:454:ILE:HB	1:F:455:PRO:HD2	1.79	0.65
1:P:454:ILE:HB	1:P:455:PRO:HD2	1.78	0.64
1:G:343:ILE:HD12	1:G:343:ILE:H	1.62	0.62
1:E:234:HIS:CD2	1:E:236:GLY:H	2.17	0.62
1:H:454:ILE:HG22	1:H:455:PRO:HD2	1.81	0.62
1:G:454:ILE:HG22	1:G:455:PRO:HD2	1.83	0.61
1:M:304:ILE:HD11	1:M:319:ALA:HB1	1.83	0.61
1:L:234:HIS:CD2	1:L:236:GLY:H	2.18	0.61
1:C:234:HIS:CD2	1:C:236:GLY:H	2.19	0.61
1:P:158:LEU:H	1:P:158:LEU:HD12	1.68	0.59
1:G:185:ILE:HG23	1:G:405:LEU:HD13	1.84	0.58
1:K:234:HIS:CD2	1:K:236:GLY:H	2.20	0.58
1:A:101:LEU:HD21	1:A:513:LEU:HD12	1.85	0.58
1:N:454:ILE:CB	1:N:455:PRO:HD2	2.34	0.58
1:N:454:ILE:HB	1:N:455:PRO:HD2	1.85	0.58
1:N:334:ALA:HB1	1:N:373:ALA:HB1	1.85	0.57
1:O:51:ILE:HD12	1:O:57:VAL:HG22	1.87	0.57
1:F:234:HIS:CD2	1:F:236:GLY:H	2.23	0.57
1:D:234:HIS:CD2	1:D:236:GLY:H	2.23	0.56
1:K:41:LEU:HD22	1:K:100:VAL:HG11	1.87	0.56
1:O:118:HIS:CD2	1:P:463:GLY:HA2	2.41	0.56
1:B:505:PRO:HG2	1:B:508:VAL:HG23	1.87	0.56
1:A:234:HIS:CD2	1:A:236:GLY:H	2.24	0.55
1:F:44:LYS:HE2	1:F:488:VAL:HG12	1.89	0.55
1:J:429:LEU:HD23	1:J:448:ALA:HB2	1.89	0.55
1:E:334:ALA:HB2	1:E:376:PRO:HB3	1.87	0.55
1:M:232:VAL:HG21	1:M:368:VAL:HG21	1.88	0.54
1:C:232:VAL:HG12	1:C:232:VAL:O	2.06	0.54
1:E:454:ILE:CB	1:E:455:PRO:HD2	2.38	0.54
1:G:469:ALA:HB1	1:G:493:ILE:HD11	1.89	0.53
1:K:266:ILE:H	1:K:266:ILE:HD13	1.73	0.53
1:M:170:PHE:CE2	1:M:172:ALA:HB3	2.44	0.53
1:G:293:ILE:HG23	1:G:348:PRO:HA	1.91	0.53
1:I:63:GLY:O	1:I:67:VAL:HG22	2.09	0.52
1:N:238:PRO:O	1:N:318:LEU:HD12	2.10	0.52
1:O:87:GLN:HA	1:O:87:GLN:HE21	1.75	0.52
1:G:246:ILE:HD12	1:G:335:LEU:HD11	1.92	0.52
1:L:233:VAL:HG21	1:L:320:VAL:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:N:415:VAL:HB	1:N:421:ILE:HG21	1.91	0.52
1:F:223:ILE:HG22	1:F:225:GLY:H	1.74	0.51
1:G:187:ALA:HB1	1:G:222:LEU:HG	1.90	0.51
1:F:118:HIS:CD2	1:G:463:GLY:HA2	2.46	0.51
1:B:304:ILE:CD1	1:B:319:ALA:HB1	2.41	0.51
1:J:424:GLU:HG2	1:J:482:THR:HG23	1.92	0.51
1:M:234:HIS:CD2	1:M:236:GLY:H	2.29	0.50
1:B:304:ILE:HD11	1:B:319:ALA:HB1	1.92	0.50
1:L:211:LYS:HB2	1:L:391:LEU:HD11	1.93	0.50
1:O:454:ILE:CB	1:O:455:PRO:HD2	2.41	0.50
1:E:497:ILE:HD13	1:E:497:ILE:H	1.75	0.50
1:F:454:ILE:CB	1:F:455:PRO:HD2	2.42	0.50
1:D:467:ILE:HD12	1:D:470:LEU:HD23	1.93	0.50
1:E:91:VAL:HG22	1:E:94:GLY:H	1.77	0.50
1:I:255:VAL:HG22	1:I:282:TYR:HB3	1.93	0.49
1:J:505:PRO:HG2	1:J:508:VAL:HG23	1.95	0.49
1:B:29:ALA:CB	1:B:74:HIS:CD2	2.95	0.49
1:G:454:ILE:CB	1:G:455:PRO:HD2	2.42	0.49
1:J:287:VAL:HG11	1:J:311:PHE:HB3	1.94	0.49
1:E:454:ILE:HB	1:E:455:PRO:HD2	1.95	0.49
1:J:454:ILE:HB	1:J:455:PRO:HD2	1.95	0.49
1:G:454:ILE:CG2	1:G:455:PRO:HD2	2.43	0.49
1:M:304:ILE:CD1	1:M:319:ALA:HB1	2.43	0.48
1:O:299:ILE:HG21	1:O:328:ILE:HD11	1.94	0.48
1:L:416:PRO:HA	1:L:503:VAL:HG12	1.94	0.48
1:C:146:VAL:HG11	1:C:198:GLY:HA2	1.95	0.48
1:G:340:ILE:HD11	1:G:350:ASP:HB2	1.94	0.48
1:F:530:ILE:HD12	1:G:50:LEU:HG	1.96	0.48
1:O:281:LYS:HZ3	1:O:281:LYS:HB3	1.79	0.48
1:G:323:VAL:HG12	1:G:328:ILE:HG12	1.96	0.48
1:K:232:VAL:HG11	1:K:368:VAL:CG2	2.43	0.48
1:A:27:ILE:HG23	1:A:106:LEU:HB3	1.95	0.48
1:K:246:ILE:HD12	1:K:335:LEU:HD13	1.94	0.48
1:N:248:VAL:HG11	1:N:328:ILE:HG23	1.95	0.48
1:B:343:ILE:H	1:B:343:ILE:HD12	1.79	0.47
1:F:180:ILE:O	1:F:184:VAL:HG23	2.15	0.47
1:H:202:VAL:HG22	1:H:203:SER:H	1.80	0.47
1:N:185:ILE:HG13	1:N:405:LEU:HD22	1.97	0.47
1:G:340:ILE:HD11	1:G:350:ASP:CB	2.45	0.47
1:N:158:LEU:HD22	1:N:158:LEU:H	1.79	0.47
1:D:462:ALA:HB2	1:D:488:VAL:HG13	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:H:287:VAL:HG11	1:H:311:PHE:HB3	1.96	0.47
1:H:334:ALA:HB1	1:H:373:ALA:HB1	1.97	0.46
1:F:287:VAL:HG11	1:F:311:PHE:HB3	1.98	0.46
1:K:454:ILE:CG2	1:K:455:PRO:HD2	2.42	0.46
1:O:454:ILE:HB	1:O:455:PRO:HD2	1.96	0.46
1:E:413:TYR:HB2	1:E:506:ILE:HG21	1.97	0.46
1:C:101:LEU:HD13	1:C:454:ILE:HD11	1.98	0.46
1:I:433:ALA:HB2	1:I:444:ILE:HG22	1.98	0.46
1:E:414:ILE:HD12	1:E:503:VAL:HG21	1.97	0.46
1:B:264:ILE:HD13	1:B:271:GLN:HB2	1.98	0.46
1:B:64:ALA:HA	1:B:67:VAL:HG22	1.97	0.46
1:C:287:VAL:HG13	1:C:312:LEU:HD23	1.98	0.46
1:A:411:GLU:CD	1:A:510:ARG:HH22	2.20	0.46
1:O:485:GLY:HA3	1:O:497:ILE:HD11	1.98	0.46
1:A:158:LEU:H	1:A:158:LEU:HD22	1.81	0.45
1:B:424:GLU:HA	1:B:477:HIS:HE1	1.80	0.45
1:L:343:ILE:H	1:L:343:ILE:CD1	2.22	0.45
1:L:427:ALA:CB	1:L:477:HIS:CE1	3.00	0.45
1:A:211:LYS:HB2	1:A:391:LEU:HD21	1.98	0.45
1:N:360:ARG:HH12	1:N:371:GLU:CD	2.19	0.45
1:L:143:LYS:HB2	1:L:413:TYR:CE2	2.52	0.45
1:M:232:VAL:HG21	1:M:368:VAL:CG2	2.46	0.45
1:G:266:ILE:HA	1:G:272:ILE:HD11	1.98	0.45
1:L:266:ILE:HA	1:L:272:ILE:HD11	1.99	0.45
1:L:494:ILE:HG13	1:L:495:ASP:N	2.31	0.45
1:M:227:VAL:HG22	1:M:369:PHE:CD2	2.52	0.45
1:F:222:LEU:HD21	1:F:379:VAL:HB	1.98	0.45
1:P:430:ARG:NH2	1:P:449:ASP:OD1	2.49	0.45
1:J:454:ILE:CB	1:J:455:PRO:HD2	2.47	0.44
1:B:106:LEU:HA	1:B:106:LEU:HD23	1.90	0.44
1:M:464:LEU:HD11	1:M:492:LYS:HA	1.98	0.44
1:E:152:ALA:HA	1:E:158:LEU:HD23	1.98	0.44
1:E:217:ILE:HG13	1:E:217:ILE:H	1.63	0.44
1:J:241:VAL:HG11	1:J:296:ASN:HB3	1.99	0.44
1:M:306:ASP:HA	1:M:309:GLN:HG2	1.99	0.44
1:O:152:ALA:HB2	1:O:189:THR:HG21	2.00	0.44
1:C:105:PHE:CZ	1:C:447:TYR:CZ	3.06	0.44
1:O:255:VAL:H	1:O:255:VAL:HG23	1.52	0.44
1:P:226:ILE:HG23	1:P:370:ILE:HB	2.00	0.44
1:B:27:ILE:HG12	1:B:106:LEU:HD22	1.98	0.44
1:P:33:LEU:HD23	1:P:80:LEU:HD23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:33:LEU:HD23	1:K:80:LEU:HD23	2.00	0.44
1:B:454:ILE:CB	1:B:455:PRO:HD2	2.48	0.43
1:G:254:GLU:HA	1:G:283:LEU:HD21	2.00	0.43
1:L:192:ALA:HB2	1:L:409:LEU:HD13	2.00	0.43
1:A:130:PHE:CZ	1:A:134:LEU:HD11	2.53	0.43
1:A:267:THR:C	1:A:269:PRO:HD3	2.39	0.43
1:A:424:GLU:HA	1:A:477:HIS:CE1	2.52	0.43
1:B:505:PRO:HG2	1:B:508:VAL:CG2	2.48	0.43
1:N:227:VAL:HG22	1:N:369:PHE:CD2	2.52	0.43
1:C:136:LEU:HD11	1:C:428:ARG:HB2	2.01	0.43
1:D:87:GLN:HB3	1:D:95:THR:HG23	2.01	0.43
1:P:343:ILE:HD12	1:P:343:ILE:H	1.84	0.43
1:A:184:VAL:O	1:A:188:VAL:HG23	2.18	0.43
1:K:343:ILE:HD12	1:K:343:ILE:H	1.84	0.43
1:F:90:GLU:HB3	1:F:511:GLN:HE22	1.83	0.43
1:E:246:ILE:HD12	1:E:335:LEU:HD13	2.00	0.43
1:H:232:VAL:HG11	1:H:318:LEU:HD11	2.01	0.43
1:D:454:ILE:HB	1:D:455:PRO:HD2	2.01	0.43
1:M:119:PRO:HA	1:M:122:ILE:HD12	2.00	0.43
1:F:331:LEU:HD12	1:F:331:LEU:HA	1.91	0.43
1:N:220:SER:HB3	1:N:383:LEU:HD12	2.01	0.43
1:E:424:GLU:HA	1:E:477:HIS:HE1	1.84	0.42
1:O:106:LEU:HA	1:O:106:LEU:HD23	1.88	0.42
1:H:233:VAL:O	1:H:234:HIS:CD2	2.73	0.42
1:L:419:GLY:HA2	1:L:455:PRO:HG3	2.01	0.42
1:G:454:ILE:HB	1:G:455:PRO:HD2	2.01	0.42
1:J:192:ALA:O	1:J:202:VAL:HG23	2.19	0.42
1:O:454:ILE:HG22	1:O:455:PRO:HD2	2.00	0.42
1:C:454:ILE:HG22	1:C:455:PRO:HD2	2.02	0.42
1:J:433:ALA:HB2	1:J:444:ILE:HG22	2.02	0.42
1:C:192:ALA:HB2	1:C:202:VAL:HG11	2.02	0.42
1:E:184:VAL:O	1:E:188:VAL:HG23	2.20	0.42
1:H:308:ALA:O	1:H:312:LEU:HG	2.20	0.42
1:M:293:ILE:HG23	1:M:348:PRO:HA	2.01	0.42
1:C:416:PRO:HA	1:C:503:VAL:HG12	2.01	0.42
1:L:475:ALA:O	1:L:479:LYS:HG2	2.19	0.41
1:C:79:LEU:HD12	1:C:79:LEU:HA	1.80	0.41
1:H:193:GLU:HA	1:H:194:PRO:HD3	1.94	0.41
1:J:421:ILE:HG23	1:J:422:GLU:N	2.35	0.41
1:I:27:ILE:HG23	1:I:106:LEU:HB3	2.02	0.41
1:M:192:ALA:HB1	1:M:200:TYR:CD2	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:454:ILE:HB	1:B:455:PRO:HD2	2.02	0.41
1:E:207:ILE:HG21	1:E:402:LEU:HD21	2.02	0.41
1:A:454:ILE:CB	1:A:455:PRO:HD2	2.51	0.41
1:L:212:LYS:O	1:L:384:ARG:HA	2.20	0.41
1:N:232:VAL:HG11	1:N:318:LEU:HG	2.02	0.41
1:M:75:PRO:HB2	1:N:49:MET:SD	2.60	0.41
1:I:402:LEU:HD23	1:I:402:LEU:HA	1.97	0.41
1:M:253:LEU:HD23	1:M:304:ILE:HG23	2.02	0.41
1:O:425:LEU:HB2	1:O:451:LEU:HD13	2.02	0.41
1:F:248:VAL:HG11	1:F:328:ILE:HG23	2.01	0.41
1:H:424:GLU:HG3	1:H:482:THR:HG23	2.02	0.41
1:J:264:ILE:HD13	1:J:272:ILE:HG12	2.02	0.41
1:I:312:LEU:HD13	1:I:319:ALA:HB2	2.02	0.41
1:I:373:ALA:O	1:I:376:PRO:HD3	2.20	0.41
1:O:193:GLU:HA	1:O:194:PRO:HD3	1.96	0.41
1:O:277:ASP:OD1	1:O:281:LYS:NZ	2.50	0.41
1:P:494:ILE:HG21	1:P:500:ILE:HD11	2.03	0.41
1:E:486:VAL:HA	1:E:493:ILE:HA	2.03	0.41
1:G:101:LEU:HD11	1:G:454:ILE:HG21	2.03	0.41
1:I:424:GLU:HA	1:I:477:HIS:CE1	2.56	0.41
1:E:133:SER:HA	1:E:425:LEU:HD22	2.03	0.41
1:G:362:VAL:HG11	1:G:382:LEU:HD11	2.03	0.41
1:P:211:LYS:HA	1:P:383:LEU:HB3	2.02	0.41
1:A:454:ILE:HG22	1:A:455:PRO:HD2	2.02	0.40
1:E:193:GLU:HA	1:E:194:PRO:HD3	1.81	0.40
1:H:506:ILE:HG23	1:H:507:ARG:N	2.36	0.40
1:M:228:LEU:HD23	1:M:228:LEU:HA	1.92	0.40
1:B:241:VAL:HG12	1:B:244:ALA:HB2	2.02	0.40
1:C:357:VAL:HG22	1:C:370:ILE:HD12	2.02	0.40
1:H:454:ILE:H	1:H:454:ILE:HG13	1.77	0.40
1:J:231:GLU:H	1:J:231:GLU:CD	2.24	0.40
1:D:267:THR:O	1:D:267:THR:HG22	2.21	0.40
1:E:227:VAL:HG22	1:E:369:PHE:CD2	2.56	0.40
1:P:234:HIS:CD2	1:P:236:GLY:H	2.39	0.40
1:D:185:ILE:HD13	1:D:185:ILE:HA	1.96	0.40
1:D:228:LEU:HA	1:D:228:LEU:HD23	1.94	0.40
1:G:247:ALA:HB3	1:G:298:VAL:HG22	2.03	0.40
1:K:246:ILE:HD12	1:K:335:LEU:CD1	2.51	0.40
1:K:299:ILE:HG21	1:K:328:ILE:CD1	2.51	0.40
1:K:340:ILE:HD12	1:K:340:ILE:C	2.42	0.40
1:L:246:ILE:HD12	1:L:335:LEU:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:K:312:LEU:HD13	1:K:319:ALA:HB2	2.04	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	A	517/563 (92%)	468 (90%)	30 (6%)	19 (4%)	4	34
1	B	517/563 (92%)	468 (90%)	37 (7%)	12 (2%)	7	44
1	C	517/563 (92%)	470 (91%)	27 (5%)	20 (4%)	3	32
1	D	517/563 (92%)	455 (88%)	38 (7%)	24 (5%)	3	29
1	E	517/563 (92%)	472 (91%)	28 (5%)	17 (3%)	4	37
1	F	517/563 (92%)	466 (90%)	28 (5%)	23 (4%)	3	30
1	G	517/563 (92%)	470 (91%)	31 (6%)	16 (3%)	5	38
1	H	517/563 (92%)	459 (89%)	38 (7%)	20 (4%)	3	32
1	I	517/563 (92%)	462 (89%)	33 (6%)	22 (4%)	3	30
1	J	517/563 (92%)	464 (90%)	33 (6%)	20 (4%)	3	32
1	K	517/563 (92%)	467 (90%)	35 (7%)	15 (3%)	5	39
1	L	517/563 (92%)	471 (91%)	29 (6%)	17 (3%)	4	37
1	M	517/563 (92%)	460 (89%)	37 (7%)	20 (4%)	3	32
1	N	517/563 (92%)	470 (91%)	32 (6%)	15 (3%)	5	39
1	O	517/563 (92%)	465 (90%)	36 (7%)	16 (3%)	5	38
1	P	517/563 (92%)	464 (90%)	41 (8%)	12 (2%)	7	44
All	All	8272/9008 (92%)	7451 (90%)	533 (6%)	288 (4%)	7	35

All (288) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	150	ASN
1	A	155	ARG
1	A	322	ARG
1	A	387	ASN
1	A	455	PRO
1	B	192	ALA
1	B	322	ARG
1	B	386	SER
1	B	455	PRO
1	C	322	ARG
1	C	347	THR
1	C	375	ASN
1	C	387	ASN
1	C	455	PRO
1	D	233	VAL
1	D	322	ARG
1	D	455	PRO
1	E	150	ASN
1	E	155	ARG
1	E	322	ARG
1	E	455	PRO
1	F	147	SER
1	F	172	ALA
1	F	322	ARG
1	F	386	SER
1	F	455	PRO
1	G	155	ARG
1	G	322	ARG
1	G	455	PRO
1	G	483	ASN
1	H	155	ARG
1	H	172	ALA
1	H	322	ARG
1	H	455	PRO
1	I	232	VAL
1	I	322	ARG
1	I	374	LYS
1	I	455	PRO
1	J	155	ARG
1	J	233	VAL
1	J	322	ARG
1	J	455	PRO
1	K	192	ALA

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Mol	Chain	Res	Type
1	K	322	ARG
1	K	455	PRO
1	L	192	ALA
1	L	322	ARG
1	L	455	PRO
1	M	147	SER
1	M	151	SER
1	M	232	VAL
1	M	322	ARG
1	M	387	ASN
1	M	455	PRO
1	N	147	SER
1	N	322	ARG
1	N	455	PRO
1	O	152	ALA
1	O	192	ALA
1	O	322	ARG
1	O	455	PRO
1	P	322	ARG
1	P	455	PRO
1	A	147	SER
1	A	192	ALA
1	A	202	VAL
1	B	150	ASN
1	B	155	ARG
1	B	156	ASP
1	C	155	ARG
1	C	156	ASP
1	C	192	ALA
1	C	233	VAL
1	D	71	GLU
1	D	155	ARG
1	D	232	VAL
1	D	267	THR
1	D	496	ASP
1	E	232	VAL
1	F	156	ASP
1	F	387	ASN
1	F	438	GLY
1	F	481	LEU
1	G	151	SER
1	G	192	ALA

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Mol	Chain	Res	Type
1	G	233	VAL
1	H	482	THR
1	H	496	ASP
1	I	152	ALA
1	I	155	ARG
1	I	170	PHE
1	I	192	ALA
1	I	431	GLU
1	J	150	ASN
1	J	156	ASP
1	J	170	PHE
1	J	192	ALA
1	J	495	ASP
1	K	156	ASP
1	K	170	PHE
1	K	483	ASN
1	K	496	ASP
1	K	501	ASN
1	L	232	VAL
1	L	375	ASN
1	L	505	PRO
1	M	156	ASP
1	M	386	SER
1	M	483	ASN
1	N	144	VAL
1	N	155	ARG
1	O	155	ARG
1	O	156	ASP
1	O	170	PHE
1	O	339	ILE
1	P	155	ARG
1	P	174	GLY
1	A	174	GLY
1	A	197	ASP
1	A	431	GLU
1	B	174	GLY
1	B	238	PRO
1	B	431	GLU
1	C	150	ASN
1	C	171	MET
1	C	174	GLY
1	C	194	PRO

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Mol	Chain	Res	Type
1	C	348	PRO
1	C	431	GLU
1	C	496	ASP
1	D	156	ASP
1	D	171	MET
1	D	174	GLY
1	D	192	ALA
1	D	194	PRO
1	D	234	HIS
1	D	269	PRO
1	D	431	GLU
1	E	156	ASP
1	E	174	GLY
1	E	192	ALA
1	E	194	PRO
1	E	233	VAL
1	E	431	GLU
1	F	20	ARG
1	F	155	ARG
1	F	204	LEU
1	F	431	GLU
1	G	387	ASN
1	G	431	GLU
1	H	149	LEU
1	H	156	ASP
1	H	192	ALA
1	H	431	GLU
1	I	42	GLY
1	I	150	ASN
1	I	151	SER
1	I	156	ASP
1	I	174	GLY
1	J	147	SER
1	J	174	GLY
1	J	232	VAL
1	J	431	GLU
1	K	155	ARG
1	K	431	GLU
1	L	155	ARG
1	L	156	ASP
1	L	431	GLU
1	L	495	ASP

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Mol	Chain	Res	Type
1	M	155	ARG
1	M	174	GLY
1	M	431	GLU
1	N	156	ASP
1	N	431	GLU
1	O	174	GLY
1	O	431	GLU
1	P	156	ASP
1	P	431	GLU
1	A	156	ASP
1	B	138	PRO
1	C	137	LEU
1	C	232	VAL
1	D	147	SER
1	D	483	ASN
1	E	193	GLU
1	E	339	ILE
1	F	137	LEU
1	F	154	ALA
1	F	193	GLU
1	F	364	ASN
1	G	156	ASP
1	G	194	PRO
1	H	170	PHE
1	H	193	GLU
1	I	137	LEU
1	I	386	SER
1	I	482	THR
1	I	501	ASN
1	J	116	ASN
1	J	138	PRO
1	J	193	GLU
1	J	348	PRO
1	K	137	LEU
1	K	238	PRO
1	L	138	PRO
1	L	170	PHE
1	L	218	GLU
1	L	233	VAL
1	M	138	PRO
1	M	150	ASN
1	N	138	PRO

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Mol	Chain	Res	Type
1	N	233	VAL
1	O	376	PRO
1	P	138	PRO
1	P	192	ALA
1	A	137	LEU
1	A	172	ALA
1	B	137	LEU
1	C	138	PRO
1	C	482	THR
1	D	20	ARG
1	E	137	LEU
1	E	348	PRO
1	F	138	PRO
1	F	171	MET
1	F	194	PRO
1	F	238	PRO
1	F	483	ASN
1	G	137	LEU
1	G	138	PRO
1	H	137	LEU
1	H	138	PRO
1	I	147	SER
1	I	149	LEU
1	I	238	PRO
1	J	137	LEU
1	J	269	PRO
1	K	138	PRO
1	L	137	LEU
1	L	147	SER
1	M	137	LEU
1	M	170	PHE
1	M	203	SER
1	M	238	PRO
1	N	137	LEU
1	N	170	PHE
1	N	218	GLU
1	O	137	LEU
1	O	138	PRO
1	O	194	PRO
1	P	193	GLU
1	A	138	PRO
1	A	232	VAL

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Mol	Chain	Res	Type
1	D	137	LEU
1	D	138	PRO
1	H	233	VAL
1	H	269	PRO
1	H	386	SER
1	I	138	PRO
1	J	194	PRO
1	L	174	GLY
1	M	375	ASN
1	M	501	ASN
1	N	150	ASN
1	N	174	GLY
1	N	232	VAL
1	P	137	LEU
1	A	339	ILE
1	A	348	PRO
1	D	146	VAL
1	G	348	PRO
1	H	238	PRO
1	K	194	PRO
1	K	233	VAL
1	O	238	PRO
1	P	348	PRO
1	A	268	SER
1	E	138	PRO
1	H	503	VAL
1	D	193	GLU
1	F	191	VAL
1	G	232	VAL
1	G	255	VAL
1	H	199	GLY
1	P	466	PRO
1	O	232	VAL
1	D	191	VAL
1	E	375	ASN

5.3.2 Protein sidechains ⓘ

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

The Analysed column shows the number of residues for which the sidechain conformation was

analysed, and the total number of residues.

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	427/453 (94%)	406 (95%)	21 (5%)	29	61
1	B	427/453 (94%)	405 (95%)	22 (5%)	27	60
1	C	427/453 (94%)	414 (97%)	13 (3%)	46	72
1	D	427/453 (94%)	401 (94%)	26 (6%)	22	56
1	E	427/453 (94%)	412 (96%)	15 (4%)	41	69
1	F	427/453 (94%)	417 (98%)	10 (2%)	56	78
1	G	427/453 (94%)	410 (96%)	17 (4%)	36	66
1	H	427/453 (94%)	411 (96%)	16 (4%)	39	68
1	I	427/453 (94%)	411 (96%)	16 (4%)	39	68
1	J	427/453 (94%)	412 (96%)	15 (4%)	41	69
1	K	427/453 (94%)	401 (94%)	26 (6%)	22	56
1	L	427/453 (94%)	406 (95%)	21 (5%)	29	61
1	M	427/453 (94%)	409 (96%)	18 (4%)	34	65
1	N	427/453 (94%)	413 (97%)	14 (3%)	43	70
1	O	427/453 (94%)	412 (96%)	15 (4%)	41	69
1	P	427/453 (94%)	414 (97%)	13 (3%)	46	72
All	All	6832/7248 (94%)	6554 (96%)	278 (4%)	40	65

All (278) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	52	ASP
1	A	97	SER
1	A	107	GLU
1	A	132	LYS
1	A	149	LEU
1	A	181	MET
1	A	196	PRO
1	A	216	THR
1	A	222	LEU
1	A	226	ILE
1	A	231	GLU
1	A	267	THR
1	A	380	ASN
1	A	391	LEU
1	A	406	ARG

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Mol	Chain	Res	Type
1	A	410	MET
1	A	415	VAL
1	A	454	ILE
1	A	472	ASP
1	A	481	LEU
1	A	528	ASP
1	B	39	SER
1	B	91	VAL
1	B	145	ASP
1	B	178	ASN
1	B	185	ILE
1	B	216	THR
1	B	219	ASP
1	B	253	LEU
1	B	258	PRO
1	B	272	ILE
1	B	282	TYR
1	B	327	ASP
1	B	345	ASP
1	B	356	LEU
1	B	386	SER
1	B	406	ARG
1	B	410	MET
1	B	415	VAL
1	B	454	ILE
1	B	455	PRO
1	B	493	ILE
1	B	499	SER
1	C	52	ASP
1	C	75	PRO
1	C	155	ARG
1	C	156	ASP
1	C	178	ASN
1	C	196	PRO
1	C	216	THR
1	C	380	ASN
1	C	382	LEU
1	C	423	LEU
1	C	454	ILE
1	C	477	HIS
1	C	484	CYS
1	D	47	ASP

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Mol	Chain	Res	Type
1	D	56	ASP
1	D	139	GLN
1	D	144	VAL
1	D	156	ASP
1	D	158	LEU
1	D	159	LYS
1	D	196	PRO
1	D	202	VAL
1	D	239	ARG
1	D	243	LYS
1	D	277	ASP
1	D	306	ASP
1	D	309	GLN
1	D	325	ARG
1	D	351	LEU
1	D	356	LEU
1	D	379	VAL
1	D	380	ASN
1	D	389	MET
1	D	415	VAL
1	D	447	TYR
1	D	454	ILE
1	D	455	PRO
1	D	458	LEU
1	D	479	LYS
1	E	20	ARG
1	E	37	LEU
1	E	101	LEU
1	E	222	LEU
1	E	253	LEU
1	E	275	PHE
1	E	282	TYR
1	E	311	PHE
1	E	380	ASN
1	E	406	ARG
1	E	415	VAL
1	E	454	ILE
1	E	455	PRO
1	E	495	ASP
1	E	497	ILE
1	F	119	PRO
1	F	145	ASP

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Mol	Chain	Res	Type
1	F	204	LEU
1	F	258	PRO
1	F	380	ASN
1	F	386	SER
1	F	441	GLN
1	F	477	HIS
1	F	482	THR
1	F	528	ASP
1	G	47	ASP
1	G	74	HIS
1	G	75	PRO
1	G	178	ASN
1	G	216	THR
1	G	222	LEU
1	G	253	LEU
1	G	306	ASP
1	G	343	ILE
1	G	380	ASN
1	G	406	ARG
1	G	434	ARG
1	G	441	GLN
1	G	447	TYR
1	G	454	ILE
1	G	455	PRO
1	G	495	ASP
1	H	21	ASP
1	H	39	SER
1	H	75	PRO
1	H	101	LEU
1	H	139	GLN
1	H	275	PHE
1	H	333	LYS
1	H	380	ASN
1	H	400	ASP
1	H	406	ARG
1	H	410	MET
1	H	434	ARG
1	H	441	GLN
1	H	454	ILE
1	H	455	PRO
1	H	476	ARG
1	I	107	GLU

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Mol	Chain	Res	Type
1	I	170	PHE
1	I	177	LEU
1	I	196	PRO
1	I	222	LEU
1	I	305	ASP
1	I	324	LYS
1	I	350	ASP
1	I	356	LEU
1	I	379	VAL
1	I	380	ASN
1	I	392	ASP
1	I	454	ILE
1	I	455	PRO
1	I	456	MET
1	I	495	ASP
1	J	52	ASP
1	J	89	SER
1	J	101	LEU
1	J	116	ASN
1	J	118	HIS
1	J	216	THR
1	J	282	TYR
1	J	306	ASP
1	J	345	ASP
1	J	380	ASN
1	J	454	ILE
1	J	455	PRO
1	J	472	ASP
1	J	476	ARG
1	J	496	ASP
1	K	16	ARG
1	K	37	LEU
1	K	52	ASP
1	K	101	LEU
1	K	132	LYS
1	K	147	SER
1	K	159	LYS
1	K	166	MET
1	K	197	ASP
1	K	200	TYR
1	K	201	ASN
1	K	218	GLU

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Mol	Chain	Res	Type
1	K	231	GLU
1	K	249	LEU
1	K	266	ILE
1	K	282	TYR
1	K	325	ARG
1	K	326	SER
1	K	341	SER
1	K	356	LEU
1	K	380	ASN
1	K	389	MET
1	K	398	ILE
1	K	441	GLN
1	K	454	ILE
1	K	477	HIS
1	L	47	ASP
1	L	75	PRO
1	L	101	LEU
1	L	119	PRO
1	L	150	ASN
1	L	177	LEU
1	L	190	THR
1	L	252	SER
1	L	269	PRO
1	L	273	LYS
1	L	282	TYR
1	L	325	ARG
1	L	341	SER
1	L	366	LYS
1	L	380	ASN
1	L	441	GLN
1	L	454	ILE
1	L	455	PRO
1	L	472	ASP
1	L	477	HIS
1	L	504	GLU
1	M	52	ASP
1	M	96	THR
1	M	156	ASP
1	M	170	PHE
1	M	205	ASP
1	M	242	GLU
1	M	310	HIS

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Mol	Chain	Res	Type
1	M	356	LEU
1	M	380	ASN
1	M	406	ARG
1	M	410	MET
1	M	434	ARG
1	M	447	TYR
1	M	454	ILE
1	M	455	PRO
1	M	456	MET
1	M	483	ASN
1	M	509	THR
1	N	75	PRO
1	N	90	GLU
1	N	142	THR
1	N	155	ARG
1	N	156	ASP
1	N	296	ASN
1	N	305	ASP
1	N	327	ASP
1	N	341	SER
1	N	368	VAL
1	N	380	ASN
1	N	454	ILE
1	N	455	PRO
1	N	509	THR
1	O	47	ASP
1	O	51	ILE
1	O	87	GLN
1	O	178	ASN
1	O	216	THR
1	O	230	LYS
1	O	281	LYS
1	O	305	ASP
1	O	359	GLU
1	O	380	ASN
1	O	406	ARG
1	O	441	GLN
1	O	454	ILE
1	O	457	ILE
1	O	495	ASP
1	P	47	ASP
1	P	52	ASP

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Mol	Chain	Res	Type
1	P	75	PRO
1	P	132	LYS
1	P	147	SER
1	P	155	ARG
1	P	212	LYS
1	P	222	LEU
1	P	356	LEU
1	P	380	ASN
1	P	423	LEU
1	P	455	PRO
1	P	497	ILE

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (38) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	234	HIS
1	A	309	GLN
1	A	477	HIS
1	A	511	GLN
1	B	74	HIS
1	B	178	ASN
1	B	234	HIS
1	B	477	HIS
1	C	17	ASN
1	C	87	GLN
1	C	234	HIS
1	D	61	ASN
1	D	118	HIS
1	D	234	HIS
1	D	477	HIS
1	E	139	GLN
1	E	234	HIS
1	E	477	HIS
1	F	118	HIS
1	F	234	HIS
1	G	178	ASN
1	G	477	HIS
1	H	234	HIS
1	I	118	HIS
1	I	234	HIS
1	I	477	HIS
1	J	87	GLN

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Mol	Chain	Res	Type
1	K	234	HIS
1	L	234	HIS
1	M	221	GLN
1	M	234	HIS
1	M	477	HIS
1	M	490	ASN
1	N	118	HIS
1	O	118	HIS
1	O	477	HIS
1	P	17	ASN
1	P	234	HIS

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no carbohydrates in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.