wwPDB EM Map/Model Validation Report (i)

Apr 10, 2016 – 01:51 PM BST

PDB ID	:	3J1C
EMDB ID:	:	EMD-5392
Title	:	Cryo-EM structure of 9-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	:	9.10 Å(reported)
Based on PDB ID	:	3KO1

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

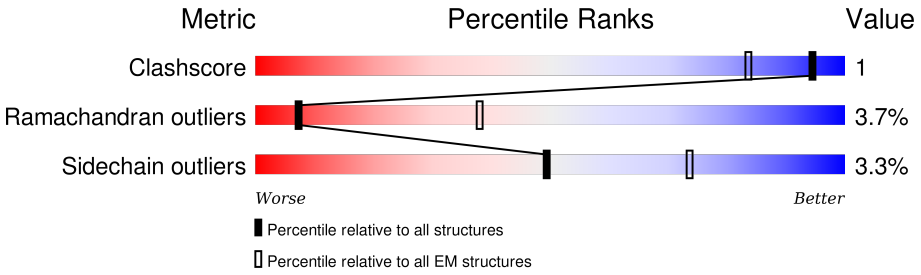
MolProbity	:	4.02b-467
Mogul	:	unknown
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et. al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk27241

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 9.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	563	66% 22% • 8%
1	B	563	68% 19% • • 8%
1	C	563	67% 21% • • 8%
1	D	563	69% 19% • 8%
1	E	563	66% 22% • • 8%
1	F	563	70% 19% • • 8%
1	G	563	69% 18% • • 8%
1	H	563	67% 20% • • 8%
1	I	563	65% 23% • 8%

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Mol	Chain	Length	Quality of chain
1	J	563	67% 21% 8%
1	K	563	72% 17% 8%
1	L	563	71% 18% 8%
1	M	563	68% 19% 5% 8%
1	N	563	67% 20% 8%
1	O	563	68% 19% 8%
1	P	563	71% 17% 8%
1	Q	563	71% 18% 8%
1	R	563	69% 19% 8%

2 Entry composition

There is only 1 type of molecule in this entry. The entry contains 70866 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		
1	Q	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		

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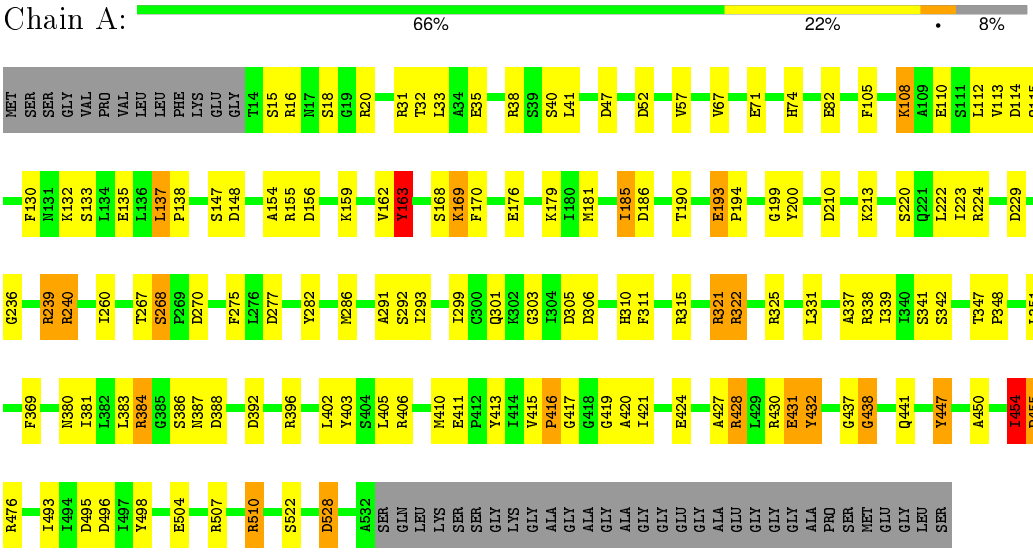
Mol	Chain	Residues	Atoms					AltConf	Trace
1	R	519	Total	C	N	O	S	0	0
			3937	2475	673	773	16		

3 Residue-property plots (i)

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

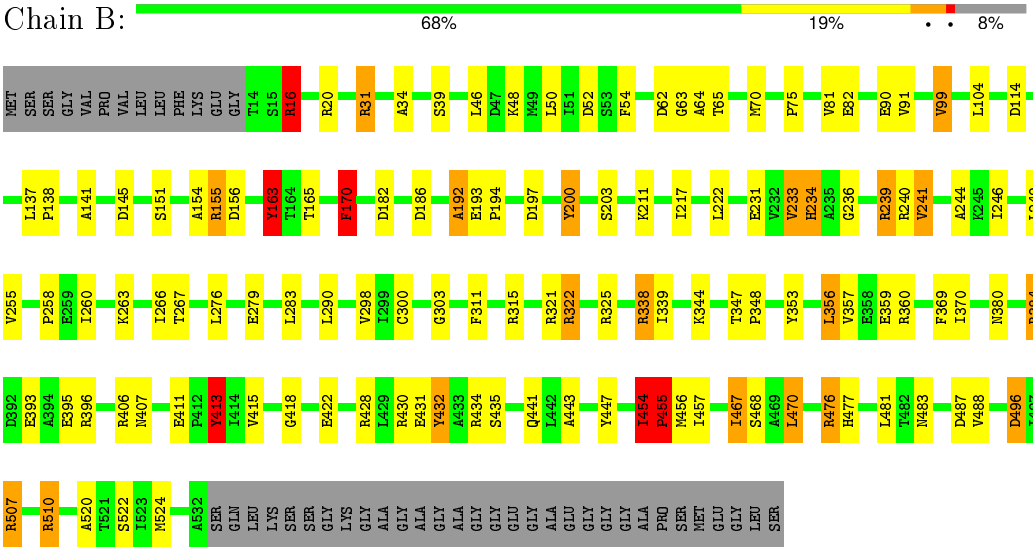
- Molecule 1: Chaperonin alpha subunit

Chain A:



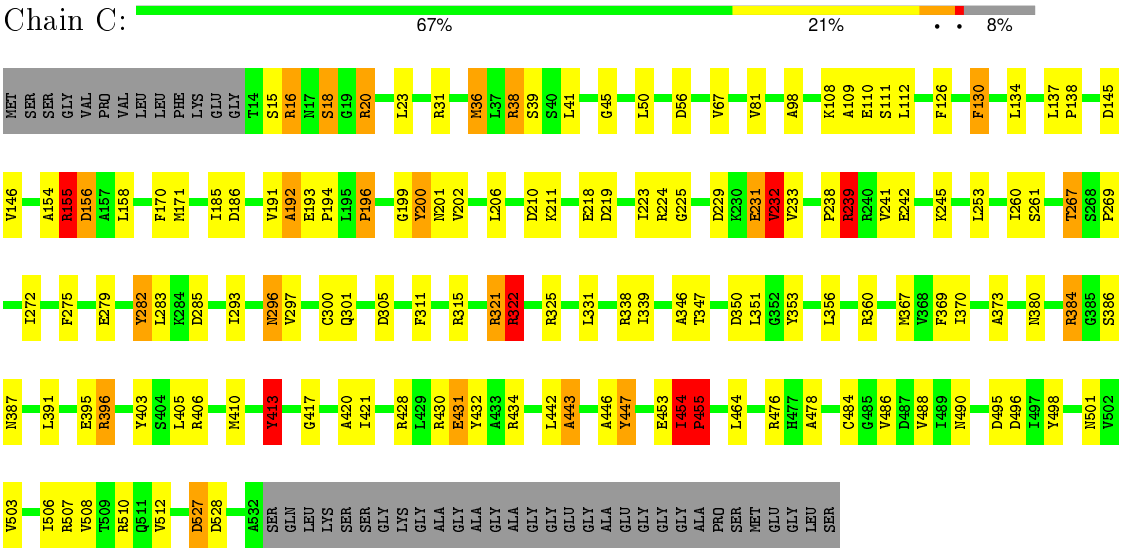
- Molecule 1: Chaperonin alpha subunit

Chain B:



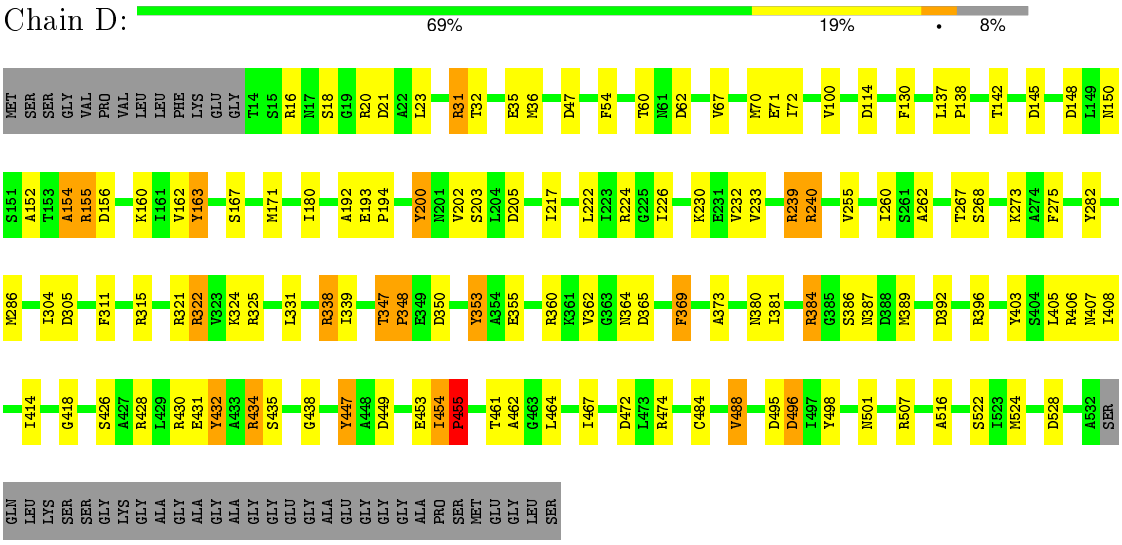
- Molecule 1: Chaperonin alpha subunit

Chain C:



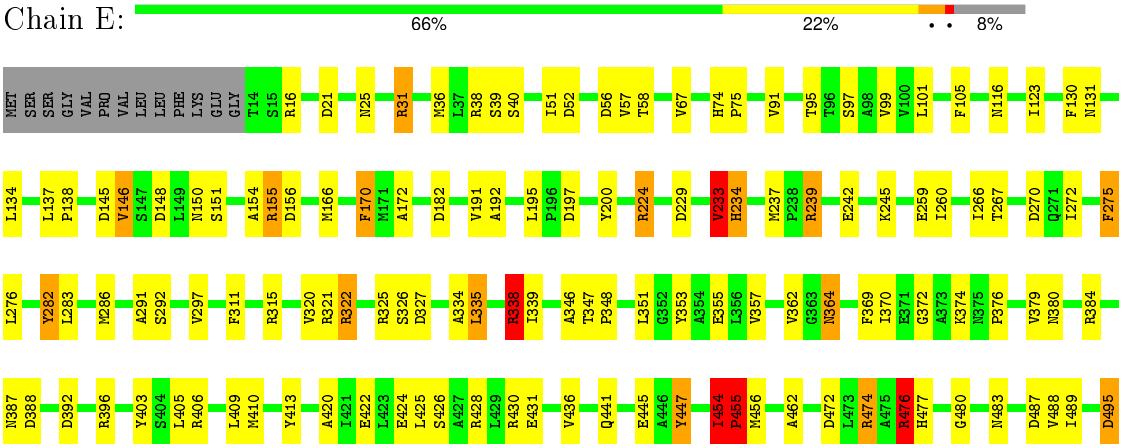
• Molecule 1: Chaperonin alpha subunit

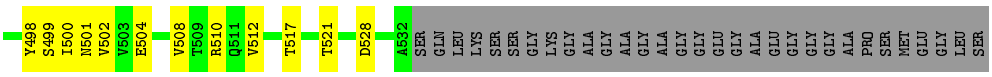
Chain D:



• Molecule 1: Chaperonin alpha subunit

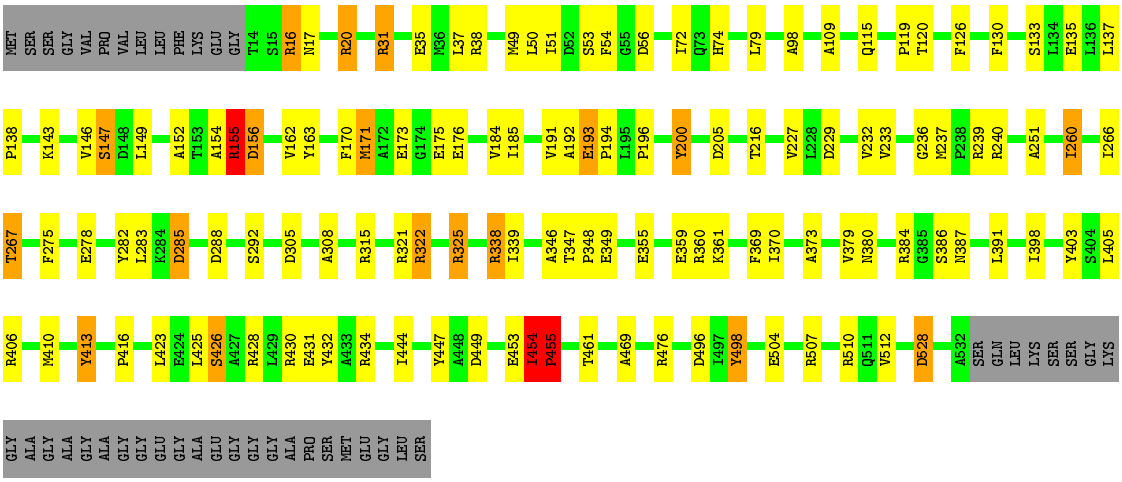
Chain E:





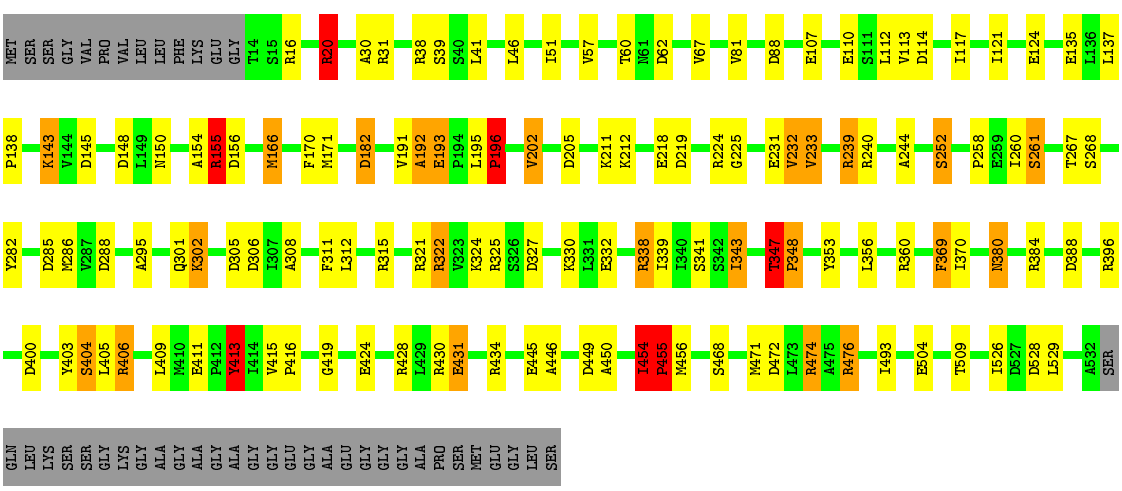
- Molecule 1: Chaperonin alpha subunit

Chain F:



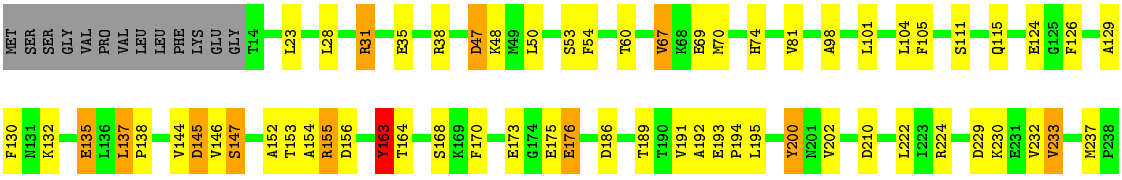
- Molecule 1: Chaperonin alpha subunit

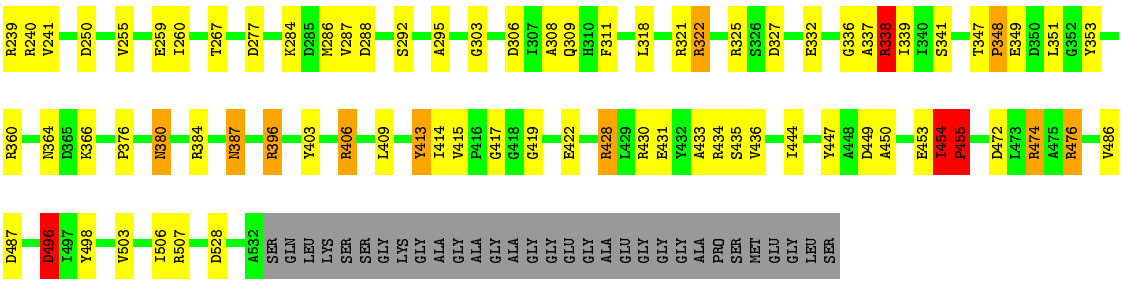
Chain G:



- Molecule 1: Chaperonin alpha subunit

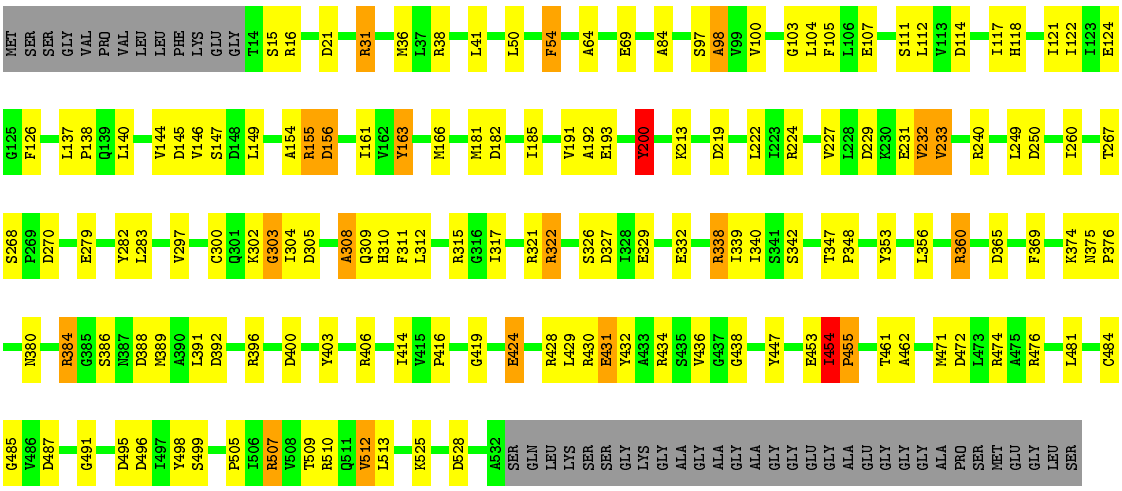
Chain H:





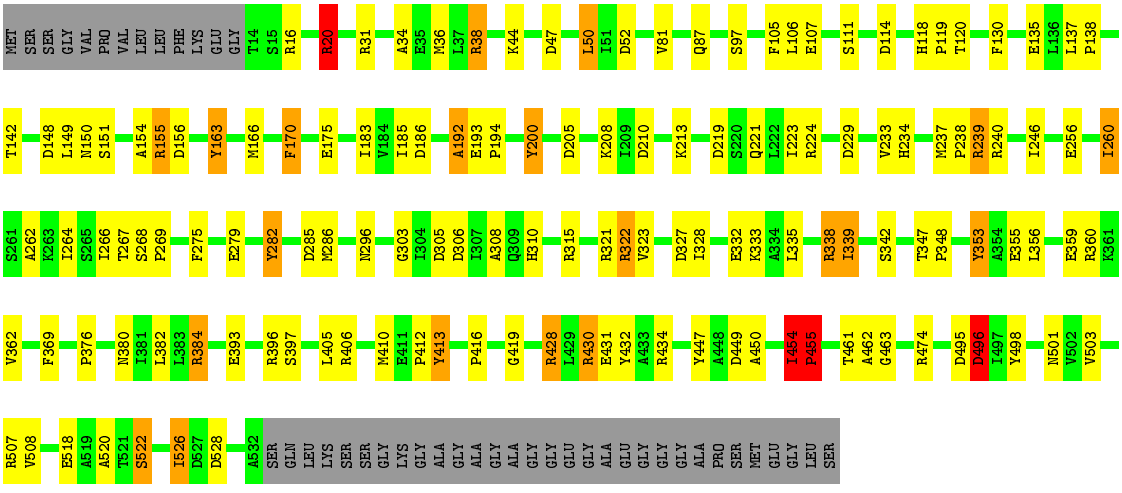
• Molecule 1: Chaperonin alpha subunit

Chain I:



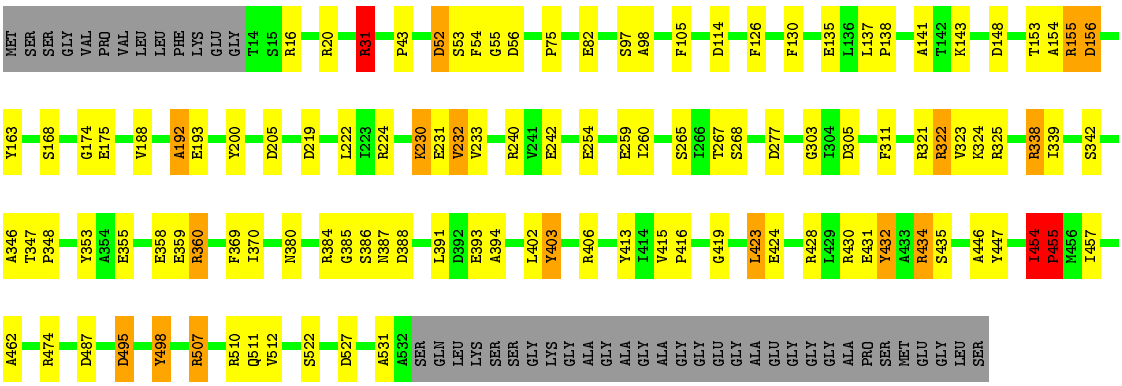
• Molecule 1: Chaperonin alpha subunit

Chain J:



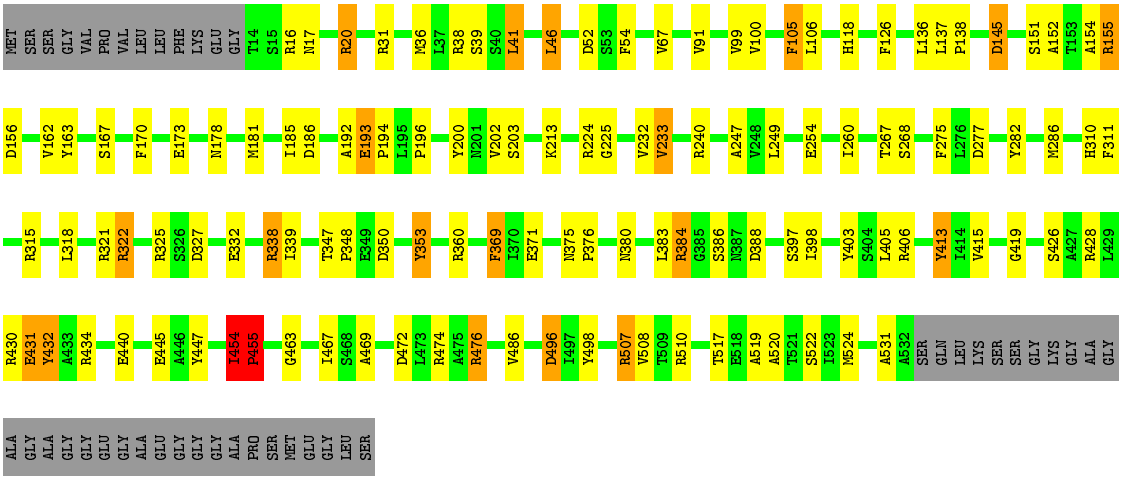
• Molecule 1: Chaperonin alpha subunit

Chain K:



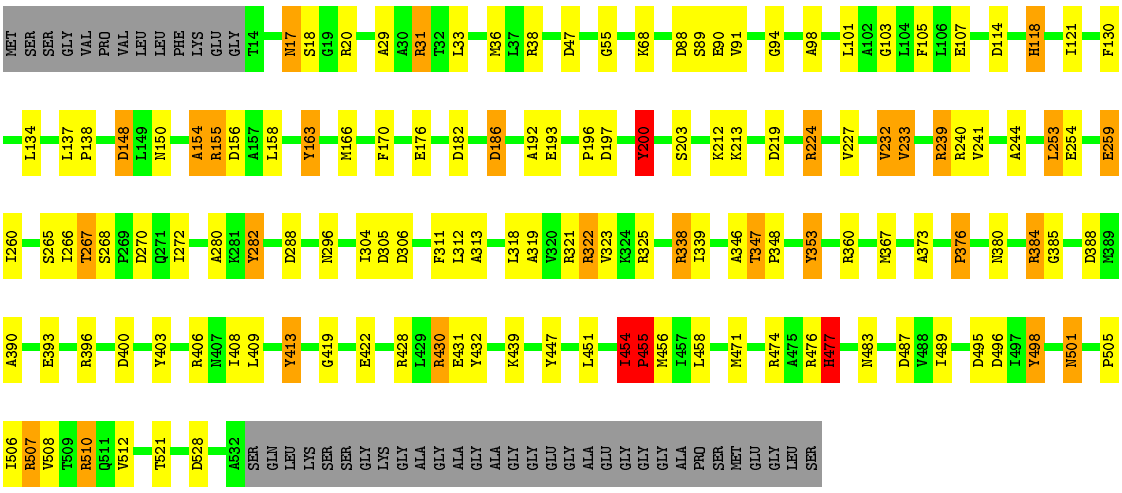
• Molecule 1: Chaperonin alpha subunit

Chain L:



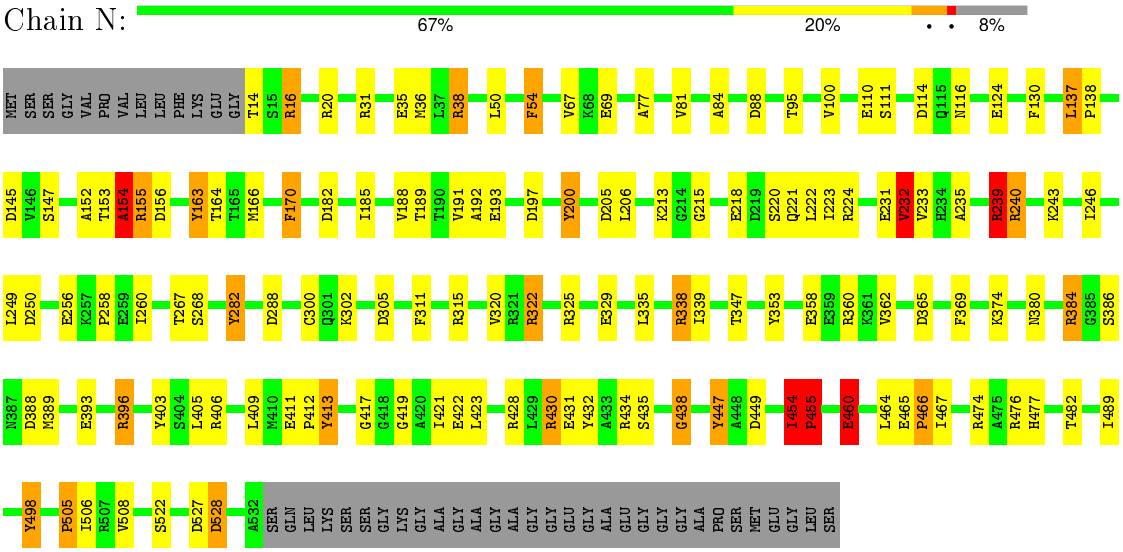
• Molecule 1: Chaperonin alpha subunit

Chain M:



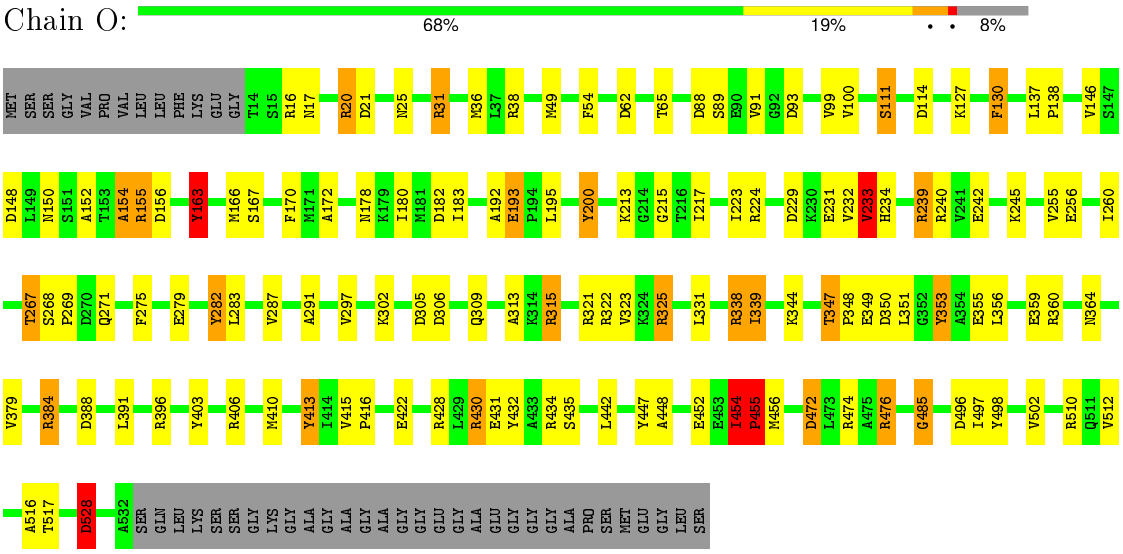
• Molecule 1: Chaperonin alpha subunit

Chain N:



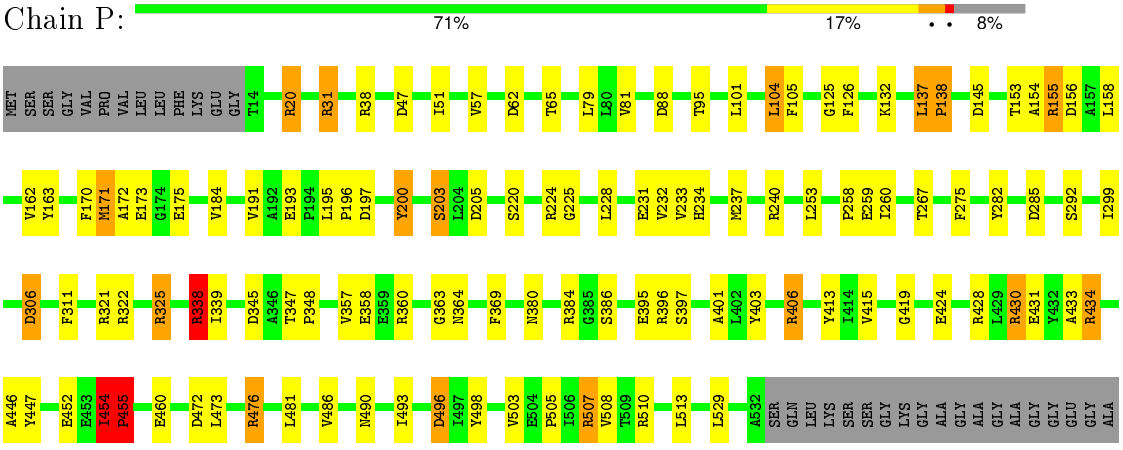
- Molecule 1: Chaperonin alpha subunit

Chain O:



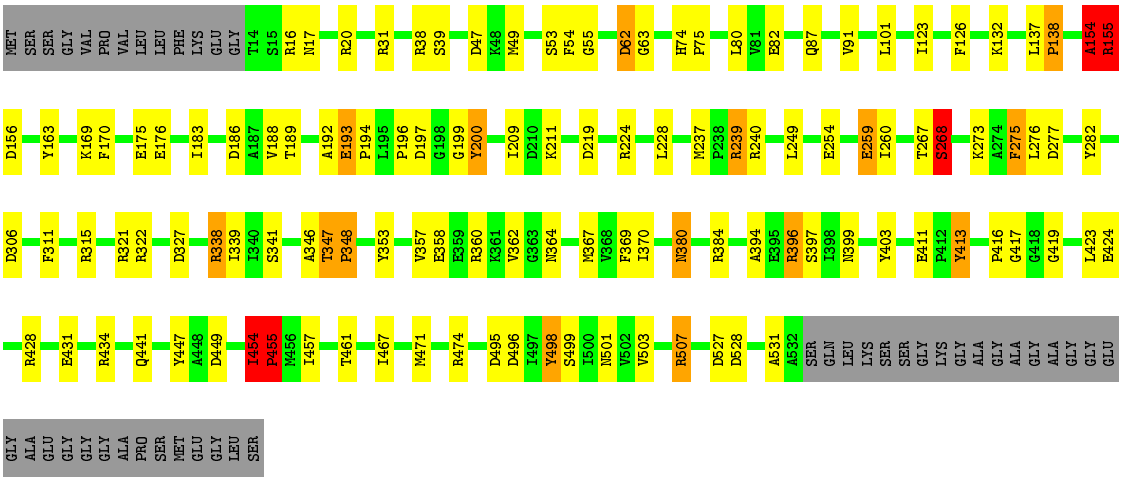
- Molecule 1: Chaperonin alpha subunit

Chain P:



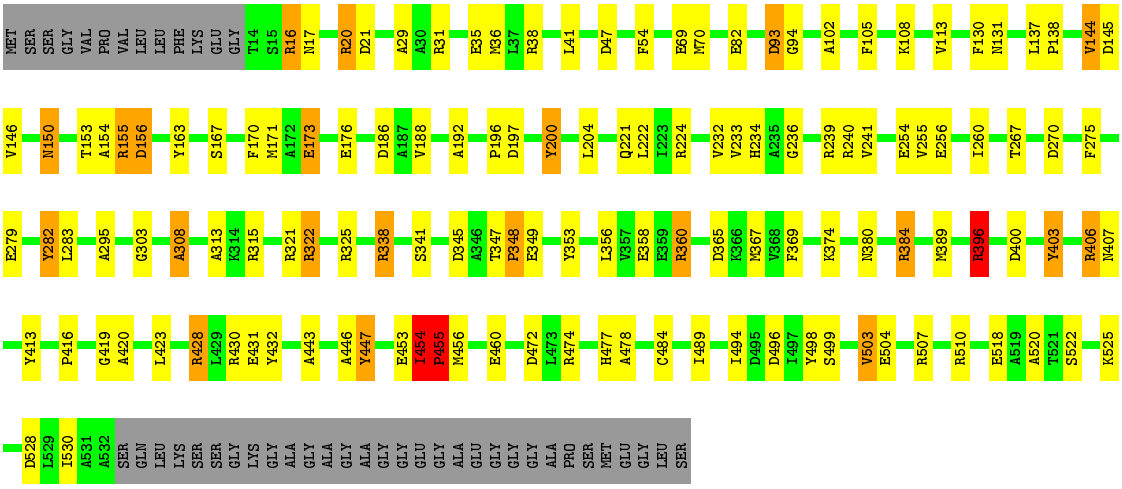
• Molecule 1: Chaperonin alpha subunit

Chain Q:



• Molecule 1: Chaperonin alpha subunit

Chain R:



4 Experimental information (i)

Property	Value	Source
Reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	Depositor
Number of images	9596	Depositor
Resolution determination method	Not provided	Depositor
CTF correction method	The whole micrograph	Depositor
Microscope	Titan Krios	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	Not provided	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	1.58	25/3974 (0.6%)	2.04	116/5360 (2.2%)
1	B	1.61	19/3974 (0.5%)	2.00	94/5360 (1.8%)
1	C	1.56	17/3974 (0.4%)	1.98	106/5360 (2.0%)
1	D	1.56	17/3974 (0.4%)	1.97	105/5360 (2.0%)
1	E	1.58	24/3974 (0.6%)	1.92	91/5360 (1.7%)
1	F	1.60	21/3974 (0.5%)	1.96	95/5360 (1.8%)
1	G	1.56	13/3974 (0.3%)	1.98	103/5360 (1.9%)
1	H	1.58	17/3974 (0.4%)	2.08	121/5360 (2.3%)
1	I	1.62	20/3974 (0.5%)	1.98	102/5360 (1.9%)
1	J	1.63	23/3974 (0.6%)	2.02	100/5360 (1.9%)
1	K	1.61	26/3974 (0.7%)	1.92	85/5360 (1.6%)
1	L	1.58	15/3974 (0.4%)	1.98	99/5360 (1.8%)
1	M	1.57	22/3974 (0.6%)	1.98	110/5360 (2.1%)
1	N	1.60	18/3974 (0.5%)	2.03	114/5360 (2.1%)
1	O	1.59	21/3974 (0.5%)	2.04	106/5360 (2.0%)
1	P	1.57	15/3974 (0.4%)	2.05	98/5360 (1.8%)
1	Q	1.59	17/3974 (0.4%)	1.94	88/5360 (1.6%)
1	R	1.62	28/3974 (0.7%)	1.97	110/5360 (2.1%)
All	All	1.59	358/71532 (0.5%)	1.99	1843/96480 (1.9%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
1	H	0	16
1	I	0	19
1	J	0	20
1	K	0	18
1	L	0	22
1	M	0	22
1	N	0	21
1	O	0	22
1	P	0	18
1	Q	0	18
1	R	0	21
All	All	0	355

All (358) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	Q	397	SER	CA-CB	10.83	1.69	1.52
1	Q	413	TYR	CE2-CZ	9.00	1.50	1.38
1	F	413	TYR	CG-CD2	8.70	1.50	1.39
1	A	15	SER	CA-CB	8.59	1.65	1.52
1	A	268	SER	CA-CB	8.57	1.65	1.52
1	R	353	TYR	CE2-CZ	8.50	1.49	1.38
1	I	311	PHE	CG-CD2	8.19	1.51	1.38
1	L	474	ARG	CD-NE	8.10	1.60	1.46
1	E	384	ARG	CD-NE	7.99	1.60	1.46
1	K	163	TYR	CE2-CZ	7.93	1.48	1.38
1	E	39	SER	CA-CB	7.87	1.64	1.52
1	P	155	ARG	CZ-NH1	-7.70	1.23	1.33
1	N	220	SER	CA-CB	7.67	1.64	1.52
1	A	437	GLY	N-CA	-7.67	1.34	1.46
1	C	111	SER	CA-CB	7.65	1.64	1.52
1	E	259	GLU	CB-CG	7.60	1.66	1.52
1	R	341	SER	CA-CB	7.58	1.64	1.52
1	B	82	GLU	CG-CD	-7.53	1.40	1.51
1	C	406	ARG	CD-NE	7.52	1.59	1.46
1	K	254	GLU	CB-CG	7.47	1.66	1.52
1	N	498	TYR	CE2-CZ	7.46	1.48	1.38
1	P	203	SER	CA-CB	7.45	1.64	1.52
1	N	215	GLY	CA-C	-7.44	1.40	1.51
1	J	97	SER	CA-CB	7.27	1.63	1.52
1	K	432	TYR	CG-CD1	7.26	1.48	1.39
1	B	395	GLU	CD-OE2	7.24	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	J	135	GLU	CD-OE2	7.24	1.33	1.25
1	J	275	PHE	CG-CD2	7.20	1.49	1.38
1	M	413	TYR	CE1-CZ	7.20	1.48	1.38
1	B	447	TYR	CE2-CZ	7.19	1.47	1.38
1	M	338	ARG	CD-NE	7.17	1.58	1.46
1	O	435	SER	CA-CB	7.03	1.63	1.52
1	O	256	GLU	CD-OE2	7.01	1.33	1.25
1	D	435	SER	CB-OG	7.01	1.51	1.42
1	G	325	ARG	CD-NE	7.00	1.58	1.46
1	M	422	GLU	CD-OE1	6.96	1.33	1.25
1	F	278	GLU	CG-CD	6.94	1.62	1.51
1	O	422	GLU	CB-CG	6.92	1.65	1.52
1	E	499	SER	CA-CB	6.89	1.63	1.52
1	A	239	ARG	CD-NE	6.82	1.58	1.46
1	I	491	GLY	CA-C	-6.82	1.41	1.51
1	R	498	TYR	CE1-CZ	6.77	1.47	1.38
1	I	505	PRO	N-CD	-6.77	1.38	1.47
1	M	458	LEU	CA-CB	6.75	1.69	1.53
1	J	163	TYR	CG-CD2	6.74	1.48	1.39
1	A	82	GLU	CD-OE1	6.73	1.33	1.25
1	E	413	TYR	CE1-CZ	6.73	1.47	1.38
1	O	355	GLU	CD-OE2	6.73	1.33	1.25
1	M	31	ARG	CD-NE	6.69	1.57	1.46
1	L	522	SER	CA-CB	6.67	1.62	1.52
1	N	522	SER	CB-OG	6.67	1.50	1.42
1	K	231	GLU	CG-CD	-6.66	1.42	1.51
1	H	321	ARG	CD-NE	6.63	1.57	1.46
1	A	431	GLU	CB-CG	6.61	1.64	1.52
1	R	353	TYR	CG-CD2	6.57	1.47	1.39
1	L	510	ARG	CD-NE	6.57	1.57	1.46
1	L	520	ALA	CA-CB	6.57	1.66	1.52
1	N	432	TYR	CG-CD1	6.55	1.47	1.39
1	M	89	SER	CA-CB	6.55	1.62	1.52
1	I	303	GLY	N-CA	6.54	1.55	1.46
1	I	15	SER	CA-CB	6.53	1.62	1.52
1	O	200	TYR	CE2-CZ	6.51	1.47	1.38
1	R	406	ARG	CD-NE	6.51	1.57	1.46
1	C	453	GLU	CB-CG	6.49	1.64	1.52
1	O	416	PRO	N-CD	6.49	1.56	1.47
1	R	358	GLU	CB-CG	6.48	1.64	1.52
1	R	94	GLY	CA-C	6.41	1.62	1.51
1	K	432	TYR	CZ-OH	6.40	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	O	498	TYR	CE2-CZ	6.39	1.46	1.38
1	B	31	ARG	CD-NE	6.38	1.57	1.46
1	N	389	MET	N-CA	6.38	1.59	1.46
1	D	71	GLU	CG-CD	-6.36	1.42	1.51
1	N	498	TYR	CZ-OH	6.35	1.48	1.37
1	M	385	GLY	CA-C	-6.32	1.41	1.51
1	P	258	PRO	N-CA	-6.32	1.36	1.47
1	R	38	ARG	CD-NE	6.31	1.57	1.46
1	B	82	GLU	CB-CG	6.30	1.64	1.52
1	E	275	PHE	CE2-CZ	6.29	1.49	1.37
1	M	200	TYR	CE2-CZ	6.29	1.46	1.38
1	N	114	ASP	CA-CB	6.29	1.67	1.53
1	J	200	TYR	CE1-CZ	6.28	1.46	1.38
1	O	485	GLY	CA-C	6.28	1.61	1.51
1	E	234	HIS	CB-CG	-6.27	1.38	1.50
1	H	292	SER	CA-CB	6.27	1.62	1.52
1	G	403	TYR	CE1-CZ	6.27	1.46	1.38
1	M	55	GLY	N-CA	-6.25	1.36	1.46
1	A	507	ARG	CD-NE	6.23	1.57	1.46
1	O	432	TYR	CE1-CZ	6.22	1.46	1.38
1	H	406	ARG	CD-NE	6.22	1.57	1.46
1	D	447	TYR	CG-CD1	6.22	1.47	1.39
1	O	178	ASN	N-CA	-6.22	1.33	1.46
1	F	444	ILE	N-CA	6.20	1.58	1.46
1	G	39	SER	CA-CB	6.20	1.62	1.52
1	R	315	ARG	CD-NE	6.20	1.56	1.46
1	B	393	GLU	CD-OE2	6.17	1.32	1.25
1	A	35	GLU	CD-OE1	6.16	1.32	1.25
1	C	110	GLU	CB-CG	6.16	1.63	1.52
1	E	282	TYR	CZ-OH	6.13	1.48	1.37
1	R	518	GLU	CG-CD	6.12	1.61	1.51
1	M	403	TYR	CG-CD1	6.11	1.47	1.39
1	N	218	GLU	N-CA	6.11	1.58	1.46
1	K	355	GLU	CG-CD	-6.10	1.42	1.51
1	O	224	ARG	CD-NE	6.10	1.56	1.46
1	R	82	GLU	CG-CD	-6.10	1.42	1.51
1	I	224	ARG	CD-NE	6.08	1.56	1.46
1	F	35	GLU	CG-CD	-6.07	1.42	1.51
1	R	358	GLU	CD-OE2	6.07	1.32	1.25
1	K	130	PHE	CG-CD2	6.07	1.47	1.38
1	A	406	ARG	CD-NE	6.07	1.56	1.46
1	K	231	GLU	CB-CG	6.07	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	I	485	GLY	N-CA	6.07	1.55	1.46
1	D	484	CYS	CB-SG	6.05	1.92	1.82
1	E	376	PRO	CA-CB	6.02	1.65	1.53
1	E	424	GLU	CB-CG	6.01	1.63	1.52
1	Q	138	PRO	N-CD	6.01	1.56	1.47
1	N	393	GLU	CB-CG	6.00	1.63	1.52
1	B	369	PHE	CG-CD1	5.98	1.47	1.38
1	I	403	TYR	CE2-CZ	5.98	1.46	1.38
1	B	395	GLU	CB-CG	5.98	1.63	1.52
1	I	326	SER	CA-CB	5.98	1.61	1.52
1	A	369	PHE	CG-CD2	5.97	1.47	1.38
1	C	45	GLY	CA-C	-5.96	1.42	1.51
1	A	40	SER	CB-OG	5.95	1.50	1.42
1	A	110	GLU	CD-OE2	-5.94	1.19	1.25
1	H	403	TYR	CG-CD1	5.94	1.46	1.39
1	C	413	TYR	CZ-OH	5.91	1.48	1.37
1	H	433	ALA	CA-CB	5.91	1.64	1.52
1	E	426	SER	CA-CB	5.90	1.61	1.52
1	J	428	ARG	CD-NE	5.90	1.56	1.46
1	J	111	SER	CA-CB	5.88	1.61	1.52
1	N	282	TYR	CE1-CZ	5.87	1.46	1.38
1	F	175	GLU	CG-CD	5.87	1.60	1.51
1	B	252	SER	CA-CB	5.87	1.61	1.52
1	Q	175	GLU	CB-CG	5.86	1.63	1.52
1	L	105	PHE	CG-CD2	-5.86	1.29	1.38
1	F	109	ALA	CA-CB	5.85	1.64	1.52
1	I	103	GLY	CA-C	-5.85	1.42	1.51
1	E	504	GLU	CD-OE2	5.82	1.32	1.25
1	R	254	GLU	CB-CG	5.81	1.63	1.52
1	L	225	GLY	CA-C	-5.81	1.42	1.51
1	B	52	ASP	CA-CB	5.80	1.66	1.53
1	K	338	ARG	CD-NE	5.80	1.56	1.46
1	H	348	PRO	CA-CB	5.79	1.65	1.53
1	L	397	SER	CA-CB	5.79	1.61	1.52
1	M	265	SER	CB-OG	5.78	1.49	1.42
1	F	176	GLU	CD-OE1	5.78	1.32	1.25
1	P	31	ARG	CD-NE	5.77	1.56	1.46
1	R	478	ALA	CA-CB	5.77	1.64	1.52
1	I	163	TYR	CG-CD1	5.77	1.46	1.39
1	B	447	TYR	CB-CG	-5.77	1.43	1.51
1	O	89	SER	CA-CB	5.76	1.61	1.52
1	D	364	ASN	CA-CB	5.76	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	R	460	GLU	CD-OE2	5.76	1.31	1.25
1	E	195	LEU	C-N	-5.75	1.23	1.34
1	M	259	GLU	CG-CD	5.74	1.60	1.51
1	O	476	ARG	CD-NE	5.74	1.56	1.46
1	H	175	GLU	CB-CG	5.73	1.63	1.52
1	J	38	ARG	CA-CB	5.71	1.66	1.53
1	J	20	ARG	CD-NE	5.70	1.56	1.46
1	B	411	GLU	CB-CG	5.68	1.62	1.52
1	D	167	SER	CA-CB	5.68	1.61	1.52
1	K	510	ARG	CD-NE	5.67	1.56	1.46
1	H	191	VAL	CB-CG1	5.67	1.64	1.52
1	A	292	SER	CA-CB	5.67	1.61	1.52
1	A	447	TYR	CB-CG	-5.66	1.43	1.51
1	L	430	ARG	CD-NE	5.66	1.56	1.46
1	N	311	PHE	CG-CD2	5.66	1.47	1.38
1	H	155	ARG	CD-NE	5.65	1.56	1.46
1	J	355	GLU	CB-CG	5.64	1.62	1.52
1	D	282	TYR	CD1-CE1	5.64	1.47	1.39
1	E	498	TYR	CD1-CE1	5.63	1.47	1.39
1	K	342	SER	CB-OG	5.63	1.49	1.42
1	P	240	ARG	CD-NE	5.63	1.56	1.46
1	Q	268	SER	CA-CB	5.62	1.61	1.52
1	E	445	GLU	CD-OE2	5.62	1.31	1.25
1	A	447	TYR	CE1-CZ	5.62	1.45	1.38
1	A	504	GLU	N-CA	-5.62	1.35	1.46
1	F	133	SER	CA-CB	5.62	1.61	1.52
1	F	163	TYR	CG-CD1	5.61	1.46	1.39
1	I	147	SER	CA-CB	5.61	1.61	1.52
1	H	168	SER	CB-OG	5.60	1.49	1.42
1	L	173	GLU	CG-CD	5.60	1.60	1.51
1	F	349	GLU	CD-OE1	5.60	1.31	1.25
1	B	90	GLU	CD-OE1	5.60	1.31	1.25
1	C	403	TYR	CG-CD1	5.59	1.46	1.39
1	I	384	ARG	NE-CZ	5.58	1.40	1.33
1	J	428	ARG	NE-CZ	5.58	1.40	1.33
1	E	282	TYR	CE2-CZ	5.58	1.45	1.38
1	P	419	GLY	CA-C	-5.56	1.43	1.51
1	N	329	GLU	CD-OE1	5.52	1.31	1.25
1	A	38	ARG	CD-NE	5.52	1.55	1.46
1	G	107	GLU	CD-OE1	5.51	1.31	1.25
1	D	347	THR	C-N	5.51	1.44	1.34
1	A	71	GLU	CD-OE2	5.51	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	498	TYR	CB-CG	-5.50	1.43	1.51
1	J	224	ARG	NE-CZ	5.50	1.40	1.33
1	M	311	PHE	CG-CD1	5.49	1.47	1.38
1	G	258	PRO	N-CD	-5.49	1.40	1.47
1	M	94	GLY	N-CA	-5.49	1.37	1.46
1	Q	341	SER	CA-CB	5.49	1.61	1.52
1	J	315	ARG	N-CA	-5.48	1.35	1.46
1	E	16	ARG	CD-NE	5.48	1.55	1.46
1	M	254	GLU	CD-OE1	5.48	1.31	1.25
1	A	41	LEU	C-N	5.47	1.42	1.33
1	H	336	GLY	CA-C	-5.47	1.43	1.51
1	J	396	ARG	CD-NE	5.47	1.55	1.46
1	B	353	TYR	CE2-CZ	5.46	1.45	1.38
1	N	147	SER	N-CA	5.46	1.57	1.46
1	R	29	ALA	CA-CB	5.46	1.64	1.52
1	G	124	GLU	CD-OE1	5.46	1.31	1.25
1	B	203	SER	CA-CB	5.46	1.61	1.52
1	C	126	PHE	CE1-CZ	5.46	1.47	1.37
1	Q	447	TYR	CE1-CZ	5.46	1.45	1.38
1	H	124	GLU	CD-OE1	-5.46	1.19	1.25
1	M	239	ARG	CD-NE	5.45	1.55	1.46
1	N	35	GLU	CG-CD	-5.45	1.43	1.51
1	N	300	CYS	CB-SG	5.45	1.91	1.82
1	C	18	SER	CA-CB	5.44	1.61	1.52
1	G	341	SER	CA-CB	5.44	1.61	1.52
1	O	384	ARG	NE-CZ	5.44	1.40	1.33
1	C	431	GLU	CB-CG	5.44	1.62	1.52
1	J	275	PHE	CB-CG	5.43	1.60	1.51
1	A	522	SER	CA-CB	5.42	1.61	1.52
1	J	175	GLU	CG-CD	5.42	1.60	1.51
1	I	321	ARG	CD-NE	5.41	1.55	1.46
1	R	173	GLU	CG-CD	5.41	1.60	1.51
1	C	218	GLU	CG-CD	-5.40	1.43	1.51
1	Q	454	ILE	C-N	5.39	1.44	1.34
1	R	522	SER	CA-CB	5.39	1.61	1.52
1	N	329	GLU	CB-CG	5.39	1.62	1.52
1	K	231	GLU	CD-OE1	5.38	1.31	1.25
1	O	268	SER	CB-OG	5.38	1.49	1.42
1	M	403	TYR	CB-CG	-5.38	1.43	1.51
1	F	403	TYR	CG-CD1	5.37	1.46	1.39
1	H	417	GLY	CA-C	-5.37	1.43	1.51
1	A	353	TYR	CG-CD1	5.37	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	426	SER	CB-OG	5.37	1.49	1.42
1	C	432	TYR	CB-CG	5.36	1.59	1.51
1	R	54	PHE	CE2-CZ	5.36	1.47	1.37
1	P	220	SER	CB-OG	5.35	1.49	1.42
1	J	338	ARG	CD-NE	5.35	1.55	1.46
1	A	430	ARG	CZ-NH2	5.33	1.40	1.33
1	A	199	GLY	N-CA	-5.33	1.38	1.46
1	K	358	GLU	CD-OE1	-5.31	1.19	1.25
1	D	454	ILE	C-N	5.31	1.44	1.34
1	Q	74	HIS	CB-CG	5.31	1.59	1.50
1	R	499	SER	CA-CB	5.30	1.60	1.52
1	Q	132	LYS	N-CA	-5.30	1.35	1.46
1	I	163	TYR	CD1-CE1	-5.30	1.31	1.39
1	Q	417	GLY	N-CA	5.30	1.53	1.46
1	A	130	PHE	CG-CD1	5.29	1.46	1.38
1	P	20	ARG	NE-CZ	5.29	1.40	1.33
1	P	292	SER	CA-CB	5.29	1.60	1.52
1	L	445	GLU	CB-CG	5.29	1.62	1.52
1	E	369	PHE	CG-CD1	5.28	1.46	1.38
1	D	426	SER	CA-CB	5.27	1.60	1.52
1	G	295	ALA	CA-CB	5.27	1.63	1.52
1	F	236	GLY	N-CA	5.27	1.53	1.46
1	F	359	GLU	CG-CD	5.27	1.59	1.51
1	P	62	ASP	CB-CG	5.26	1.62	1.51
1	H	422	GLU	CB-CG	5.26	1.62	1.52
1	P	175	GLU	CD-OE2	-5.26	1.19	1.25
1	I	431	GLU	CD-OE2	5.25	1.31	1.25
1	J	522	SER	CB-OG	5.24	1.49	1.42
1	K	31	ARG	CD-NE	5.24	1.55	1.46
1	D	130	PHE	CG-CD2	5.24	1.46	1.38
1	H	54	PHE	CG-CD2	5.24	1.46	1.38
1	O	111	SER	CA-CB	5.23	1.60	1.52
1	A	325	ARG	CA-CB	5.23	1.65	1.53
1	C	39	SER	CA-CB	5.23	1.60	1.52
1	L	426	SER	CB-OG	5.23	1.49	1.42
1	O	155	ARG	CD-NE	5.23	1.55	1.46
1	B	63	GLY	CA-C	-5.23	1.43	1.51
1	R	484	CYS	C-N	5.23	1.42	1.33
1	G	110	GLU	CG-CD	-5.22	1.44	1.51
1	Q	358	GLU	CD-OE1	5.22	1.31	1.25
1	B	82	GLU	CD-OE1	5.22	1.31	1.25
1	C	199	GLY	CA-C	-5.22	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	K	435	SER	CA-CB	5.22	1.60	1.52
1	K	369	PHE	CE1-CZ	5.21	1.47	1.37
1	R	176	GLU	CD-OE1	5.20	1.31	1.25
1	P	493	ILE	CA-C	5.20	1.66	1.52
1	K	522	SER	CA-CB	5.20	1.60	1.52
1	B	413	TYR	CG-CD1	5.20	1.46	1.39
1	N	353	TYR	CE1-CZ	5.20	1.45	1.38
1	L	38	ARG	NE-CZ	5.19	1.39	1.33
1	Q	55	GLY	CA-C	-5.19	1.43	1.51
1	I	462	ALA	N-CA	-5.19	1.35	1.46
1	F	31	ARG	CD-NE	5.19	1.55	1.46
1	J	397	SER	CA-CB	5.19	1.60	1.52
1	F	173	GLU	CB-CG	5.18	1.62	1.52
1	R	348	PRO	N-CD	-5.18	1.40	1.47
1	G	225	GLY	CA-C	-5.18	1.43	1.51
1	M	353	TYR	CG-CD2	5.18	1.45	1.39
1	M	103	GLY	N-CA	5.18	1.53	1.46
1	K	527	ASP	CA-CB	5.17	1.65	1.53
1	P	403	TYR	CE2-CZ	5.17	1.45	1.38
1	R	200	TYR	CE2-CZ	5.17	1.45	1.38
1	H	453	GLU	CB-CG	5.17	1.61	1.52
1	K	175	GLU	CA-CB	5.17	1.65	1.53
1	B	300	CYS	CB-SG	5.17	1.91	1.82
1	Q	360	ARG	C-O	5.16	1.33	1.23
1	E	441	GLN	CA-CB	5.16	1.65	1.53
1	R	31	ARG	CD-NE	5.16	1.55	1.46
1	P	397	SER	CB-OG	-5.15	1.35	1.42
1	E	422	GLU	CG-CD	5.15	1.59	1.51
1	F	453	GLU	CB-CG	5.15	1.61	1.52
1	K	55	GLY	CA-C	5.15	1.60	1.51
1	K	268	SER	N-CA	5.14	1.56	1.46
1	G	302	LYS	C-N	5.14	1.42	1.33
1	D	32	THR	N-CA	-5.14	1.36	1.46
1	E	224	ARG	CD-NE	5.13	1.55	1.46
1	Q	259	GLU	CB-CG	5.13	1.61	1.52
1	G	20	ARG	CZ-NH2	5.13	1.39	1.33
1	L	52	ASP	CA-CB	5.13	1.65	1.53
1	O	353	TYR	CG-CD1	5.12	1.45	1.39
1	G	31	ARG	CD-NE	5.12	1.55	1.46
1	I	396	ARG	CZ-NH2	-5.12	1.26	1.33
1	O	339	ILE	CA-CB	-5.11	1.43	1.54
1	K	242	GLU	CB-CG	5.10	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	498	TYR	CG-CD1	5.10	1.45	1.39
1	E	410	MET	N-CA	-5.09	1.36	1.46
1	R	167	SER	CB-OG	5.09	1.48	1.42
1	F	355	GLU	CB-CG	5.09	1.61	1.52
1	J	16	ARG	CD-NE	5.09	1.55	1.46
1	D	522	SER	CA-CB	5.09	1.60	1.52
1	K	265	SER	C-N	5.09	1.45	1.34
1	K	424	GLU	CG-CD	5.08	1.59	1.51
1	M	18	SER	CA-CB	5.08	1.60	1.52
1	C	478	ALA	CA-CB	5.08	1.63	1.52
1	E	498	TYR	CG-CD2	5.08	1.45	1.39
1	L	413	TYR	CB-CG	-5.08	1.44	1.51
1	J	332	GLU	CA-CB	5.07	1.65	1.53
1	E	326	SER	CA-CB	5.07	1.60	1.52
1	F	454	ILE	C-N	5.07	1.43	1.34
1	Q	282	TYR	CE2-CZ	5.07	1.45	1.38
1	D	35	GLU	CD-OE2	5.06	1.31	1.25
1	F	426	SER	CA-CB	5.06	1.60	1.52
1	D	355	GLU	CG-CD	5.06	1.59	1.51
1	F	193	GLU	CD-OE2	5.05	1.31	1.25
1	O	338	ARG	NE-CZ	-5.05	1.26	1.33
1	D	453	GLU	CD-OE1	5.05	1.31	1.25
1	O	359	GLU	CA-CB	5.05	1.65	1.53
1	R	504	GLU	CD-OE1	-5.05	1.20	1.25
1	K	53	SER	CA-CB	5.04	1.60	1.52
1	Q	53	SER	CA-CB	5.04	1.60	1.52
1	H	341	SER	CB-OG	-5.04	1.35	1.42
1	C	110	GLU	CD-OE1	5.03	1.31	1.25
1	P	413	TYR	CG-CD2	5.02	1.45	1.39
1	I	69	GLU	CD-OE1	5.02	1.31	1.25
1	M	105	PHE	CG-CD2	5.02	1.46	1.38
1	R	349	GLU	CB-CG	5.02	1.61	1.52
1	C	353	TYR	CD1-CE1	5.01	1.46	1.39
1	J	462	ALA	CA-CB	5.01	1.62	1.52
1	J	305	ASP	CA-CB	5.01	1.65	1.53
1	I	54	PHE	CE2-CZ	5.00	1.46	1.37
1	L	388	ASP	C-O	5.00	1.32	1.23
1	M	176	GLU	CB-CG	5.00	1.61	1.52

All (1843) bond angle outliers are listed below:

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	384	ARG	NE-CZ-NH2	22.41	131.51	120.30
1	P	224	ARG	NE-CZ-NH2	20.40	130.50	120.30
1	D	406	ARG	NE-CZ-NH2	20.01	130.31	120.30
1	P	325	ARG	NE-CZ-NH1	-19.55	110.52	120.30
1	O	510	ARG	NE-CZ-NH2	19.31	129.96	120.30
1	M	325	ARG	NE-CZ-NH2	18.70	129.65	120.30
1	P	384	ARG	NE-CZ-NH2	18.29	129.44	120.30
1	P	224	ARG	NE-CZ-NH1	-18.28	111.16	120.30
1	H	430	ARG	NE-CZ-NH1	-18.00	111.30	120.30
1	A	498	TYR	CB-CG-CD2	-17.99	110.21	121.00
1	P	434	ARG	NE-CZ-NH2	17.78	129.19	120.30
1	N	338	ARG	NE-CZ-NH1	-17.60	111.50	120.30
1	P	428	ARG	NE-CZ-NH1	-17.50	111.55	120.30
1	H	384	ARG	NE-CZ-NH1	-17.47	111.57	120.30
1	G	315	ARG	NE-CZ-NH2	17.39	129.00	120.30
1	G	384	ARG	NE-CZ-NH2	17.04	128.82	120.30
1	M	240	ARG	NE-CZ-NH2	17.03	128.82	120.30
1	O	20	ARG	NE-CZ-NH2	17.00	128.80	120.30
1	J	428	ARG	NE-CZ-NH1	-16.99	111.81	120.30
1	R	155	ARG	NE-CZ-NH2	16.70	128.65	120.30
1	R	507	ARG	NE-CZ-NH1	-16.47	112.07	120.30
1	P	430	ARG	NE-CZ-NH2	16.37	128.48	120.30
1	P	325	ARG	NE-CZ-NH2	16.28	128.44	120.30
1	A	403	TYR	CB-CG-CD1	-16.26	111.25	121.00
1	N	428	ARG	NE-CZ-NH2	16.24	128.42	120.30
1	A	338	ARG	NE-CZ-NH2	16.21	128.41	120.30
1	B	16	ARG	NE-CZ-NH2	16.04	128.32	120.30
1	I	396	ARG	NE-CZ-NH2	15.87	128.23	120.30
1	B	240	ARG	NE-CZ-NH1	-15.42	112.59	120.30
1	L	474	ARG	NE-CZ-NH2	15.20	127.90	120.30
1	O	31	ARG	NE-CZ-NH2	15.16	127.88	120.30
1	H	430	ARG	NE-CZ-NH2	15.05	127.83	120.30
1	Q	338	ARG	NE-CZ-NH1	-15.03	112.78	120.30
1	C	510	ARG	NE-CZ-NH1	-14.94	112.83	120.30
1	C	434	ARG	NE-CZ-NH1	-14.82	112.89	120.30
1	F	498	TYR	CB-CG-CD2	-14.76	112.15	121.00
1	H	240	ARG	NE-CZ-NH1	-14.74	112.93	120.30
1	F	428	ARG	NE-CZ-NH2	14.72	127.66	120.30
1	K	434	ARG	NE-CZ-NH1	-14.68	112.96	120.30
1	J	321	ARG	NE-CZ-NH2	14.65	127.63	120.30
1	F	406	ARG	NE-CZ-NH2	14.54	127.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	239	ARG	NE-CZ-NH2	14.54	127.57	120.30
1	I	360	ARG	NE-CZ-NH1	-14.49	113.06	120.30
1	O	38	ARG	NE-CZ-NH2	14.09	127.34	120.30
1	M	507	ARG	NE-CZ-NH1	-14.08	113.26	120.30
1	C	428	ARG	NE-CZ-NH2	13.99	127.30	120.30
1	B	239	ARG	NE-CZ-NH2	13.96	127.28	120.30
1	J	434	ARG	NE-CZ-NH2	13.90	127.25	120.30
1	O	510	ARG	NE-CZ-NH1	-13.85	113.38	120.30
1	A	403	TYR	CB-CG-CD2	13.79	129.28	121.00
1	C	476	ARG	NE-CZ-NH2	13.73	127.17	120.30
1	J	360	ARG	NE-CZ-NH2	13.71	127.16	120.30
1	K	510	ARG	NE-CZ-NH1	-13.67	113.47	120.30
1	D	403	TYR	CB-CG-CD2	13.64	129.19	121.00
1	B	510	ARG	NE-CZ-NH1	-13.64	113.48	120.30
1	Q	126	PHE	CB-CG-CD1	-13.64	111.25	120.80
1	D	403	TYR	CB-CG-CD1	-13.57	112.86	121.00
1	N	322	ARG	NE-CZ-NH2	13.55	127.08	120.30
1	B	498	TYR	CB-CG-CD2	-13.55	112.87	121.00
1	E	428	ARG	NE-CZ-NH2	13.52	127.06	120.30
1	O	240	ARG	NE-CZ-NH1	-13.51	113.55	120.30
1	A	455	PRO	CA-N-CD	-13.38	92.77	111.50
1	M	510	ARG	NE-CZ-NH2	13.36	126.98	120.30
1	O	434	ARG	NE-CZ-NH2	13.33	126.97	120.30
1	A	498	TYR	CB-CG-CD1	13.32	128.99	121.00
1	F	31	ARG	NE-CZ-NH2	13.23	126.91	120.30
1	G	384	ARG	NE-CZ-NH1	-13.21	113.69	120.30
1	H	428	ARG	NE-CZ-NH2	13.13	126.87	120.30
1	P	476	ARG	NE-CZ-NH2	13.13	126.86	120.30
1	N	239	ARG	NE-CZ-NH2	13.12	126.86	120.30
1	Q	239	ARG	NE-CZ-NH1	-13.11	113.75	120.30
1	A	16	ARG	NE-CZ-NH2	13.09	126.84	120.30
1	H	338	ARG	NE-CZ-NH2	13.07	126.83	120.30
1	E	384	ARG	NE-CZ-NH2	13.06	126.83	120.30
1	D	322	ARG	NE-CZ-NH2	13.03	126.82	120.30
1	B	170	PHE	CB-CG-CD2	-12.94	111.74	120.80
1	M	31	ARG	NE-CZ-NH2	12.93	126.77	120.30
1	N	54	PHE	CB-CG-CD2	-12.83	111.82	120.80
1	P	338	ARG	NE-CZ-NH2	12.79	126.70	120.30
1	B	240	ARG	NE-CZ-NH2	12.78	126.69	120.30
1	O	240	ARG	NE-CZ-NH2	12.76	126.68	120.30
1	I	240	ARG	NE-CZ-NH2	12.75	126.67	120.30
1	B	434	ARG	NE-CZ-NH2	12.71	126.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	163	TYR	CB-CG-CD2	-12.65	113.41	121.00
1	H	224	ARG	NE-CZ-NH1	-12.65	113.97	120.30
1	F	155	ARG	NE-CZ-NH2	12.53	126.56	120.30
1	C	321	ARG	NE-CZ-NH2	12.46	126.53	120.30
1	K	455	PRO	CA-N-CD	-12.44	94.08	111.50
1	L	430	ARG	NE-CZ-NH2	12.41	126.50	120.30
1	F	338	ARG	NE-CZ-NH1	12.36	126.48	120.30
1	G	430	ARG	NE-CZ-NH1	-12.32	114.14	120.30
1	Q	338	ARG	NE-CZ-NH2	12.32	126.46	120.30
1	H	434	ARG	NE-CZ-NH2	12.32	126.46	120.30
1	O	396	ARG	NE-CZ-NH2	12.30	126.45	120.30
1	N	311	PHE	CB-CG-CD2	12.21	129.35	120.80
1	J	432	TYR	CB-CG-CD2	12.20	128.32	121.00
1	P	321	ARG	NE-CZ-NH2	12.19	126.39	120.30
1	B	16	ARG	NE-CZ-NH1	-12.18	114.21	120.30
1	F	428	ARG	NE-CZ-NH1	-12.16	114.22	120.30
1	D	338	ARG	NE-CZ-NH1	-12.14	114.23	120.30
1	F	16	ARG	NE-CZ-NH2	12.12	126.36	120.30
1	F	455	PRO	CA-N-CD	-12.10	94.56	111.50
1	B	430	ARG	NE-CZ-NH2	12.08	126.34	120.30
1	H	396	ARG	NE-CZ-NH2	12.08	126.34	120.30
1	I	126	PHE	CB-CG-CD1	12.08	129.26	120.80
1	I	224	ARG	NE-CZ-NH2	12.05	126.33	120.30
1	O	360	ARG	NE-CZ-NH1	-12.01	114.30	120.30
1	B	396	ARG	NE-CZ-NH2	12.00	126.30	120.30
1	L	224	ARG	NE-CZ-NH2	11.99	126.29	120.30
1	D	322	ARG	NE-CZ-NH1	-11.96	114.32	120.30
1	E	239	ARG	NE-CZ-NH1	-11.96	114.32	120.30
1	D	455	PRO	CA-N-CD	-11.92	94.81	111.50
1	Q	31	ARG	NE-CZ-NH2	11.85	126.22	120.30
1	N	406	ARG	NE-CZ-NH2	11.84	126.22	120.30
1	L	498	TYR	CB-CG-CD1	11.83	128.10	121.00
1	C	16	ARG	NE-CZ-NH1	-11.82	114.39	120.30
1	A	413	TYR	CB-CG-CD2	-11.77	113.94	121.00
1	P	455	PRO	CA-N-CD	-11.73	95.08	111.50
1	Q	126	PHE	CB-CG-CD2	11.72	129.01	120.80
1	G	311	PHE	CB-CG-CD2	11.72	129.00	120.80
1	H	455	PRO	CA-N-CD	-11.72	95.09	111.50
1	Q	498	TYR	CB-CG-CD2	-11.69	113.99	121.00
1	C	38	ARG	NE-CZ-NH2	11.65	126.12	120.30
1	D	148	ASP	CB-CG-OD1	11.65	128.78	118.30
1	N	315	ARG	NE-CZ-NH1	-11.65	114.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	507	ARG	NE-CZ-NH2	11.63	126.11	120.30
1	P	338	ARG	NE-CZ-NH1	-11.60	114.50	120.30
1	K	428	ARG	NE-CZ-NH1	-11.55	114.52	120.30
1	J	474	ARG	NE-CZ-NH2	11.54	126.07	120.30
1	H	155	ARG	NE-CZ-NH2	11.52	126.06	120.30
1	M	239	ARG	NE-CZ-NH2	11.50	126.05	120.30
1	N	311	PHE	CB-CG-CD1	-11.47	112.77	120.80
1	Q	360	ARG	NE-CZ-NH2	11.45	126.02	120.30
1	H	474	ARG	NE-CZ-NH1	-11.43	114.58	120.30
1	H	498	TYR	CB-CG-CD2	-11.42	114.15	121.00
1	F	325	ARG	NE-CZ-NH2	11.34	125.97	120.30
1	O	474	ARG	NE-CZ-NH2	11.34	125.97	120.30
1	B	396	ARG	NE-CZ-NH1	-11.34	114.63	120.30
1	L	455	PRO	CA-N-CD	-11.28	95.71	111.50
1	P	170	PHE	CB-CG-CD2	-11.28	112.91	120.80
1	H	240	ARG	NE-CZ-NH2	11.25	125.93	120.30
1	L	20	ARG	NE-CZ-NH2	11.24	125.92	120.30
1	R	455	PRO	CA-N-CD	-11.23	95.78	111.50
1	L	498	TYR	CB-CG-CD2	-11.20	114.28	121.00
1	C	510	ARG	NE-CZ-NH2	11.18	125.89	120.30
1	E	275	PHE	CB-CG-CD2	11.14	128.60	120.80
1	P	430	ARG	NE-CZ-NH1	-11.13	114.74	120.30
1	B	322	ARG	NE-CZ-NH1	-11.10	114.75	120.30
1	I	474	ARG	NE-CZ-NH2	11.07	125.83	120.30
1	A	338	ARG	NE-CZ-NH1	-11.06	114.77	120.30
1	Q	200	TYR	CB-CG-CD2	-11.05	114.37	121.00
1	Q	455	PRO	CA-N-CD	-11.02	96.07	111.50
1	N	170	PHE	CB-CG-CD1	-11.01	113.09	120.80
1	H	476	ARG	NE-CZ-NH2	11.01	125.80	120.30
1	J	455	PRO	CA-N-CD	-11.01	96.09	111.50
1	B	170	PHE	CB-CG-CD1	10.99	128.49	120.80
1	E	338	ARG	NE-CZ-NH2	10.98	125.79	120.30
1	H	322	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	D	315	ARG	NE-CZ-NH2	10.95	125.78	120.30
1	L	403	TYR	CB-CG-CD1	-10.95	114.43	121.00
1	K	31	ARG	NE-CZ-NH2	10.93	125.77	120.30
1	G	455	PRO	CA-N-CD	-10.93	96.19	111.50
1	C	455	PRO	CA-N-CD	-10.93	96.20	111.50
1	N	455	PRO	CA-N-CD	-10.91	96.22	111.50
1	O	455	PRO	CA-N-CD	-10.91	96.23	111.50
1	L	325	ARG	NE-CZ-NH1	-10.89	114.85	120.30
1	F	239	ARG	NE-CZ-NH2	10.88	125.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	434	ARG	NE-CZ-NH1	-10.86	114.87	120.30
1	L	360	ARG	NE-CZ-NH1	-10.86	114.87	120.30
1	R	20	ARG	NE-CZ-NH1	-10.81	114.90	120.30
1	J	239	ARG	NE-CZ-NH2	10.80	125.70	120.30
1	D	360	ARG	NE-CZ-NH1	-10.80	114.90	120.30
1	R	105	PHE	CB-CG-CD2	-10.78	113.26	120.80
1	L	406	ARG	NE-CZ-NH2	10.74	125.67	120.30
1	B	455	PRO	CA-N-CD	-10.66	96.57	111.50
1	M	428	ARG	NE-CZ-NH1	-10.63	114.99	120.30
1	Q	507	ARG	NE-CZ-NH1	-10.61	114.99	120.30
1	Q	282	TYR	CB-CG-CD2	-10.59	114.64	121.00
1	A	210	ASP	CB-CG-OD2	10.59	127.83	118.30
1	K	507	ARG	NE-CZ-NH2	10.56	125.58	120.30
1	G	430	ARG	NE-CZ-NH2	10.56	125.58	120.30
1	J	327	ASP	CB-CG-OD1	10.54	127.79	118.30
1	H	487	ASP	CB-CG-OD2	10.54	127.78	118.30
1	J	240	ARG	NE-CZ-NH1	-10.52	115.04	120.30
1	E	321	ARG	NE-CZ-NH2	10.52	125.56	120.30
1	E	282	TYR	CB-CG-CD2	10.50	127.30	121.00
1	A	282	TYR	CB-CG-CD1	-10.50	114.70	121.00
1	F	240	ARG	NE-CZ-NH1	-10.44	115.08	120.30
1	I	126	PHE	CB-CG-CD2	-10.43	113.50	120.80
1	G	406	ARG	NE-CZ-NH1	-10.43	115.09	120.30
1	I	200	TYR	CB-CG-CD2	10.42	127.25	121.00
1	E	155	ARG	NE-CZ-NH1	-10.41	115.10	120.30
1	I	434	ARG	NE-CZ-NH2	10.41	125.50	120.30
1	D	325	ARG	NE-CZ-NH2	10.38	125.49	120.30
1	F	315	ARG	NE-CZ-NH2	10.37	125.49	120.30
1	K	430	ARG	NE-CZ-NH1	-10.38	115.11	120.30
1	K	163	TYR	CZ-CE2-CD2	-10.28	110.54	119.80
1	O	163	TYR	CB-CG-CD1	-10.27	114.84	121.00
1	Q	434	ARG	NE-CZ-NH2	10.25	125.43	120.30
1	N	476	ARG	NE-CZ-NH2	10.24	125.42	120.30
1	P	282	TYR	CB-CG-CD2	-10.22	114.87	121.00
1	I	396	ARG	NE-CZ-NH1	-10.18	115.21	120.30
1	L	432	TYR	CB-CG-CD2	-10.17	114.90	121.00
1	J	474	ARG	NE-CZ-NH1	-10.15	115.22	120.30
1	D	305	ASP	CB-CG-OD1	-10.14	109.17	118.30
1	E	239	ARG	NE-CZ-NH2	10.14	125.37	120.30
1	I	487	ASP	CB-CG-OD2	-10.11	109.20	118.30
1	D	31	ARG	NE-CZ-NH1	-10.11	115.25	120.30
1	G	321	ARG	NE-CZ-NH2	-10.09	115.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	K	430	ARG	NE-CZ-NH2	10.08	125.34	120.30
1	J	495	ASP	CB-CG-OD2	10.06	127.36	118.30
1	M	270	ASP	CB-CG-OD2	10.06	127.36	118.30
1	I	200	TYR	CB-CG-CD1	-10.06	114.97	121.00
1	N	200	TYR	CB-CG-CD1	-10.05	114.97	121.00
1	O	282	TYR	CB-CG-CD1	-10.05	114.97	121.00
1	K	311	PHE	CB-CG-CD1	-10.05	113.77	120.80
1	N	224	ARG	NE-CZ-NH2	10.04	125.32	120.30
1	Q	31	ARG	NE-CZ-NH1	-10.04	115.28	120.30
1	C	338	ARG	NE-CZ-NH2	10.03	125.31	120.30
1	O	155	ARG	NE-CZ-NH2	10.00	125.30	120.30
1	J	275	PHE	CB-CG-CD2	9.98	127.78	120.80
1	R	200	TYR	CB-CG-CD2	-9.96	115.02	121.00
1	I	430	ARG	NE-CZ-NH2	9.92	125.26	120.30
1	K	321	ARG	NE-CZ-NH2	9.92	125.26	120.30
1	M	31	ARG	NE-CZ-NH1	-9.91	115.34	120.30
1	P	396	ARG	NE-CZ-NH2	9.91	125.25	120.30
1	P	447	TYR	CB-CG-CD1	-9.88	115.07	121.00
1	H	434	ARG	NE-CZ-NH1	-9.86	115.37	120.30
1	L	321	ARG	NE-CZ-NH2	9.86	125.23	120.30
1	M	476	ARG	NE-CZ-NH2	9.85	125.23	120.30
1	C	31	ARG	NE-CZ-NH2	9.85	125.22	120.30
1	P	428	ARG	NE-CZ-NH2	9.83	125.22	120.30
1	O	315	ARG	NE-CZ-NH1	-9.81	115.39	120.30
1	J	322	ARG	NE-CZ-NH1	9.80	125.20	120.30
1	A	411	GLU	OE1-CD-OE2	-9.79	111.55	123.30
1	R	338	ARG	NE-CZ-NH1	-9.76	115.42	120.30
1	D	474	ARG	NE-CZ-NH1	-9.75	115.43	120.30
1	G	322	ARG	NE-CZ-NH2	9.71	125.16	120.30
1	F	240	ARG	NE-CZ-NH2	9.70	125.15	120.30
1	C	350	ASP	CB-CG-OD2	9.68	127.01	118.30
1	A	315	ARG	NE-CZ-NH2	9.68	125.14	120.30
1	K	432	TYR	CB-CG-CD2	9.68	126.81	121.00
1	A	476	ARG	NE-CZ-NH1	-9.66	115.47	120.30
1	O	434	ARG	NE-CZ-NH1	-9.65	115.47	120.30
1	J	396	ARG	NE-CZ-NH1	-9.62	115.49	120.30
1	D	224	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	K	495	ASP	CB-CG-OD2	9.60	126.94	118.30
1	P	434	ARG	NE-CZ-NH1	-9.60	115.50	120.30
1	R	413	TYR	CB-CG-CD1	-9.58	115.25	121.00
1	A	126	PHE	CB-CG-CD1	9.58	127.50	120.80
1	M	510	ARG	NE-CZ-NH1	-9.58	115.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	322	ARG	NE-CZ-NH2	9.57	125.08	120.30
1	A	38	ARG	NE-CZ-NH2	9.55	125.08	120.30
1	I	338	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	J	353	TYR	CB-CG-CD1	-9.54	115.28	121.00
1	A	430	ARG	NE-CZ-NH2	9.54	125.07	120.30
1	F	16	ARG	NE-CZ-NH1	-9.54	115.53	120.30
1	A	360	ARG	NE-CZ-NH1	-9.52	115.54	120.30
1	H	130	PHE	CB-CG-CD2	-9.51	114.14	120.80
1	N	360	ARG	NE-CZ-NH2	9.50	125.05	120.30
1	B	507	ARG	NE-CZ-NH2	9.49	125.05	120.30
1	A	413	TYR	CB-CG-CD1	9.48	126.69	121.00
1	F	434	ARG	NE-CZ-NH1	-9.47	115.56	120.30
1	C	434	ARG	NE-CZ-NH2	9.45	125.02	120.30
1	A	430	ARG	NE-CZ-NH1	-9.44	115.58	120.30
1	G	16	ARG	NE-CZ-NH1	-9.43	115.58	120.30
1	C	155	ARG	NE-CZ-NH1	-9.43	115.58	120.30
1	G	31	ARG	NE-CZ-NH2	9.43	125.02	120.30
1	F	325	ARG	NE-CZ-NH1	-9.41	115.59	120.30
1	R	474	ARG	NE-CZ-NH1	9.41	125.00	120.30
1	J	410	MET	CG-SD-CE	-9.39	85.17	100.20
1	G	315	ARG	NE-CZ-NH1	-9.37	115.62	120.30
1	B	510	ARG	NE-CZ-NH2	9.35	124.97	120.30
1	D	16	ARG	NE-CZ-NH2	9.35	124.97	120.30
1	O	282	TYR	CB-CG-CD2	9.33	126.60	121.00
1	G	476	ARG	NE-CZ-NH2	9.33	124.96	120.30
1	C	495	ASP	CB-CG-OD1	9.32	126.69	118.30
1	P	275	PHE	CB-CG-CD2	-9.28	114.30	120.80
1	A	275	PHE	CB-CG-CD1	9.26	127.28	120.80
1	R	186	ASP	CB-CG-OD1	9.26	126.63	118.30
1	C	126	PHE	CB-CG-CD2	-9.25	114.33	120.80
1	J	36	MET	CG-SD-CE	-9.25	85.41	100.20
1	I	455	PRO	CA-N-CD	-9.21	98.61	111.50
1	A	528	ASP	CB-CG-OD1	9.20	126.58	118.30
1	K	224	ARG	NE-CZ-NH1	9.19	124.89	120.30
1	K	369	PHE	CB-CG-CD2	-9.18	114.37	120.80
1	O	476	ARG	NE-CZ-NH1	-9.18	115.71	120.30
1	K	240	ARG	NE-CZ-NH2	9.15	124.87	120.30
1	A	322	ARG	NE-CZ-NH2	9.14	124.87	120.30
1	P	170	PHE	CB-CG-CD1	9.14	127.20	120.80
1	R	396	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	J	285	ASP	CB-CG-OD1	9.13	126.52	118.30
1	P	384	ARG	NE-CZ-NH1	-9.11	115.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	219	ASP	CB-CG-OD2	-9.10	110.11	118.30
1	O	384	ARG	NE-CZ-NH1	-9.07	115.76	120.30
1	E	282	TYR	CB-CG-CD1	-9.05	115.57	121.00
1	C	396	ARG	NE-CZ-NH2	9.04	124.82	120.30
1	J	52	ASP	CB-CG-OD2	-9.03	110.18	118.30
1	N	250	ASP	CB-CG-OD2	9.02	126.42	118.30
1	M	224	ARG	NE-CZ-NH2	9.01	124.81	120.30
1	H	474	ARG	NE-CZ-NH2	9.01	124.80	120.30
1	J	322	ARG	NE-CZ-NH2	-9.00	115.80	120.30
1	D	305	ASP	CB-CG-OD2	8.98	126.39	118.30
1	A	282	TYR	CB-CG-CD2	8.98	126.39	121.00
1	A	210	ASP	CB-CG-OD1	-8.96	110.24	118.30
1	G	434	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	R	240	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	E	388	ASP	CB-CG-OD2	8.95	126.36	118.30
1	F	275	PHE	CB-CG-CD1	8.95	127.06	120.80
1	A	321	ARG	NE-CZ-NH1	-8.93	115.83	120.30
1	H	126	PHE	CB-CG-CD1	8.93	127.05	120.80
1	H	455	PRO	CB-CA-C	8.93	134.32	112.00
1	R	186	ASP	CB-CG-OD2	-8.93	110.27	118.30
1	R	528	ASP	CB-CG-OD2	8.90	126.31	118.30
1	J	275	PHE	CB-CG-CD1	-8.88	114.58	120.80
1	Q	200	TYR	CB-CG-CD1	8.88	126.33	121.00
1	F	507	ARG	NE-CZ-NH1	8.87	124.74	120.30
1	A	126	PHE	CB-CG-CD2	-8.87	114.59	120.80
1	P	507	ARG	NE-CZ-NH2	8.83	124.71	120.30
1	B	432	TYR	CB-CG-CD2	-8.81	115.72	121.00
1	D	21	ASP	CB-CG-OD1	-8.81	110.37	118.30
1	B	130	PHE	CB-CG-CD2	-8.79	114.65	120.80
1	N	528	ASP	CB-CG-OD1	8.79	126.21	118.30
1	M	384	ARG	NE-CZ-NH1	8.78	124.69	120.30
1	L	507	ARG	NE-CZ-NH2	8.76	124.68	120.30
1	F	20	ARG	NE-CZ-NH2	8.75	124.67	120.30
1	L	181	MET	CG-SD-CE	-8.73	86.23	100.20
1	F	360	ARG	NE-CZ-NH1	-8.71	115.94	120.30
1	L	432	TYR	CB-CG-CD1	8.70	126.22	121.00
1	A	275	PHE	CB-CG-CD2	-8.70	114.71	120.80
1	Q	327	ASP	CB-CG-OD1	8.69	126.12	118.30
1	D	171	MET	CG-SD-CE	-8.69	86.30	100.20
1	M	200	TYR	CB-CG-CD1	8.69	126.21	121.00
1	A	148	ASP	CB-CG-OD1	-8.68	110.49	118.30
1	E	476	ARG	NE-CZ-NH1	-8.68	115.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	406	ARG	NE-CZ-NH2	8.66	124.63	120.30
1	C	321	ARG	NE-CZ-NH1	-8.65	115.98	120.30
1	N	305	ASP	CB-CG-OD2	-8.65	110.52	118.30
1	D	524	MET	CG-SD-CE	-8.64	86.37	100.20
1	K	163	TYR	CB-CG-CD2	-8.62	115.83	121.00
1	I	114	ASP	CB-CG-OD1	8.62	126.06	118.30
1	Q	16	ARG	NE-CZ-NH1	-8.61	116.00	120.30
1	G	311	PHE	CB-CG-CD1	-8.60	114.78	120.80
1	I	16	ARG	NE-CZ-NH2	8.60	124.60	120.30
1	Q	321	ARG	NE-CZ-NH1	-8.59	116.00	120.30
1	D	406	ARG	NE-CZ-NH1	-8.56	116.02	120.30
1	R	413	TYR	CB-CG-CD2	8.54	126.13	121.00
1	D	350	ASP	CB-CG-OD2	8.52	125.97	118.30
1	L	476	ARG	NE-CZ-NH2	8.52	124.56	120.30
1	F	360	ARG	NE-CZ-NH2	8.50	124.55	120.30
1	J	384	ARG	NE-CZ-NH2	8.48	124.54	120.30
1	D	496	ASP	CB-CG-OD2	8.48	125.93	118.30
1	N	498	TYR	CB-CG-CD2	8.45	126.07	121.00
1	R	155	ARG	NE-CZ-NH1	-8.45	116.08	120.30
1	I	455	PRO	CB-CA-C	8.44	133.09	112.00
1	R	315	ARG	NE-CZ-NH2	8.43	124.52	120.30
1	O	338	ARG	NE-CZ-NH2	8.43	124.51	120.30
1	D	338	ARG	NE-CZ-NH2	8.42	124.51	120.30
1	L	474	ARG	NE-CZ-NH1	-8.41	116.09	120.30
1	J	38	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	A	388	ASP	CB-CG-OD1	8.41	125.87	118.30
1	C	156	ASP	CB-CG-OD1	-8.40	110.74	118.30
1	I	338	ARG	NE-CZ-NH1	-8.40	116.10	120.30
1	O	130	PHE	CB-CG-CD1	-8.39	114.93	120.80
1	Q	403	TYR	CB-CG-CD1	8.39	126.03	121.00
1	D	20	ARG	NE-CZ-NH1	-8.39	116.11	120.30
1	N	476	ARG	NE-CZ-NH1	-8.38	116.11	120.30
1	B	62	ASP	CB-CG-OD2	8.36	125.82	118.30
1	Q	327	ASP	CB-CG-OD2	-8.36	110.78	118.30
1	D	21	ASP	CB-CG-OD2	8.35	125.82	118.30
1	R	400	ASP	CB-CG-OD2	8.35	125.81	118.30
1	N	282	TYR	CG-CD2-CE2	-8.33	114.63	121.30
1	R	384	ARG	NE-CZ-NH2	8.30	124.45	120.30
1	R	282	TYR	CB-CG-CD1	-8.30	116.02	121.00
1	E	455	PRO	CA-N-CD	-8.29	99.89	111.50
1	K	141	ALA	N-CA-CB	8.28	121.70	110.10
1	M	455	PRO	CA-N-CD	-8.28	99.91	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	239	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	I	321	ARG	NE-CZ-NH2	8.26	124.43	120.30
1	O	413	TYR	CB-CG-CD1	-8.25	116.05	121.00
1	O	410	MET	CG-SD-CE	-8.22	87.04	100.20
1	H	163	TYR	CB-CG-CD2	-8.21	116.08	121.00
1	G	145	ASP	CB-CG-OD1	-8.19	110.93	118.30
1	J	315	ARG	NE-CZ-NH2	8.17	124.39	120.30
1	L	369	PHE	CB-CG-CD1	-8.17	115.08	120.80
1	J	432	TYR	CB-CG-CD1	-8.15	116.11	121.00
1	L	126	PHE	CB-CG-CD1	8.15	126.51	120.80
1	L	510	ARG	NE-CZ-NH2	8.15	124.37	120.30
1	A	114	ASP	CB-CG-OD2	8.13	125.62	118.30
1	C	406	ARG	NE-CZ-NH2	8.13	124.36	120.30
1	J	285	ASP	CB-CG-OD2	-8.12	110.99	118.30
1	N	155	ARG	NE-CZ-NH2	8.12	124.36	120.30
1	Q	428	ARG	NE-CZ-NH1	-8.12	116.24	120.30
1	G	474	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	I	365	ASP	CB-CG-OD1	8.11	125.60	118.30
1	J	430	ARG	NE-CZ-NH1	-8.11	116.25	120.30
1	N	282	TYR	CB-CG-CD2	-8.10	116.14	121.00
1	D	20	ARG	NE-CZ-NH2	8.10	124.35	120.30
1	D	205	ASP	CB-CG-OD2	8.10	125.59	118.30
1	D	240	ARG	NE-CZ-NH2	8.09	124.35	120.30
1	R	510	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	B	413	TYR	CB-CG-CD1	8.08	125.85	121.00
1	J	240	ARG	NE-CZ-NH2	8.08	124.34	120.30
1	R	369	PHE	CB-CG-CD1	8.08	126.45	120.80
1	Q	62	ASP	CB-CG-OD1	8.07	125.56	118.30
1	C	410	MET	CG-SD-CE	-8.05	87.33	100.20
1	D	325	ARG	NE-CZ-NH1	-8.05	116.28	120.30
1	R	153	THR	CA-CB-CG2	-8.03	101.16	112.40
1	L	350	ASP	CB-CG-OD1	8.02	125.52	118.30
1	M	396	ARG	NE-CZ-NH2	8.01	124.30	120.30
1	L	353	TYR	CZ-CE2-CD2	-7.99	112.61	119.80
1	M	163	TYR	CB-CG-CD2	-7.98	116.21	121.00
1	R	510	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	D	62	ASP	CB-CG-OD1	7.95	125.46	118.30
1	Q	155	ARG	NE-CZ-NH1	-7.95	116.33	120.30
1	E	447	TYR	CB-CG-CD1	-7.93	116.24	121.00
1	J	360	ARG	NE-CZ-NH1	-7.93	116.33	120.30
1	H	338	ARG	NE-CZ-NH1	-7.91	116.34	120.30
1	Q	16	ARG	NE-CZ-NH2	7.91	124.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	384	ARG	NE-CZ-NH2	7.89	124.25	120.30
1	I	327	ASP	CB-CG-OD1	7.89	125.40	118.30
1	C	285	ASP	CB-CG-OD1	7.88	125.39	118.30
1	Q	498	TYR	CB-CG-CD1	7.88	125.73	121.00
1	D	360	ARG	NE-CZ-NH2	7.88	124.24	120.30
1	E	105	PHE	CB-CG-CD2	-7.87	115.29	120.80
1	N	38	ARG	NE-CZ-NH2	-7.87	116.36	120.30
1	M	166	MET	CG-SD-CE	-7.86	87.62	100.20
1	B	353	TYR	CB-CG-CD2	7.85	125.71	121.00
1	J	369	PHE	CB-CG-CD1	7.85	126.30	120.80
1	N	315	ARG	NE-CZ-NH2	7.85	124.23	120.30
1	H	498	TYR	CB-CG-CD1	7.84	125.71	121.00
1	L	508	VAL	CA-CB-CG2	7.84	122.66	110.90
1	R	20	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	N	434	ARG	NE-CZ-NH2	7.83	124.21	120.30
1	N	396	ARG	NE-CZ-NH2	7.83	124.21	120.30
1	E	286	MET	CG-SD-CE	-7.82	87.69	100.20
1	N	240	ARG	NE-CZ-NH1	7.82	124.21	120.30
1	L	277	ASP	CB-CG-OD2	7.81	125.33	118.30
1	M	38	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	O	516	ALA	N-CA-CB	-7.80	99.18	110.10
1	C	360	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	G	282	TYR	CB-CG-CD1	7.78	125.67	121.00
1	E	170	PHE	CB-CG-CD2	7.78	126.25	120.80
1	N	353	TYR	CB-CG-CD1	-7.78	116.33	121.00
1	M	360	ARG	NE-CZ-NH2	7.78	124.19	120.30
1	Q	454	ILE	CB-CA-C	7.77	127.14	111.60
1	H	54	PHE	CB-CG-CD2	-7.77	115.36	120.80
1	N	432	TYR	CB-CG-CD2	-7.76	116.34	121.00
1	R	360	ARG	NE-CZ-NH2	-7.76	116.42	120.30
1	Q	449	ASP	CB-CG-OD2	7.75	125.28	118.30
1	K	54	PHE	CB-CG-CD2	7.75	126.22	120.80
1	E	52	ASP	CB-CG-OD2	7.73	125.26	118.30
1	O	21	ASP	CB-CG-OD2	7.72	125.25	118.30
1	O	403	TYR	CB-CG-CD2	-7.72	116.37	121.00
1	J	114	ASP	CB-CG-OD2	7.71	125.24	118.30
1	L	454	ILE	CB-CA-C	7.71	127.01	111.60
1	J	495	ASP	CB-CG-OD1	-7.70	111.37	118.30
1	O	430	ARG	NE-CZ-NH2	7.70	124.15	120.30
1	K	141	ALA	CB-CA-C	-7.70	98.55	110.10
1	M	155	ARG	NE-CZ-NH2	7.69	124.14	120.30
1	H	353	TYR	CB-CG-CD1	7.68	125.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	454	ILE	CB-CA-C	7.67	126.95	111.60
1	F	155	ARG	NE-CZ-NH1	-7.67	116.46	120.30
1	I	38	ARG	NE-CZ-NH1	-7.67	116.47	120.30
1	L	322	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	Q	154	ALA	N-CA-CB	7.66	120.82	110.10
1	B	315	ARG	NE-CZ-NH1	-7.65	116.47	120.30
1	A	105	PHE	CB-CG-CD1	7.64	126.15	120.80
1	D	392	ASP	CB-CG-OD2	7.61	125.15	118.30
1	N	31	ARG	NE-CZ-NH2	7.61	124.11	120.30
1	N	432	TYR	CB-CG-CD1	7.61	125.57	121.00
1	R	443	ALA	CB-CA-C	7.60	121.50	110.10
1	F	282	TYR	CG-CD1-CE1	-7.59	115.22	121.30
1	F	498	TYR	CB-CG-CD1	7.58	125.55	121.00
1	C	403	TYR	CB-CG-CD2	-7.58	116.45	121.00
1	L	105	PHE	CB-CG-CD2	-7.58	115.50	120.80
1	N	454	ILE	CB-CA-C	7.57	126.75	111.60
1	J	105	PHE	CB-CG-CD2	-7.57	115.50	120.80
1	Q	224	ARG	NE-CZ-NH1	-7.57	116.52	120.30
1	F	126	PHE	CB-CG-CD2	-7.57	115.50	120.80
1	Q	38	ARG	NE-CZ-NH2	7.56	124.08	120.30
1	B	498	TYR	CG-CD1-CE1	-7.56	115.25	121.30
1	R	345	ASP	CB-CG-OD2	7.55	125.10	118.30
1	G	88	ASP	CB-CG-OD2	7.55	125.09	118.30
1	J	47	ASP	CB-CG-OD1	-7.55	111.51	118.30
1	F	126	PHE	CB-CG-CD1	7.53	126.07	120.80
1	B	163	TYR	CB-CG-CD1	7.53	125.52	121.00
1	A	67	VAL	CA-CB-CG2	7.51	122.17	110.90
1	P	396	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	A	16	ARG	NE-CZ-NH1	-7.51	116.55	120.30
1	A	277	ASP	O-C-N	-7.50	110.70	122.70
1	N	282	TYR	CD1-CG-CD2	7.50	126.15	117.90
1	O	20	ARG	NE-CZ-NH1	-7.49	116.56	120.30
1	D	222	LEU	CB-CG-CD2	7.49	123.73	111.00
1	J	205	ASP	CB-CG-OD1	7.49	125.04	118.30
1	P	237	MET	CG-SD-CE	-7.48	88.23	100.20
1	Q	403	TYR	CB-CG-CD2	-7.48	116.51	121.00
1	K	324	LYS	O-C-N	-7.47	110.75	122.70
1	A	325	ARG	NE-CZ-NH1	-7.46	116.57	120.30
1	K	388	ASP	CB-CG-OD1	-7.45	111.59	118.30
1	A	510	ARG	NE-CZ-NH2	7.45	124.03	120.30
1	G	471	MET	CG-SD-CE	-7.45	88.28	100.20
1	L	16	ARG	NE-CZ-NH2	-7.44	116.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	275	PHE	CB-CG-CD1	7.43	126.00	120.80
1	M	163	TYR	CB-CG-CD1	7.41	125.45	121.00
1	Q	54	PHE	CB-CG-CD1	-7.41	115.61	120.80
1	P	240	ARG	NE-CZ-NH2	7.41	124.01	120.30
1	Q	54	PHE	CB-CG-CD2	7.41	125.99	120.80
1	C	315	ARG	NE-CZ-NH2	7.38	123.99	120.30
1	A	476	ARG	CD-NE-CZ	7.38	133.93	123.60
1	G	409	LEU	O-C-N	-7.37	110.90	122.70
1	A	428	ARG	N-CA-CB	7.37	123.87	110.60
1	I	124	GLU	OE1-CD-OE2	-7.37	114.46	123.30
1	R	430	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	C	305	ASP	CB-CG-OD1	7.37	124.93	118.30
1	Q	471	MET	CG-SD-CE	-7.36	88.42	100.20
1	N	388	ASP	CB-CG-OD2	-7.35	111.68	118.30
1	G	327	ASP	CB-CG-OD1	7.34	124.91	118.30
1	A	392	ASP	CB-CG-OD2	7.34	124.91	118.30
1	J	105	PHE	CB-CG-CD1	7.33	125.94	120.80
1	G	20	ARG	NE-CZ-NH2	-7.33	116.63	120.30
1	K	20	ARG	NE-CZ-NH2	7.33	123.97	120.30
1	R	455	PRO	CB-CA-C	7.33	130.31	112.00
1	K	510	ARG	NE-CZ-NH2	7.32	123.96	120.30
1	L	170	PHE	CB-CG-CD2	-7.32	115.68	120.80
1	D	432	TYR	CB-CG-CD2	-7.31	116.62	121.00
1	M	305	ASP	CB-CG-OD1	7.29	124.86	118.30
1	E	455	PRO	CB-CA-C	7.29	130.24	112.00
1	Q	447	TYR	CB-CG-CD2	-7.29	116.63	121.00
1	H	487	ASP	CB-CG-OD1	-7.28	111.75	118.30
1	K	338	ARG	NE-CZ-NH1	-7.28	116.66	120.30
1	F	391	LEU	CB-CG-CD1	7.27	123.37	111.00
1	J	518	GLU	N-CA-CB	-7.27	97.51	110.60
1	I	432	TYR	CG-CD2-CE2	-7.27	115.48	121.30
1	K	474	ARG	NE-CZ-NH1	7.27	123.93	120.30
1	O	325	ARG	NE-CZ-NH2	7.27	123.94	120.30
1	P	205	ASP	CB-CG-OD1	7.27	124.84	118.30
1	G	454	ILE	CB-CA-C	7.27	126.13	111.60
1	B	46	LEU	CB-CG-CD2	7.26	123.35	111.00
1	G	380	ASN	CB-CA-C	7.26	124.93	110.40
1	R	530	ILE	O-C-N	-7.26	111.09	122.70
1	M	406	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	D	311	PHE	CB-CG-CD1	-7.25	115.73	120.80
1	E	403	TYR	CB-CG-CD2	-7.23	116.66	121.00
1	E	229	ASP	CB-CG-OD2	7.23	124.81	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	447	TYR	CB-CG-CD2	-7.22	116.67	121.00
1	K	446	ALA	CB-CA-C	-7.22	99.28	110.10
1	J	186	ASP	N-CA-CB	-7.21	97.61	110.60
1	L	240	ARG	NE-CZ-NH2	7.21	123.91	120.30
1	R	93	ASP	CB-CG-OD2	-7.21	111.81	118.30
1	M	376	PRO	N-CD-CG	7.21	114.02	103.20
1	P	455	PRO	CB-CA-C	7.21	130.01	112.00
1	K	277	ASP	N-CA-CB	-7.20	97.63	110.60
1	C	421	ILE	O-C-N	-7.20	111.18	122.70
1	C	413	TYR	CG-CD1-CE1	-7.20	115.54	121.30
1	C	311	PHE	CB-CG-CD2	-7.20	115.76	120.80
1	P	171	MET	CG-SD-CE	-7.20	88.69	100.20
1	B	454	ILE	CB-CA-C	7.19	125.99	111.60
1	E	498	TYR	CB-CG-CD2	-7.19	116.69	121.00
1	O	16	ARG	CD-NE-CZ	7.19	133.66	123.60
1	M	413	TYR	CG-CD2-CE2	7.18	127.05	121.30
1	P	345	ASP	CB-CG-OD1	7.18	124.77	118.30
1	I	487	ASP	CB-CG-OD1	7.18	124.76	118.30
1	M	280	ALA	CB-CA-C	-7.18	99.34	110.10
1	I	428	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	P	486	VAL	CG1-CB-CG2	-7.17	99.42	110.90
1	N	365	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	B	200	TYR	CB-CG-CD2	-7.17	116.70	121.00
1	N	465	GLU	OE1-CD-OE2	-7.17	114.70	123.30
1	K	454	ILE	C-N-CD	-7.16	104.85	120.60
1	L	275	PHE	CB-CG-CD2	7.16	125.81	120.80
1	M	114	ASP	CB-CG-OD1	7.15	124.73	118.30
1	M	90	GLU	OE1-CD-OE2	-7.14	114.73	123.30
1	M	447	TYR	CB-CG-CD1	7.14	125.29	121.00
1	D	282	TYR	CB-CG-CD2	-7.14	116.72	121.00
1	P	20	ARG	NE-CZ-NH2	7.13	123.86	120.30
1	N	205	ASP	CB-CG-OD2	7.13	124.71	118.30
1	E	237	MET	CG-SD-CE	-7.11	88.82	100.20
1	A	311	PHE	CA-CB-CG	-7.11	96.83	113.90
1	K	393	GLU	O-C-N	-7.11	111.33	122.70
1	E	67	VAL	CA-CB-CG1	-7.11	100.24	110.90
1	I	315	ARG	NE-CZ-NH1	-7.11	116.75	120.30
1	D	496	ASP	CB-CG-OD1	-7.11	111.91	118.30
1	B	241	VAL	CA-CB-CG1	7.10	121.55	110.90
1	Q	369	PHE	CB-CG-CD1	7.10	125.77	120.80
1	N	325	ARG	NE-CZ-NH2	7.10	123.85	120.30
1	B	81	VAL	CA-CB-CG1	7.09	121.54	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	J	384	ARG	NE-CZ-NH1	-7.09	116.75	120.30
1	P	498	TYR	CB-CG-CD2	-7.09	116.75	121.00
1	Q	275	PHE	CB-CG-CD2	-7.09	115.84	120.80
1	A	163	TYR	CB-CG-CD2	-7.08	116.75	121.00
1	H	322	ARG	NH1-CZ-NH2	-7.08	111.61	119.40
1	N	474	ARG	NE-CZ-NH2	7.07	123.84	120.30
1	O	166	MET	CG-SD-CE	-7.07	88.88	100.20
1	Q	63	GLY	O-C-N	-7.07	111.39	122.70
1	L	428	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	C	296	ASN	CB-CG-OD1	-7.06	107.48	121.60
1	G	456	MET	CA-CB-CG	7.06	125.30	113.30
1	I	434	ARG	NE-CZ-NH1	-7.05	116.77	120.30
1	B	454	ILE	C-N-CD	-7.05	105.09	120.60
1	M	474	ARG	NE-CZ-NH2	-7.04	116.78	120.30
1	L	36	MET	CG-SD-CE	7.03	111.45	100.20
1	C	369	PHE	CB-CG-CD2	-7.03	115.88	120.80
1	E	130	PHE	CB-CG-CD1	7.03	125.72	120.80
1	K	311	PHE	CB-CG-CD2	7.03	125.72	120.80
1	J	305	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	I	166	MET	CG-SD-CE	-7.02	88.97	100.20
1	D	100	VAL	CG1-CB-CG2	-7.01	99.68	110.90
1	G	233	VAL	CB-CA-C	7.00	124.70	111.40
1	H	145	ASP	CB-CG-OD2	7.00	124.60	118.30
1	B	321	ARG	N-CA-CB	-7.00	98.01	110.60
1	H	130	PHE	CB-CG-CD1	6.99	125.69	120.80
1	H	173	GLU	O-C-N	-6.99	111.32	123.20
1	B	200	TYR	CB-CG-CD1	6.98	125.19	121.00
1	K	219	ASP	CB-CG-OD2	-6.98	112.02	118.30
1	D	516	ALA	CB-CA-C	-6.98	99.63	110.10
1	F	322	ARG	NE-CZ-NH1	-6.98	116.81	120.30
1	I	510	ARG	NE-CZ-NH2	6.98	123.79	120.30
1	O	447	TYR	CB-CG-CD1	-6.97	116.82	121.00
1	L	126	PHE	CB-CG-CD2	-6.97	115.92	120.80
1	A	305	ASP	CB-CG-OD2	-6.96	112.04	118.30
1	J	528	ASP	CB-CG-OD1	6.96	124.56	118.30
1	H	360	ARG	NE-CZ-NH2	6.96	123.78	120.30
1	J	155	ARG	NE-CZ-NH2	6.95	123.78	120.30
1	D	155	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	H	396	ARG	NE-CZ-NH1	-6.94	116.83	120.30
1	J	16	ARG	NE-CZ-NH1	6.93	123.77	120.30
1	C	367	MET	N-CA-CB	6.93	123.07	110.60
1	M	388	ASP	CB-CG-OD2	6.92	124.53	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	367	MET	CG-SD-CE	-6.92	89.13	100.20
1	A	163	TYR	CZ-CE2-CD2	6.92	126.02	119.80
1	B	487	ASP	CB-CG-OD2	6.90	124.51	118.30
1	D	455	PRO	CB-CA-C	6.89	129.22	112.00
1	B	428	ARG	NE-CZ-NH2	6.88	123.74	120.30
1	Q	169	LYS	N-CA-CB	-6.87	98.23	110.60
1	E	242	GLU	OE1-CD-OE2	-6.87	115.05	123.30
1	K	455	PRO	CB-CA-C	6.87	129.18	112.00
1	E	38	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	H	413	TYR	CZ-CE2-CD2	6.87	125.98	119.80
1	M	390	ALA	CB-CA-C	-6.87	99.80	110.10
1	G	325	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	A	474	ARG	NE-CZ-NH2	6.86	123.73	120.30
1	B	415	VAL	CA-CB-CG2	6.86	121.19	110.90
1	I	454	ILE	CB-CA-C	6.86	125.32	111.60
1	K	369	PHE	CB-CG-CD1	6.86	125.60	120.80
1	E	454	ILE	CB-CA-C	6.85	125.30	111.60
1	J	498	TYR	CG-CD2-CE2	-6.84	115.83	121.30
1	H	153	THR	CA-CB-CG2	-6.83	102.84	112.40
1	M	323	VAL	CA-CB-CG2	-6.83	100.66	110.90
1	A	179	LYS	O-C-N	-6.83	111.78	122.70
1	N	322	ARG	NH1-CZ-NH2	-6.83	111.89	119.40
1	F	305	ASP	CB-CG-OD1	6.82	124.44	118.30
1	N	182	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	E	148	ASP	CB-CG-OD1	-6.81	112.17	118.30
1	H	126	PHE	CB-CG-CD2	-6.80	116.04	120.80
1	N	54	PHE	CB-CG-CD1	6.80	125.56	120.80
1	G	286	MET	CG-SD-CE	-6.79	89.33	100.20
1	B	389	MET	CG-SD-CE	-6.79	89.33	100.20
1	M	495	ASP	CB-CG-OD2	-6.79	112.19	118.30
1	G	450	ALA	N-CA-CB	-6.78	100.60	110.10
1	J	430	ARG	NE-CZ-NH2	6.77	123.69	120.30
1	E	56	ASP	CB-CG-OD1	6.76	124.39	118.30
1	O	271	GLN	O-C-N	-6.76	111.88	122.70
1	E	224	ARG	NE-CZ-NH1	6.76	123.68	120.30
1	E	315	ARG	NE-CZ-NH1	-6.76	116.92	120.30
1	B	163	TYR	CB-CG-CD2	-6.75	116.95	121.00
1	O	472	ASP	CB-CG-OD1	6.74	124.36	118.30
1	J	428	ARG	NH1-CZ-NH2	6.74	126.81	119.40
1	J	327	ASP	CB-CG-OD2	-6.74	112.24	118.30
1	Q	315	ARG	NE-CZ-NH1	6.74	123.67	120.30
1	I	360	ARG	CD-NE-CZ	6.73	133.02	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	N	163	TYR	CB-CG-CD1	6.73	125.04	121.00
1	E	275	PHE	CB-CG-CD1	-6.72	116.09	120.80
1	L	233	VAL	CA-CB-CG1	6.72	120.98	110.90
1	E	388	ASP	CB-CG-OD1	-6.72	112.25	118.30
1	P	498	TYR	CB-CG-CD1	6.71	125.03	121.00
1	N	430	ARG	CD-NE-CZ	-6.71	114.21	123.60
1	H	60	THR	CA-CB-OG1	6.70	123.08	109.00
1	L	338	ARG	NE-CZ-NH2	-6.70	116.95	120.30
1	K	454	ILE	CB-CA-C	6.70	124.99	111.60
1	L	203	SER	N-CA-CB	6.70	120.54	110.50
1	Q	321	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	O	428	ARG	NE-CZ-NH1	-6.69	116.96	120.30
1	J	454	ILE	CB-CA-C	6.69	124.97	111.60
1	F	38	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	M	88	ASP	CB-CG-OD1	6.68	124.31	118.30
1	R	38	ARG	NE-CZ-NH1	-6.68	116.96	120.30
1	J	229	ASP	CB-CG-OD1	6.67	124.31	118.30
1	D	114	ASP	CB-CG-OD2	6.67	124.31	118.30
1	C	490	ASN	O-C-N	-6.67	111.86	123.20
1	R	472	ASP	CB-CG-OD2	-6.67	112.30	118.30
1	C	16	ARG	CD-NE-CZ	6.66	132.93	123.60
1	I	499	SER	N-CA-CB	6.66	120.49	110.50
1	M	325	ARG	NH1-CZ-NH2	-6.65	112.08	119.40
1	R	494	ILE	CA-CB-CG1	6.65	123.63	111.00
1	D	162	VAL	CA-CB-CG2	-6.64	100.93	110.90
1	M	455	PRO	N-CA-CB	6.64	111.27	103.30
1	H	67	VAL	CA-CB-CG1	-6.64	100.94	110.90
1	K	394	ALA	N-CA-CB	6.64	119.39	110.10
1	E	116	ASN	CB-CG-OD1	-6.63	108.33	121.60
1	F	321	ARG	NE-CZ-NH1	-6.63	116.98	120.30
1	F	146	VAL	CG1-CB-CG2	-6.63	100.30	110.90
1	F	454	ILE	CA-C-N	6.61	135.61	117.10
1	J	338	ARG	NE-CZ-NH2	6.61	123.61	120.30
1	L	434	ARG	CG-CD-NE	-6.61	97.92	111.80
1	N	369	PHE	CB-CG-CD2	-6.61	116.17	120.80
1	G	195	LEU	CB-CG-CD1	-6.61	99.77	111.00
1	E	392	ASP	CB-CG-OD1	-6.61	112.36	118.30
1	O	88	ASP	CB-CG-OD2	6.61	124.25	118.30
1	D	365	ASP	CB-CG-OD1	6.60	124.24	118.30
1	R	494	ILE	CB-CA-C	6.59	124.79	111.60
1	R	16	ARG	NE-CZ-NH2	6.59	123.59	120.30
1	R	38	ARG	NE-CZ-NH2	6.59	123.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	360	ARG	NE-CZ-NH1	-6.59	117.01	120.30
1	L	224	ARG	NH1-CZ-NH2	-6.59	112.15	119.40
1	K	406	ARG	CD-NE-CZ	6.58	132.81	123.60
1	E	166	MET	CG-SD-CE	-6.57	89.68	100.20
1	I	155	ARG	N-CA-CB	-6.57	98.77	110.60
1	N	396	ARG	NE-CZ-NH1	-6.57	117.01	120.30
1	G	468	SER	CB-CA-C	-6.57	97.62	110.10
1	N	200	TYR	CB-CG-CD2	6.57	124.94	121.00
1	L	286	MET	CG-SD-CE	-6.57	89.69	100.20
1	P	472	ASP	CB-CG-OD2	6.57	124.21	118.30
1	R	443	ALA	N-CA-CB	-6.57	100.91	110.10
1	I	353	TYR	CB-CG-CD2	-6.56	117.06	121.00
1	K	305	ASP	CB-CG-OD1	6.56	124.20	118.30
1	R	130	PHE	CB-CG-CD2	-6.56	116.21	120.80
1	G	252	SER	N-CA-CB	6.56	120.33	110.50
1	G	261	SER	N-CA-CB	6.55	120.33	110.50
1	Q	197	ASP	CB-CG-OD1	6.55	124.20	118.30
1	K	434	ARG	NE-CZ-NH2	6.55	123.58	120.30
1	G	182	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	G	434	ARG	NH1-CZ-NH2	-6.55	112.19	119.40
1	H	486	VAL	CG1-CB-CG2	-6.55	100.42	110.90
1	Q	239	ARG	NE-CZ-NH2	6.55	123.57	120.30
1	I	16	ARG	NE-CZ-NH1	-6.55	117.03	120.30
1	O	403	TYR	CB-CG-CD1	6.54	124.92	121.00
1	R	489	ILE	O-C-N	-6.54	112.23	122.70
1	N	498	TYR	CB-CG-CD1	-6.54	117.08	121.00
1	H	327	ASP	CB-CG-OD1	6.54	124.18	118.30
1	I	481	LEU	CB-CG-CD2	6.54	122.11	111.00
1	P	47	ASP	CB-CG-OD2	-6.53	112.42	118.30
1	J	81	VAL	CG1-CB-CG2	-6.52	100.46	110.90
1	M	240	ARG	NE-CZ-NH1	-6.52	117.04	120.30
1	B	182	ASP	CB-CG-OD1	-6.52	112.44	118.30
1	D	464	LEU	CB-CG-CD1	-6.52	99.92	111.00
1	G	113	VAL	CG1-CB-CG2	-6.52	100.47	110.90
1	G	60	THR	CA-CB-CG2	-6.51	103.28	112.40
1	J	455	PRO	CB-CA-C	6.51	128.28	112.00
1	A	38	ARG	NH1-CZ-NH2	-6.51	112.24	119.40
1	E	353	TYR	CB-CG-CD2	-6.50	117.10	121.00
1	L	20	ARG	NH1-CZ-NH2	-6.50	112.25	119.40
1	L	240	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	C	476	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	M	29	ALA	N-CA-CB	-6.50	101.00	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	360	ARG	NE-CZ-NH1	-6.50	117.05	120.30
1	L	17	ASN	CB-CA-C	-6.50	97.41	110.40
1	G	330	LYS	O-C-N	-6.49	112.31	122.70
1	J	507	ARG	NE-CZ-NH1	6.49	123.55	120.30
1	O	455	PRO	CB-CA-C	6.49	128.24	112.00
1	H	155	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	E	224	ARG	NH1-CZ-NH2	-6.49	112.27	119.40
1	K	155	ARG	N-CA-CB	-6.48	98.93	110.60
1	E	472	ASP	CB-CG-OD2	6.48	124.13	118.30
1	F	434	ARG	NE-CZ-NH2	6.48	123.54	120.30
1	M	36	MET	CG-SD-CE	-6.47	89.85	100.20
1	P	200	TYR	CB-CG-CD2	-6.47	117.12	121.00
1	K	52	ASP	CB-CG-OD2	6.46	124.11	118.30
1	K	259	GLU	OE1-CD-OE2	-6.46	115.55	123.30
1	C	239	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	113	VAL	CG1-CB-CG2	-6.45	100.58	110.90
1	N	428	ARG	NH1-CZ-NH2	-6.45	112.30	119.40
1	A	148	ASP	CB-CG-OD2	6.45	124.11	118.30
1	B	311	PHE	CB-CG-CD1	-6.45	116.28	120.80
1	R	16	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	F	285	ASP	CB-CG-OD2	6.45	124.10	118.30
1	G	446	ALA	CB-CA-C	6.45	119.77	110.10
1	O	428	ARG	CD-NE-CZ	6.44	132.62	123.60
1	Q	276	LEU	CB-CG-CD2	-6.44	100.05	111.00
1	H	288	ASP	CB-CG-OD2	6.42	124.08	118.30
1	H	295	ALA	O-C-N	-6.42	112.42	122.70
1	C	31	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	O	325	ARG	NE-CZ-NH1	-6.42	117.09	120.30
1	Q	240	ARG	NE-CZ-NH2	6.41	123.51	120.30
1	H	353	TYR	CB-CG-CD2	-6.41	117.15	121.00
1	F	496	ASP	CB-CG-OD2	6.41	124.07	118.30
1	B	31	ARG	NE-CZ-NH1	-6.41	117.10	120.30
1	C	15	SER	O-C-N	-6.40	112.46	122.70
1	N	20	ARG	NE-CZ-NH2	6.39	123.50	120.30
1	L	498	TYR	CA-CB-CG	6.39	125.54	113.40
1	A	222	LEU	CB-CG-CD2	6.39	121.86	111.00
1	E	353	TYR	CB-CG-CD1	6.39	124.83	121.00
1	A	415	VAL	CG1-CB-CG2	6.38	121.11	110.90
1	L	403	TYR	CG-CD1-CE1	-6.37	116.20	121.30
1	M	476	ARG	NE-CZ-NH1	-6.37	117.11	120.30
1	R	35	GLU	OE1-CD-OE2	-6.37	115.65	123.30
1	P	363	GLY	C-N-CA	6.37	137.62	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	249	LEU	C-N-CA	6.37	137.62	121.70
1	Q	200	TYR	CG-CD1-CE1	-6.35	116.22	121.30
1	H	325	ARG	NE-CZ-NH2	6.35	123.47	120.30
1	A	432	TYR	CB-CG-CD2	-6.35	117.19	121.00
1	G	244	ALA	N-CA-CB	-6.34	101.22	110.10
1	I	21	ASP	CB-CG-OD2	6.34	124.01	118.30
1	K	428	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	G	396	ARG	NE-CZ-NH1	-6.34	117.13	120.30
1	H	308	ALA	CB-CA-C	-6.34	100.59	110.10
1	N	221	GLN	CG-CD-OE1	-6.34	108.92	121.60
1	E	148	ASP	CB-CG-OD2	6.34	124.00	118.30
1	N	67	VAL	CA-CB-CG1	-6.33	101.40	110.90
1	E	405	LEU	CB-CG-CD2	6.33	121.76	111.00
1	L	200	TYR	CB-CG-CD1	-6.33	117.20	121.00
1	R	472	ASP	CB-CG-OD1	6.33	123.99	118.30
1	P	406	ARG	NE-CZ-NH1	-6.32	117.14	120.30
1	G	305	ASP	CB-CG-OD2	-6.32	112.61	118.30
1	I	447	TYR	CB-CG-CD2	-6.32	117.21	121.00
1	A	522	SER	CB-CA-C	-6.32	98.10	110.10
1	P	406	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	R	474	ARG	NH1-CZ-NH2	-6.31	112.46	119.40
1	C	267	THR	O-C-N	-6.31	112.61	122.70
1	F	56	ASP	CB-CG-OD2	6.31	123.98	118.30
1	I	163	TYR	CB-CG-CD2	6.31	124.78	121.00
1	L	315	ARG	NE-CZ-NH2	6.31	123.45	120.30
1	E	327	ASP	CB-CG-OD1	6.30	123.97	118.30
1	P	503	VAL	CA-CB-CG1	-6.29	101.46	110.90
1	P	496	ASP	CB-CG-OD1	6.29	123.96	118.30
1	E	320	VAL	CA-CB-CG2	-6.28	101.48	110.90
1	N	455	PRO	CB-CA-C	6.28	127.71	112.00
1	O	242	GLU	CB-CA-C	6.28	122.96	110.40
1	C	484	CYS	O-C-N	-6.28	112.53	123.20
1	F	275	PHE	CB-CG-CD2	-6.27	116.41	120.80
1	M	346	ALA	N-CA-CB	-6.26	101.33	110.10
1	P	473	LEU	CB-CG-CD1	6.26	121.65	111.00
1	P	170	PHE	CB-CA-C	-6.26	97.89	110.40
1	G	282	TYR	CG-CD2-CE2	6.25	126.30	121.30
1	K	126	PHE	CB-CG-CD1	6.25	125.18	120.80
1	O	233	VAL	CA-CB-CG1	6.25	120.28	110.90
1	C	126	PHE	CB-CG-CD1	6.25	125.17	120.80
1	L	338	ARG	NE-CZ-NH1	-6.25	117.18	120.30
1	C	498	TYR	CB-CG-CD2	-6.24	117.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	212	LYS	N-CA-CB	6.24	121.83	110.60
1	L	163	TYR	CG-CD2-CE2	-6.24	116.31	121.30
1	D	163	TYR	CG-CD1-CE1	6.24	126.29	121.30
1	E	182	ASP	CB-CG-OD1	-6.24	112.69	118.30
1	E	428	ARG	NE-CZ-NH1	-6.23	117.19	120.30
1	Q	369	PHE	CB-CG-CD2	-6.23	116.44	120.80
1	D	202	VAL	CB-CA-C	-6.22	99.57	111.40
1	B	356	LEU	CB-CG-CD2	-6.22	100.43	111.00
1	I	338	ARG	CD-NE-CZ	6.22	132.30	123.60
1	O	182	ASP	CB-CG-OD2	6.21	123.89	118.30
1	C	186	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	O	65	THR	O-C-N	-6.21	112.77	122.70
1	D	23	LEU	CB-CG-CD1	6.20	121.53	111.00
1	H	69	GLU	CG-CD-OE2	6.19	130.69	118.30
1	P	125	GLY	O-C-N	-6.19	112.80	122.70
1	C	428	ARG	NH1-CZ-NH2	-6.18	112.60	119.40
1	C	464	LEU	O-C-N	-6.18	112.81	122.70
1	G	413	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	H	28	LEU	O-C-N	-6.18	112.81	122.70
1	H	380	ASN	O-C-N	-6.18	112.81	122.70
1	I	432	TYR	CB-CG-CD2	-6.18	117.29	121.00
1	Q	394	ALA	N-CA-CB	-6.18	101.44	110.10
1	G	155	ARG	N-CA-C	6.18	127.69	111.00
1	I	282	TYR	CB-CG-CD2	6.18	124.71	121.00
1	Q	20	ARG	N-CA-CB	6.18	121.73	110.60
1	F	373	ALA	O-C-N	-6.18	112.81	122.70
1	B	430	ARG	NH1-CZ-NH2	-6.18	112.61	119.40
1	K	487	ASP	CB-CG-OD2	6.18	123.86	118.30
1	A	432	TYR	CG-CD1-CE1	6.17	126.24	121.30
1	P	401	ALA	N-CA-CB	-6.17	101.46	110.10
1	K	168	SER	O-C-N	-6.17	112.83	122.70
1	F	98	ALA	CB-CA-C	-6.16	100.85	110.10
1	H	496	ASP	N-CA-CB	-6.16	99.51	110.60
1	C	527	ASP	CB-CG-OD2	-6.16	112.76	118.30
1	R	295	ALA	CB-CA-C	6.16	119.33	110.10
1	K	360	ARG	CD-NE-CZ	6.15	132.21	123.60
1	O	231	GLU	OE1-CD-OE2	-6.15	115.92	123.30
1	B	99	VAL	CA-CB-CG2	-6.14	101.69	110.90
1	H	496	ASP	CB-CG-OD1	6.14	123.83	118.30
1	P	395	GLU	OE1-CD-OE2	-6.14	115.93	123.30
1	E	487	ASP	CB-CG-OD2	6.14	123.82	118.30
1	F	430	ARG	NE-CZ-NH2	6.14	123.37	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	70	MET	CA-CB-CG	6.13	123.72	113.30
1	P	306	ASP	CB-CG-OD2	6.13	123.82	118.30
1	M	413	TYR	CZ-CE2-CD2	-6.13	114.28	119.80
1	O	347	THR	O-C-N	-6.13	109.46	121.10
1	A	224	ARG	NE-CZ-NH1	-6.12	117.24	120.30
1	Q	189	THR	CA-CB-CG2	-6.12	103.83	112.40
1	I	447	TYR	CB-CG-CD1	6.12	124.67	121.00
1	G	232	VAL	C-N-CA	6.12	137.00	121.70
1	P	162	VAL	CA-CB-CG2	-6.12	101.72	110.90
1	F	251	ALA	N-CA-CB	-6.12	101.54	110.10
1	H	454	ILE	CB-CA-C	6.12	123.83	111.60
1	F	288	ASP	CB-CG-OD2	6.11	123.80	118.30
1	P	104	LEU	CB-CG-CD2	6.11	121.39	111.00
1	G	338	ARG	NE-CZ-NH2	6.11	123.35	120.30
1	O	146	VAL	CA-CB-CG1	-6.11	101.74	110.90
1	N	224	ARG	CG-CD-NE	-6.11	98.98	111.80
1	I	507	ARG	NE-CZ-NH1	-6.10	117.25	120.30
1	H	47	ASP	CB-CG-OD2	6.10	123.79	118.30
1	G	305	ASP	CB-CG-OD1	6.10	123.79	118.30
1	G	528	ASP	CB-CG-OD2	-6.09	112.81	118.30
1	N	124	GLU	O-C-N	-6.09	112.84	123.20
1	F	205	ASP	CB-CG-OD1	-6.09	112.82	118.30
1	C	369	PHE	CB-CG-CD1	6.09	125.06	120.80
1	E	99	VAL	CA-CB-CG2	-6.09	101.77	110.90
1	K	16	ARG	NE-CZ-NH1	-6.08	117.26	120.30
1	R	400	ASP	CB-CG-OD1	-6.08	112.83	118.30
1	N	130	PHE	N-CA-CB	-6.08	99.67	110.60
1	N	388	ASP	CB-CG-OD1	6.07	123.77	118.30
1	R	200	TYR	CG-CD2-CE2	-6.07	116.44	121.30
1	L	440	GLU	O-C-N	-6.07	112.99	122.70
1	L	106	LEU	O-C-N	-6.07	112.99	122.70
1	K	359	GLU	CA-CB-CG	6.07	126.74	113.40
1	G	360	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	A	33	LEU	O-C-N	-6.06	113.01	122.70
1	R	47	ASP	CB-CG-OD1	6.05	123.75	118.30
1	B	498	TYR	CB-CG-CD1	6.05	124.63	121.00
1	P	126	PHE	CB-CG-CD2	-6.05	116.57	120.80
1	G	396	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	H	164	THR	CA-CB-CG2	6.04	120.86	112.40
1	K	188	VAL	CA-CB-CG2	-6.04	101.84	110.90
1	H	286	MET	CG-SD-CE	-6.04	90.53	100.20
1	Q	467	ILE	CA-CB-CG1	6.04	122.48	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	322	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	A	286	MET	CG-SD-CE	-6.04	90.54	100.20
1	I	38	ARG	O-C-N	-6.04	113.04	122.70
1	L	353	TYR	CB-CG-CD1	-6.04	117.38	121.00
1	R	308	ALA	CB-CA-C	-6.04	101.05	110.10
1	R	321	ARG	NE-CZ-NH2	6.04	123.32	120.30
1	D	472	ASP	CB-CG-OD2	6.03	123.73	118.30
1	E	21	ASP	CB-CG-OD1	6.03	123.73	118.30
1	L	327	ASP	CB-CG-OD1	6.03	123.72	118.30
1	N	325	ARG	NH1-CZ-NH2	-6.03	112.77	119.40
1	O	99	VAL	CG1-CB-CG2	-6.02	101.26	110.90
1	G	400	ASP	CB-CG-OD2	-6.02	112.88	118.30
1	H	74	HIS	CA-CB-CG	-6.02	103.36	113.60
1	E	425	LEU	CB-CG-CD2	6.02	121.24	111.00
1	D	155	ARG	C-N-CA	6.02	136.75	121.70
1	A	438	GLY	N-CA-C	6.01	128.14	113.10
1	E	36	MET	CG-SD-CE	-6.01	90.58	100.20
1	A	432	TYR	CB-CG-CD1	6.01	124.61	121.00
1	I	389	MET	CA-CB-CG	6.01	123.52	113.30
1	B	338	ARG	CG-CD-NE	-6.01	99.18	111.80
1	N	527	ASP	CB-CG-OD1	-6.01	112.89	118.30
1	B	233	VAL	CA-CB-CG1	-6.01	101.89	110.90
1	D	200	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	G	455	PRO	CB-CA-C	6.01	127.02	112.00
1	I	229	ASP	CB-CG-OD1	6.01	123.71	118.30
1	L	384	ARG	NE-CZ-NH1	6.01	123.30	120.30
1	M	305	ASP	CB-CG-OD2	-6.01	112.89	118.30
1	M	454	ILE	C-N-CD	-6.01	107.39	120.60
1	A	200	TYR	CB-CA-C	-6.00	98.39	110.40
1	H	349	GLU	OE1-CD-OE2	-6.00	116.09	123.30
1	G	219	ASP	CB-CG-OD1	-6.00	112.90	118.30
1	I	429	LEU	CB-CG-CD2	6.00	121.20	111.00
1	O	528	ASP	CB-CG-OD1	6.00	123.70	118.30
1	N	325	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	B	65	THR	OG1-CB-CG2	-6.00	96.21	110.00
1	L	163	TYR	CB-CG-CD1	5.99	124.60	121.00
1	M	403	TYR	CB-CG-CD1	5.99	124.60	121.00
1	R	130	PHE	CB-CG-CD1	5.99	125.00	120.80
1	N	256	GLU	OE1-CD-OE2	-5.99	116.11	123.30
1	A	186	ASP	CB-CG-OD2	-5.99	112.91	118.30
1	G	148	ASP	CB-CG-OD1	5.99	123.69	118.30
1	P	81	VAL	O-C-N	-5.99	113.12	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	196	PRO	N-CA-CB	-5.99	96.02	102.60
1	L	496	ASP	N-CA-CB	-5.98	99.83	110.60
1	L	67	VAL	CG1-CB-CG2	-5.98	101.33	110.90
1	N	249	LEU	CB-CA-C	-5.98	98.83	110.20
1	H	240	ARG	O-C-N	5.98	132.27	122.70
1	R	389	MET	CG-SD-CE	-5.98	90.63	100.20
1	B	407	ASN	CA-CB-CG	-5.98	100.25	113.40
1	B	413	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	A	507	ARG	NE-CZ-NH1	5.97	123.29	120.30
1	I	144	VAL	CG1-CB-CG2	5.97	120.45	110.90
1	A	455	PRO	N-CA-CB	5.97	110.46	103.30
1	K	224	ARG	NE-CZ-NH2	-5.97	117.32	120.30
1	C	210	ASP	CB-CG-OD1	5.96	123.67	118.30
1	J	406	ARG	NE-CZ-NH2	5.96	123.28	120.30
1	L	151	SER	CB-CA-C	-5.96	98.77	110.10
1	D	353	TYR	CB-CG-CD1	5.96	124.58	121.00
1	F	406	ARG	CG-CD-NE	-5.96	99.29	111.80
1	G	192	ALA	CB-CA-C	5.96	119.04	110.10
1	K	31	ARG	NE-CZ-NH1	-5.96	117.32	120.30
1	N	110	GLU	O-C-N	-5.96	113.17	122.70
1	H	288	ASP	CB-CG-OD1	-5.95	112.94	118.30
1	R	16	ARG	CD-NE-CZ	5.95	131.93	123.60
1	C	443	ALA	CB-CA-C	5.95	119.03	110.10
1	N	305	ASP	CB-CG-OD1	5.95	123.66	118.30
1	Q	101	LEU	CB-CG-CD2	5.95	121.12	111.00
1	C	403	TYR	CG-CD2-CE2	-5.95	116.54	121.30
1	L	311	PHE	CB-CG-CD2	-5.95	116.64	120.80
1	G	62	ASP	CB-CG-OD2	-5.95	112.95	118.30
1	O	415	VAL	CB-CA-C	-5.95	100.10	111.40
1	P	105	PHE	CB-CG-CD2	-5.95	116.64	120.80
1	J	166	MET	CA-C-O	5.94	132.58	120.10
1	O	517	THR	CA-CB-CG2	-5.94	104.08	112.40
1	M	203	SER	N-CA-CB	5.94	119.41	110.50
1	I	360	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	D	282	TYR	CG-CD2-CE2	-5.94	116.55	121.30
1	G	41	LEU	CB-CG-CD1	5.93	121.09	111.00
1	L	38	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	F	360	ARG	N-CA-CB	5.93	121.28	110.60
1	Q	360	ARG	NH1-CZ-NH2	-5.93	112.88	119.40
1	A	57	VAL	O-C-N	-5.93	113.22	122.70
1	C	196	PRO	N-CD-CG	5.93	112.09	103.20
1	O	267	THR	N-CA-CB	5.92	121.56	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	O	403	TYR	CZ-CE2-CD2	-5.92	114.47	119.80
1	H	111	SER	CB-CA-C	-5.92	98.86	110.10
1	J	262	ALA	N-CA-CB	5.92	118.38	110.10
1	B	468	SER	N-CA-CB	5.92	119.37	110.50
1	C	206	LEU	CB-CG-CD1	-5.91	100.95	111.00
1	D	36	MET	CA-CB-CG	5.91	123.35	113.30
1	F	229	ASP	CB-CG-OD1	5.91	123.62	118.30
1	L	155	ARG	NE-CZ-NH2	5.91	123.26	120.30
1	F	171	MET	O-C-N	-5.91	113.24	122.70
1	K	130	PHE	CB-CG-CD2	5.91	124.94	120.80
1	Q	367	MET	N-CA-CB	5.91	121.23	110.60
1	K	527	ASP	CB-CG-OD2	5.90	123.61	118.30
1	B	46	LEU	CB-CG-CD1	-5.90	100.97	111.00
1	O	287	VAL	CA-CB-CG2	-5.90	102.05	110.90
1	R	155	ARG	NH1-CZ-NH2	-5.90	112.91	119.40
1	K	423	LEU	O-C-N	-5.90	113.26	122.70
1	C	442	LEU	CB-CG-CD1	-5.89	100.98	111.00
1	I	181	MET	CG-SD-CE	-5.89	90.77	100.20
1	M	114	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	A	32	THR	CA-CB-CG2	5.89	120.65	112.40
1	C	16	ARG	NE-CZ-NH2	5.89	123.25	120.30
1	D	353	TYR	CD1-CE1-CZ	5.89	125.10	119.80
1	R	432	TYR	CZ-CE2-CD2	-5.89	114.50	119.80
1	E	364	ASN	N-CA-CB	5.89	121.20	110.60
1	M	454	ILE	CB-CA-C	5.88	123.37	111.60
1	D	16	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	K	462	ALA	N-CA-CB	-5.88	101.87	110.10
1	A	402	LEU	CB-CG-CD1	-5.88	101.01	111.00
1	D	163	TYR	CD1-CE1-CZ	-5.88	114.51	119.80
1	P	369	PHE	CB-CG-CD1	5.88	124.92	120.80
1	H	53	SER	CB-CA-C	-5.88	98.93	110.10
1	I	156	ASP	CB-CG-OD2	5.88	123.59	118.30
1	F	498	TYR	CG-CD2-CE2	-5.87	116.60	121.30
1	G	285	ASP	CB-CG-OD1	5.87	123.58	118.30
1	H	176	GLU	OE1-CD-OE2	5.87	130.34	123.30
1	E	197	ASP	CB-CG-OD1	5.87	123.58	118.30
1	E	430	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	J	205	ASP	O-C-N	-5.86	113.32	122.70
1	M	306	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	O	178	ASN	O-C-N	-5.86	113.32	122.70
1	Q	197	ASP	CB-CG-OD2	-5.86	113.02	118.30
1	B	311	PHE	CB-CG-CD2	5.86	124.90	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	31	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	O	31	ARG	NH1-CZ-NH2	-5.86	112.95	119.40
1	A	342	SER	N-CA-CB	5.86	119.29	110.50
1	J	219	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	K	114	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	P	510	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	D	430	ARG	C-N-CA	5.86	136.35	121.70
1	M	393	GLU	OE1-CD-OE2	-5.86	116.27	123.30
1	H	230	LYS	O-C-N	-5.86	113.33	122.70
1	G	411	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	J	20	ARG	NE-CZ-NH2	5.85	123.23	120.30
1	I	388	ASP	CB-CG-OD2	5.85	123.57	118.30
1	K	402	LEU	CB-CG-CD1	-5.85	101.05	111.00
1	Q	454	ILE	C-N-CD	-5.85	107.72	120.60
1	J	31	ARG	NE-CZ-NH2	5.85	123.22	120.30
1	N	411	GLU	OE1-CD-OE2	-5.85	116.28	123.30
1	J	308	ALA	O-C-N	-5.85	113.34	122.70
1	O	291	ALA	O-C-N	-5.84	113.35	122.70
1	M	458	LEU	CB-CG-CD2	-5.84	101.07	111.00
1	M	17	ASN	N-CA-CB	5.84	121.11	110.60
1	M	213	LYS	C-N-CA	5.84	134.56	122.30
1	M	428	ARG	NE-CZ-NH2	5.84	123.22	120.30
1	I	474	ARG	NE-CZ-NH1	-5.84	117.38	120.30
1	A	114	ASP	CB-CG-OD1	-5.84	113.05	118.30
1	N	14	THR	CA-CB-OG1	5.84	121.25	109.00
1	P	454	ILE	CB-CA-C	5.84	123.27	111.60
1	D	407	ASN	CA-CB-CG	-5.83	100.57	113.40
1	I	322	ARG	N-CA-C	5.83	126.75	111.00
1	I	424	GLU	OE1-CD-OE2	-5.83	116.30	123.30
1	M	483	ASN	N-CA-CB	5.83	121.10	110.60
1	G	454	ILE	C-N-CD	-5.83	107.78	120.60
1	J	163	TYR	CG-CD1-CE1	-5.83	116.64	121.30
1	M	347	THR	CA-C-N	5.83	133.42	117.10
1	E	413	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	F	406	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
1	K	388	ASP	CB-CG-OD2	5.83	123.54	118.30
1	I	105	PHE	CB-CG-CD2	-5.82	116.72	120.80
1	K	370	ILE	O-C-N	-5.82	113.39	122.70
1	B	192	ALA	CB-CA-C	5.82	118.83	110.10
1	E	292	SER	N-CA-CB	5.82	119.23	110.50
1	R	413	TYR	CZ-CE2-CD2	-5.82	114.56	119.80
1	E	321	ARG	NH1-CZ-NH2	-5.81	113.01	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Q	163	TYR	CB-CA-C	-5.81	98.77	110.40
1	C	350	ASP	CB-CG-OD1	-5.81	113.07	118.30
1	P	454	ILE	C-N-CD	-5.81	107.82	120.60
1	G	46	LEU	CB-CG-CD2	5.81	120.88	111.00
1	H	195	LEU	CB-CA-C	5.81	121.24	110.20
1	D	226	ILE	CA-C-O	5.81	132.30	120.10
1	O	396	ARG	NE-CZ-NH1	-5.80	117.40	120.30
1	L	170	PHE	CG-CD2-CE2	-5.80	114.42	120.80
1	K	322	ARG	O-C-N	-5.80	113.42	122.70
1	M	282	TYR	CB-CG-CD2	-5.80	117.52	121.00
1	R	241	VAL	CA-CB-CG2	-5.79	102.21	110.90
1	J	286	MET	CG-SD-CE	-5.79	90.94	100.20
1	C	134	LEU	CB-CG-CD1	-5.78	101.17	111.00
1	H	277	ASP	CB-CG-OD2	5.78	123.50	118.30
1	O	502	VAL	CG1-CB-CG2	-5.78	101.65	110.90
1	R	453	GLU	CB-CA-C	-5.78	98.85	110.40
1	K	205	ASP	CB-CG-OD2	-5.78	113.10	118.30
1	M	321	ARG	C-N-CA	5.78	136.14	121.70
1	O	344	LYS	O-C-N	-5.78	113.46	122.70
1	C	56	ASP	CB-CG-OD2	5.77	123.49	118.30
1	D	275	PHE	CB-CG-CD1	-5.77	116.76	120.80
1	O	388	ASP	O-C-N	-5.77	113.47	122.70
1	B	91	VAL	C-N-CA	5.77	134.41	122.30
1	G	308	ALA	N-CA-CB	-5.76	102.03	110.10
1	M	224	ARG	NH1-CZ-NH2	-5.76	113.06	119.40
1	P	205	ASP	CB-CG-OD2	-5.76	113.11	118.30
1	F	200	TYR	CD1-CE1-CZ	-5.76	114.62	119.80
1	R	150	ASN	CB-CA-C	5.76	121.91	110.40
1	G	219	ASP	CB-CG-OD2	5.75	123.48	118.30
1	H	318	LEU	O-C-N	-5.75	113.49	122.70
1	Q	507	ARG	NE-CZ-NH2	5.75	123.18	120.30
1	L	371	GLU	OE1-CD-OE2	-5.75	116.40	123.30
1	N	154	ALA	C-N-CA	5.75	136.08	121.70
1	N	374	LYS	O-C-N	-5.75	113.50	122.70
1	N	239	ARG	NH1-CZ-NH2	-5.75	113.08	119.40
1	E	406	ARG	N-CA-CB	-5.75	100.26	110.60
1	J	166	MET	O-C-N	-5.74	113.51	122.70
1	R	105	PHE	CB-CG-CD1	5.74	124.82	120.80
1	R	131	ASN	CB-CG-OD1	-5.74	110.12	121.60
1	N	403	TYR	CG-CD1-CE1	5.74	125.89	121.30
1	P	191	VAL	CG1-CB-CG2	-5.74	101.72	110.90
1	R	454	ILE	CB-CA-C	5.74	123.08	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	186	ASP	CB-CG-OD2	-5.74	113.14	118.30
1	F	321	ARG	CD-NE-CZ	5.74	131.63	123.60
1	G	252	SER	O-C-N	-5.74	113.52	122.70
1	L	91	VAL	CA-CB-CG2	5.73	119.50	110.90
1	D	488	VAL	O-C-N	-5.73	113.53	122.70
1	F	135	GLU	OE1-CD-OE2	5.73	130.18	123.30
1	J	342	SER	N-CA-CB	5.73	119.10	110.50
1	P	384	ARG	N-CA-CB	5.73	120.91	110.60
1	B	91	VAL	CB-CA-C	-5.73	100.52	111.40
1	H	255	VAL	O-C-N	-5.73	113.54	122.70
1	P	282	TYR	CG-CD1-CE1	-5.73	116.72	121.30
1	H	200	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	M	338	ARG	NE-CZ-NH1	5.72	123.16	120.30
1	P	490	ASN	C-N-CA	5.72	134.32	122.30
1	G	107	GLU	O-C-N	-5.72	113.55	122.70
1	N	232	VAL	CG1-CB-CG2	-5.72	101.75	110.90
1	H	23	LEU	CB-CG-CD1	5.72	120.72	111.00
1	M	498	TYR	CB-CG-CD2	-5.72	117.57	121.00
1	I	322	ARG	NE-CZ-NH2	-5.71	117.44	120.30
1	L	193	GLU	N-CA-CB	-5.71	100.33	110.60
1	O	442	LEU	CB-CG-CD2	5.71	120.70	111.00
1	C	454	ILE	C-N-CD	-5.71	108.05	120.60
1	M	487	ASP	CB-CG-OD2	-5.71	113.17	118.30
1	Q	311	PHE	CB-CG-CD2	5.70	124.79	120.80
1	B	455	PRO	CB-CA-C	5.70	126.25	112.00
1	C	200	TYR	CB-CG-CD1	-5.70	117.58	121.00
1	P	88	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	192	ALA	N-CA-CB	5.70	118.07	110.10
1	R	360	ARG	NE-CZ-NH1	-5.70	117.45	120.30
1	P	447	TYR	CG-CD1-CE1	-5.69	116.75	121.30
1	F	237	MET	CG-SD-CE	-5.68	91.10	100.20
1	R	407	ASN	O-C-N	-5.68	113.61	122.70
1	C	410	MET	CA-CB-CG	-5.68	103.64	113.30
1	H	54	PHE	CG-CD2-CE2	-5.68	114.55	120.80
1	F	130	PHE	CB-CG-CD2	-5.67	116.83	120.80
1	Q	49	MET	O-C-N	-5.67	113.62	122.70
1	B	430	ARG	CD-NE-CZ	5.67	131.54	123.60
1	G	239	ARG	NE-CZ-NH1	-5.67	117.47	120.30
1	O	428	ARG	NE-CZ-NH2	5.67	123.14	120.30
1	N	305	ASP	O-C-N	-5.67	113.63	122.70
1	O	338	ARG	NH1-CZ-NH2	-5.67	113.17	119.40
1	P	357	VAL	CA-CB-CG1	-5.67	102.40	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	451	LEU	CB-CG-CD2	5.66	120.63	111.00
1	M	182	ASP	N-CA-CB	5.66	120.79	110.60
1	J	359	GLU	O-C-N	-5.66	113.64	122.70
1	O	454	ILE	CA-C-N	5.66	132.94	117.10
1	F	476	ARG	NE-CZ-NH2	5.66	123.13	120.30
1	O	163	TYR	CB-CG-CD2	5.66	124.39	121.00
1	D	528	ASP	CB-CG-OD1	-5.66	113.21	118.30
1	K	82	GLU	OE1-CD-OE2	-5.66	116.51	123.30
1	R	365	ASP	CB-CG-OD1	5.65	123.39	118.30
1	J	321	ARG	NE-CZ-NH1	-5.65	117.47	120.30
1	M	477	HIS	CA-CB-CG	5.65	123.21	113.60
1	Q	396	ARG	NE-CZ-NH1	5.65	123.13	120.30
1	P	184	VAL	O-C-N	-5.65	113.66	122.70
1	A	402	LEU	CB-CG-CD2	-5.65	101.40	111.00
1	C	36	MET	CG-SD-CE	-5.65	91.16	100.20
1	P	158	LEU	CB-CG-CD2	-5.65	101.40	111.00
1	J	447	TYR	N-CA-CB	-5.65	100.44	110.60
1	G	324	LYS	O-C-N	-5.64	113.67	122.70
1	C	430	ARG	NE-CZ-NH2	5.64	123.12	120.30
1	F	31	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	M	148	ASP	CB-CG-OD1	5.64	123.38	118.30
1	M	227	VAL	O-C-N	-5.64	113.67	122.70
1	A	306	ASP	CB-CG-OD2	5.64	123.38	118.30
1	A	392	ASP	CB-CG-OD1	-5.64	113.22	118.30
1	D	406	ARG	NH1-CZ-NH2	-5.64	113.20	119.40
1	N	36	MET	N-CA-CB	-5.64	100.45	110.60
1	A	381	ILE	CA-CB-CG1	5.64	121.71	111.00
1	R	503	VAL	CB-CA-C	-5.64	100.69	111.40
1	C	432	TYR	CB-CG-CD1	5.64	124.38	121.00
1	I	484	CYS	CA-CB-SG	-5.64	103.86	114.00
1	M	33	LEU	CB-CG-CD1	5.64	120.58	111.00
1	C	272	ILE	CA-CB-CG1	-5.63	100.30	111.00
1	D	142	THR	CA-CB-CG2	5.63	120.29	112.40
1	H	191	VAL	CA-CB-CG2	-5.63	102.45	110.90
1	A	169	LYS	N-CA-CB	-5.63	100.46	110.60
1	H	105	PHE	CB-CG-CD1	-5.63	116.86	120.80
1	G	528	ASP	O-C-N	-5.63	113.69	122.70
1	C	109	ALA	CB-CA-C	5.63	118.54	110.10
1	C	130	PHE	CB-CG-CD2	-5.63	116.86	120.80
1	H	38	ARG	NE-CZ-NH2	5.63	123.11	120.30
1	E	474	ARG	NE-CZ-NH1	5.63	123.11	120.30
1	C	231	GLU	OE1-CD-OE2	-5.62	116.56	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	160	LYS	O-C-N	-5.62	113.71	122.70
1	P	153	THR	OG1-CB-CG2	-5.62	97.07	110.00
1	E	40	SER	CB-CA-C	-5.62	99.42	110.10
1	Q	399	ASN	O-C-N	-5.62	113.71	122.70
1	C	158	LEU	CB-CG-CD2	5.62	120.55	111.00
1	C	420	ALA	C-N-CA	5.62	135.74	121.70
1	K	387	ASN	N-CA-CB	5.62	120.71	110.60
1	N	100	VAL	CA-CB-CG1	5.62	119.32	110.90
1	C	413	TYR	N-CA-CB	5.61	120.71	110.60
1	E	353	TYR	CZ-CE2-CD2	5.61	124.85	119.80
1	Q	82	GLU	OE1-CD-OE2	-5.61	116.56	123.30
1	P	253	LEU	CB-CG-CD1	5.61	120.54	111.00
1	D	18	SER	CB-CA-C	-5.61	99.45	110.10
1	O	305	ASP	O-C-N	-5.61	113.73	122.70
1	A	311	PHE	CB-CG-CD2	-5.61	116.88	120.80
1	L	186	ASP	CB-CG-OD1	5.61	123.34	118.30
1	R	144	VAL	CG1-CB-CG2	-5.60	101.93	110.90
1	B	447	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	A	510	ARG	NH1-CZ-NH2	-5.59	113.25	119.40
1	M	396	ARG	CD-NE-CZ	5.59	131.43	123.60
1	N	430	ARG	NH1-CZ-NH2	-5.59	113.25	119.40
1	I	250	ASP	CB-CG-OD1	5.59	123.33	118.30
1	N	111	SER	N-CA-CB	5.58	118.88	110.50
1	R	341	SER	O-C-N	-5.58	113.76	122.70
1	C	219	ASP	CB-CG-OD1	5.58	123.33	118.30
1	F	216	THR	N-CA-CB	5.58	120.91	110.30
1	G	405	LEU	CB-CG-CD2	5.58	120.49	111.00
1	R	275	PHE	CB-CG-CD2	-5.58	116.89	120.80
1	Q	527	ASP	CB-CG-OD1	5.58	123.32	118.30
1	O	456	MET	CG-SD-CE	5.58	109.13	100.20
1	C	454	ILE	CA-C-N	5.58	132.71	117.10
1	H	144	VAL	CA-CB-CG1	-5.57	102.54	110.90
1	G	388	ASP	CB-CG-OD2	5.57	123.31	118.30
1	G	472	ASP	CB-CG-OD1	5.57	123.31	118.30
1	M	219	ASP	CB-CG-OD1	5.57	123.31	118.30
1	B	432	TYR	CB-CG-CD1	5.57	124.34	121.00
1	F	346	ALA	N-CA-CB	-5.57	102.30	110.10
1	J	508	VAL	CA-CB-CG2	5.57	119.25	110.90
1	K	531	ALA	CB-CA-C	5.57	118.45	110.10
1	P	200	TYR	CB-CG-CD1	5.57	124.34	121.00
1	A	163	TYR	CG-CD2-CE2	-5.57	116.85	121.30
1	C	417	GLY	O-C-N	-5.57	113.74	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	410	MET	O-C-N	-5.56	113.81	122.70
1	C	396	ARG	CG-CD-NE	-5.56	100.12	111.80
1	N	464	LEU	O-C-N	-5.56	113.81	122.70
1	Q	176	GLU	CB-CA-C	-5.56	99.28	110.40
1	F	162	VAL	CG1-CB-CG2	-5.56	102.01	110.90
1	R	496	ASP	CB-CG-OD2	5.56	123.30	118.30
1	M	471	MET	CG-SD-CE	-5.55	91.31	100.20
1	R	102	ALA	N-CA-CB	5.55	117.88	110.10
1	D	396	ARG	NE-CZ-NH1	-5.55	117.52	120.30
1	Q	188	VAL	CA-CB-CG2	-5.55	102.57	110.90
1	J	239	ARG	NH1-CZ-NH2	-5.55	113.30	119.40
1	B	250	ASP	CB-CG-OD2	5.55	123.29	118.30
1	J	223	ILE	CA-CB-CG1	5.55	121.54	111.00
1	J	449	ASP	CB-CG-OD1	5.55	123.29	118.30
1	B	54	PHE	CB-CG-CD1	-5.54	116.92	120.80
1	N	164	THR	O-C-N	-5.54	113.83	122.70
1	O	239	ARG	NH1-CZ-NH2	-5.54	113.30	119.40
1	J	413	TYR	CG-CD1-CE1	5.54	125.73	121.30
1	E	445	GLU	OE1-CD-OE2	-5.54	116.65	123.30
1	A	454	ILE	C-N-CD	-5.54	108.41	120.60
1	J	296	ASN	N-CA-CB	5.54	120.57	110.60
1	I	436	VAL	CA-CB-CG2	5.53	119.20	110.90
1	P	47	ASP	CB-CG-OD1	5.53	123.28	118.30
1	D	369	PHE	CB-CG-CD2	-5.53	116.93	120.80
1	E	512	VAL	CG1-CB-CG2	5.53	119.75	110.90
1	Q	499	SER	N-CA-CB	5.53	118.80	110.50
1	K	230	LYS	N-CA-C	5.53	125.93	111.00
1	D	434	ARG	NE-CZ-NH1	-5.53	117.54	120.30
1	R	423	LEU	CB-CG-CD2	5.53	120.39	111.00
1	I	31	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	M	400	ASP	CB-CG-OD2	5.52	123.27	118.30
1	P	38	ARG	NE-CZ-NH2	5.52	123.06	120.30
1	M	197	ASP	CB-CG-OD2	5.52	123.27	118.30
1	B	435	SER	CB-CA-C	-5.52	99.61	110.10
1	I	84	ALA	N-CA-CB	-5.52	102.37	110.10
1	M	489	ILE	O-C-N	-5.52	113.87	122.70
1	N	282	TYR	CB-CG-CD1	-5.52	117.69	121.00
1	A	162	VAL	CA-CB-CG1	5.52	119.18	110.90
1	D	405	LEU	O-C-N	-5.51	113.88	122.70
1	K	126	PHE	CB-CG-CD2	-5.51	116.94	120.80
1	R	153	THR	O-C-N	-5.51	113.88	122.70
1	M	373	ALA	CB-CA-C	5.51	118.36	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	501	ASN	CA-CB-CG	-5.51	101.28	113.40
1	R	163	TYR	CG-CD1-CE1	-5.51	116.89	121.30
1	H	428	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	L	454	ILE	C-N-CD	-5.50	108.49	120.60
1	N	353	TYR	CG-CD1-CE1	-5.50	116.90	121.30
1	P	446	ALA	N-CA-CB	-5.50	102.39	110.10
1	P	507	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
1	E	384	ARG	NE-CZ-NH1	-5.50	117.55	120.30
1	F	267	THR	N-CA-CB	5.50	120.75	110.30
1	A	163	TYR	CB-CG-CD1	5.50	124.30	121.00
1	O	448	ALA	N-CA-CB	-5.50	102.40	110.10
1	P	282	TYR	CB-CG-CD1	5.50	124.30	121.00
1	O	167	SER	O-C-N	-5.50	113.91	122.70
1	H	449	ASP	O-C-N	-5.49	113.92	122.70
1	A	232	VAL	CG1-CB-CG2	-5.49	102.12	110.90
1	B	114	ASP	CB-CG-OD1	5.49	123.24	118.30
1	E	58	THR	CA-CB-CG2	-5.49	104.72	112.40
1	J	412	PRO	N-CD-CG	5.49	111.43	103.20
1	M	376	PRO	CA-N-CD	-5.49	103.82	111.50
1	D	130	PHE	CB-CG-CD2	-5.48	116.97	120.80
1	A	240	ARG	CD-NE-CZ	5.48	131.27	123.60
1	C	395	GLU	OE1-CD-OE2	-5.48	116.73	123.30
1	H	105	PHE	CG-CD1-CE1	-5.48	114.78	120.80
1	K	148	ASP	CB-CG-OD1	5.47	123.23	118.30
1	P	145	ASP	CB-CG-OD1	5.47	123.23	118.30
1	F	512	VAL	CG1-CB-CG2	5.47	119.65	110.90
1	H	153	THR	CA-CB-OG1	5.47	120.48	109.00
1	K	205	ASP	CB-CG-OD1	5.47	123.22	118.30
1	R	163	TYR	CG-CD2-CE2	-5.47	116.93	121.30
1	N	430	ARG	NE-CZ-NH1	5.47	123.03	120.30
1	B	126	PHE	CB-CG-CD1	5.46	124.62	120.80
1	M	233	VAL	N-CA-C	5.46	125.75	111.00
1	H	325	ARG	NE-CZ-NH1	-5.46	117.57	120.30
1	C	253	LEU	C-N-CA	5.46	135.35	121.70
1	C	455	PRO	CB-CA-C	5.46	125.64	112.00
1	M	182	ASP	CA-CB-CG	5.46	125.40	113.40
1	O	454	ILE	O-C-N	-5.46	110.73	121.10
1	F	449	ASP	CB-CG-OD2	5.45	123.21	118.30
1	M	88	ASP	CB-CG-OD2	-5.45	113.39	118.30
1	L	277	ASP	CB-CG-OD1	-5.45	113.39	118.30
1	O	93	ASP	CB-CG-OD2	5.45	123.20	118.30
1	Q	306	ASP	CB-CG-OD2	-5.45	113.39	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	R	224	ARG	NE-CZ-NH1	-5.45	117.58	120.30
1	D	47	ASP	O-C-N	-5.45	113.98	122.70
1	O	240	ARG	CG-CD-NE	-5.45	100.36	111.80
1	N	166	MET	CG-SD-CE	-5.45	91.48	100.20
1	D	70	MET	CG-SD-CE	5.45	108.91	100.20
1	J	34	ALA	O-C-N	-5.45	113.99	122.70
1	M	528	ASP	CB-CG-OD1	5.45	123.20	118.30
1	F	322	ARG	O-C-N	-5.44	113.99	122.70
1	B	266	ILE	CA-CB-CG1	5.44	121.34	111.00
1	C	38	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	C	373	ALA	CB-CA-C	5.44	118.26	110.10
1	D	255	VAL	CA-CB-CG2	-5.44	102.73	110.90
1	E	283	LEU	CB-CG-CD1	-5.44	101.75	111.00
1	B	263	LYS	O-C-N	-5.44	114.00	122.70
1	L	247	ALA	N-CA-CB	-5.44	102.48	110.10
1	C	282	TYR	CB-CG-CD2	5.44	124.26	121.00
1	N	466	PRO	N-CD-CG	5.44	111.36	103.20
1	M	495	ASP	CB-CG-OD1	5.43	123.19	118.30
1	N	88	ASP	CB-CG-OD2	5.43	123.19	118.30
1	R	156	ASP	CB-CG-OD1	-5.43	113.41	118.30
1	I	279	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	J	256	GLU	OE1-CD-OE2	-5.43	116.78	123.30
1	O	476	ARG	N-CA-CB	-5.43	100.83	110.60
1	R	221	GLN	CB-CA-C	5.42	121.25	110.40
1	C	507	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	N	489	ILE	CB-CA-C	-5.42	100.76	111.60
1	Q	20	ARG	NE-CZ-NH2	5.42	123.01	120.30
1	A	32	THR	OG1-CB-CG2	-5.42	97.54	110.00
1	F	17	ASN	N-CA-CB	5.42	120.35	110.60
1	H	434	ARG	CG-CD-NE	-5.42	100.43	111.80
1	E	233	VAL	CG1-CB-CG2	5.41	119.56	110.90
1	B	325	ARG	NE-CZ-NH2	5.41	123.01	120.30
1	A	270	ASP	CB-CG-OD2	5.41	123.17	118.30
1	D	226	ILE	O-C-N	-5.41	114.04	122.70
1	R	367	MET	CG-SD-CE	-5.41	91.54	100.20
1	E	413	TYR	CB-CG-CD1	5.41	124.25	121.00
1	M	322	ARG	NE-CZ-NH2	5.41	123.00	120.30
1	Q	411	GLU	CB-CA-C	5.41	121.21	110.40
1	A	18	SER	N-CA-C	-5.41	96.40	111.00
1	O	150	ASN	N-CA-CB	5.41	120.33	110.60
1	H	241	VAL	O-C-N	-5.40	114.06	122.70
1	Q	455	PRO	CB-CA-C	5.40	125.50	112.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	L	99	VAL	CG1-CB-CG2	-5.39	102.27	110.90
1	L	524	MET	CG-SD-CE	-5.39	91.57	100.20
1	A	229	ASP	N-CA-CB	-5.39	100.89	110.60
1	D	67	VAL	CA-CB-CG2	5.39	118.99	110.90
1	D	262	ALA	N-CA-CB	5.39	117.65	110.10
1	N	235	ALA	N-CA-CB	5.39	117.65	110.10
1	R	41	LEU	CB-CG-CD2	5.39	120.17	111.00
1	D	362	VAL	CA-CB-CG2	-5.39	102.82	110.90
1	K	495	ASP	CB-CG-OD1	-5.39	113.45	118.30
1	N	114	ASP	CB-CG-OD2	5.39	123.15	118.30
1	L	472	ASP	CB-CG-OD2	-5.39	113.45	118.30
1	I	305	ASP	CB-CG-OD2	-5.38	113.45	118.30
1	Q	362	VAL	CA-CB-CG1	-5.38	102.82	110.90
1	R	498	TYR	CB-CG-CD1	-5.38	117.77	121.00
1	D	461	THR	CA-CB-CG2	-5.38	104.86	112.40
1	R	197	ASP	O-C-N	-5.38	114.05	123.20
1	N	188	VAL	CG1-CB-CG2	-5.38	102.29	110.90
1	D	230	LYS	O-C-N	-5.38	114.09	122.70
1	J	463	GLY	O-C-N	-5.38	114.09	122.70
1	Q	273	LYS	CB-CA-C	-5.38	99.64	110.40
1	F	147	SER	N-CA-CB	5.38	118.56	110.50
1	N	69	GLU	OE1-CD-OE2	-5.38	116.85	123.30
1	N	476	ARG	CB-CG-CD	5.38	125.58	111.60
1	P	233	VAL	N-CA-C	5.38	125.52	111.00
1	C	156	ASP	CB-CG-OD2	5.37	123.13	118.30
1	I	232	VAL	CG1-CB-CG2	5.37	119.49	110.90
1	R	155	ARG	N-CA-C	5.37	125.50	111.00
1	D	54	PHE	CB-CG-CD2	-5.37	117.04	120.80
1	M	155	ARG	N-CA-C	5.37	125.49	111.00
1	Q	254	GLU	N-CA-CB	-5.37	100.94	110.60
1	P	275	PHE	CZ-CE2-CD2	5.37	126.54	120.10
1	H	322	ARG	N-CA-C	5.36	125.48	111.00
1	I	384	ARG	CG-CD-NE	-5.36	100.54	111.80
1	Q	474	ARG	NE-CZ-NH2	5.36	122.98	120.30
1	H	135	GLU	CG-CD-OE2	5.36	129.02	118.30
1	L	162	VAL	CA-CB-CG2	5.36	118.94	110.90
1	J	393	GLU	OE1-CD-OE2	-5.36	116.87	123.30
1	M	306	ASP	CB-CG-OD1	5.36	123.12	118.30
1	E	369	PHE	CG-CD2-CE2	5.35	126.69	120.80
1	E	327	ASP	CB-CG-OD2	-5.35	113.48	118.30
1	H	422	GLU	O-C-N	-5.35	114.14	122.70
1	E	97	SER	CB-CA-C	-5.35	99.93	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	432	TYR	CD1-CE1-CZ	-5.35	114.99	119.80
1	H	210	ASP	CB-CG-OD2	5.35	123.11	118.30
1	I	124	GLU	CA-C-N	5.35	126.89	116.20
1	F	413	TYR	CB-CG-CD2	-5.35	117.79	121.00
1	G	30	ALA	N-CA-CB	-5.35	102.62	110.10
1	L	31	ARG	CD-NE-CZ	-5.35	116.12	123.60
1	D	321	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	M	200	TYR	CB-CG-CD2	-5.34	117.79	121.00
1	P	228	LEU	N-CA-CB	5.34	121.09	110.40
1	O	349	GLU	OE1-CD-OE2	-5.34	116.89	123.30
1	R	428	ARG	NE-CZ-NH1	-5.34	117.63	120.30
1	A	341	SER	N-CA-CB	5.34	118.51	110.50
1	F	370	ILE	O-C-N	-5.34	114.15	122.70
1	B	488	VAL	CA-CB-CG1	-5.34	102.89	110.90
1	E	155	ARG	NE-CZ-NH2	5.34	122.97	120.30
1	L	454	ILE	O-C-N	-5.34	110.96	121.10
1	B	170	PHE	CD1-CE1-CZ	-5.34	113.70	120.10
1	D	304	ILE	O-C-N	-5.34	114.16	122.70
1	B	165	THR	CA-CB-CG2	-5.33	104.93	112.40
1	E	335	LEU	CB-CG-CD2	5.33	120.07	111.00
1	F	455	PRO	N-CA-CB	5.33	109.70	103.30
1	L	455	PRO	CB-CA-C	5.33	125.33	112.00
1	L	519	ALA	O-C-N	-5.33	114.17	122.70
1	A	396	ARG	NE-CZ-NH1	5.33	122.97	120.30
1	F	455	PRO	CB-CA-C	5.33	125.33	112.00
1	J	142	THR	O-C-N	-5.33	114.17	122.70
1	F	37	LEU	O-C-N	-5.33	114.18	122.70
1	M	240	ARG	NH1-CZ-NH2	-5.33	113.54	119.40
1	N	384	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	R	270	ASP	O-C-N	-5.33	114.18	122.70
1	C	486	VAL	CA-CB-CG2	-5.32	102.91	110.90
1	I	400	ASP	N-CA-CB	-5.32	101.02	110.60
1	M	38	ARG	CD-NE-CZ	5.32	131.05	123.60
1	H	364	ASN	N-CA-CB	5.32	120.18	110.60
1	M	430	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	N	16	ARG	NE-CZ-NH2	5.32	122.96	120.30
1	N	428	ARG	CG-CD-NE	-5.32	100.63	111.80
1	R	420	ALA	N-CA-CB	-5.32	102.65	110.10
1	J	353	TYR	CB-CG-CD2	5.32	124.19	121.00
1	M	521	THR	N-CA-CB	5.32	120.40	110.30
1	C	242	GLU	CB-CA-C	5.31	121.02	110.40
1	A	20	ARG	NE-CZ-NH1	-5.31	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	470	LEU	O-C-N	-5.31	114.21	122.70
1	Q	423	LEU	CB-CG-CD2	5.31	120.03	111.00
1	J	183	ILE	O-C-N	-5.31	114.21	122.70
1	O	305	ASP	CB-CG-OD2	5.31	123.08	118.30
1	O	379	VAL	CA-CB-CG1	-5.31	102.94	110.90
1	R	313	ALA	CB-CA-C	5.31	118.06	110.10
1	F	426	SER	N-CA-CB	5.30	118.45	110.50
1	K	507	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	B	481	LEU	CB-CG-CD2	5.30	120.00	111.00
1	N	338	ARG	NH1-CZ-NH2	5.30	125.23	119.40
1	P	447	TYR	CD1-CG-CD2	5.30	123.72	117.90
1	C	488	VAL	O-C-N	-5.29	114.23	122.70
1	L	254	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	O	476	ARG	NE-CZ-NH2	5.29	122.95	120.30
1	P	65	THR	O-C-N	-5.29	114.23	122.70
1	P	424	GLU	OE1-CD-OE2	-5.29	116.95	123.30
1	B	522	SER	CA-C-N	5.29	128.84	117.20
1	B	155	ARG	N-CA-C	5.29	125.28	111.00
1	I	438	GLY	N-CA-C	5.29	126.33	113.10
1	B	246	ILE	O-C-N	-5.29	114.24	122.70
1	L	486	VAL	CA-CB-CG1	5.29	118.83	110.90
1	M	288	ASP	O-C-N	-5.29	114.24	122.70
1	P	197	ASP	CB-CG-OD1	5.29	123.06	118.30
1	Q	39	SER	CB-CA-C	-5.29	100.06	110.10
1	R	236	GLY	C-N-CA	5.29	134.91	121.70
1	E	362	VAL	O-C-N	-5.28	114.22	123.20
1	R	507	ARG	N-CA-CB	-5.28	101.09	110.60
1	I	191	VAL	CA-CB-CG2	-5.28	102.98	110.90
1	N	302	LYS	O-C-N	-5.28	114.22	123.20
1	O	331	LEU	CB-CG-CD2	5.28	119.98	111.00
1	P	433	ALA	N-CA-C	5.28	125.26	111.00
1	A	528	ASP	CB-CG-OD2	-5.28	113.55	118.30
1	O	38	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
1	R	113	VAL	O-C-N	-5.28	114.26	122.70
1	M	239	ARG	NE-CZ-NH1	-5.27	117.66	120.30
1	D	273	LYS	O-C-N	-5.27	114.27	122.70
1	I	219	ASP	O-C-N	-5.27	114.26	122.70
1	R	146	VAL	O-C-N	-5.27	114.26	122.70
1	G	211	LYS	CB-CA-C	5.27	120.94	110.40
1	F	292	SER	CB-CA-C	-5.27	100.09	110.10
1	L	517	THR	CA-CB-CG2	-5.27	105.02	112.40
1	Q	219	ASP	CB-CG-OD2	5.27	123.04	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	311	PHE	CB-CG-CD2	5.27	124.49	120.80
1	O	62	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	C	202	VAL	CB-CA-C	-5.26	101.40	111.40
1	D	373	ALA	O-C-N	-5.26	114.28	122.70
1	E	396	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	I	310	HIS	CA-C-O	5.26	131.15	120.10
1	E	436	VAL	CG1-CB-CG2	-5.26	102.48	110.90
1	R	456	MET	CG-SD-CE	-5.26	91.78	100.20
1	A	291	ALA	N-CA-CB	5.26	117.46	110.10
1	D	72	ILE	CA-CB-CG2	-5.26	100.38	110.90
1	E	517	THR	CA-CB-CG2	-5.26	105.04	112.40
1	H	31	ARG	NE-CZ-NH2	5.26	122.93	120.30
1	C	350	ASP	C-N-CA	5.26	134.85	121.70
1	R	360	ARG	NH1-CZ-NH2	5.26	125.18	119.40
1	F	79	LEU	CB-CG-CD2	5.26	119.94	111.00
1	P	138	PRO	C-N-CA	5.26	134.84	121.70
1	A	315	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
1	B	186	ASP	CB-CG-OD1	5.25	123.03	118.30
1	G	135	GLU	O-C-N	-5.25	114.30	122.70
1	H	287	VAL	CA-CB-CG1	5.25	118.78	110.90
1	O	313	ALA	CA-C-O	-5.25	109.07	120.10
1	R	239	ARG	NE-CZ-NH1	5.25	122.93	120.30
1	P	79	LEU	CB-CG-CD1	-5.25	102.08	111.00
1	K	360	ARG	NE-CZ-NH2	5.25	122.92	120.30
1	A	223	ILE	CA-CB-CG1	5.25	120.97	111.00
1	D	406	ARG	N-CA-CB	-5.25	101.16	110.60
1	I	461	THR	CA-CB-CG2	-5.25	105.05	112.40
1	O	223	ILE	CA-CB-CG1	5.25	120.97	111.00
1	C	41	LEU	O-C-N	-5.24	114.29	123.20
1	M	170	PHE	CB-CG-CD1	5.24	124.47	120.80
1	I	353	TYR	CG-CD2-CE2	-5.24	117.11	121.30
1	N	460	GLU	CB-CA-C	-5.24	99.92	110.40
1	O	297	VAL	CG1-CB-CG2	-5.24	102.52	110.90
1	P	225	GLY	O-C-N	-5.24	114.32	122.70
1	R	256	GLU	OE1-CD-OE2	-5.24	117.01	123.30
1	E	16	ARG	NE-CZ-NH2	5.24	122.92	120.30
1	P	195	LEU	CB-CG-CD2	5.24	119.90	111.00
1	F	447	TYR	CG-CD2-CE2	-5.24	117.11	121.30
1	I	117	ILE	CB-CA-C	5.23	122.07	111.60
1	C	275	PHE	CB-CG-CD1	-5.23	117.14	120.80
1	G	403	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	K	153	THR	OG1-CB-CG2	-5.23	97.97	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	H	189	THR	O-C-N	-5.23	114.33	122.70
1	R	188	VAL	O-C-N	-5.23	114.33	122.70
1	R	275	PHE	CB-CG-CD1	5.23	124.46	120.80
1	J	498	TYR	CB-CG-CD1	-5.23	117.86	121.00
1	R	69	GLU	O-C-N	-5.23	114.34	122.70
1	A	168	SER	O-C-N	-5.22	114.34	122.70
1	A	303	GLY	N-CA-C	5.22	126.16	113.10
1	H	229	ASP	CB-CG-OD1	-5.22	113.60	118.30
1	I	512	VAL	CA-CB-CG1	-5.22	103.06	110.90
1	M	347	THR	O-C-N	-5.22	111.17	121.10
1	N	369	PHE	CB-CA-C	-5.22	99.95	110.40
1	H	286	MET	O-C-N	-5.22	114.34	122.70
1	N	384	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	M	496	ASP	O-C-N	-5.22	114.35	122.70
1	A	52	ASP	O-C-N	-5.22	114.35	122.70
1	E	447	TYR	CB-CG-CD2	5.22	124.13	121.00
1	F	72	ILE	CB-CA-C	-5.22	101.16	111.60
1	H	147	SER	N-CA-CB	5.22	118.33	110.50
1	I	392	ASP	CB-CG-OD2	5.22	123.00	118.30
1	F	149	LEU	N-CA-CB	5.22	120.84	110.40
1	M	38	ARG	NE-CZ-NH2	5.22	122.91	120.30
1	C	360	ARG	O-C-N	-5.22	114.35	122.70
1	J	192	ALA	CB-CA-C	5.22	117.92	110.10
1	P	299	ILE	CB-CA-C	-5.22	101.17	111.60
1	Q	209	ILE	CB-CA-C	-5.22	101.17	111.60
1	N	147	SER	O-C-N	-5.21	114.36	122.70
1	C	297	VAL	CA-CB-CG1	5.21	118.72	110.90
1	C	498	TYR	CB-CG-CD1	5.21	124.13	121.00
1	F	469	ALA	CB-CA-C	-5.21	102.28	110.10
1	I	282	TYR	CB-CG-CD1	-5.21	117.87	121.00
1	A	455	PRO	CB-CA-C	5.21	125.02	112.00
1	F	184	VAL	CA-CB-CG2	-5.21	103.09	110.90
1	H	476	ARG	CB-CA-C	-5.21	99.98	110.40
1	K	105	PHE	CG-CD2-CE2	-5.21	115.07	120.80
1	D	331	LEU	CB-CG-CD1	-5.21	102.15	111.00
1	G	62	ASP	CB-CG-OD1	5.21	122.99	118.30
1	P	285	ASP	CB-CG-OD2	-5.21	113.61	118.30
1	E	291	ALA	CB-CA-C	-5.20	102.30	110.10
1	H	146	VAL	CB-CA-C	-5.20	101.52	111.40
1	A	190	THR	N-CA-CB	5.20	120.18	110.30
1	C	170	PHE	CG-CD1-CE1	5.20	126.52	120.80
1	L	469	ALA	CB-CA-C	-5.20	102.31	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	M	313	ALA	CB-CA-C	-5.20	102.31	110.10
1	D	203	SER	N-CA-CB	5.19	118.29	110.50
1	H	332	GLU	OE1-CD-OE2	-5.19	117.07	123.30
1	N	505	PRO	N-CA-CB	5.19	109.53	103.30
1	L	531	ALA	O-C-N	-5.19	114.40	122.70
1	O	114	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	G	306	ASP	CB-CG-OD1	5.18	122.97	118.30
1	A	115	GLN	O-C-N	-5.18	114.41	122.70
1	M	253	LEU	CB-CG-CD2	-5.18	102.19	111.00
1	P	430	ARG	CD-NE-CZ	5.18	130.86	123.60
1	B	70	MET	CA-CB-CG	5.18	122.11	113.30
1	B	75	PRO	N-CA-CB	5.18	109.52	103.30
1	C	232	VAL	CA-CB-CG1	5.18	118.67	110.90
1	C	322	ARG	N-CA-C	5.18	124.98	111.00
1	L	38	ARG	O-C-N	-5.18	114.41	122.70
1	N	449	ASP	CB-CG-OD2	-5.18	113.64	118.30
1	Q	531	ALA	N-CA-CB	5.18	117.35	110.10
1	E	501	ASN	CA-CB-CG	-5.18	102.01	113.40
1	H	435	SER	C-N-CA	5.18	134.64	121.70
1	C	384	ARG	NE-CZ-NH1	-5.18	117.71	120.30
1	D	389	MET	CG-SD-CE	-5.18	91.92	100.20
1	I	329	GLU	CA-CB-CG	-5.18	102.01	113.40
1	D	501	ASN	O-C-N	-5.17	114.42	122.70
1	F	425	LEU	O-C-N	-5.17	114.42	122.70
1	H	507	ARG	CD-NE-CZ	5.17	130.84	123.60
1	I	308	ALA	CB-CA-C	-5.17	102.34	110.10
1	H	186	ASP	CB-CG-OD1	5.17	122.96	118.30
1	F	156	ASP	O-C-N	-5.17	114.42	122.70
1	A	337	ALA	N-CA-CB	5.17	117.34	110.10
1	B	249	LEU	CB-CA-C	-5.17	100.38	110.20
1	G	504	GLU	O-C-N	-5.17	111.28	121.10
1	O	100	VAL	O-C-N	-5.17	114.43	122.70
1	J	450	ALA	O-C-N	-5.17	114.43	122.70
1	K	403	TYR	CA-CB-CG	-5.17	103.58	113.40
1	D	200	TYR	CB-CG-CD2	5.17	124.10	121.00
1	R	396	ARG	NH1-CZ-NH2	-5.17	113.72	119.40
1	J	107	GLU	CB-CA-C	-5.16	100.07	110.40
1	J	260	ILE	N-CA-CB	5.16	122.67	110.80
1	E	495	ASP	CB-CG-OD2	-5.16	113.65	118.30
1	H	306	ASP	CB-CG-OD2	5.16	122.94	118.30
1	B	384	ARG	NE-CZ-NH2	5.16	122.88	120.30
1	D	31	ARG	NE-CZ-NH2	5.16	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	334	ALA	N-CA-CB	-5.16	102.88	110.10
1	H	259	GLU	OE1-CD-OE2	-5.16	117.11	123.30
1	O	474	ARG	NH1-CZ-NH2	-5.16	113.73	119.40
1	O	498	TYR	CB-CG-CD2	-5.16	117.91	121.00
1	C	261	SER	N-CA-CB	5.16	118.24	110.50
1	G	166	MET	N-CA-CB	-5.16	101.32	110.60
1	M	512	VAL	CA-CB-CG2	5.16	118.63	110.90
1	Q	123	ILE	O-C-N	-5.16	114.45	122.70
1	L	447	TYR	CB-CG-CD2	-5.15	117.91	121.00
1	O	498	TYR	CG-CD2-CE2	-5.15	117.18	121.30
1	A	108	LYS	CA-C-O	5.15	130.92	120.10
1	L	170	PHE	CD1-CG-CD2	5.15	124.99	118.30
1	C	134	LEU	CB-CG-CD2	5.15	119.75	111.00
1	I	227	VAL	CA-CB-CG2	5.14	118.62	110.90
1	O	172	ALA	N-CA-CB	-5.14	102.90	110.10
1	Q	183	ILE	O-C-N	-5.14	114.47	122.70
1	B	384	ARG	NE-CZ-NH1	-5.14	117.73	120.30
1	D	23	LEU	N-CA-CB	-5.14	100.12	110.40
1	L	315	ARG	CB-CA-C	-5.14	100.12	110.40
1	A	31	ARG	NE-CZ-NH2	-5.14	117.73	120.30
1	A	186	ASP	CB-CG-OD1	5.14	122.92	118.30
1	F	163	TYR	CB-CG-CD2	-5.14	117.92	121.00
1	K	353	TYR	CG-CD2-CE2	-5.14	117.19	121.30
1	D	449	ASP	CB-CG-OD1	5.14	122.92	118.30
1	G	431	GLU	OE1-CD-OE2	-5.14	117.14	123.30
1	H	351	LEU	O-C-N	-5.14	114.47	123.20
1	B	64	ALA	O-C-N	5.13	130.92	122.70
1	F	406	ARG	O-C-N	-5.13	114.48	122.70
1	I	432	TYR	CZ-CE2-CD2	5.13	124.42	119.80
1	I	472	ASP	CB-CG-OD2	5.13	122.92	118.30
1	K	360	ARG	NH1-CZ-NH2	-5.13	113.75	119.40
1	M	400	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	N	369	PHE	CB-CG-CD1	5.13	124.39	120.80
1	P	476	ARG	NE-CZ-NH1	-5.13	117.73	120.30
1	F	453	GLU	CB-CA-C	-5.13	100.13	110.40
1	I	64	ALA	N-CA-CB	-5.13	102.92	110.10
1	K	232	VAL	CA-CB-CG2	5.13	118.60	110.90
1	L	522	SER	O-C-N	-5.13	114.49	122.70
1	N	206	LEU	CB-CG-CD2	5.13	119.72	111.00
1	O	406	ARG	CD-NE-CZ	5.13	130.78	123.60
1	I	121	ILE	CA-CB-CG2	-5.13	100.64	110.90
1	K	384	ARG	NE-CZ-NH2	-5.13	117.74	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	105	PHE	CB-CG-CD1	5.12	124.39	120.80
1	A	311	PHE	CB-CG-CD1	5.12	124.39	120.80
1	A	321	ARG	CD-NE-CZ	5.12	130.77	123.60
1	B	104	LEU	N-CA-CB	5.12	120.64	110.40
1	N	413	TYR	CG-CD2-CE2	-5.12	117.20	121.30
1	G	88	ASP	O-C-N	-5.12	114.51	122.70
1	A	112	LEU	O-C-N	-5.12	114.51	122.70
1	F	266	ILE	O-C-N	-5.12	114.51	122.70
1	F	410	MET	CG-SD-CE	-5.12	92.01	100.20
1	L	318	LEU	CB-CG-CD2	5.12	119.70	111.00
1	A	235	ALA	CA-C-N	5.12	126.43	116.20
1	D	428	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	C	447	TYR	CB-CG-CD1	-5.11	117.93	121.00
1	O	54	PHE	CG-CD1-CE1	-5.11	115.18	120.80
1	G	143	LYS	CA-CB-CG	5.11	124.64	113.40
1	I	392	ASP	CB-CA-C	5.11	120.62	110.40
1	K	358	GLU	OE1-CD-OE2	-5.11	117.17	123.30
1	J	282	TYR	CZ-CE2-CD2	-5.11	115.20	119.80
1	R	170	PHE	CB-CA-C	-5.11	100.19	110.40
1	H	414	ILE	CA-CB-CG2	-5.11	100.69	110.90
1	I	182	ASP	O-C-N	-5.10	114.53	122.70
1	J	170	PHE	CB-CG-CD1	-5.10	117.23	120.80
1	B	283	LEU	N-CA-CB	5.10	120.60	110.40
1	C	229	ASP	CB-CG-OD1	5.10	122.89	118.30
1	L	178	ASN	CB-CA-C	-5.10	100.19	110.40
1	N	223	ILE	O-C-N	-5.10	114.54	122.70
1	O	91	VAL	CB-CA-C	-5.10	101.71	111.40
1	F	447	TYR	CB-CG-CD1	-5.10	117.94	121.00
1	G	240	ARG	NE-CZ-NH1	5.10	122.85	120.30
1	K	20	ARG	NH1-CZ-NH2	-5.10	113.79	119.40
1	R	315	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	L	17	ASN	N-CA-CB	5.10	119.77	110.60
1	O	391	LEU	CB-CG-CD1	-5.10	102.33	111.00
1	H	450	ALA	N-CA-CB	-5.10	102.97	110.10
1	I	342	SER	N-CA-CB	5.10	118.14	110.50
1	B	344	LYS	CA-CB-CG	5.09	124.61	113.40
1	H	168	SER	CB-CA-C	-5.09	100.42	110.10
1	J	87	GLN	CG-CD-OE1	-5.09	111.41	121.60
1	M	212	LYS	N-CA-CB	5.09	119.77	110.60
1	N	498	TYR	O-C-N	-5.09	114.55	122.70
1	C	223	ILE	O-C-N	-5.09	114.55	122.70
1	N	320	VAL	CA-C-N	5.09	128.40	117.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	181	MET	CG-SD-CE	5.09	108.34	100.20
1	N	288	ASP	CB-CG-OD2	5.09	122.88	118.30
1	O	315	ARG	CG-CD-NE	-5.09	101.11	111.80
1	R	70	MET	CA-CB-CG	5.09	121.95	113.30
1	H	503	VAL	O-C-N	-5.09	114.56	122.70
1	R	520	ALA	N-CA-CB	-5.09	102.98	110.10
1	E	131	ASN	CA-CB-CG	-5.09	102.21	113.40
1	E	134	LEU	CB-CG-CD2	5.09	119.65	111.00
1	F	74	HIS	CB-CA-C	-5.09	100.23	110.40
1	I	200	TYR	CZ-CE2-CD2	-5.09	115.22	119.80
1	G	369	PHE	CB-CG-CD2	5.08	124.36	120.80
1	J	496	ASP	N-CA-C	5.08	124.73	111.00
1	G	166	MET	CA-CB-CG	5.08	121.94	113.30
1	I	406	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	L	54	PHE	CB-CG-CD1	5.08	124.36	120.80
1	R	21	ASP	CB-CG-OD2	5.08	122.87	118.30
1	N	430	ARG	NE-CZ-NH2	5.08	122.84	120.30
1	A	384	ARG	NE-CZ-NH1	5.08	122.84	120.30
1	E	379	VAL	N-CA-CB	5.08	122.67	111.50
1	J	130	PHE	CB-CG-CD1	-5.08	117.24	120.80
1	Q	397	SER	N-CA-CB	5.08	118.11	110.50
1	C	23	LEU	CB-CG-CD2	-5.08	102.37	111.00
1	G	404	SER	O-C-N	-5.08	114.58	122.70
1	H	129	ALA	N-CA-CB	-5.08	103.00	110.10
1	D	324	LYS	CB-CA-C	-5.07	100.25	110.40
1	H	237	MET	N-CA-CB	-5.07	101.47	110.60
1	O	148	ASP	CB-CG-OD2	5.07	122.86	118.30
1	F	461	THR	CA-CB-CG2	-5.07	105.30	112.40
1	L	406	ARG	NH1-CZ-NH2	-5.07	113.82	119.40
1	E	462	ALA	CB-CA-C	-5.07	102.50	110.10
1	I	240	ARG	NH1-CZ-NH2	-5.07	113.83	119.40
1	R	403	TYR	CG-CD1-CE1	-5.07	117.25	121.30
1	G	114	ASP	CB-CG-OD2	5.07	122.86	118.30
1	H	98	ALA	CB-CA-C	-5.07	102.50	110.10
1	L	31	ARG	O-C-N	-5.07	114.60	122.70
1	O	215	GLY	O-C-N	-5.07	114.59	122.70
1	J	526	ILE	C-N-CA	5.06	134.36	121.70
1	D	286	MET	CA-CB-CG	5.06	121.91	113.30
1	F	507	ARG	NH1-CZ-NH2	-5.06	113.83	119.40
1	G	356	LEU	CB-CG-CD2	5.06	119.61	111.00
1	P	95	THR	CA-CB-CG2	5.06	119.49	112.40
1	P	384	ARG	CB-CA-C	-5.06	100.28	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	P	137	LEU	CA-C-N	5.06	131.26	117.10
1	G	261	SER	N-CA-C	-5.06	97.35	111.00
1	H	35	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	J	279	GLU	OE1-CD-OE2	-5.06	117.23	123.30
1	L	249	LEU	CB-CG-CD1	5.06	119.59	111.00
1	K	56	ASP	CB-CG-OD1	5.05	122.85	118.30
1	I	297	VAL	CA-CB-CG1	5.05	118.48	110.90
1	M	353	TYR	CG-CD2-CE2	-5.05	117.26	121.30
1	R	454	ILE	C-N-CD	-5.05	109.48	120.60
1	Q	498	TYR	CZ-CE2-CD2	5.05	124.35	119.80
1	F	321	ARG	NE-CZ-NH2	5.05	122.83	120.30
1	J	339	ILE	O-C-N	-5.05	114.62	122.70
1	K	457	ILE	CB-CA-C	5.05	121.70	111.60
1	E	322	ARG	N-CA-C	5.05	124.63	111.00
1	I	369	PHE	CG-CD1-CE1	-5.05	115.25	120.80
1	J	221	GLN	CA-CB-CG	5.05	124.51	113.40
1	M	186	ASP	CA-CB-CG	5.05	124.51	113.40
1	I	98	ALA	N-CA-CB	5.05	117.17	110.10
1	M	244	ALA	CB-CA-C	5.05	117.67	110.10
1	G	205	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	I	476	ARG	NE-CZ-NH1	-5.04	117.78	120.30
1	N	338	ARG	CD-NE-CZ	-5.04	116.54	123.60
1	O	229	ASP	CB-CG-OD1	5.04	122.84	118.30
1	R	70	MET	CG-SD-CE	-5.04	92.13	100.20
1	A	186	ASP	N-CA-CB	-5.04	101.53	110.60
1	I	38	ARG	CG-CD-NE	-5.04	101.21	111.80
1	C	387	ASN	CA-CB-CG	-5.04	102.32	113.40
1	P	513	LEU	CB-CG-CD1	-5.04	102.44	111.00
1	A	176	GLU	OE1-CD-OE2	-5.04	117.25	123.30
1	B	163	TYR	CG-CD2-CE2	-5.04	117.27	121.30
1	E	369	PHE	CB-CG-CD1	5.04	124.33	120.80
1	H	70	MET	CG-SD-CE	-5.04	92.14	100.20
1	N	358	GLU	N-CA-CB	-5.04	101.53	110.60
1	Q	237	MET	CG-SD-CE	-5.04	92.14	100.20
1	A	47	ASP	O-C-N	-5.03	114.64	122.70
1	H	472	ASP	N-CA-CB	-5.03	101.54	110.60
1	G	170	PHE	CB-CG-CD2	-5.03	117.28	120.80
1	H	155	ARG	N-CA-C	5.03	124.58	111.00
1	L	428	ARG	CD-NE-CZ	5.03	130.64	123.60
1	A	135	GLU	CA-CB-CG	5.03	124.46	113.40
1	L	431	GLU	N-CA-CB	5.03	119.65	110.60
1	G	288	ASP	CB-CG-OD1	5.03	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	445	GLU	CA-CB-CG	5.03	124.45	113.40
1	O	512	VAL	CA-CB-CG1	-5.03	103.36	110.90
1	H	115	GLN	C-N-CA	5.02	134.26	121.70
1	J	50	LEU	CB-CG-CD2	-5.02	102.46	111.00
1	A	427	ALA	N-CA-CB	-5.02	103.07	110.10
1	D	54	PHE	O-C-N	-5.02	114.66	123.20
1	H	145	ASP	CB-CA-C	5.02	120.45	110.40
1	B	276	LEU	CB-CG-CD2	-5.02	102.47	111.00
1	I	107	GLU	N-CA-CB	-5.02	101.57	110.60
1	O	452	GLU	OE1-CD-OE2	-5.02	117.28	123.30
1	B	325	ARG	O-C-N	-5.02	114.67	122.70
1	B	239	ARG	NE-CZ-NH1	-5.01	117.79	120.30
1	C	170	PHE	CD1-CE1-CZ	-5.01	114.08	120.10
1	C	403	TYR	CG-CD1-CE1	-5.01	117.29	121.30
1	G	321	ARG	NH1-CZ-NH2	5.01	124.92	119.40
1	B	441	GLN	CG-CD-OE1	-5.01	111.58	121.60
1	G	218	GLU	CG-CD-OE2	-5.01	108.28	118.30
1	G	312	LEU	CB-CA-C	-5.01	100.68	110.20
1	M	107	GLU	O-C-N	-5.01	114.68	122.70
1	Q	380	ASN	CB-CG-OD1	-5.01	111.58	121.60
1	A	115	GLN	C-N-CA	5.01	134.22	121.70
1	F	51	ILE	CB-CA-C	-5.01	101.58	111.60
1	G	347	THR	CA-CB-CG2	5.01	119.41	112.40
1	I	231	GLU	CB-CA-C	-5.01	100.38	110.40
1	J	454	ILE	C-N-CD	-5.01	109.58	120.60
1	M	323	VAL	CA-CB-CG1	5.01	118.41	110.90
1	N	362	VAL	CA-CB-CG2	-5.01	103.39	110.90
1	Q	228	LEU	CB-CG-CD1	-5.01	102.48	111.00
1	H	366	LYS	N-CA-CB	5.01	119.61	110.60
1	K	360	ARG	CB-CA-C	-5.01	100.38	110.40
1	H	239	ARG	NE-CZ-NH1	-5.01	117.80	120.30
1	H	507	ARG	O-C-N	-5.01	114.69	122.70
1	R	173	GLU	O-C-N	-5.01	114.69	123.20
1	O	432	TYR	CB-CG-CD2	-5.00	118.00	121.00
1	F	510	ARG	NE-CZ-NH2	5.00	122.80	120.30
1	I	146	VAL	CG1-CB-CG2	5.00	118.91	110.90
1	K	323	VAL	CA-CB-CG2	-5.00	103.39	110.90
1	L	338	ARG	NH1-CZ-NH2	5.00	124.90	119.40

There are no chirality outliers.

All (355) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	126	PHE	Sidechain
1	A	147	SER	Peptide
1	A	154	ALA	Peptide
1	A	163	TYR	Sidechain
1	A	169	LYS	Mainchain
1	A	193	GLU	Peptide
1	A	213	LYS	Peptide
1	A	239	ARG	Sidechain
1	A	260	ILE	Peptide
1	A	267	THR	Peptide
1	A	321	ARG	Sidechain
1	A	347	THR	Peptide
1	A	353	TYR	Sidechain
1	A	360	ARG	Sidechain
1	A	384	ARG	Sidechain
1	A	428	ARG	Sidechain
1	A	432	TYR	Sidechain
1	A	447	TYR	Sidechain
1	A	454	ILE	Mainchain
1	A	510	ARG	Sidechain
1	A	74	HIS	Sidechain
1	B	154	ALA	Peptide
1	B	16	ARG	Sidechain
1	B	163	TYR	Sidechain
1	B	170	PHE	Sidechain
1	B	193	GLU	Peptide
1	B	234	HIS	Sidechain
1	B	239	ARG	Sidechain
1	B	260	ILE	Peptide
1	B	267	THR	Peptide
1	B	31	ARG	Sidechain
1	B	338	ARG	Peptide
1	B	347	THR	Peptide
1	B	360	ARG	Sidechain
1	B	413	TYR	Sidechain
1	B	432	TYR	Sidechain
1	B	454	ILE	Mainchain
1	B	476	ARG	Sidechain
1	B	507	ARG	Sidechain
1	B	510	ARG	Sidechain
1	C	130	PHE	Sidechain
1	C	154	ALA	Peptide
1	C	155	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	C	191	VAL	Peptide
1	C	193	GLU	Peptide
1	C	20	ARG	Sidechain
1	C	201	ASN	Mainchain
1	C	224	ARG	Sidechain
1	C	232	VAL	Peptide
1	C	239	ARG	Sidechain
1	C	260	ILE	Peptide
1	C	267	THR	Peptide
1	C	282	TYR	Sidechain
1	C	321	ARG	Sidechain
1	C	322	ARG	Sidechain
1	C	325	ARG	Sidechain
1	C	347	THR	Peptide
1	C	38	ARG	Sidechain
1	C	384	ARG	Sidechain
1	C	396	ARG	Sidechain
1	C	413	TYR	Sidechain
1	C	447	TYR	Sidechain
1	C	454	ILE	Mainchain
1	D	154	ALA	Mainchain,Peptide
1	D	193	GLU	Peptide
1	D	200	TYR	Sidechain
1	D	239	ARG	Sidechain
1	D	240	ARG	Sidechain
1	D	260	ILE	Peptide
1	D	267	THR	Peptide
1	D	268	SER	Peptide
1	D	31	ARG	Sidechain
1	D	338	ARG	Sidechain
1	D	347	THR	Peptide
1	D	353	TYR	Sidechain
1	D	369	PHE	Sidechain
1	D	384	ARG	Sidechain
1	D	432	TYR	Sidechain
1	D	434	ARG	Sidechain
1	D	447	TYR	Sidechain
1	D	495	ASP	Peptide
1	D	498	TYR	Sidechain
1	D	507	ARG	Sidechain
1	E	154	ALA	Peptide
1	E	191	VAL	Peptide

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Mol	Chain	Res	Type	Group
1	E	224	ARG	Sidechain
1	E	239	ARG	Sidechain
1	E	260	ILE	Peptide
1	E	267	THR	Peptide
1	E	275	PHE	Sidechain
1	E	282	TYR	Sidechain
1	E	311	PHE	Sidechain
1	E	325	ARG	Sidechain
1	E	338	ARG	Peptide
1	E	346	ALA	Peptide
1	E	347	THR	Peptide
1	E	447	TYR	Sidechain
1	E	454	ILE	Mainchain
1	E	474	ARG	Sidechain
1	E	476	ARG	Sidechain
1	E	510	ARG	Sidechain
1	E	95	THR	Mainchain
1	F	154	ALA	Peptide
1	F	16	ARG	Sidechain
1	F	193	GLU	Peptide
1	F	200	TYR	Sidechain
1	F	260	ILE	Peptide
1	F	267	THR	Peptide
1	F	31	ARG	Sidechain
1	F	325	ARG	Sidechain
1	F	338	ARG	Peptide
1	F	347	THR	Peptide
1	F	384	ARG	Sidechain
1	F	432	TYR	Sidechain
1	F	498	TYR	Sidechain
1	F	504	GLU	Peptide
1	F	54	PHE	Sidechain
1	G	154	ALA	Peptide
1	G	191	VAL	Peptide
1	G	193	GLU	Peptide
1	G	196	PRO	Peptide
1	G	20	ARG	Sidechain
1	G	202	VAL	Mainchain
1	G	224	ARG	Sidechain
1	G	232	VAL	Peptide
1	G	239	ARG	Sidechain
1	G	260	ILE	Peptide

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Mol	Chain	Res	Type	Group
1	G	267	THR	Peptide
1	G	338	ARG	Peptide
1	G	347	THR	Peptide
1	G	353	TYR	Sidechain
1	G	369	PHE	Sidechain
1	G	413	TYR	Sidechain
1	G	428	ARG	Sidechain
1	G	454	ILE	Mainchain
1	G	474	ARG	Sidechain
1	G	476	ARG	Sidechain
1	H	154	ALA	Peptide
1	H	163	TYR	Sidechain
1	H	193	GLU	Peptide
1	H	232	VAL	Peptide
1	H	260	ILE	Peptide
1	H	267	THR	Peptide
1	H	31	ARG	Sidechain
1	H	338	ARG	Sidechain,Peptide
1	H	347	THR	Peptide
1	H	396	ARG	Sidechain
1	H	406	ARG	Sidechain
1	H	428	ARG	Sidechain
1	H	447	TYR	Sidechain
1	H	474	ARG	Sidechain
1	H	476	ARG	Sidechain
1	I	154	ALA	Peptide
1	I	163	TYR	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	302	LYS	Peptide
1	I	31	ARG	Sidechain
1	I	338	ARG	Peptide
1	I	347	THR	Peptide
1	I	360	ARG	Sidechain
1	I	384	ARG	Sidechain
1	I	454	ILE	Mainchain
1	I	498	TYR	Sidechain
1	I	507	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	I	525	LYS	Mainchain
1	I	54	PHE	Sidechain
1	J	151	SER	Peptide
1	J	154	ALA	Peptide
1	J	163	TYR	Sidechain
1	J	170	PHE	Sidechain
1	J	193	GLU	Peptide
1	J	20	ARG	Sidechain
1	J	213	LYS	Peptide
1	J	239	ARG	Sidechain
1	J	260	ILE	Peptide
1	J	267	THR	Peptide
1	J	282	TYR	Sidechain
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	413	TYR	Sidechain
1	J	428	ARG	Sidechain
1	J	430	ARG	Sidechain
1	J	454	ILE	Mainchain
1	K	154	ALA	Peptide
1	K	193	GLU	Peptide
1	K	232	VAL	Peptide
1	K	260	ILE	Peptide
1	K	267	THR	Peptide
1	K	31	ARG	Sidechain
1	K	325	ARG	Sidechain
1	K	338	ARG	Sidechain,Peptide
1	K	346	ALA	Peptide
1	K	347	THR	Peptide
1	K	360	ARG	Sidechain
1	K	403	TYR	Sidechain
1	K	432	TYR	Sidechain
1	K	434	ARG	Sidechain
1	K	447	TYR	Sidechain
1	K	454	ILE	Mainchain
1	K	498	TYR	Sidechain
1	L	105	PHE	Sidechain
1	L	154	ALA	Peptide
1	L	193	GLU	Peptide

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Mol	Chain	Res	Type	Group
1	L	196	PRO	Peptide
1	L	20	ARG	Sidechain
1	L	213	LYS	Peptide
1	L	232	VAL	Peptide
1	L	260	ILE	Peptide
1	L	267	THR	Peptide
1	L	268	SER	Peptide
1	L	282	TYR	Sidechain
1	L	310	HIS	Sidechain
1	L	338	ARG	Peptide
1	L	347	THR	Peptide
1	L	353	TYR	Sidechain
1	L	369	PHE	Sidechain
1	L	384	ARG	Sidechain
1	L	413	TYR	Sidechain
1	L	432	TYR	Sidechain
1	L	454	ILE	Mainchain
1	L	476	ARG	Sidechain
1	L	507	ARG	Sidechain
1	M	154	ALA	Peptide
1	M	163	TYR	Sidechain
1	M	193	GLU	Peptide
1	M	196	PRO	Peptide
1	M	200	TYR	Sidechain
1	M	224	ARG	Sidechain
1	M	239	ARG	Sidechain
1	M	260	ILE	Peptide
1	M	267	THR	Peptide
1	M	282	TYR	Sidechain
1	M	31	ARG	Sidechain
1	M	338	ARG	Peptide
1	M	347	THR	Peptide
1	M	353	TYR	Sidechain
1	M	384	ARG	Sidechain
1	M	430	ARG	Sidechain
1	M	432	TYR	Sidechain
1	M	454	ILE	Mainchain
1	M	477	HIS	Sidechain
1	M	498	TYR	Sidechain
1	M	507	ARG	Sidechain
1	M	510	ARG	Sidechain
1	N	116	ASN	Mainchain

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Mol	Chain	Res	Type	Group
1	N	154	ALA	Peptide
1	N	191	VAL	Peptide
1	N	193	GLU	Peptide
1	N	213	LYS	Peptide
1	N	231	GLU	Peptide
1	N	232	VAL	Peptide
1	N	239	ARG	Sidechain
1	N	240	ARG	Sidechain
1	N	260	ILE	Peptide
1	N	267	THR	Peptide
1	N	282	TYR	Sidechain
1	N	338	ARG	Sidechain
1	N	347	THR	Peptide
1	N	38	ARG	Sidechain
1	N	384	ARG	Sidechain
1	N	396	ARG	Sidechain
1	N	430	ARG	Sidechain
1	N	447	TYR	Sidechain
1	N	454	ILE	Mainchain
1	N	498	TYR	Sidechain
1	O	154	ALA	Peptide
1	O	163	TYR	Sidechain
1	O	193	GLU	Peptide
1	O	20	ARG	Sidechain
1	O	213	LYS	Peptide
1	O	232	VAL	Peptide
1	O	234	HIS	Sidechain
1	O	239	ARG	Sidechain
1	O	260	ILE	Peptide
1	O	267	THR	Peptide
1	O	302	LYS	Peptide
1	O	31	ARG	Sidechain
1	O	315	ARG	Sidechain
1	O	325	ARG	Sidechain
1	O	338	ARG	Peptide
1	O	347	THR	Peptide
1	O	350	ASP	Mainchain
1	O	353	TYR	Sidechain
1	O	384	ARG	Sidechain
1	O	430	ARG	Sidechain
1	O	454	ILE	Mainchain
1	O	476	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	P	154	ALA	Mainchain,Peptide
1	P	163	TYR	Sidechain
1	P	196	PRO	Mainchain
1	P	200	TYR	Sidechain
1	P	232	VAL	Mainchain
1	P	234	HIS	Sidechain
1	P	260	ILE	Peptide
1	P	267	THR	Peptide
1	P	31	ARG	Sidechain
1	P	311	PHE	Sidechain
1	P	325	ARG	Sidechain
1	P	338	ARG	Sidechain
1	P	347	THR	Peptide
1	P	406	ARG	Sidechain
1	P	454	ILE	Mainchain
1	P	476	ARG	Sidechain
1	P	507	ARG	Sidechain
1	Q	154	ALA	Peptide
1	Q	193	GLU	Peptide
1	Q	196	PRO	Peptide
1	Q	200	TYR	Sidechain
1	Q	239	ARG	Sidechain
1	Q	260	ILE	Peptide
1	Q	267	THR	Peptide
1	Q	268	SER	Peptide
1	Q	275	PHE	Sidechain
1	Q	338	ARG	Peptide
1	Q	346	ALA	Peptide
1	Q	347	THR	Peptide
1	Q	353	TYR	Sidechain
1	Q	384	ARG	Sidechain
1	Q	396	ARG	Sidechain
1	Q	413	TYR	Sidechain
1	Q	498	TYR	Sidechain
1	Q	507	ARG	Sidechain
1	R	154	ALA	Peptide
1	R	196	PRO	Peptide
1	R	200	TYR	Sidechain
1	R	232	VAL	Peptide
1	R	234	HIS	Sidechain
1	R	260	ILE	Peptide
1	R	267	THR	Peptide

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Mol	Chain	Res	Type	Group
1	R	282	TYR	Sidechain
1	R	322	ARG	Sidechain
1	R	325	ARG	Sidechain
1	R	338	ARG	Mainchain
1	R	347	THR	Peptide
1	R	360	ARG	Sidechain
1	R	384	ARG	Sidechain
1	R	396	ARG	Sidechain
1	R	403	TYR	Sidechain
1	R	428	ARG	Sidechain
1	R	447	TYR	Sidechain
1	R	454	ILE	Mainchain
1	R	477	HIS	Sidechain
1	R	525	LYS	Mainchain

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	11	0
1	B	3937	0	4104	18	0
1	C	3937	0	4104	17	0
1	D	3937	0	4104	5	0
1	E	3937	0	4104	19	0
1	F	3937	0	4104	8	0
1	G	3937	0	4104	15	0
1	H	3937	0	4104	11	0
1	I	3937	0	4104	16	0
1	J	3937	0	4104	13	0
1	K	3937	0	4104	9	0
1	L	3937	0	4104	9	0
1	M	3937	0	4104	17	0
1	N	3937	0	4104	14	0
1	O	3937	0	4104	13	0
1	P	3937	0	4104	8	0
1	Q	3937	0	4104	9	0
1	R	3937	0	4104	8	0
All	All	70866	0	73872	214	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 1.

All (214) 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:J:454:ILE:HG22	1:J:455:PRO:HD2	1.66	0.78
1:D:454:ILE:HB	1:D:455:PRO:HD2	1.75	0.69
1:O:255:VAL:HG21	1:O:279:GLU:HG3	1.74	0.69
1:E:233:VAL:HG13	1:E:234:HIS:H	1.60	0.66
1:J:362:VAL:HG11	1:J:382:LEU:HD21	1.77	0.66
1:G:67:VAL:HB	1:G:81:VAL:HG22	1.79	0.64
1:P:454:ILE:HB	1:P:455:PRO:HD2	1.80	0.63
1:E:335:LEU:HD11	1:E:370:ILE:HG21	1.81	0.62
1:I:41:LEU:HD11	1:I:97:SER:HA	1.82	0.61
1:C:279:GLU:O	1:C:283:LEU:HD22	2.01	0.60
1:M:130:PHE:CE2	1:M:134:LEU:HD11	2.35	0.60
1:O:454:ILE:HG22	1:O:455:PRO:HD2	1.82	0.59
1:C:67:VAL:CG1	1:C:81:VAL:HG13	2.32	0.59
1:A:417:GLY:HA2	1:A:421:ILE:HG22	1.84	0.59
1:O:233:VAL:HG13	1:O:309:GLN:HE22	1.67	0.59
1:K:98:ALA:HB2	1:K:512:VAL:HB	1.85	0.58
1:F:283:LEU:HD22	1:F:308:ALA:HB2	1.84	0.58
1:F:454:ILE:HG22	1:F:455:PRO:HD2	1.86	0.58
1:I:98:ALA:HB2	1:I:512:VAL:HG12	1.84	0.58
1:M:232:VAL:HG22	1:M:318:LEU:HD21	1.86	0.57
1:H:67:VAL:HB	1:H:81:VAL:HG22	1.86	0.57
1:C:108:LYS:HB3	1:C:446:ALA:HB1	1.87	0.57
1:C:185:ILE:HG23	1:C:405:LEU:HD22	1.87	0.56
1:N:137:LEU:HB3	1:N:506:ILE:HD11	1.86	0.56
1:B:255:VAL:HG21	1:B:279:GLU:HG3	1.88	0.56
1:H:454:ILE:HG22	1:H:455:PRO:HD2	1.88	0.55
1:I:233:VAL:HG13	1:I:309:GLN:HE22	1.71	0.55
1:C:293:ILE:HD11	1:C:346:ALA:HA	1.88	0.54
1:A:293:ILE:HD12	1:A:351:LEU:HD21	1.88	0.54
1:L:454:ILE:HB	1:L:455:PRO:HD2	1.90	0.54
1:J:454:ILE:CG2	1:J:455:PRO:HD2	2.38	0.53
1:N:185:ILE:HG23	1:N:405:LEU:HD22	1.90	0.53
1:B:454:ILE:CB	1:B:455:PRO:HD2	2.39	0.53
1:I:283:LEU:HD22	1:I:308:ALA:HB2	1.91	0.52
1:E:454:ILE:HG22	1:E:455:PRO:HD2	1.91	0.52
1:I:391:LEU:N	1:I:391:LEU:HD12	2.24	0.52
1:R:454:ILE:HG22	1:R:455:PRO:HD2	1.92	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:J:44:LYS:HB2	1:J:461:THR:HG22	1.91	0.52
1:K:454:ILE:HB	1:K:455:PRO:HD2	1.92	0.52
1:N:454:ILE:HG22	1:N:455:PRO:HD2	1.91	0.51
1:O:245:LYS:HB3	1:O:351:LEU:HD21	1.92	0.51
1:N:77:ALA:O	1:N:81:VAL:HG23	2.09	0.51
1:B:241:VAL:HG12	1:B:244:ALA:HB2	1.92	0.51
1:K:385:GLY:HA3	1:K:391:LEU:HD13	1.92	0.51
1:M:267:THR:HA	1:M:272:ILE:HD11	1.93	0.51
1:J:234:HIS:CE1	1:J:310:HIS:CD2	2.98	0.51
1:O:127:LYS:HA	1:O:130:PHE:CE2	2.46	0.51
1:P:454:ILE:CB	1:P:455:PRO:HD2	2.40	0.50
1:E:476:ARG:NH2	1:E:480:GLY:HA3	2.27	0.50
1:C:67:VAL:HG12	1:C:81:VAL:HG13	1.93	0.50
1:L:41:LEU:HD22	1:L:100:VAL:HG21	1.93	0.50
1:E:91:VAL:HG12	1:E:508:VAL:HG12	1.93	0.50
1:G:343:ILE:HD12	1:G:343:ILE:H	1.77	0.50
1:H:101:LEU:HA	1:H:104:LEU:HD12	1.94	0.50
1:M:266:ILE:HG13	1:M:268:SER:H	1.76	0.50
1:C:241:VAL:HG11	1:C:296:ASN:HB3	1.93	0.49
1:K:143:LYS:HB2	1:K:413:TYR:CE2	2.47	0.49
1:K:454:ILE:CB	1:K:455:PRO:HD2	2.42	0.49
1:B:125:GLY:HA3	1:B:443:ALA:HB3	1.94	0.49
1:R:283:LEU:HD22	1:R:308:ALA:HB2	1.95	0.49
1:O:180:ILE:HA	1:O:183:ILE:HD12	1.95	0.49
1:G:143:LYS:HB2	1:G:413:TYR:CE2	2.46	0.49
1:P:51:ILE:HG12	1:P:57:VAL:HG13	1.95	0.49
1:E:355:GLU:HB2	1:E:372:GLY:HA3	1.95	0.49
1:E:51:ILE:HG23	1:E:57:VAL:HG22	1.94	0.49
1:L:454:ILE:CB	1:L:455:PRO:HD2	2.43	0.49
1:Q:259:GLU:CD	1:Q:259:GLU:H	2.16	0.49
1:M:121:ILE:HG21	1:M:439:LYS:HB2	1.94	0.48
1:H:284:LYS:HB2	1:H:311:PHE:CE1	2.47	0.48
1:M:505:PRO:O	1:M:508:VAL:HG22	2.13	0.48
1:N:417:GLY:HA2	1:N:421:ILE:HG22	1.95	0.48
1:F:227:VAL:HG22	1:F:369:PHE:CE2	2.47	0.48
1:J:246:ILE:HD13	1:J:335:LEU:HD13	1.95	0.48
1:E:297:VAL:HG21	1:E:357:VAL:HG21	1.94	0.48
1:C:225:GLY:HA3	1:C:370:ILE:O	2.13	0.48
1:D:462:ALA:HB2	1:D:488:VAL:HG23	1.95	0.48
1:F:185:ILE:HG23	1:F:405:LEU:HD13	1.96	0.47
1:D:232:VAL:HG12	1:D:233:VAL:O	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:234:HIS:CD2	1:B:236:GLY:H	2.33	0.47
1:E:145:ASP:CG	1:E:146:VAL:H	2.17	0.47
1:F:49:MET:HB2	1:G:526:ILE:HD11	1.97	0.47
1:G:454:ILE:CB	1:G:455:PRO:HD2	2.44	0.47
1:Q:357:VAL:HG22	1:Q:370:ILE:HD13	1.95	0.47
1:A:185:ILE:HG13	1:A:405:LEU:HD22	1.97	0.46
1:N:477:HIS:CD2	1:N:482:THR:HG22	2.51	0.46
1:B:454:ILE:HG22	1:B:455:PRO:HD2	1.97	0.46
1:A:473:LEU:HD13	1:A:493:ILE:HG23	1.98	0.46
1:Q:457:ILE:O	1:Q:461:THR:HG23	2.15	0.46
1:M:98:ALA:HA	1:M:101:LEU:HD12	1.98	0.46
1:H:132:LYS:HA	1:H:135:GLU:HG2	1.98	0.46
1:C:67:VAL:HG13	1:C:81:VAL:HG22	1.97	0.46
1:E:200:TYR:CD1	1:E:409:LEU:HD22	2.50	0.45
1:E:500:ILE:HG23	1:E:502:VAL:HG22	1.98	0.45
1:N:505:PRO:O	1:N:508:VAL:HG22	2.17	0.45
1:B:456:MET:SD	1:B:470:LEU:HD22	2.56	0.45
1:C:245:LYS:HB3	1:C:351:LEU:HD21	1.98	0.45
1:P:430:ARG:HH12	1:P:452:GLU:CD	2.19	0.45
1:I:509:THR:HG22	1:I:513:LEU:HD12	1.98	0.45
1:B:211:LYS:HG3	1:B:391:LEU:HD11	1.98	0.45
1:L:39:SER:HB2	1:L:46:LEU:HD12	1.99	0.45
1:N:246:ILE:HG13	1:N:335:LEU:HD13	1.98	0.45
1:P:358:GLU:CD	1:P:360:ARG:HE	2.21	0.45
1:Q:454:ILE:HG22	1:Q:455:PRO:HD2	1.99	0.45
1:N:84:ALA:HA	1:N:95:THR:HG23	1.99	0.45
1:M:454:ILE:HG22	1:M:455:PRO:HD2	1.99	0.44
1:M:454:ILE:CB	1:M:455:PRO:HD2	2.47	0.44
1:H:337:ALA:O	1:H:338:ARG:HD3	2.16	0.44
1:B:520:ALA:O	1:B:524:MET:HG2	2.18	0.44
1:R:204:LEU:HD12	1:R:406:ARG:HD3	1.99	0.44
1:A:159:LYS:O	1:A:163:TYR:HB2	2.18	0.44
1:L:136:LEU:HA	1:L:136:LEU:HD23	1.92	0.44
1:R:144:VAL:O	1:R:145:ASP:HB2	2.18	0.44
1:E:420:ALA:HB1	1:E:483:ASN:HA	1.99	0.44
1:C:112:LEU:HD11	1:C:443:ALA:HA	1.99	0.44
1:G:202:VAL:HG11	1:G:406:ARG:HG3	2.00	0.44
1:O:321:ARG:O	1:O:323:VAL:HG23	2.18	0.44
1:A:299:ILE:HD13	1:A:331:LEU:HD13	2.00	0.44
1:Q:416:PRO:HA	1:Q:503:VAL:HG12	2.00	0.44
1:M:253:LEU:HB2	1:M:304:ILE:HG23	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:G:347:THR:HA	1:G:348:PRO:HD3	1.90	0.44
1:E:74:HIS:HA	1:E:75:PRO:HD3	1.87	0.43
1:O:49:MET:O	1:P:529:LEU:HA	2.17	0.43
1:I:112:LEU:HD12	1:I:122:ILE:HG23	2.00	0.43
1:G:51:ILE:HD13	1:G:57:VAL:HG22	1.99	0.43
1:J:106:LEU:HD21	1:J:520:ALA:HA	1.99	0.43
1:B:467:ILE:H	1:B:467:ILE:HD13	1.83	0.43
1:M:413:TYR:HB2	1:M:506:ILE:HG21	1.99	0.43
1:B:48:LYS:HA	1:C:527:ASP:O	2.18	0.43
1:E:245:LYS:HB3	1:E:351:LEU:HD21	2.00	0.43
1:J:208:LYS:NZ	1:J:210:ASP:OD1	2.44	0.43
1:I:471:MET:SD	1:N:438:GLY:HA2	2.57	0.43
1:C:454:ILE:HB	1:C:455:PRO:HD2	2.00	0.43
1:H:436:VAL:HG11	1:H:444:ILE:CD1	2.49	0.43
1:B:34:ALA:HA	1:B:99:VAL:HG12	2.00	0.43
1:M:241:VAL:HG11	1:M:296:ASN:HB3	2.01	0.43
1:H:176:GLU:H	1:H:176:GLU:CD	2.23	0.43
1:A:133:SER:O	1:A:137:LEU:HG	2.19	0.43
1:O:485:GLY:HA3	1:O:497:ILE:HD13	2.00	0.43
1:Q:347:THR:HA	1:Q:348:PRO:HD3	1.87	0.43
1:J:185:ILE:HG23	1:J:405:LEU:HD13	2.00	0.43
1:G:155:ARG:HD2	1:G:182:ASP:OD2	2.19	0.43
1:N:189:THR:HG23	1:N:409:LEU:HD11	2.00	0.43
1:J:522:SER:O	1:J:526:ILE:HG13	2.18	0.43
1:I:414:ILE:HD13	1:I:414:ILE:HG21	1.78	0.43
1:R:16:ARG:HG3	1:R:17:ASN:H	1.83	0.43
1:L:185:ILE:HG23	1:L:405:LEU:HD22	2.01	0.43
1:E:101:LEU:HD21	1:E:454:ILE:HD13	2.01	0.42
1:I:509:THR:HG22	1:I:513:LEU:CD1	2.49	0.42
1:C:413:TYR:HB2	1:C:506:ILE:HG21	2.00	0.42
1:L:383:LEU:HD22	1:L:398:ILE:HD12	2.01	0.42
1:D:180:ILE:HG13	1:D:217:ILE:HB	2.01	0.42
1:P:505:PRO:O	1:P:508:VAL:HG22	2.18	0.42
1:L:375:ASN:N	1:L:376:PRO:HD3	2.34	0.42
1:B:454:ILE:HB	1:B:455:PRO:HD2	2.01	0.42
1:A:220:SER:HB3	1:A:383:LEU:HD12	2.01	0.42
1:A:416:PRO:HG2	1:A:420:ALA:HB3	2.00	0.42
1:H:200:TYR:HB2	1:H:409:LEU:HB3	2.01	0.42
1:C:98:ALA:HB2	1:C:512:VAL:HB	2.01	0.42
1:I:312:LEU:HD22	1:I:317:ILE:HG21	2.02	0.42
1:R:16:ARG:NE	1:R:16:ARG:HA	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:O:195:LEU:HD12	1:O:195:LEU:HA	1.97	0.42
1:C:211:LYS:HB2	1:C:391:LEU:HD23	2.01	0.42
1:C:454:ILE:CB	1:C:455:PRO:HD2	2.50	0.42
1:K:192:ALA:HB1	1:K:200:TYR:HB3	2.02	0.42
1:F:191:VAL:HG21	1:F:379:VAL:HG11	2.02	0.42
1:K:98:ALA:CB	1:K:512:VAL:HB	2.49	0.41
1:O:245:LYS:HD2	1:O:351:LEU:HD21	2.02	0.41
1:G:117:ILE:CG2	1:G:121:ILE:HB	2.49	0.41
1:G:415:VAL:HG21	1:G:509:THR:HG21	2.01	0.41
1:I:300:CYS:HB3	1:I:304:ILE:HD11	2.02	0.41
1:J:323:VAL:HG12	1:J:328:ILE:HG12	2.03	0.41
1:B:290:LEU:HD13	1:B:298:VAL:HG11	2.01	0.41
1:I:375:ASN:N	1:I:376:PRO:HD3	2.35	0.41
1:B:217:ILE:HA	1:B:384:ARG:O	2.20	0.41
1:O:255:VAL:HG23	1:O:283:LEU:HD21	2.02	0.41
1:O:180:ILE:HG21	1:O:217:ILE:HG22	2.02	0.41
1:M:200:TYR:CD1	1:M:409:LEU:HD22	2.55	0.41
1:E:266:ILE:HB	1:E:272:ILE:HD11	2.02	0.41
1:B:357:VAL:HG22	1:B:370:ILE:HG12	2.02	0.41
1:J:264:ILE:HG22	1:J:266:ILE:HG12	2.03	0.41
1:E:123:ILE:HG23	1:E:521:THR:HG23	2.01	0.41
1:B:422:GLU:CD	1:B:422:GLU:H	2.23	0.41
1:Q:80:LEU:HD23	1:Q:80:LEU:HA	1.83	0.41
1:N:460:GLU:HG3	1:N:466:PRO:HG3	2.03	0.41
1:E:456:MET:HG3	1:E:456:MET:H	1.71	0.41
1:M:148:ASP:HB2	1:M:154:ALA:HB3	2.03	0.41
1:I:140:LEU:HD13	1:I:424:GLU:HG3	2.03	0.41
1:M:312:LEU:HD13	1:M:319:ALA:HB2	2.03	0.41
1:R:255:VAL:HG21	1:R:279:GLU:HG3	2.02	0.41
1:G:252:SER:HB3	1:G:302:LYS:HB2	2.03	0.41
1:D:408:ILE:HD11	1:D:414:ILE:HG21	2.02	0.41
1:A:234:HIS:CE1	1:A:236:GLY:H	2.39	0.41
1:R:108:LYS:HB3	1:R:446:ALA:HB1	2.02	0.41
1:G:112:LEU:HD22	1:G:117:ILE:HD12	2.04	0.41
1:J:237:MET:HA	1:J:238:PRO:HD3	1.89	0.41
1:Q:155:ARG:NH2	1:Q:186:ASP:OD2	2.54	0.41
1:F:143:LYS:HB2	1:F:413:TYR:CE2	2.56	0.41
1:N:421:ILE:HG23	1:N:422:GLU:N	2.35	0.40
1:K:507:ARG:O	1:K:511:GLN:HB2	2.21	0.40
1:G:370:ILE:HG21	1:G:370:ILE:HD13	1.79	0.40
1:M:158:LEU:HD23	1:M:408:ILE:HD13	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:P:101:LEU:HA	1:P:104:LEU:HD12	2.03	0.40
1:I:41:LEU:HD22	1:I:100:VAL:HG21	2.03	0.40
1:G:454:ILE:HB	1:G:455:PRO:HD2	2.04	0.40
1:I:249:LEU:HD23	1:I:340:ILE:HB	2.03	0.40
1:H:233:VAL:HG13	1:H:309:GLN:HE22	1.85	0.40
1:Q:454:ILE:CB	1:Q:455:PRO:HD2	2.51	0.40
1:E:276:LEU:HD13	1:F:260:ILE:HG12	2.04	0.40
1:N:153:THR:O	1:N:154:ALA:HB3	2.21	0.40
1:L:463:GLY:HA2	1:M:118:HIS:CE1	2.56	0.40
1:K:454:ILE:H	1:K:454:ILE:HG13	1.69	0.40
1:A:108:LYS:HG3	1:A:450:ALA:HB2	2.04	0.40
1:B:483:ASN:O	1:B:496:ASP:HA	2.21	0.40
1:H:413:TYR:HB2	1:H:506:ILE:HG21	2.03	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%)	456 (88%)	40 (8%)	21 (4%)	3	35
1	B	517/563 (92%)	455 (88%)	40 (8%)	22 (4%)	3	34
1	C	517/563 (92%)	459 (89%)	38 (7%)	20 (4%)	4	36
1	D	517/563 (92%)	461 (89%)	36 (7%)	20 (4%)	4	36
1	E	517/563 (92%)	456 (88%)	42 (8%)	19 (4%)	4	38
1	F	517/563 (92%)	456 (88%)	40 (8%)	21 (4%)	3	35
1	G	517/563 (92%)	461 (89%)	37 (7%)	19 (4%)	4	38
1	H	517/563 (92%)	460 (89%)	37 (7%)	20 (4%)	4	36
1	I	517/563 (92%)	463 (90%)	33 (6%)	21 (4%)	3	35
1	J	517/563 (92%)	468 (90%)	29 (6%)	20 (4%)	4	36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	K	517/563 (92%)	464 (90%)	35 (7%)	18 (4%)	4	39
1	L	517/563 (92%)	459 (89%)	39 (8%)	19 (4%)	4	38
1	M	517/563 (92%)	468 (90%)	33 (6%)	16 (3%)	5	42
1	N	517/563 (92%)	454 (88%)	44 (8%)	19 (4%)	4	38
1	O	517/563 (92%)	461 (89%)	37 (7%)	19 (4%)	4	38
1	P	517/563 (92%)	465 (90%)	34 (7%)	18 (4%)	4	39
1	Q	517/563 (92%)	464 (90%)	33 (6%)	20 (4%)	4	36
1	R	517/563 (92%)	463 (90%)	38 (7%)	16 (3%)	5	42
All	All	9306/10134 (92%)	8293 (89%)	665 (7%)	348 (4%)	7	38

All (348) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	233	VAL
1	A	322	ARG
1	A	455	PRO
1	B	145	ASP
1	B	155	ARG
1	B	322	ARG
1	B	348	PRO
1	B	455	PRO
1	C	192	ALA
1	C	322	ARG
1	C	455	PRO
1	D	322	ARG
1	D	348	PRO
1	D	455	PRO
1	E	233	VAL
1	E	322	ARG
1	E	387	ASN
1	E	455	PRO
1	E	495	ASP
1	F	232	VAL
1	F	233	VAL
1	F	322	ARG
1	F	455	PRO
1	G	322	ARG
1	G	455	PRO
1	H	322	ARG

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Mol	Chain	Res	Type
1	H	455	PRO
1	H	528	ASP
1	I	155	ARG
1	I	322	ARG
1	I	455	PRO
1	I	528	ASP
1	J	233	VAL
1	J	322	ARG
1	J	455	PRO
1	K	155	ARG
1	K	192	ALA
1	K	322	ARG
1	K	455	PRO
1	L	322	ARG
1	L	455	PRO
1	M	233	VAL
1	M	322	ARG
1	M	455	PRO
1	N	152	ALA
1	N	192	ALA
1	N	322	ARG
1	N	455	PRO
1	O	322	ARG
1	O	455	PRO
1	P	322	ARG
1	P	364	ASN
1	P	455	PRO
1	Q	154	ALA
1	Q	268	SER
1	Q	322	ARG
1	Q	455	PRO
1	R	155	ARG
1	R	192	ALA
1	R	322	ARG
1	R	455	PRO
1	A	155	ARG
1	A	387	ASN
1	A	416	PRO
1	A	438	GLY
1	A	496	ASP
1	B	192	ALA
1	B	197	ASP

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Mol	Chain	Res	Type
1	B	418	GLY
1	B	496	ASP
1	C	146	VAL
1	C	155	ARG
1	C	156	ASP
1	C	233	VAL
1	C	386	SER
1	C	496	ASP
1	C	528	ASP
1	D	152	ALA
1	D	496	ASP
1	E	150	ASN
1	E	155	ARG
1	E	172	ALA
1	E	192	ALA
1	E	348	PRO
1	F	147	SER
1	F	152	ALA
1	F	192	ALA
1	F	339	ILE
1	F	431	GLU
1	G	150	ASN
1	G	156	ASP
1	G	192	ALA
1	G	233	VAL
1	G	348	PRO
1	G	416	PRO
1	H	170	PHE
1	H	303	GLY
1	H	496	ASP
1	I	192	ALA
1	I	303	GLY
1	I	339	ILE
1	J	150	ASN
1	J	155	ARG
1	J	192	ALA
1	J	194	PRO
1	J	339	ILE
1	K	230	LYS
1	K	233	VAL
1	K	339	ILE
1	L	152	ALA

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Mol	Chain	Res	Type
1	L	339	ILE
1	L	386	SER
1	L	496	ASP
1	M	155	ARG
1	M	192	ALA
1	M	339	ILE
1	M	348	PRO
1	M	419	GLY
1	N	145	ASP
1	N	155	ARG
1	N	197	ASP
1	N	233	VAL
1	N	386	SER
1	O	155	ARG
1	O	156	ASP
1	O	170	PHE
1	O	233	VAL
1	O	496	ASP
1	O	528	ASP
1	P	155	ARG
1	P	156	ASP
1	P	338	ARG
1	P	386	SER
1	P	496	ASP
1	Q	170	PHE
1	Q	192	ALA
1	Q	199	GLY
1	Q	339	ILE
1	Q	496	ASP
1	R	374	LYS
1	A	138	PRO
1	A	170	PHE
1	A	339	ILE
1	A	386	SER
1	A	431	GLU
1	B	20	ARG
1	B	138	PRO
1	B	156	ASP
1	B	339	ILE
1	B	431	GLU
1	C	138	PRO
1	C	431	GLU

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Mol	Chain	Res	Type
1	D	138	PRO
1	D	150	ASN
1	D	155	ARG
1	D	156	ASP
1	D	194	PRO
1	D	387	ASN
1	D	431	GLU
1	E	156	ASP
1	E	338	ARG
1	E	339	ILE
1	E	364	ASN
1	E	431	GLU
1	F	138	PRO
1	F	155	ARG
1	F	156	ASP
1	F	170	PHE
1	F	387	ASN
1	F	528	ASP
1	G	155	ARG
1	G	261	SER
1	G	431	GLU
1	G	493	ILE
1	H	137	LEU
1	H	147	SER
1	H	155	ARG
1	H	156	ASP
1	H	339	ILE
1	H	431	GLU
1	I	138	PRO
1	I	145	ASP
1	I	156	ASP
1	I	348	PRO
1	I	386	SER
1	I	416	PRO
1	I	431	GLU
1	J	156	ASP
1	J	419	GLY
1	J	431	GLU
1	K	138	PRO
1	K	156	ASP
1	K	303	GLY
1	K	348	PRO

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Mol	Chain	Res	Type
1	K	386	SER
1	K	431	GLU
1	L	155	ARG
1	L	156	ASP
1	L	348	PRO
1	L	431	GLU
1	M	118	HIS
1	M	156	ASP
1	M	232	VAL
1	M	431	GLU
1	N	154	ALA
1	N	156	ASP
1	N	232	VAL
1	N	431	GLU
1	O	138	PRO
1	O	192	ALA
1	O	431	GLU
1	P	431	GLU
1	Q	138	PRO
1	Q	155	ARG
1	Q	156	ASP
1	Q	348	PRO
1	Q	419	GLY
1	Q	431	GLU
1	Q	495	ASP
1	R	138	PRO
1	R	156	ASP
1	R	233	VAL
1	R	348	PRO
1	R	431	GLU
1	A	156	ASP
1	A	528	ASP
1	B	141	ALA
1	B	233	VAL
1	C	194	PRO
1	C	339	ILE
1	D	137	LEU
1	D	192	ALA
1	E	138	PRO
1	E	528	ASP
1	F	115	GLN
1	F	348	PRO

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Mol	Chain	Res	Type
1	F	386	SER
1	G	193	GLU
1	G	268	SER
1	G	339	ILE
1	H	138	PRO
1	H	152	ALA
1	H	194	PRO
1	H	387	ASN
1	I	118	HIS
1	I	149	LEU
1	I	419	GLY
1	I	496	ASP
1	J	118	HIS
1	J	138	PRO
1	J	303	GLY
1	J	496	ASP
1	L	41	LEU
1	L	137	LEU
1	L	419	GLY
1	M	138	PRO
1	N	137	LEU
1	N	138	PRO
1	N	339	ILE
1	N	438	GLY
1	O	152	ALA
1	O	154	ALA
1	P	172	ALA
1	P	203	SER
1	P	339	ILE
1	R	150	ASN
1	R	173	GLU
1	R	303	GLY
1	A	137	LEU
1	A	419	GLY
1	B	137	LEU
1	B	151	SER
1	B	258	PRO
1	C	20	ARG
1	C	137	LEU
1	C	145	ASP
1	C	238	PRO
1	C	501	ASN

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Mol	Chain	Res	Type
1	D	339	ILE
1	D	438	GLY
1	E	137	LEU
1	E	170	PHE
1	F	137	LEU
1	F	194	PRO
1	G	20	ARG
1	G	138	PRO
1	H	192	ALA
1	H	419	GLY
1	I	137	LEU
1	J	137	LEU
1	J	269	PRO
1	J	501	ASN
1	K	137	LEU
1	K	416	PRO
1	L	138	PRO
1	L	145	ASP
1	M	137	LEU
1	M	150	ASN
1	N	268	SER
1	N	419	GLY
1	O	269	PRO
1	O	339	ILE
1	O	364	ASN
1	P	20	ARG
1	P	137	LEU
1	P	138	PRO
1	P	171	MET
1	P	193	GLU
1	P	348	PRO
1	R	137	LEU
1	A	348	PRO
1	B	170	PHE
1	B	194	PRO
1	C	232	VAL
1	D	145	ASP
1	D	154	ALA
1	D	386	SER
1	G	137	LEU
1	J	416	PRO
1	K	43	PRO

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Mol	Chain	Res	Type
1	K	174	GLY
1	L	118	HIS
1	L	192	ALA
1	M	501	ASN
1	O	137	LEU
1	O	193	GLU
1	Q	364	ASN
1	R	416	PRO
1	F	416	PRO
1	H	348	PRO
1	J	348	PRO
1	L	194	PRO
1	L	233	VAL
1	O	348	PRO
1	A	193	GLU
1	H	233	VAL
1	I	233	VAL
1	I	268	SER
1	Q	137	LEU
1	B	303	GLY
1	G	419	GLY
1	Q	194	PRO
1	R	419	GLY
1	A	194	PRO
1	Q	193	GLU
1	A	268	SER
1	D	418	GLY
1	K	419	GLY

5.3.2 Protein sidechains (i)

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%)	416 (97%)	11 (3%)	54 80
1	B	427/453 (94%)	406 (95%)	21 (5%)	31 67
1	C	427/453 (94%)	408 (96%)	19 (4%)	35 69

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	427/453 (94%)	420 (98%)	7 (2%)	70 88
1	E	427/453 (94%)	416 (97%)	11 (3%)	54 80
1	F	427/453 (94%)	410 (96%)	17 (4%)	38 71
1	G	427/453 (94%)	412 (96%)	15 (4%)	43 74
1	H	427/453 (94%)	412 (96%)	15 (4%)	43 74
1	I	427/453 (94%)	411 (96%)	16 (4%)	41 73
1	J	427/453 (94%)	410 (96%)	17 (4%)	38 71
1	K	427/453 (94%)	415 (97%)	12 (3%)	51 78
1	L	427/453 (94%)	417 (98%)	10 (2%)	58 83
1	M	427/453 (94%)	415 (97%)	12 (3%)	51 78
1	N	427/453 (94%)	407 (95%)	20 (5%)	32 68
1	O	427/453 (94%)	413 (97%)	14 (3%)	45 76
1	P	427/453 (94%)	416 (97%)	11 (3%)	54 80
1	Q	427/453 (94%)	412 (96%)	15 (4%)	43 74
1	R	427/453 (94%)	416 (97%)	11 (3%)	54 80
All	All	7686/8154 (94%)	7432 (97%)	254 (3%)	49 76

All (254) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	119	PRO
1	A	132	LYS
1	A	185	ILE
1	A	240	ARG
1	A	301	GLN
1	A	310	HIS
1	A	380	ASN
1	A	424	GLU
1	A	441	GLN
1	A	454	ILE
1	A	495	ASP
1	B	16	ARG
1	B	39	SER
1	B	50	LEU
1	B	130	PHE
1	B	163	TYR
1	B	170	PHE

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Mol	Chain	Res	Type
1	B	200	TYR
1	B	222	LEU
1	B	231	GLU
1	B	356	LEU
1	B	359	GLU
1	B	380	ASN
1	B	391	LEU
1	B	413	TYR
1	B	454	ILE
1	B	455	PRO
1	B	457	ILE
1	B	467	ILE
1	B	476	ARG
1	B	477	HIS
1	B	503	VAL
1	C	16	ARG
1	C	18	SER
1	C	36	MET
1	C	50	LEU
1	C	171	MET
1	C	196	PRO
1	C	200	TYR
1	C	231	GLU
1	C	239	ARG
1	C	269	PRO
1	C	300	CYS
1	C	301	GLN
1	C	331	LEU
1	C	356	LEU
1	C	380	ASN
1	C	454	ILE
1	C	455	PRO
1	C	503	VAL
1	C	508	VAL
1	D	60	THR
1	D	163	TYR
1	D	348	PRO
1	D	380	ASN
1	D	381	ILE
1	D	455	PRO
1	D	467	ILE
1	E	25	ASN

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Mol	Chain	Res	Type
1	E	31	ARG
1	E	146	VAL
1	E	151	SER
1	E	270	ASP
1	E	374	LYS
1	E	380	ASN
1	E	454	ILE
1	E	477	HIS
1	E	488	VAL
1	E	489	ILE
1	F	20	ARG
1	F	50	LEU
1	F	53	SER
1	F	119	PRO
1	F	120	THR
1	F	155	ARG
1	F	171	MET
1	F	196	PRO
1	F	285	ASP
1	F	361	LYS
1	F	380	ASN
1	F	398	ILE
1	F	423	LEU
1	F	426	SER
1	F	454	ILE
1	F	455	PRO
1	F	528	ASP
1	G	38	ARG
1	G	166	MET
1	G	171	MET
1	G	196	PRO
1	G	231	GLU
1	G	301	GLN
1	G	332	GLU
1	G	343	ILE
1	G	380	ASN
1	G	404	SER
1	G	424	GLU
1	G	449	ASP
1	G	454	ILE
1	G	455	PRO
1	G	529	LEU

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Mol	Chain	Res	Type
1	H	47	ASP
1	H	48	LYS
1	H	50	LEU
1	H	137	LEU
1	H	145	ASP
1	H	163	TYR
1	H	202	VAL
1	H	222	LEU
1	H	250	ASP
1	H	376	PRO
1	H	380	ASN
1	H	387	ASN
1	H	415	VAL
1	H	454	ILE
1	H	496	ASP
1	I	36	MET
1	I	50	LEU
1	I	104	LEU
1	I	111	SER
1	I	161	ILE
1	I	185	ILE
1	I	200	TYR
1	I	222	LEU
1	I	270	ASP
1	I	332	GLU
1	I	356	LEU
1	I	374	LYS
1	I	380	ASN
1	I	453	GLU
1	I	454	ILE
1	I	495	ASP
1	J	20	ARG
1	J	50	LEU
1	J	119	PRO
1	J	120	THR
1	J	148	ASP
1	J	149	LEU
1	J	200	TYR
1	J	268	SER
1	J	306	ASP
1	J	333	LYS
1	J	356	LEU

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Mol	Chain	Res	Type
1	J	376	PRO
1	J	380	ASN
1	J	454	ILE
1	J	455	PRO
1	J	496	ASP
1	J	503	VAL
1	K	31	ARG
1	K	52	ASP
1	K	75	PRO
1	K	97	SER
1	K	135	GLU
1	K	156	ASP
1	K	222	LEU
1	K	380	ASN
1	K	415	VAL
1	K	423	LEU
1	K	454	ILE
1	K	495	ASP
1	L	46	LEU
1	L	145	ASP
1	L	167	SER
1	L	202	VAL
1	L	332	GLU
1	L	380	ASN
1	L	415	VAL
1	L	454	ILE
1	L	455	PRO
1	L	467	ILE
1	M	17	ASN
1	M	20	ARG
1	M	47	ASP
1	M	68	LYS
1	M	91	VAL
1	M	186	ASP
1	M	259	GLU
1	M	376	PRO
1	M	380	ASN
1	M	454	ILE
1	M	456	MET
1	M	477	HIS
1	N	16	ARG
1	N	50	LEU

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Mol	Chain	Res	Type
1	N	54	PHE
1	N	163	TYR
1	N	170	PHE
1	N	200	TYR
1	N	222	LEU
1	N	239	ARG
1	N	243	LYS
1	N	258	PRO
1	N	380	ASN
1	N	412	PRO
1	N	413	TYR
1	N	423	LEU
1	N	435	SER
1	N	454	ILE
1	N	455	PRO
1	N	460	GLU
1	N	467	ILE
1	N	528	ASP
1	O	17	ASN
1	O	25	ASN
1	O	36	MET
1	O	111	SER
1	O	163	TYR
1	O	200	TYR
1	O	282	TYR
1	O	306	ASP
1	O	356	LEU
1	O	413	TYR
1	O	454	ILE
1	O	455	PRO
1	O	472	ASP
1	O	528	ASP
1	P	132	LYS
1	P	173	GLU
1	P	231	GLU
1	P	259	GLU
1	P	306	ASP
1	P	380	ASN
1	P	415	VAL
1	P	434	ARG
1	P	455	PRO
1	P	460	GLU

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Mol	Chain	Res	Type
1	P	481	LEU
1	Q	17	ASN
1	Q	47	ASP
1	Q	62	ASP
1	Q	75	PRO
1	Q	87	GLN
1	Q	91	VAL
1	Q	211	LYS
1	Q	277	ASP
1	Q	380	ASN
1	Q	424	GLU
1	Q	441	GLN
1	Q	454	ILE
1	Q	455	PRO
1	Q	501	ASN
1	Q	528	ASP
1	R	20	ARG
1	R	36	MET
1	R	93	ASP
1	R	171	MET
1	R	222	LEU
1	R	356	LEU
1	R	380	ASN
1	R	396	ARG
1	R	447	TYR
1	R	454	ILE
1	R	503	VAL

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (19) such sidechains are listed below:

Mol	Chain	Res	Type
1	B	234	HIS
1	C	477	HIS
1	D	234	HIS
1	F	201	ASN
1	H	234	HIS
1	H	441	GLN
1	I	301	GLN
1	I	309	GLN
1	J	118	HIS
1	J	234	HIS
1	K	477	HIS

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Mol	Chain	Res	Type
1	L	477	HIS
1	M	150	ASN
1	M	234	HIS
1	M	477	HIS
1	M	490	ASN
1	O	309	GLN
1	P	73	GLN
1	Q	501	ASN

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.