



Full wwPDB EM Validation Report ⓘ

Mar 15, 2025 – 06:54 am GMT

PDB ID : 9I8N
EMDB ID : EMD-52730
Title : NEDD1-bound native vertebrate gamma-tubulin ring complex from *Xenopus laevis*
Authors : Vermeulen, B.J.A.; Pfeffer, S.
Deposited on : 2025-02-05
Resolution : 4.60 Å(reported)

This is a Full wwPDB EM Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

The following versions of software and data (see [references ⓘ](#)) were used in the production of this report:

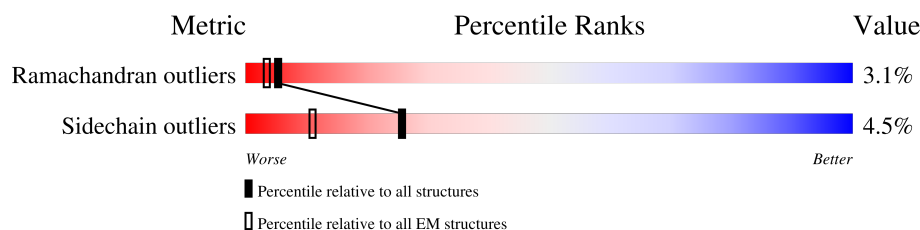
EMDB validation analysis : 0.0.1.dev117
MolProbity : 4.02b-467
Percentile statistics : 20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ : 1.9.13
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.41

1 Overall quality at a glance

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

The reported resolution of this entry is 4.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	896	
1	C	896	
1	E	896	
1	G	896	
1	M	896	
2	B	906	
2	D	906	
2	F	906	
2	H	906	

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Mol	Chain	Length	Quality of chain
2	N	906	
2	O	906	
2	Q	906	
2	R	906	
2	S	906	
2	T	906	
3	I	666	
3	K	666	
4	J	1019	
5	L	1698	
6	P	375	
7	U	671	
7	V	671	
7	W	671	
7	X	671	
8	a	451	
8	b	451	
8	c	451	
8	d	451	
8	e	451	
8	f	451	
8	g	451	
8	h	451	
8	i	451	
8	j	451	

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Mol	Chain	Length	Quality of chain
8	k	451	
8	l	451	
8	m	451	
8	n	451	
9	o	72	
9	p	72	
9	q	72	
9	r	72	
9	s	72	
9	t	72	

2 Entry composition [i](#)

There are 9 unique types of molecules in this entry. The entry contains 129788 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 Gamma-tubulin complex component.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	553	Total	C	N	O	S	0	0
			4519	2904	742	841	32		
1	C	553	Total	C	N	O	S	0	0
			4519	2904	742	841	32		
1	E	551	Total	C	N	O	S	0	0
			4508	2898	740	838	32		
1	G	553	Total	C	N	O	S	0	0
			4519	2904	742	841	32		
1	M	551	Total	C	N	O	S	0	0
			4503	2894	739	838	32		

- Molecule 2 is a protein called Gamma-tubulin complex component 3 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	625	Total	C	N	O	S	0	0
			5118	3276	880	936	26		
2	D	625	Total	C	N	O	S	0	0
			5118	3276	880	936	26		
2	F	625	Total	C	N	O	S	0	0
			5118	3276	880	936	26		
2	H	625	Total	C	N	O	S	0	0
			5118	3276	880	936	26		
2	N	625	Total	C	N	O	S	0	0
			5118	3276	880	936	26		
2	O	93	Total	C	N	O	S	0	0
			753	480	137	134	2		
2	Q	109	Total	C	N	O	S	0	0
			878	557	160	159	2		
2	R	98	Total	C	N	O	S	0	0
			794	503	144	145	2		
2	S	109	Total	C	N	O	S	0	0
			878	557	160	159	2		
2	T	93	Total	C	N	O	S	0	0
			753	480	137	134	2		

- Molecule 3 is a protein called Gamma-tubulin complex component.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	I	571	Total	C	N	O	S	0	0
			4635	2993	790	831	21		
3	K	571	Total	C	N	O	S	0	0
			4635	2993	790	831	21		

- Molecule 4 is a protein called Gamma-tubulin complex component.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	J	636	Total	C	N	O	S	0	0
			5252	3406	890	930	26		

- Molecule 5 is a protein called Gamma-tubulin complex component 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	L	780	Total	C	N	O	S	0	0
			6303	4088	1029	1155	31		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
L	392	ASP	GLU	conflict	UNP A0A974HT83
L	394	VAL	ILE	conflict	UNP A0A974HT83

- Molecule 6 is a protein called Actin, cytoplasmic 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	P	371	Total	C	N	O	S	0	0
			2892	1828	486	557	21		

- Molecule 7 is a protein called NEDD1 gamma-tubulin ring complex targeting factor L homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	U	75	Total	C	N	O	S	0	0
			634	396	112	122	4		
7	V	75	Total	C	N	O	S	0	0
			634	396	112	122	4		
7	W	75	Total	C	N	O	S	0	0
			634	396	112	122	4		
7	X	75	Total	C	N	O	S	0	0
			634	396	112	122	4		

- Molecule 8 is a protein called Tubulin gamma-1 chain.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	a	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	b	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	c	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	d	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	e	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	f	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	g	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	h	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	i	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	j	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	k	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	l	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	m	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		
8	n	436	Total	C	N	O	S	0	0
			3479	2188	615	662	14		

- Molecule 9 is a protein called Mitotic-spindle organizing protein 1.

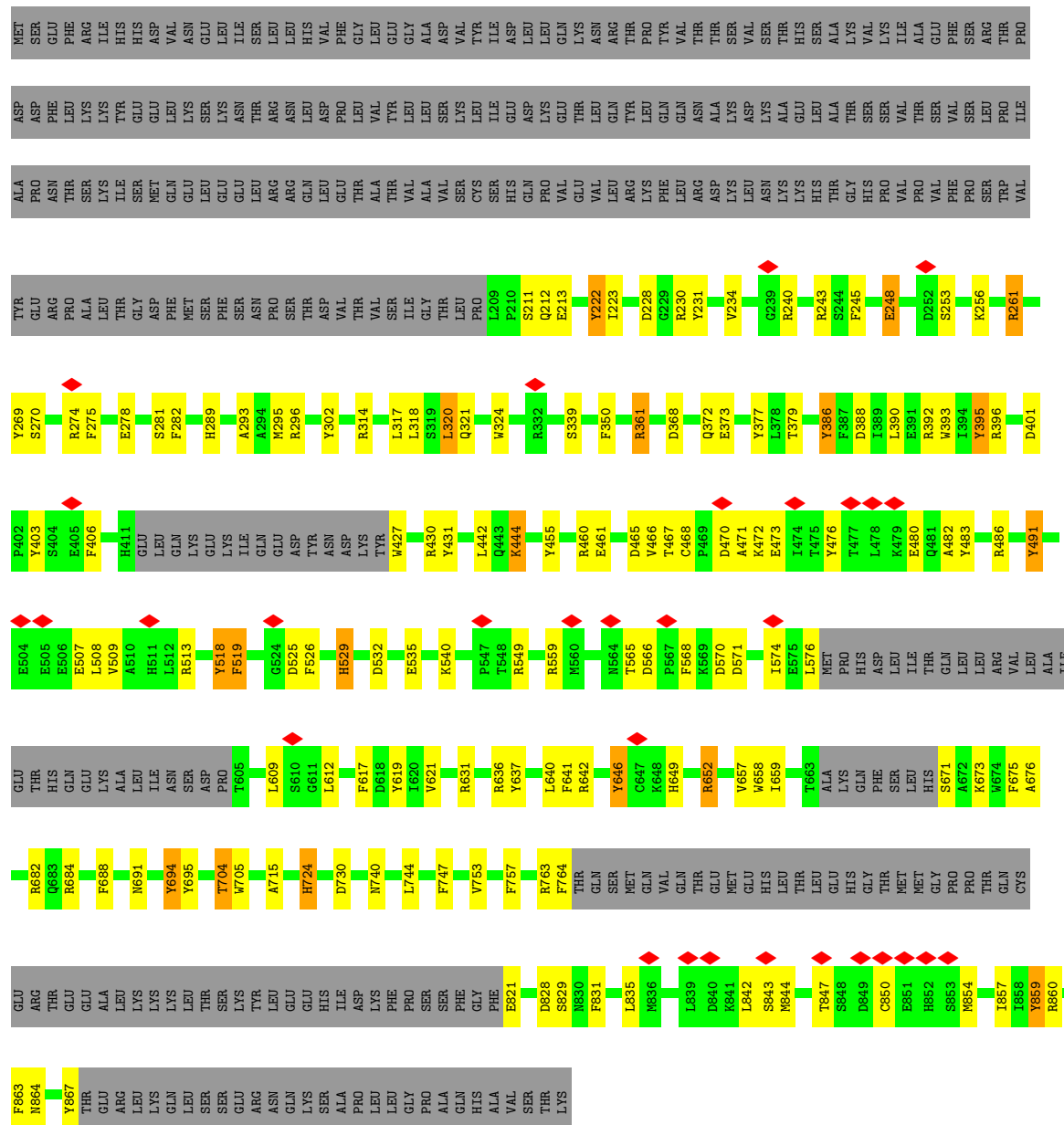
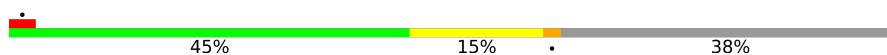
Mol	Chain	Residues	Atoms					AltConf	Trace
9	o	52	Total	C	N	O	S	0	0
			403	248	71	79	5		
9	p	56	Total	C	N	O	S	0	0
			429	263	73	89	4		
9	q	56	Total	C	N	O	S	0	0
			432	266	76	86	4		
9	r	59	Total	C	N	O	S	0	0
			454	278	80	91	5		
9	s	59	Total	C	N	O	S	0	0
			451	277	79	90	5		

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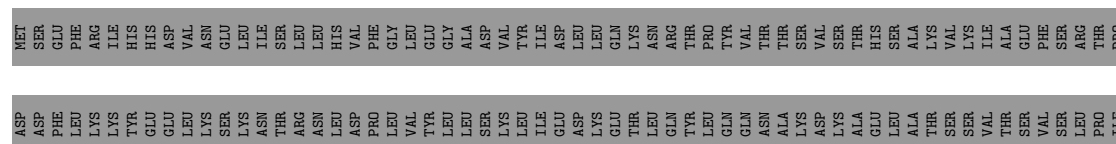
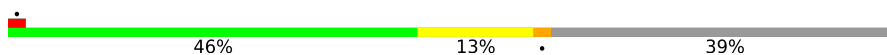
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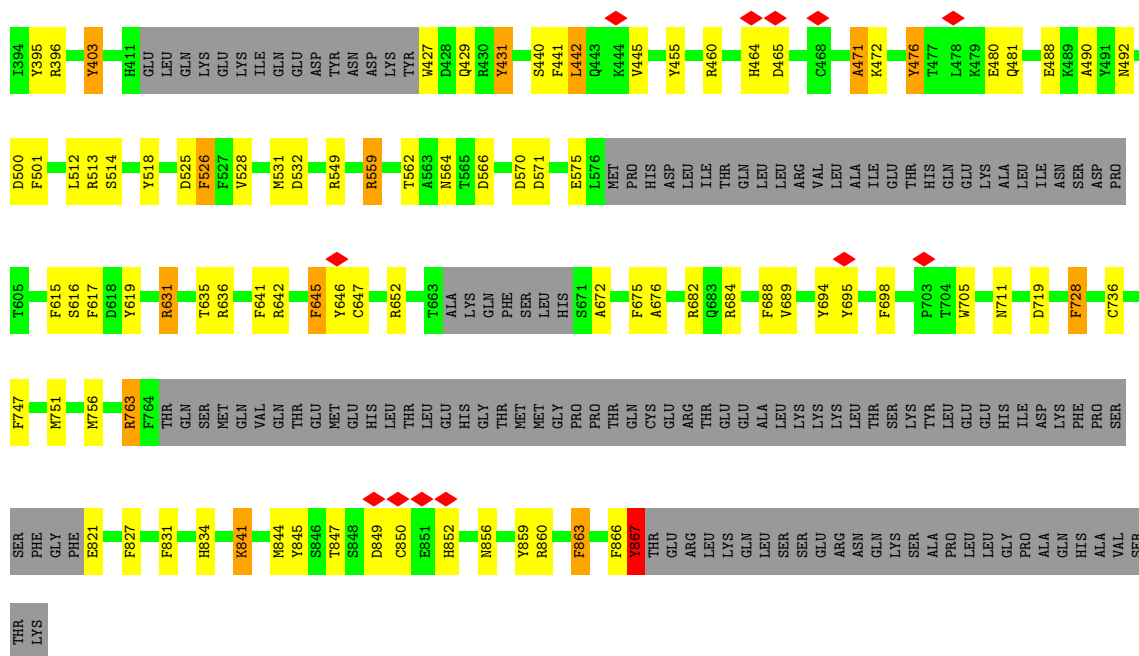
Mol	Chain	Residues	Atoms					AltConf	Trace
9	t	58	Total	C	N	O	S	0	0
			446	274	78	89	5		

Chain C:

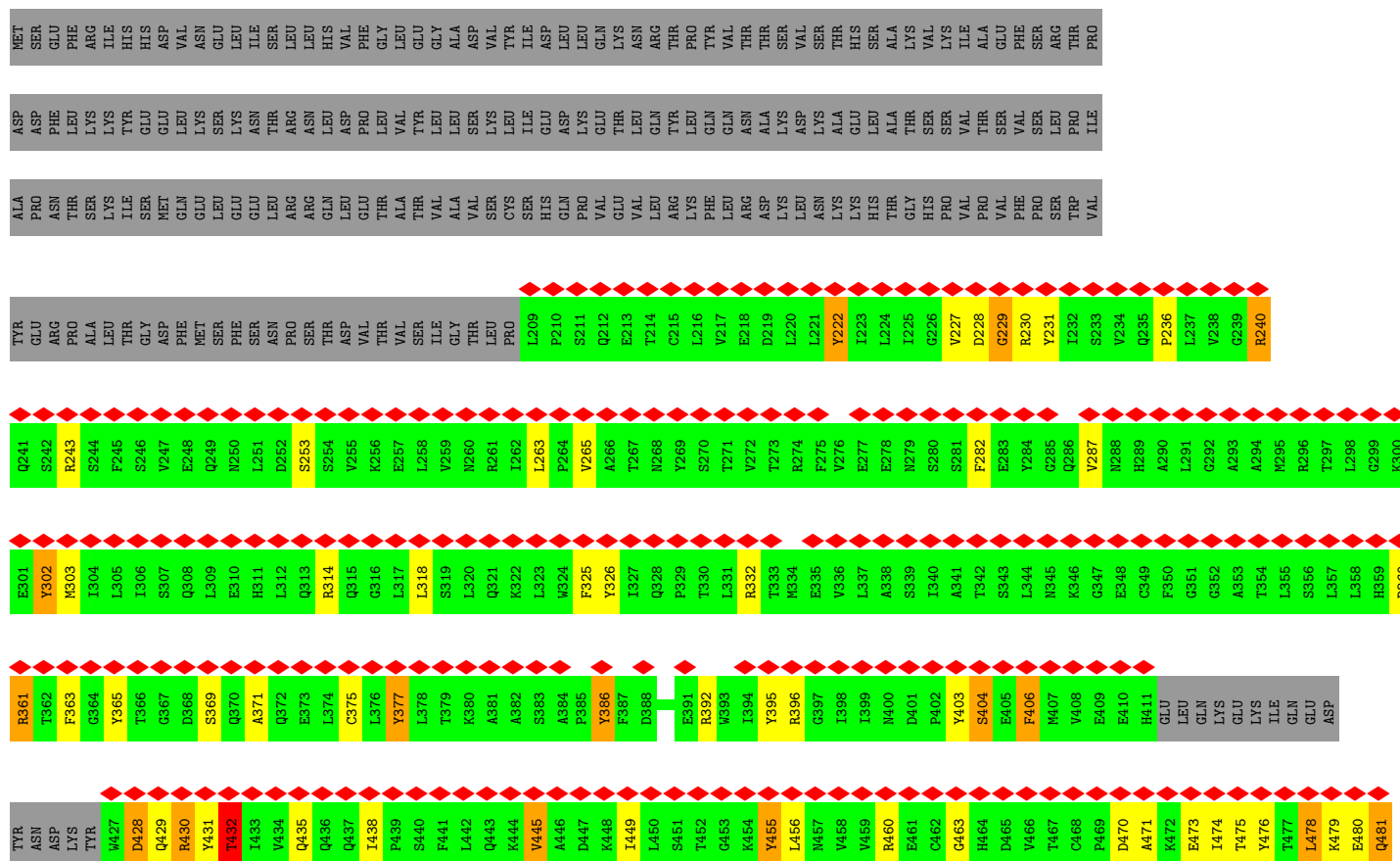


Chain E:

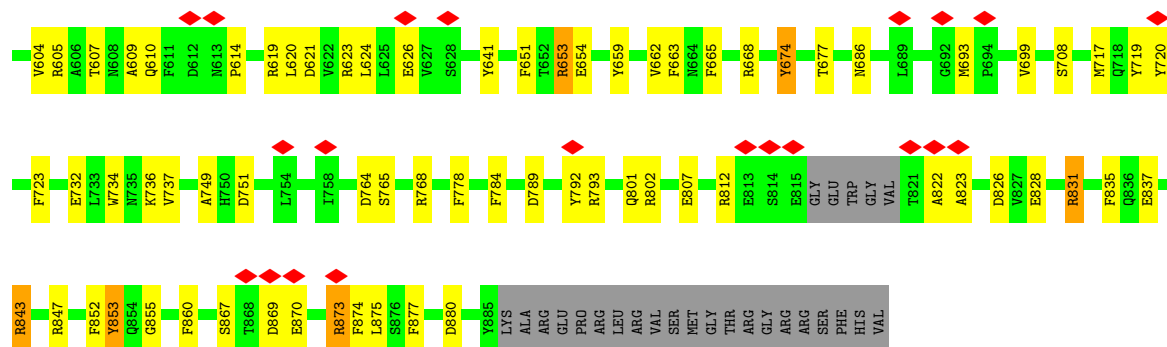




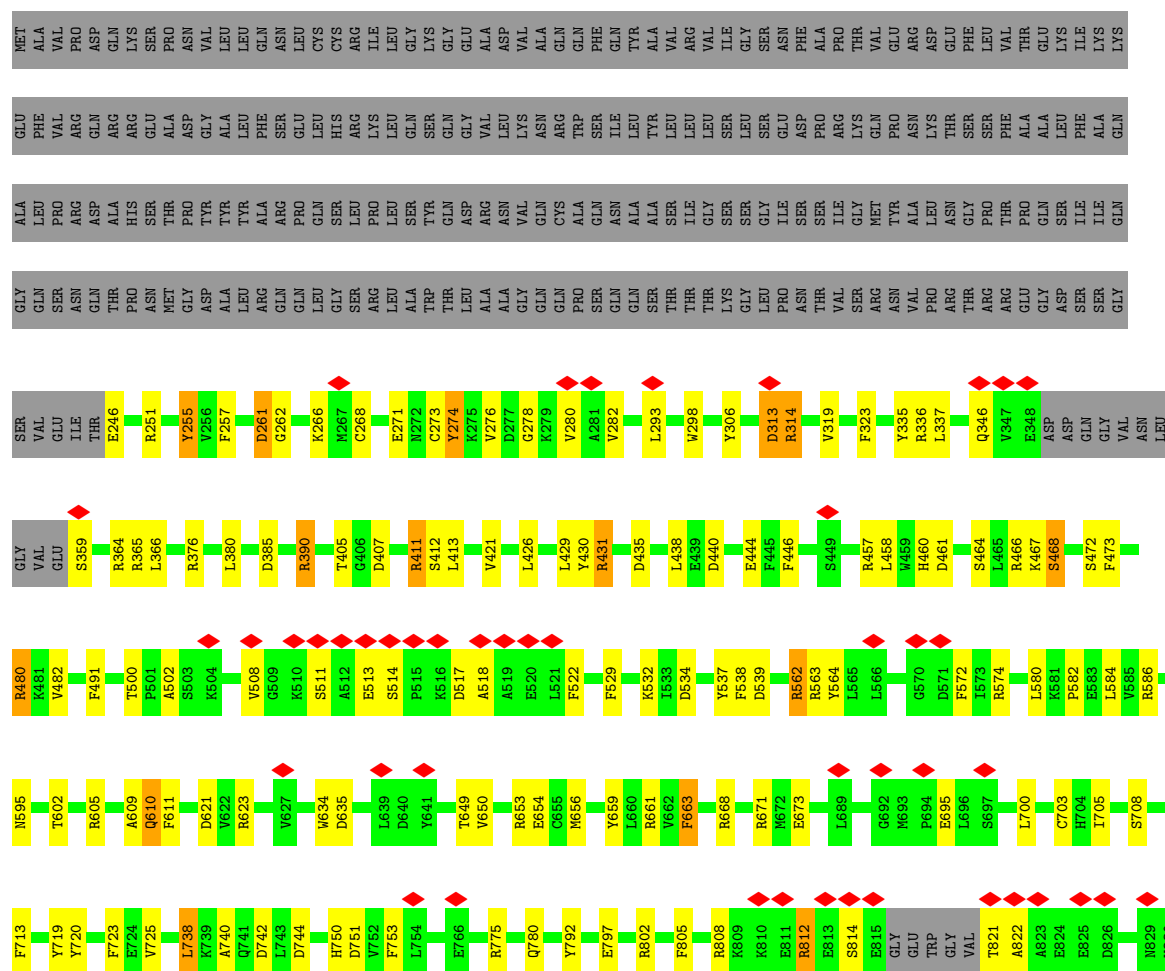
• Molecule 1: Gamma-tubulin complex component





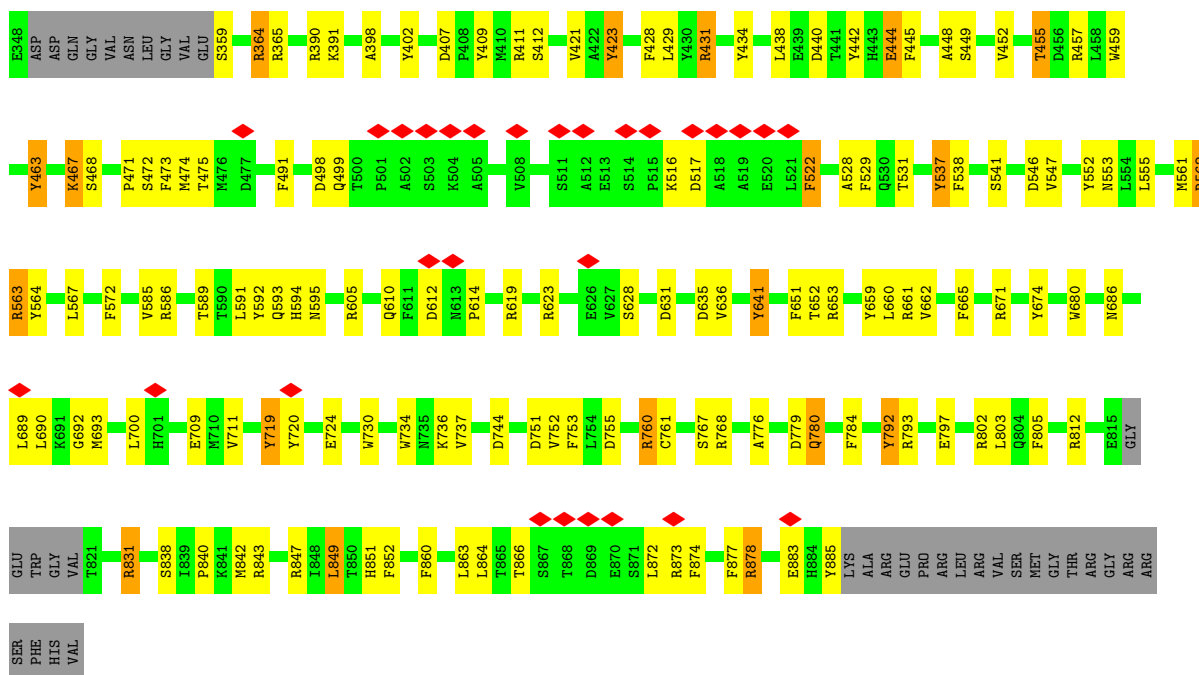


• Molecule 2: Gamma-tubulin complex component 3 homolog

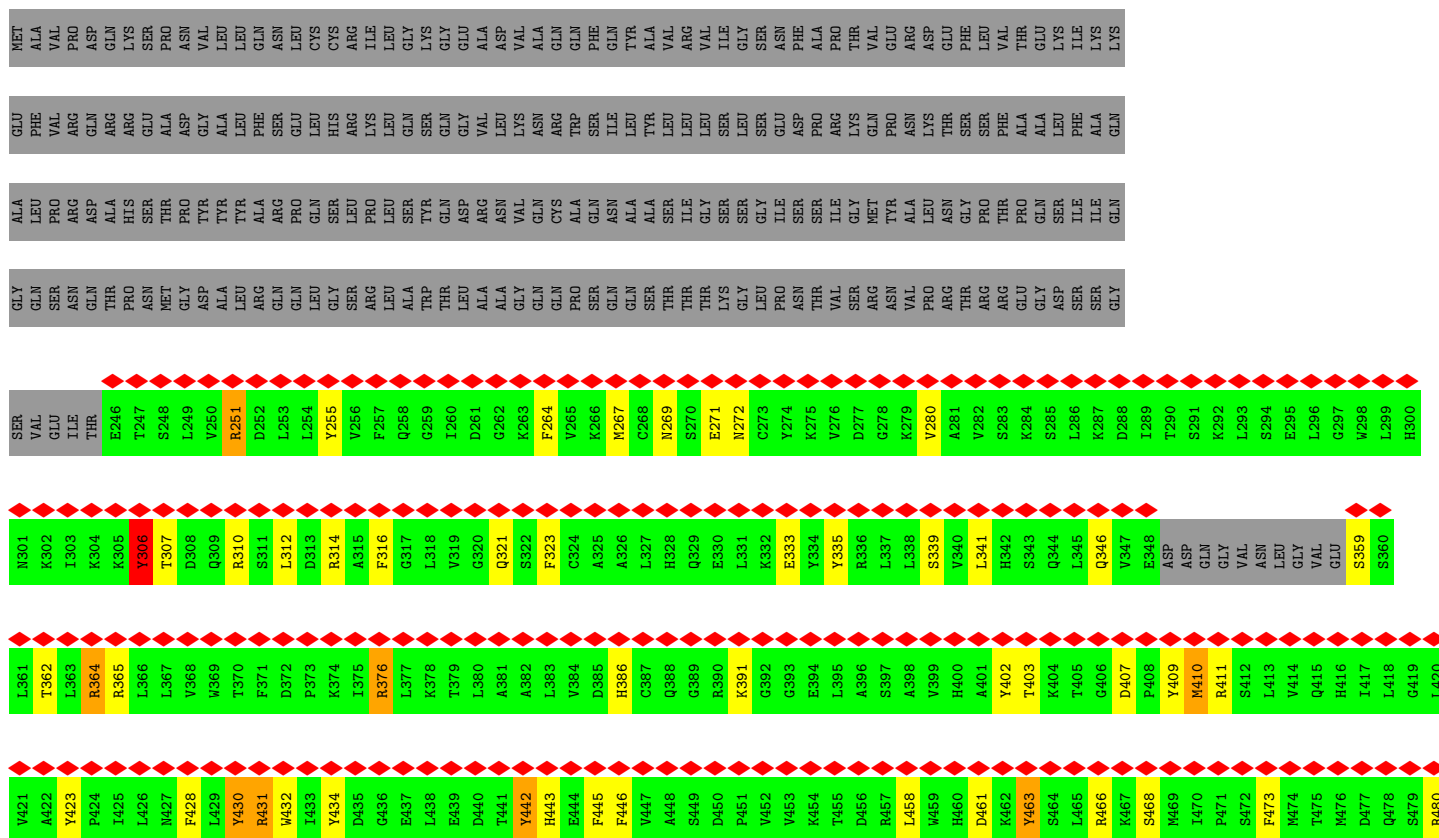


• Molecule 2: Gamma-tubulin complex component 3 homolog





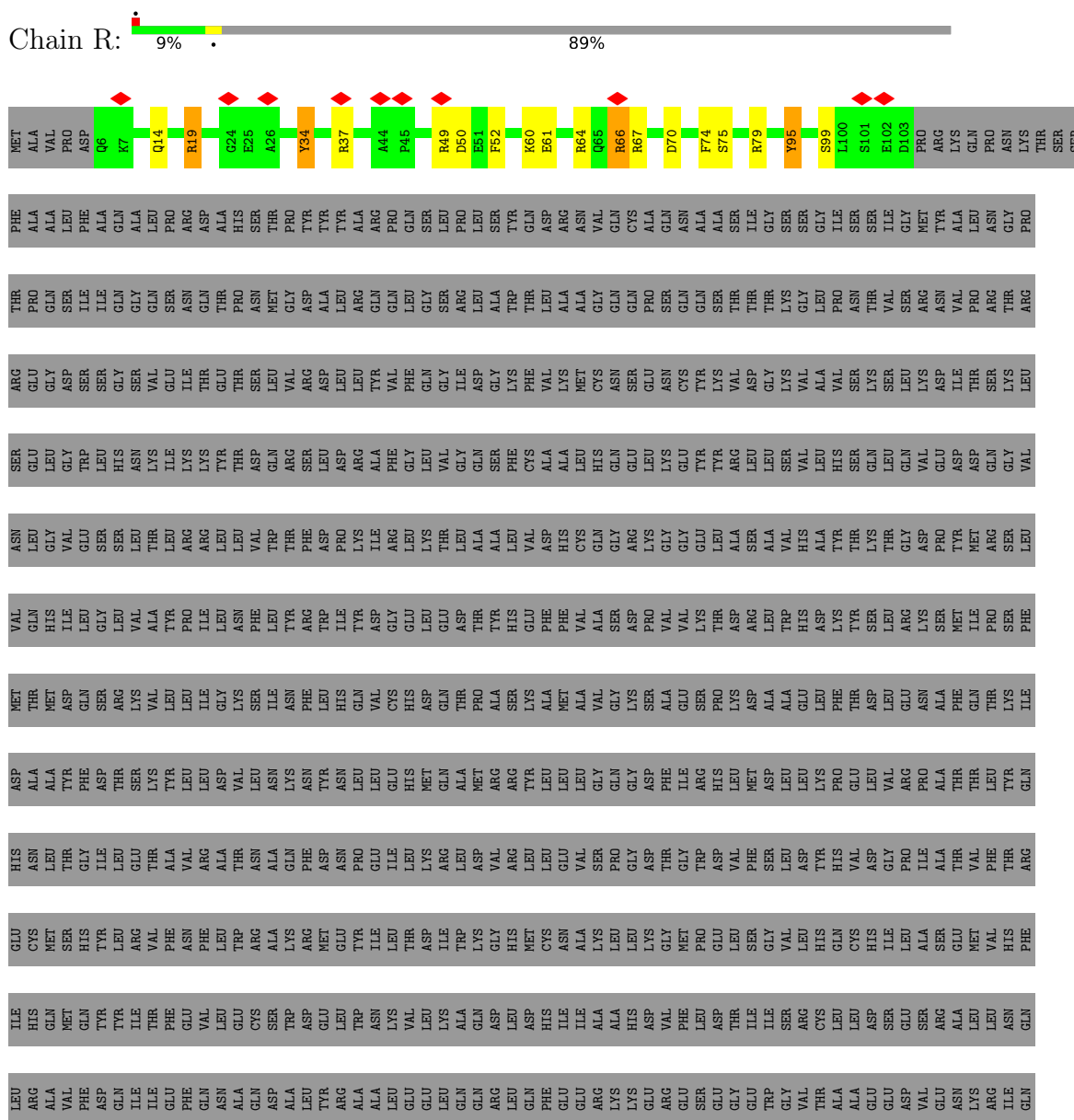
- Molecule 2: Gamma-tubulin complex component 3 homolog





[illegible]

- Molecule 2: Gamma-tubulin complex component 3 homolog

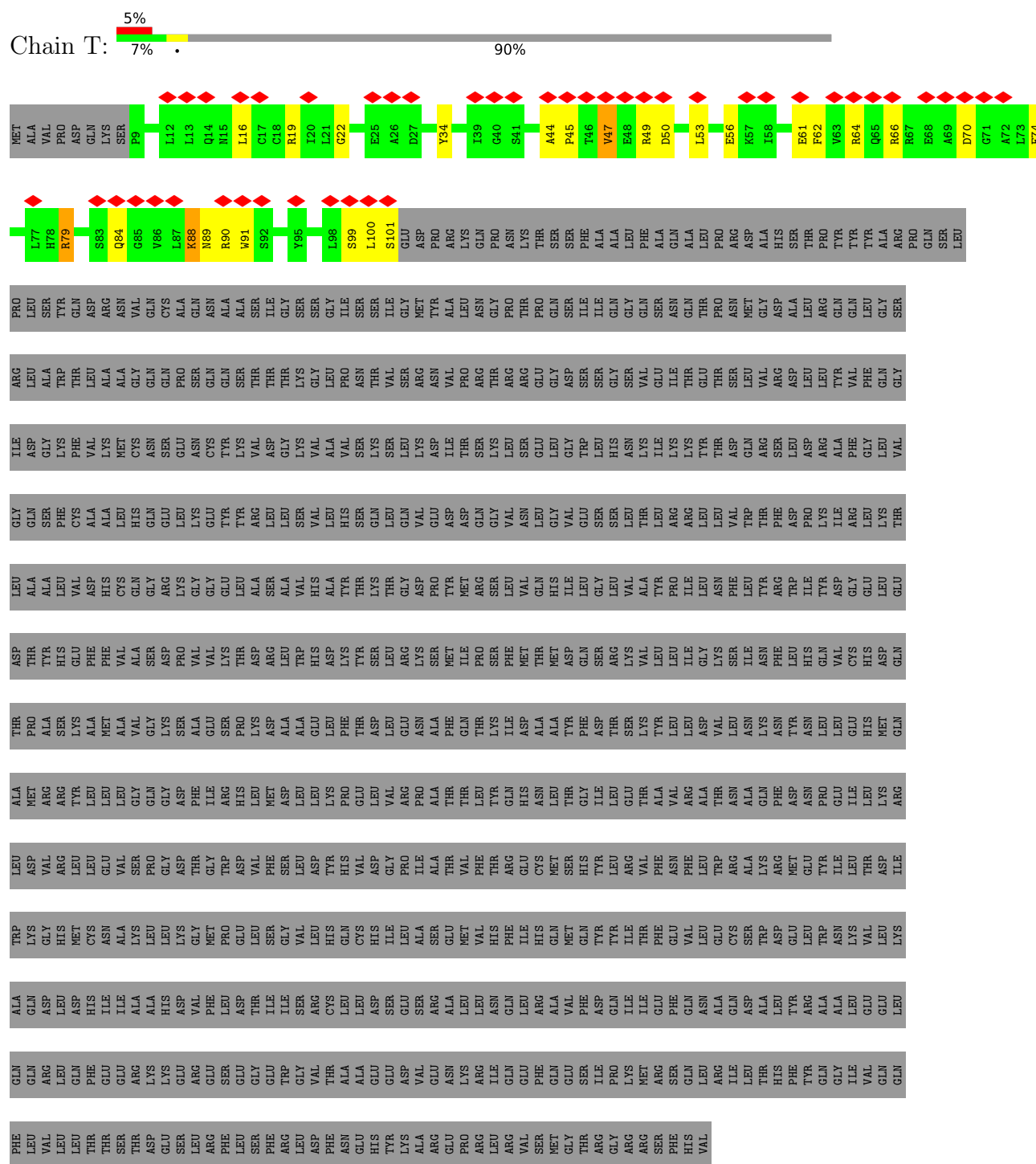


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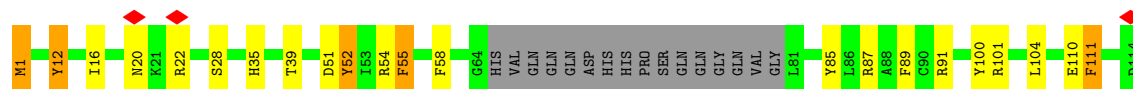
- Molecule 2: Gamma-tubulin complex component 3 homolog

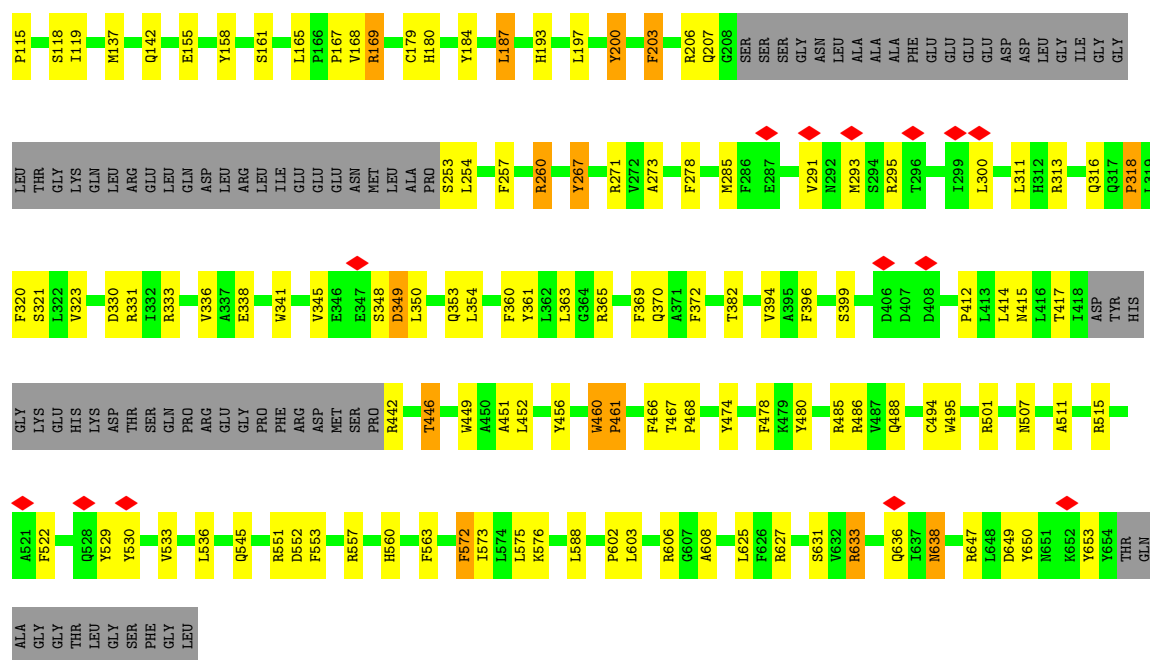
[illegible]

- Molecule 2: Gamma-tubulin complex component 3 homolog

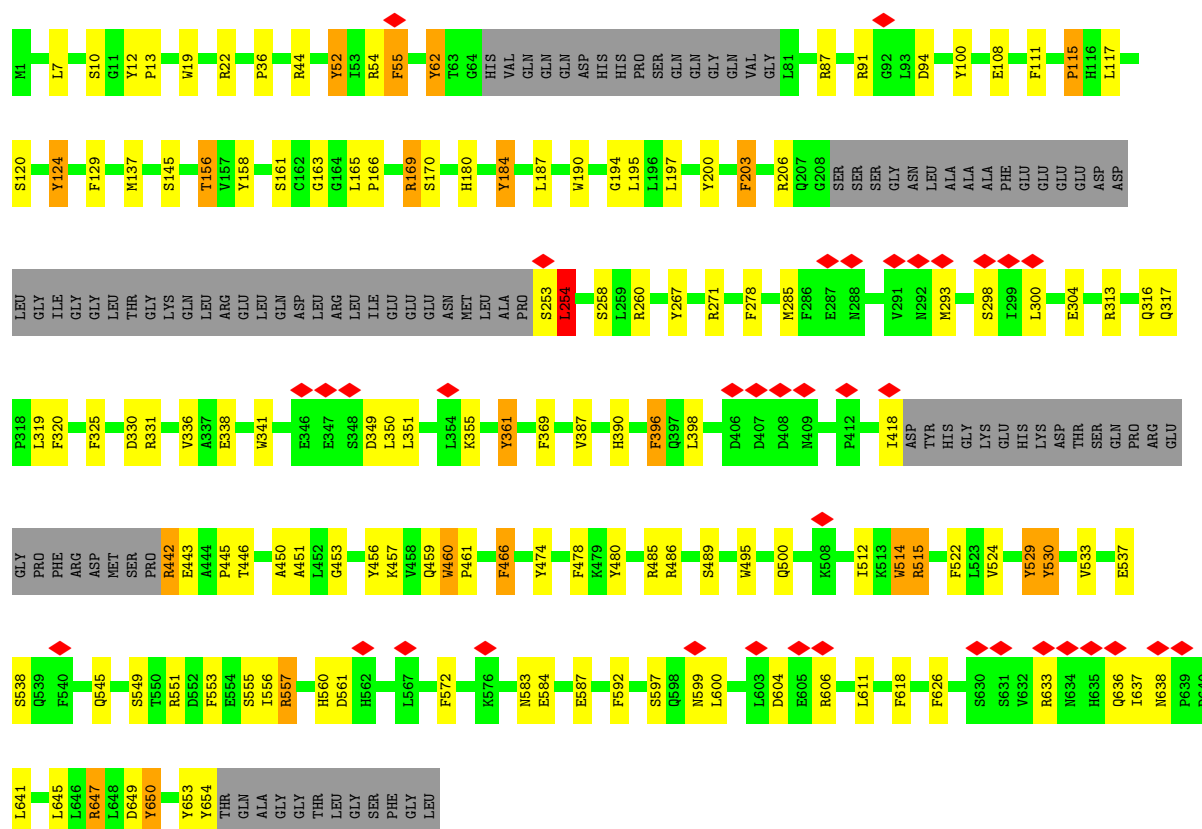


• Molecule 3: Gamma-tubulin complex component



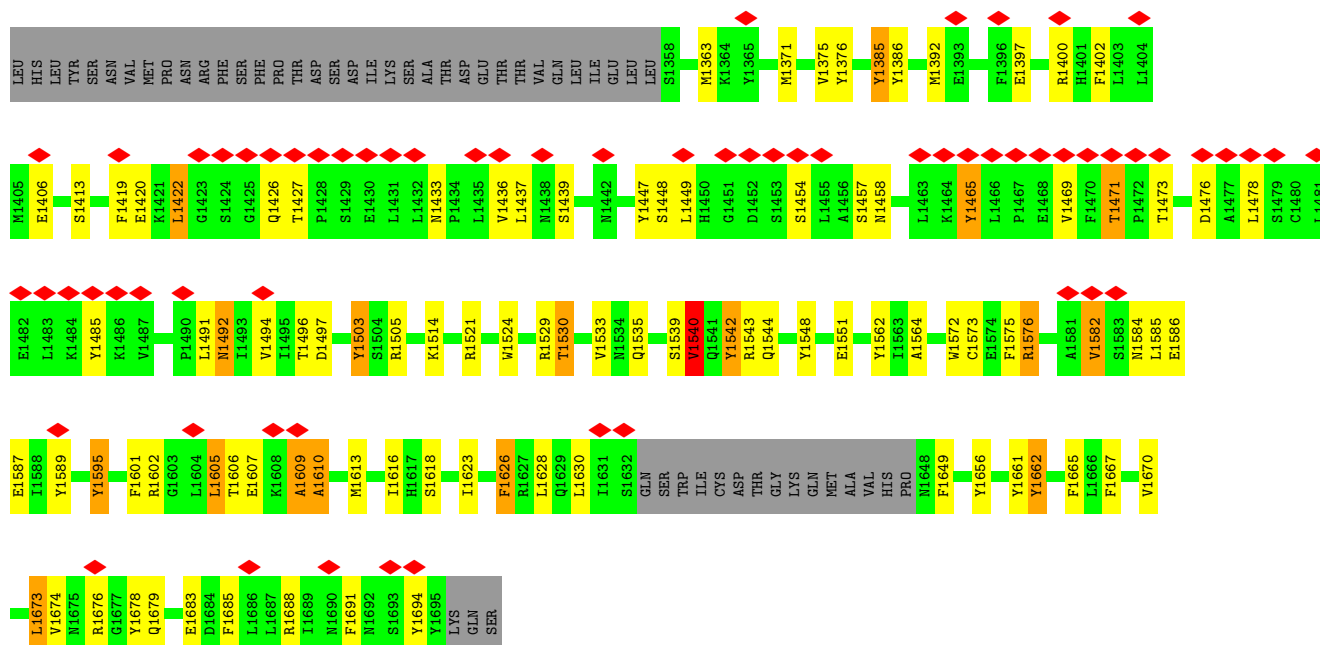


• Molecule 3: Gamma-tubulin complex component

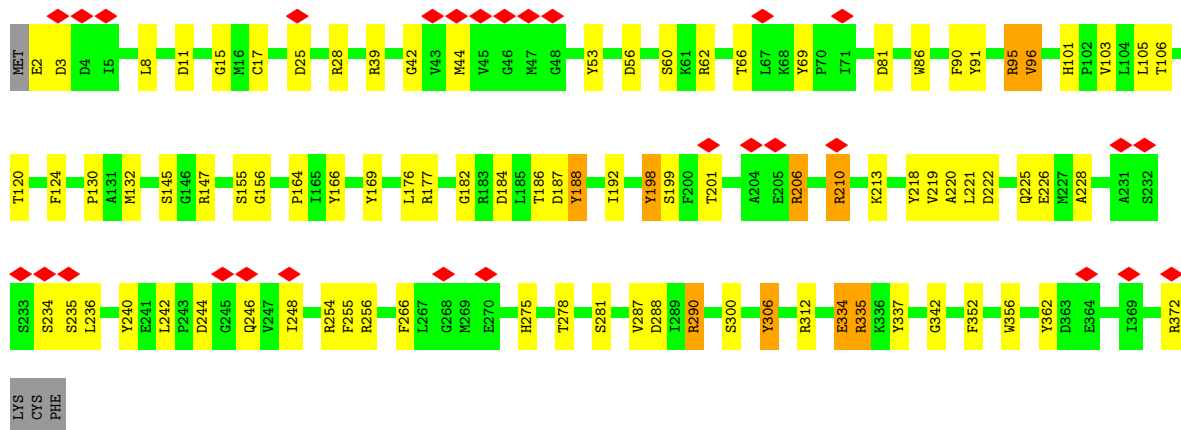
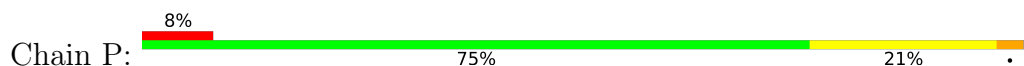


• Molecule 4: Gamma-tubulin complex component

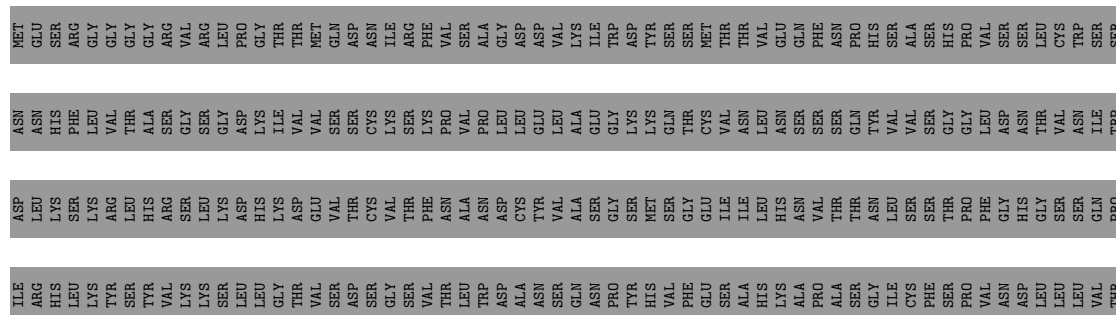


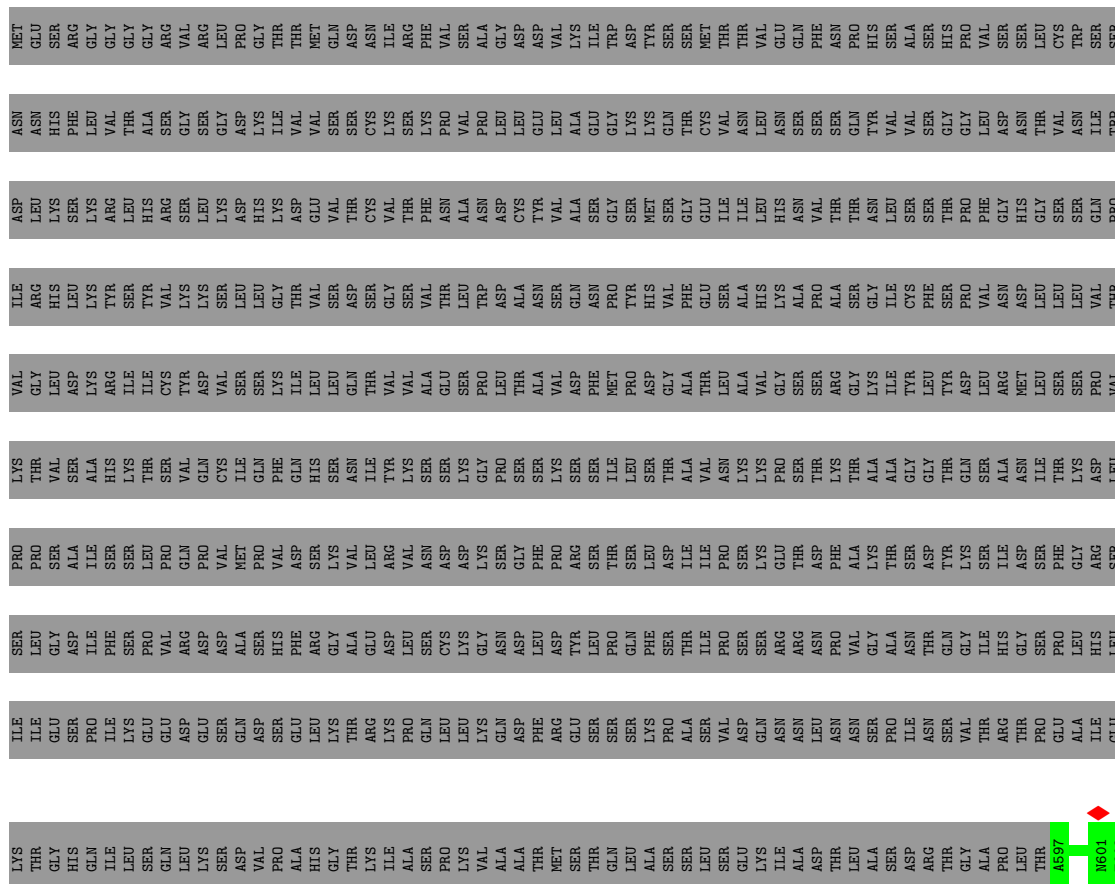


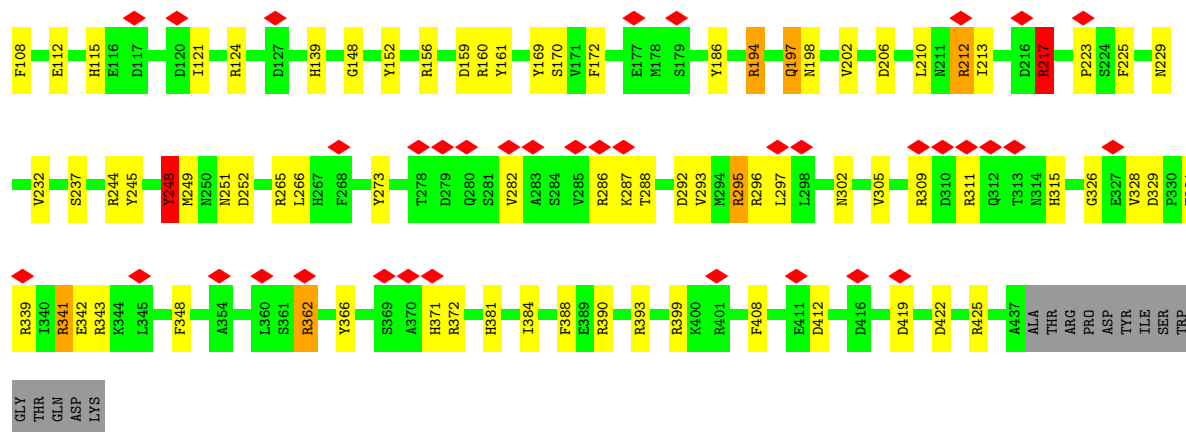
• Molecule 6: Actin, cytoplasmic 1



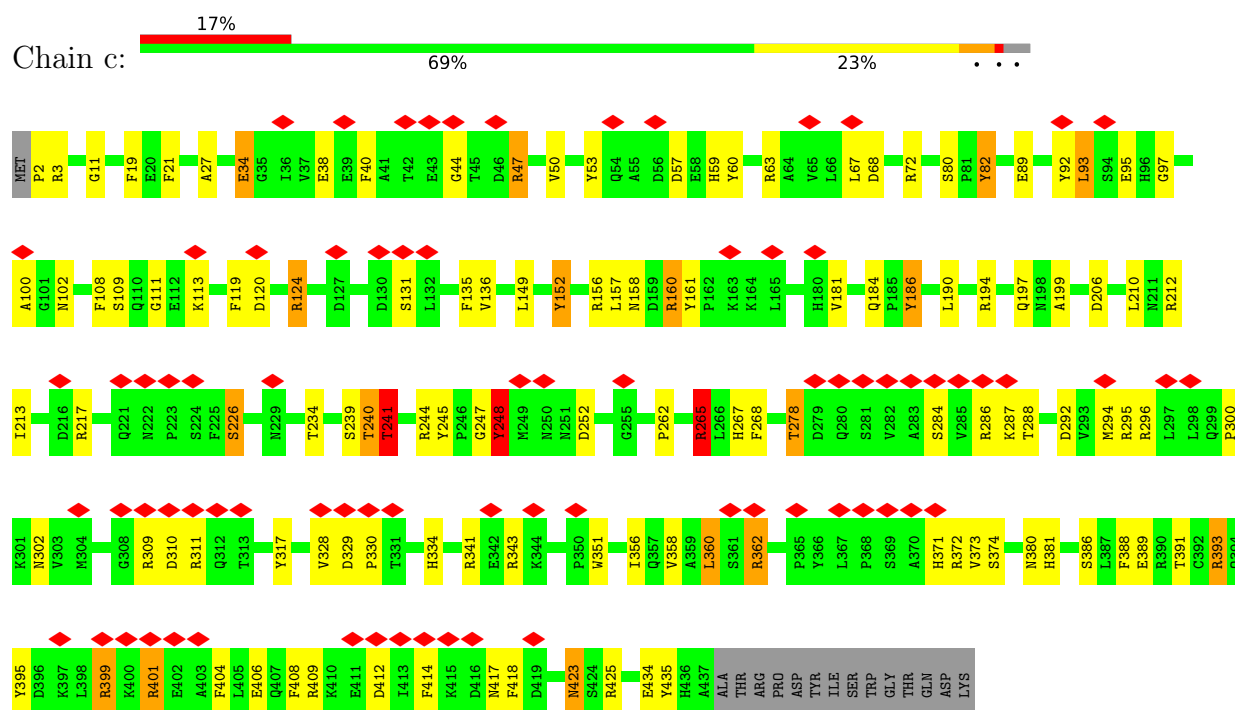
• Molecule 7: NEDD1 gamma-tubulin ring complex targeting factor L homeolog



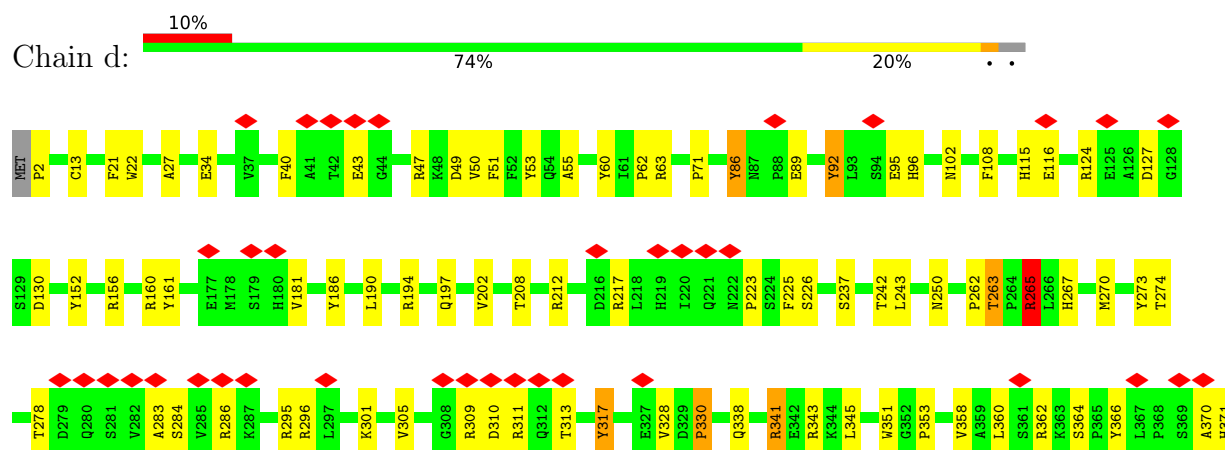




• Molecule 8: Tubulin gamma-1 chain

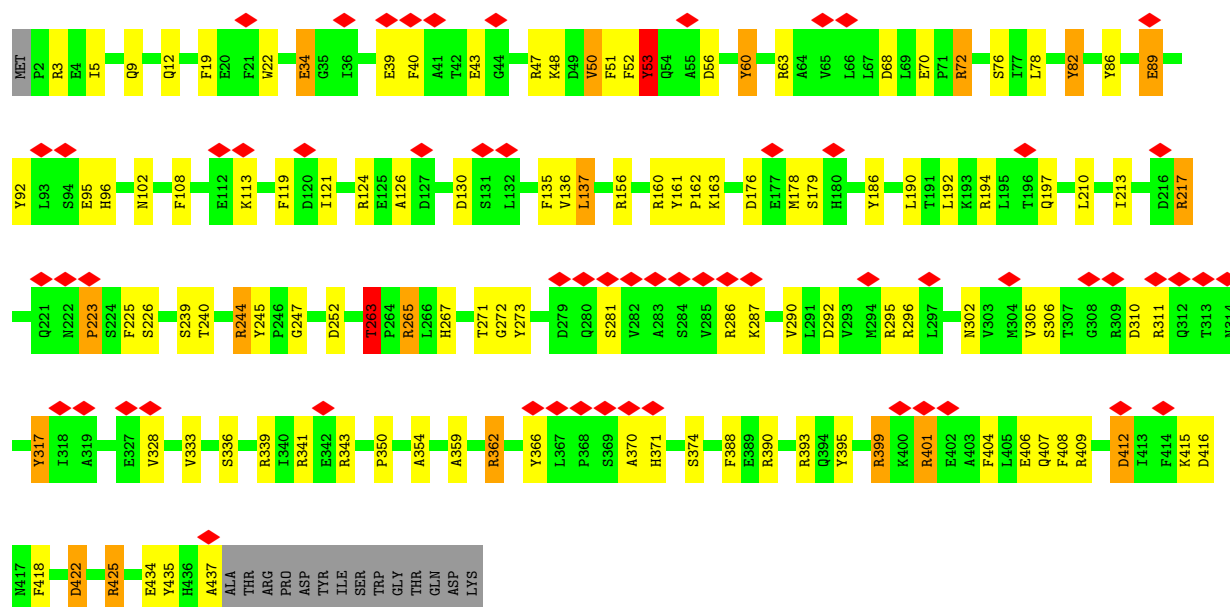


• Molecule 8: Tubulin gamma-1 chain

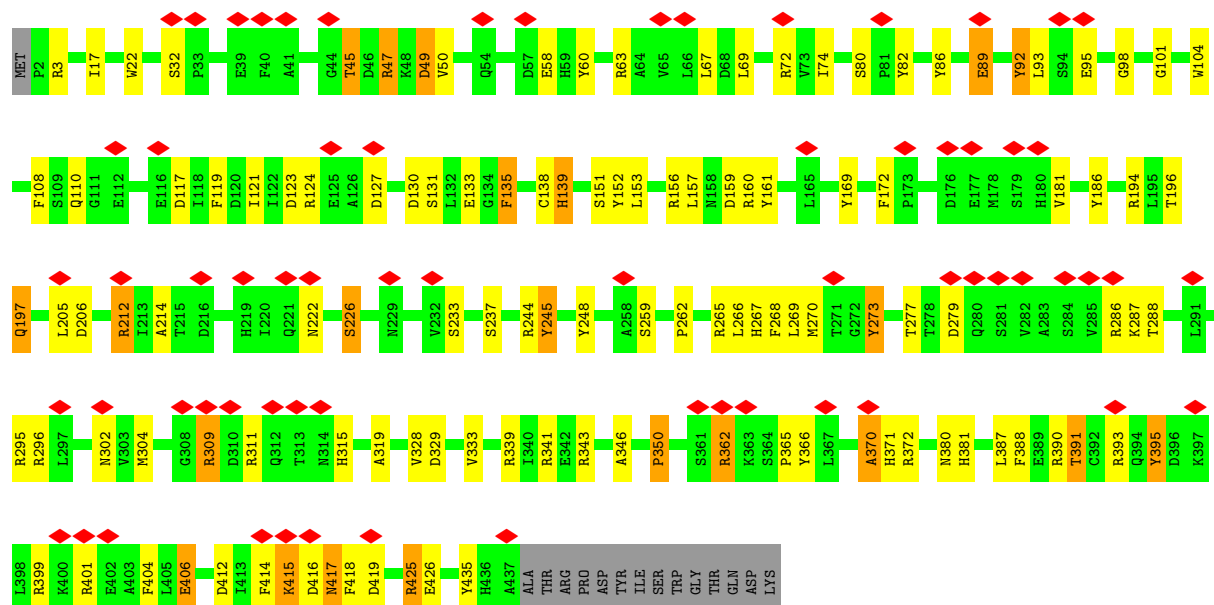




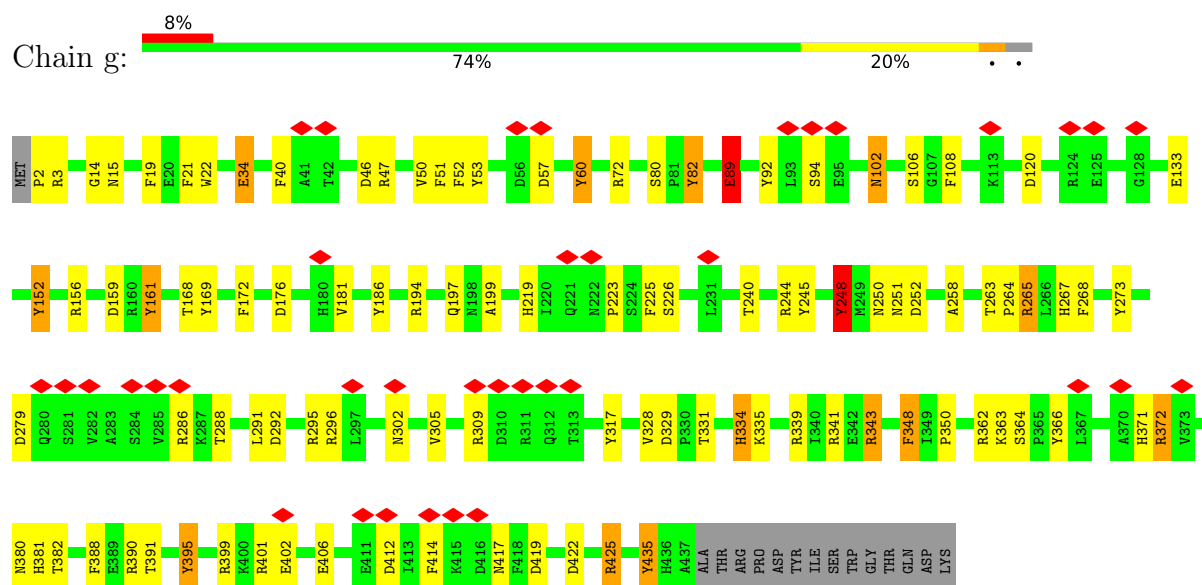
• Molecule 8: Tubulin gamma-1 chain



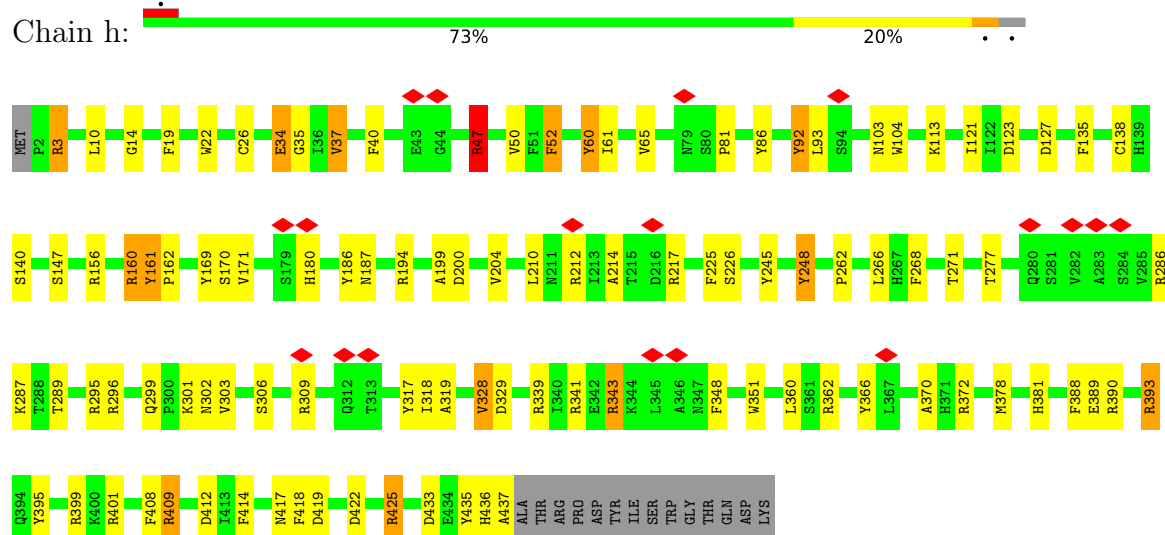
• Molecule 8: Tubulin gamma-1 chain



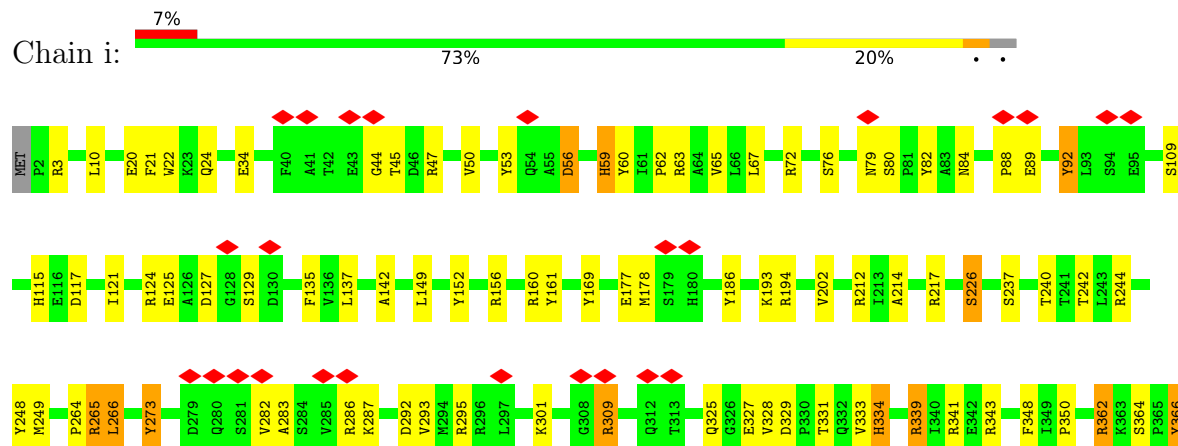
• Molecule 8: Tubulin gamma-1 chain

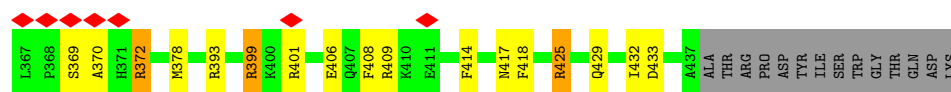


• Molecule 8: Tubulin gamma-1 chain

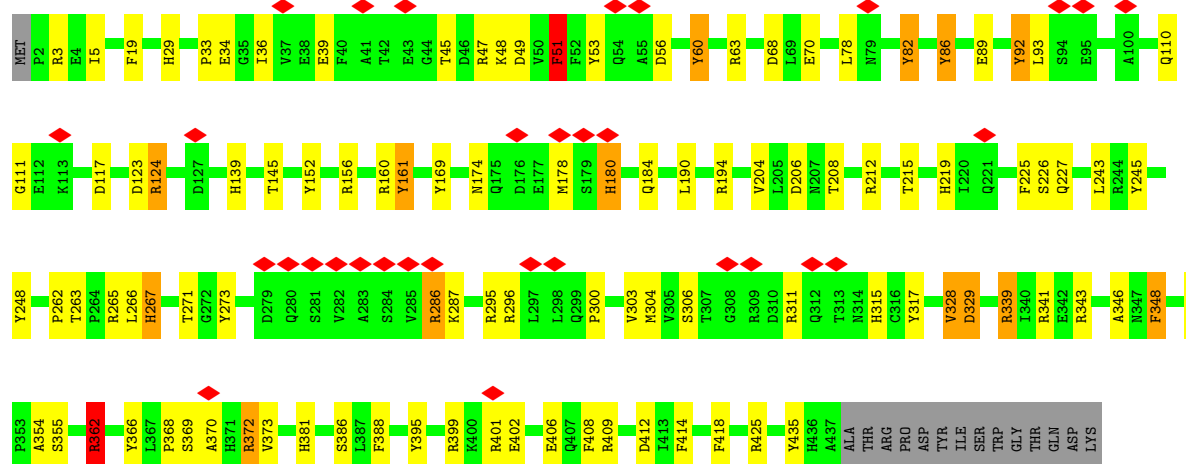
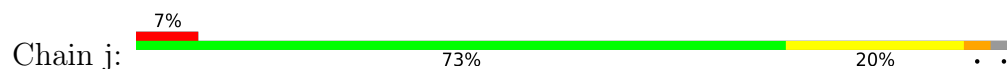


• Molecule 8: Tubulin gamma-1 chain

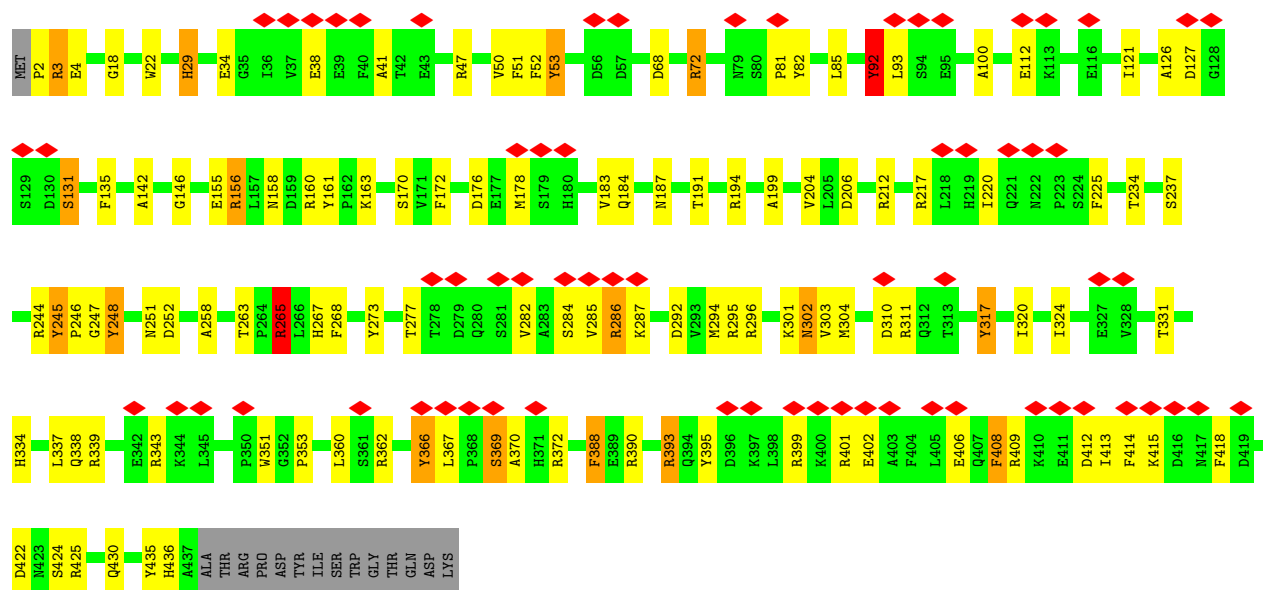




• Molecule 8: Tubulin gamma-1 chain

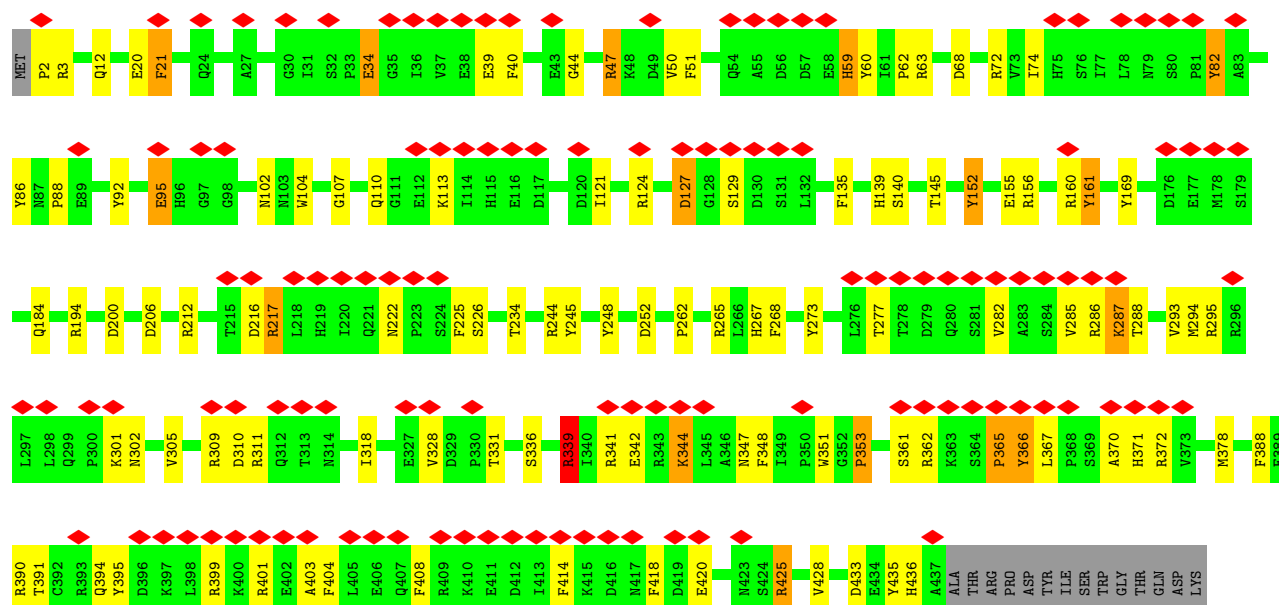


• Molecule 8: Tubulin gamma-1 chain

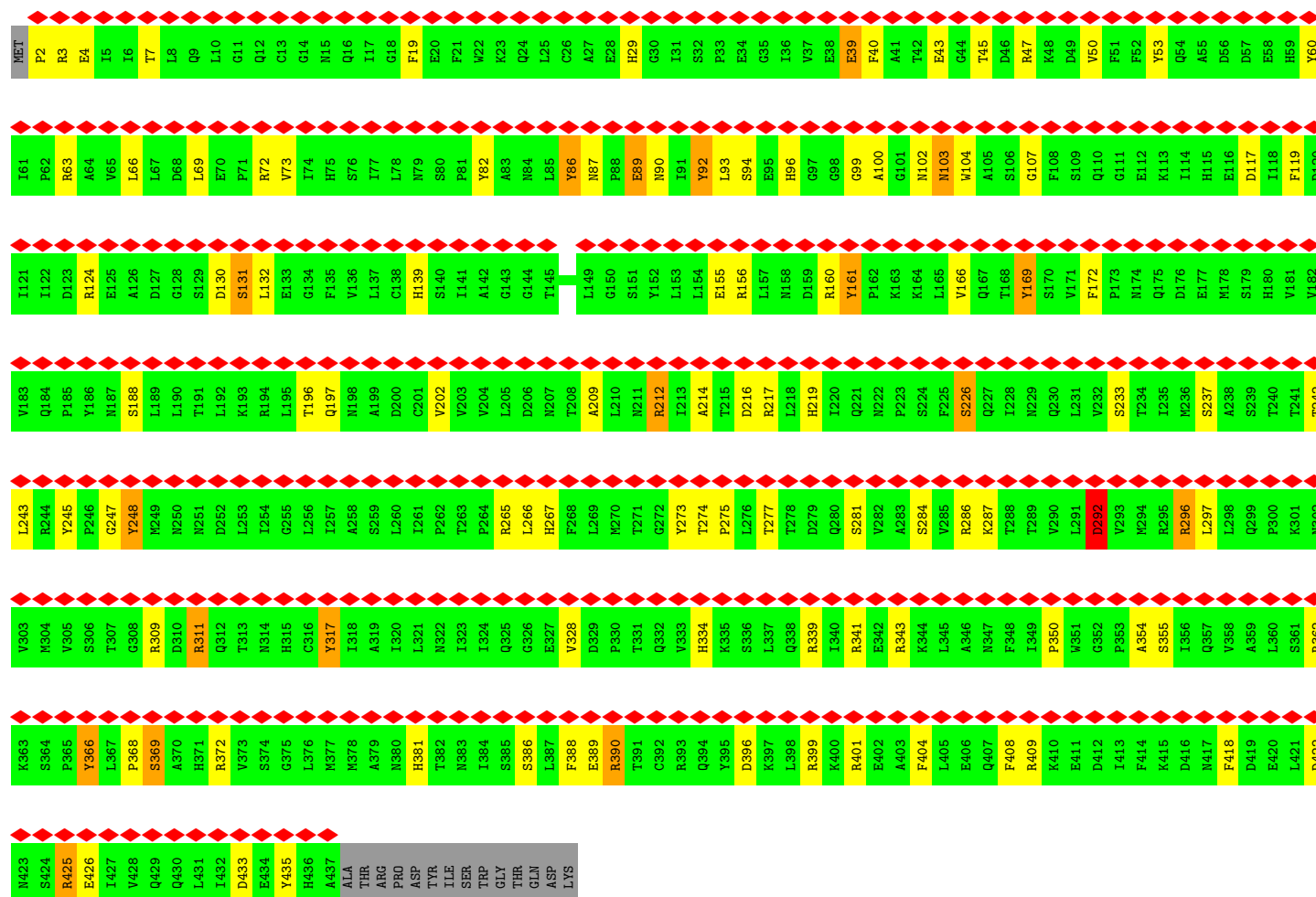
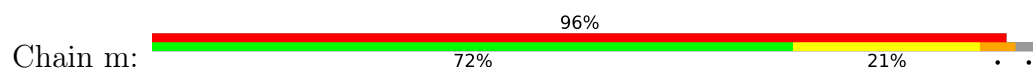


• Molecule 8: Tubulin gamma-1 chain

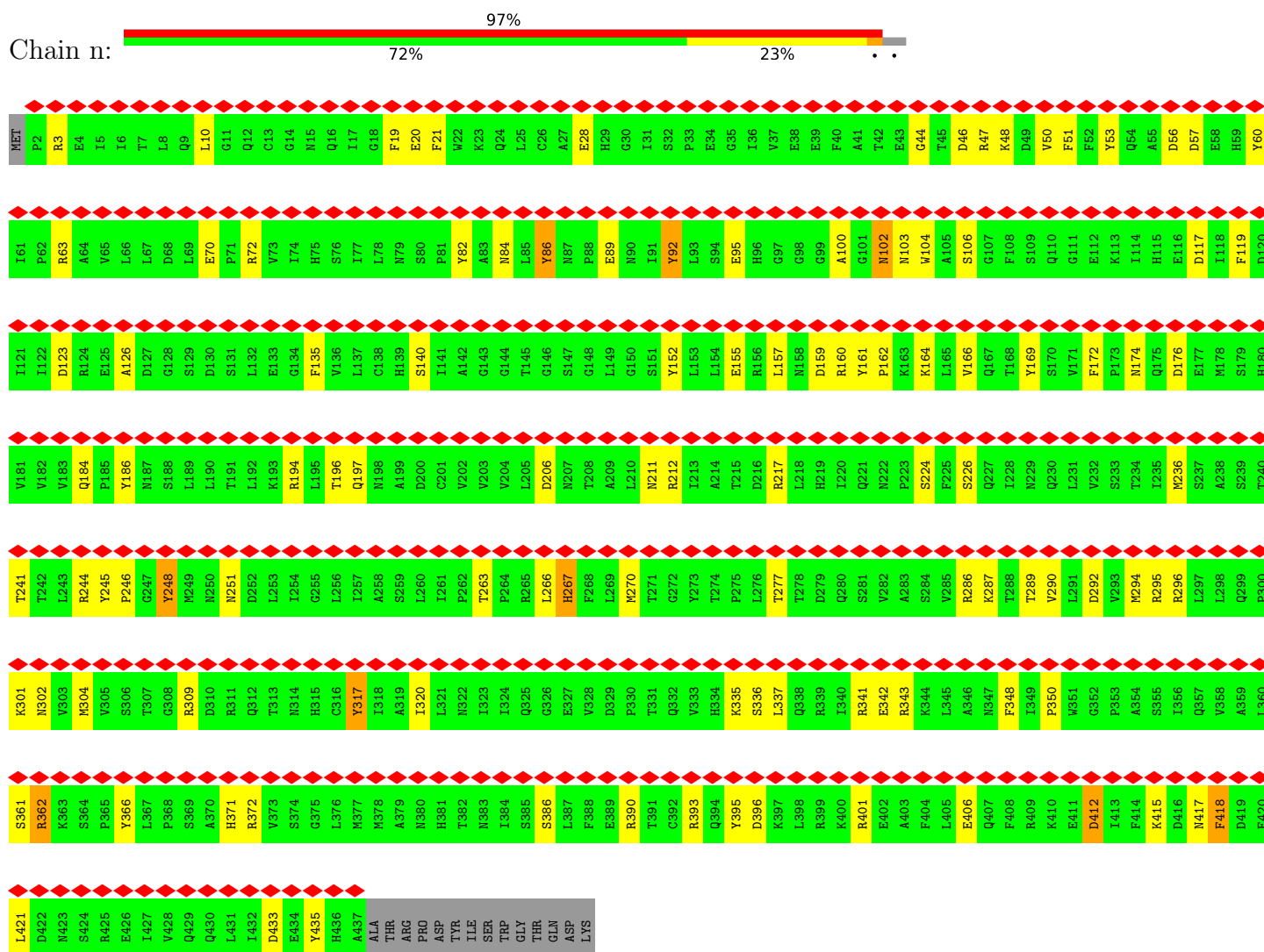




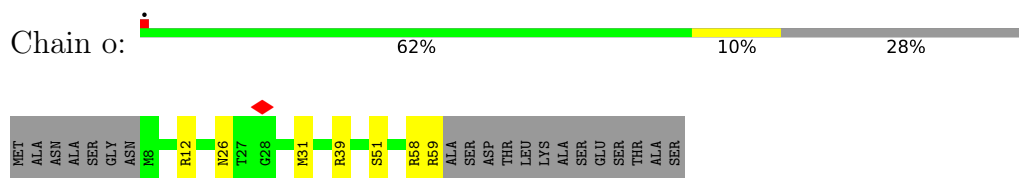
• Molecule 8: Tubulin gamma-1 chain



- Molecule 8: Tubulin gamma-1 chain



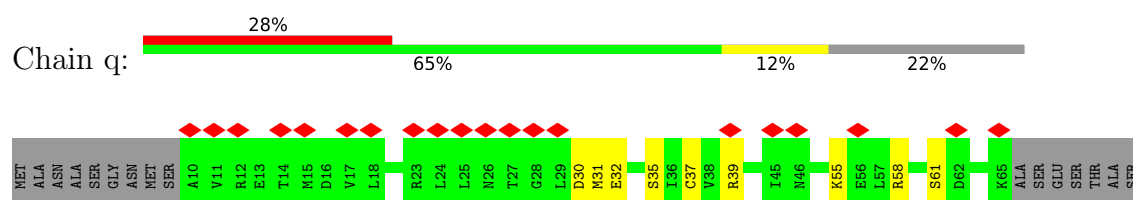
- Molecule 9: Mitotic-spindle organizing protein 1



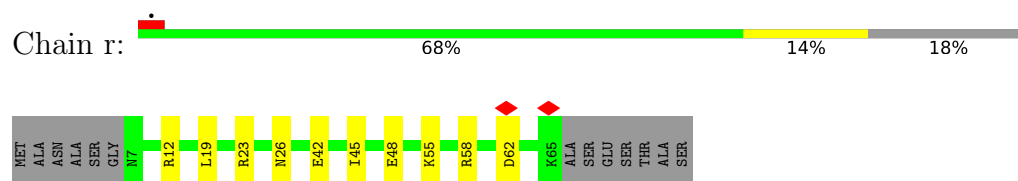
- Molecule 9: Mitotic-spindle organizing protein 1



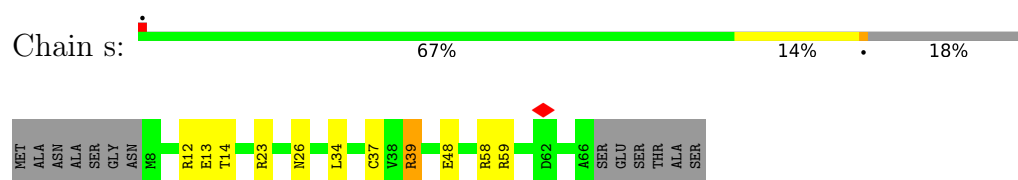
- Molecule 9: Mitotic-spindle organizing protein 1



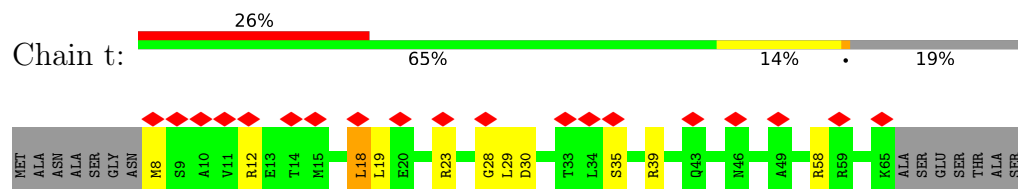
- Molecule 9: Mitotic-spindle organizing protein 1



- Molecule 9: Mitotic-spindle organizing protein 1



- Molecule 9: Mitotic-spindle organizing protein 1



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	299022	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	51	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.276	Depositor
Minimum map value	-0.152	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0217	Depositor
Map size (Å)	547.8528, 547.8528, 547.8528	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.4267, 1.4267, 1.4267	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 >5	RMSZ	# Z >5
1	A	1.72	38/4614 (0.8%)	1.90	107/6236 (1.7%)
1	C	1.70	39/4614 (0.8%)	1.98	127/6236 (2.0%)
1	E	1.72	41/4603 (0.9%)	1.94	119/6221 (1.9%)
1	G	1.73	37/4614 (0.8%)	2.00	138/6236 (2.2%)
1	M	1.72	37/4598 (0.8%)	1.93	126/6215 (2.0%)
2	B	1.69	28/5227 (0.5%)	1.95	115/7060 (1.6%)
2	D	1.71	38/5227 (0.7%)	1.94	122/7060 (1.7%)
2	F	1.71	39/5227 (0.7%)	1.98	136/7060 (1.9%)
2	H	1.71	40/5227 (0.8%)	1.91	143/7060 (2.0%)
2	N	1.73	45/5227 (0.9%)	1.95	136/7060 (1.9%)
2	O	1.77	5/764 (0.7%)	1.89	18/1026 (1.8%)
2	Q	1.73	6/892 (0.7%)	1.98	24/1199 (2.0%)
2	R	1.78	5/805 (0.6%)	2.00	21/1081 (1.9%)
2	S	1.72	6/892 (0.7%)	2.01	17/1199 (1.4%)
2	T	1.76	9/764 (1.2%)	1.89	21/1026 (2.0%)
3	I	1.73	37/4738 (0.8%)	1.91	115/6416 (1.8%)
3	K	1.95	48/4738 (1.0%)	2.04	109/6416 (1.7%)
4	J	1.95	41/5372 (0.8%)	1.94	132/7271 (1.8%)
5	L	1.70	49/6435 (0.8%)	1.95	163/8710 (1.9%)
6	P	1.74	25/2954 (0.8%)	1.92	73/4003 (1.8%)
7	U	1.71	7/640 (1.1%)	1.83	11/854 (1.3%)
7	V	1.67	4/640 (0.6%)	1.97	18/854 (2.1%)
7	W	1.68	3/640 (0.5%)	1.85	11/854 (1.3%)
7	X	1.71	10/640 (1.6%)	1.95	17/854 (2.0%)
8	a	1.70	25/3551 (0.7%)	1.93	85/4815 (1.8%)
8	b	1.71	22/3551 (0.6%)	1.91	79/4815 (1.6%)
8	c	1.78	41/3551 (1.2%)	1.97	93/4815 (1.9%)
8	d	1.74	27/3551 (0.8%)	1.93	69/4815 (1.4%)
8	e	1.73	35/3551 (1.0%)	1.99	100/4815 (2.1%)
8	f	1.73	26/3551 (0.7%)	1.96	97/4815 (2.0%)
8	g	1.69	16/3551 (0.5%)	1.95	86/4815 (1.8%)
8	h	1.71	27/3551 (0.8%)	1.98	94/4815 (2.0%)
8	i	1.73	31/3551 (0.9%)	1.96	89/4815 (1.8%)
8	j	1.74	33/3551 (0.9%)	2.02	79/4815 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
8	k	2.60	31/3551 (0.9%)	1.96	102/4815 (2.1%)
8	l	1.72	36/3551 (1.0%)	1.97	96/4815 (2.0%)
8	m	1.73	40/3551 (1.1%)	1.95	81/4815 (1.7%)
8	n	1.75	34/3551 (1.0%)	1.96	96/4815 (2.0%)
9	o	1.68	0/403	1.88	8/541 (1.5%)
9	p	1.67	3/429 (0.7%)	1.85	4/577 (0.7%)
9	q	1.67	2/432 (0.5%)	1.90	7/581 (1.2%)
9	r	1.64	1/454 (0.2%)	1.97	8/610 (1.3%)
9	s	1.65	3/451 (0.7%)	2.03	14/606 (2.3%)
9	t	1.64	4/446 (0.9%)	1.91	11/599 (1.8%)
All	All	1.77	1074/132421 (0.8%)	1.95	3317/179131 (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	17
1	C	0	20
1	E	0	17
1	G	0	18
1	M	0	19
2	B	0	24
2	D	0	12
2	F	0	19
2	H	0	27
2	N	0	23
2	O	0	2
2	Q	0	5
2	R	0	3
2	S	0	3
2	T	0	1
3	I	0	16
3	K	0	19
4	J	0	21
5	L	0	31
6	P	0	8
7	U	0	1
7	V	0	2
7	W	0	1
7	X	0	3

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Mol	Chain	#Chirality outliers	#Planarity outliers
8	a	0	12
8	b	0	13
8	c	0	10
8	d	0	9
8	e	0	13
8	f	0	12
8	g	0	12
8	h	0	13
8	i	0	7
8	j	0	15
8	k	0	13
8	l	0	10
8	m	0	14
8	n	0	8
All	All	0	473

All (1074) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	515	ARG	CZ-NH2	63.49	2.15	1.33
8	k	435	TYR	CG-CD2	53.64	2.08	1.39
8	k	435	TYR	CE1-CZ	52.86	2.07	1.38
8	k	435	TYR	CG-CD1	48.86	2.02	1.39
8	k	435	TYR	CE2-CZ	47.12	1.99	1.38
8	k	435	TYR	CD1-CE1	43.18	2.04	1.39
8	k	435	TYR	CD2-CE2	39.35	1.98	1.39
4	J	242	TRP	CD2-CE3	33.42	1.90	1.40
4	J	242	TRP	CE2-CZ2	32.88	1.95	1.39
4	J	242	TRP	CD2-CE2	32.66	1.80	1.41
4	J	242	TRP	CZ3-CH2	24.35	1.79	1.40
4	J	242	TRP	CZ2-CH2	23.34	1.81	1.37
4	J	242	TRP	CE3-CZ3	22.95	1.77	1.38
3	I	16	ILE	CG1-CD1	20.52	2.92	1.50
2	N	730	TRP	NE1-CE2	-10.31	1.24	1.37
8	a	104	TRP	NE1-CE2	9.44	1.49	1.37
1	E	642	ARG	NE-CZ	8.95	1.44	1.33
8	j	306	SER	CA-CB	8.89	1.66	1.52
8	i	364	SER	CA-CB	8.83	1.66	1.52
8	g	14	GLY	N-CA	-8.82	1.32	1.46
8	b	311	ARG	CD-NE	8.70	1.61	1.46
4	J	275	SER	CA-CB	8.65	1.66	1.52
8	c	97	GLY	N-CA	-8.61	1.33	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	366	TYR	CG-CD1	8.60	1.50	1.39
5	L	366	SER	CA-CB	8.59	1.65	1.52
2	D	844	SER	CA-CB	8.35	1.65	1.52
1	M	369	SER	CA-CB	8.33	1.65	1.52
3	K	653	TYR	CG-CD2	8.22	1.49	1.39
3	I	161	SER	CA-CB	8.21	1.65	1.52
8	b	237	SER	CA-CB	8.20	1.65	1.52
8	i	124	ARG	NE-CZ	8.12	1.43	1.33
4	J	1011	SER	CA-CB	8.00	1.65	1.52
3	K	361	TYR	CE2-CZ	7.95	1.48	1.38
4	J	816	TYR	CG-CD1	7.91	1.49	1.39
8	m	226	SER	CA-CB	7.89	1.64	1.52
4	J	413	SER	CA-CB	7.89	1.64	1.52
2	F	853	TYR	CE2-CZ	7.79	1.48	1.38
2	B	466	ARG	NE-CZ	7.79	1.43	1.33
1	A	211	SER	CA-CB	7.77	1.64	1.52
1	M	365	TYR	CZ-OH	7.77	1.51	1.37
3	K	258	SER	CA-CB	7.76	1.64	1.52
2	N	659	TYR	CE2-CZ	7.72	1.48	1.38
8	m	245	TYR	CG-CD2	7.70	1.49	1.39
1	C	695	TYR	CE1-CZ	7.69	1.48	1.38
3	K	267	TYR	CE1-CZ	7.68	1.48	1.38
8	j	372	ARG	CZ-NH2	7.67	1.43	1.33
6	P	90	PHE	CG-CD1	7.66	1.50	1.38
2	H	311	SER	CA-CB	7.66	1.64	1.52
1	G	282	PHE	CG-CD1	7.60	1.50	1.38
1	E	332	ARG	NE-CZ	7.60	1.43	1.33
5	L	34	ARG	CD-NE	7.60	1.59	1.46
1	M	229	GLY	N-CA	-7.59	1.34	1.46
8	f	194	ARG	CZ-NH2	7.56	1.42	1.33
8	a	169	TYR	CE1-CZ	7.53	1.48	1.38
7	U	648	SER	CA-CB	7.52	1.64	1.52
2	F	838	SER	CA-CB	7.50	1.64	1.52
8	c	409	ARG	CD-NE	7.50	1.59	1.46
1	A	486	ARG	CZ-NH1	7.48	1.42	1.33
3	K	551	ARG	NE-CZ	7.44	1.42	1.33
8	d	237	SER	CA-CB	7.42	1.64	1.52
2	Q	64	ARG	CD-NE	7.42	1.59	1.46
8	c	53	TYR	CG-CD1	7.40	1.48	1.39
2	F	562	ARG	CZ-NH2	7.38	1.42	1.33
4	J	703	TYR	CG-CD2	7.37	1.48	1.39
5	L	1595	TYR	CZ-OH	7.36	1.50	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	j	53	TYR	CE2-CZ	7.35	1.48	1.38
8	f	133	GLU	CG-CD	7.34	1.62	1.51
5	L	511	GLU	CG-CD	7.33	1.62	1.51
1	E	455	TYR	CE1-CZ	7.31	1.48	1.38
1	A	364	GLY	N-CA	-7.30	1.35	1.46
8	j	82	TYR	CB-CG	-7.29	1.40	1.51
8	f	372	ARG	NE-CZ	7.17	1.42	1.33
1	C	671	SER	CA-CB	7.17	1.63	1.52
8	c	47	ARG	CZ-NH2	7.17	1.42	1.33
8	l	107	GLY	CA-C	-7.14	1.40	1.51
8	g	80	SER	CA-CB	7.13	1.63	1.52
2	O	98	LEU	N-CA	-7.13	1.32	1.46
8	b	388	PHE	CE1-CZ	7.13	1.50	1.37
1	G	242	SER	CA-CB	7.12	1.63	1.52
8	f	151	SER	CA-CB	7.11	1.63	1.52
8	m	4	GLU	CD-OE1	7.11	1.33	1.25
2	R	75	SER	CA-CB	7.09	1.63	1.52
8	n	224	SER	CB-OG	7.08	1.51	1.42
8	e	425	ARG	NE-CZ	7.07	1.42	1.33
3	K	443	GLU	CD-OE2	7.07	1.33	1.25
2	H	295	GLU	CD-OE1	7.06	1.33	1.25
8	i	273	TYR	CE2-CZ	7.06	1.47	1.38
5	L	1524	TRP	NE1-CE2	-7.06	1.28	1.37
8	f	63	ARG	NE-CZ	7.06	1.42	1.33
1	M	832	SER	CA-CB	7.05	1.63	1.52
8	i	334	HIS	CB-CG	-7.05	1.37	1.50
3	I	295	ARG	CZ-NH1	7.04	1.42	1.33
2	F	317	GLY	CA-C	-7.03	1.40	1.51
1	A	575	GLU	CD-OE2	7.03	1.33	1.25
2	N	673	GLU	CB-CG	7.02	1.65	1.52
2	H	390	ARG	CZ-NH2	7.02	1.42	1.33
2	N	310	ARG	CZ-NH2	7.01	1.42	1.33
8	n	336	SER	CA-CB	6.99	1.63	1.52
2	D	457	ARG	CD-NE	6.96	1.58	1.46
2	H	274	TYR	CZ-OH	6.96	1.49	1.37
3	K	19	TRP	NE1-CE2	-6.95	1.28	1.37
4	J	690	ILE	C-N	6.94	1.45	1.33
1	C	361	ARG	CZ-NH2	6.93	1.42	1.33
1	E	763	ARG	CZ-NH2	6.91	1.42	1.33
8	b	172	PHE	CG-CD1	6.91	1.49	1.38
8	e	265	ARG	CZ-NH1	6.90	1.42	1.33
9	s	12	ARG	CZ-NH1	6.87	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	695	TYR	CB-CG	6.87	1.61	1.51
1	M	822	SER	CA-CB	6.87	1.63	1.52
3	I	553	PHE	CG-CD2	6.86	1.49	1.38
8	j	194	ARG	NE-CZ	6.86	1.42	1.33
2	N	784	PHE	CG-CD1	6.86	1.49	1.38
8	i	20	GLU	CB-CG	6.86	1.65	1.52
5	L	34	ARG	NE-CZ	6.83	1.42	1.33
8	m	369	SER	CA-CB	6.82	1.63	1.52
8	k	146	GLY	CA-C	-6.81	1.41	1.51
8	l	245	TYR	CE1-CZ	6.81	1.47	1.38
2	S	62	PHE	C-N	6.81	1.49	1.34
8	d	284	SER	CA-CB	6.79	1.63	1.52
8	g	364	SER	CA-CB	6.79	1.63	1.52
3	I	295	ARG	CZ-NH2	6.77	1.41	1.33
3	I	551	ARG	CZ-NH2	6.77	1.41	1.33
8	i	169	TYR	CE2-CZ	6.77	1.47	1.38
7	X	627	VAL	CB-CG1	6.76	1.67	1.52
8	e	9	GLN	CG-CD	6.75	1.66	1.51
5	L	506	TYR	CG-CD1	6.75	1.48	1.39
5	L	1542	TYR	CB-CG	6.75	1.61	1.51
1	C	261	ARG	CD-NE	6.74	1.57	1.46
3	K	480	TYR	CG-CD2	6.74	1.48	1.39
8	j	89	GLU	CG-CD	6.73	1.62	1.51
2	H	283	SER	CA-CB	6.73	1.63	1.52
2	N	775	ARG	NE-CZ	6.72	1.41	1.33
8	h	3	ARG	CZ-NH1	6.72	1.41	1.33
5	L	1420	GLU	CB-CG	6.71	1.65	1.52
8	l	169	TYR	CB-CG	-6.71	1.41	1.51
8	g	194	ARG	NE-CZ	6.71	1.41	1.33
1	M	848	SER	CA-CB	6.70	1.63	1.52
2	T	74	PHE	CB-CG	6.70	1.62	1.51
2	N	583	GLU	CB-CG	6.70	1.64	1.52
1	M	705	TRP	NE1-CE2	-6.69	1.28	1.37
2	D	412	SER	CA-CB	6.69	1.62	1.52
1	E	559	ARG	CZ-NH2	6.69	1.41	1.33
1	C	526	PHE	CG-CD1	6.68	1.48	1.38
3	I	267	TYR	CG-CD1	6.67	1.47	1.39
2	F	322	SER	CA-CB	6.67	1.62	1.52
8	m	372	ARG	NE-CZ	6.67	1.41	1.33
4	J	719	ARG	CZ-NH1	6.67	1.41	1.33
8	m	311	ARG	CZ-NH2	6.66	1.41	1.33
1	A	845	TYR	CG-CD1	6.66	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	631	ARG	CZ-NH2	6.66	1.41	1.33
2	D	538	PHE	CG-CD1	6.65	1.48	1.38
1	G	619	TYR	CE1-CZ	6.65	1.47	1.38
5	L	408	TYR	CB-CG	-6.65	1.41	1.51
2	Q	95	TYR	CZ-OH	6.65	1.49	1.37
1	A	211	SER	CB-OG	6.64	1.50	1.42
2	H	537	TYR	CG-CD2	6.64	1.47	1.39
8	c	124	ARG	CZ-NH1	6.63	1.41	1.33
1	E	288	ASN	CB-CG	6.61	1.66	1.51
6	P	91	TYR	CG-CD1	6.61	1.47	1.39
8	d	401	ARG	CD-NE	6.61	1.57	1.46
1	G	264	PRO	N-CD	-6.60	1.38	1.47
3	I	321	SER	CA-CB	6.59	1.62	1.52
8	b	293	VAL	CB-CG1	6.59	1.66	1.52
7	U	628	GLU	CG-CD	6.58	1.61	1.51
1	M	513	ARG	CZ-NH1	6.57	1.41	1.33
1	E	361	ARG	CZ-NH1	6.57	1.41	1.33
8	k	38	GLU	CD-OE1	6.55	1.32	1.25
8	a	309	ARG	NE-CZ	6.55	1.41	1.33
8	h	372	ARG	CZ-NH2	6.55	1.41	1.33
7	X	647	TYR	CG-CD2	6.53	1.47	1.39
8	n	140	SER	CB-OG	-6.53	1.33	1.42
6	P	281	SER	CB-OG	6.53	1.50	1.42
8	h	14	GLY	CA-C	6.52	1.62	1.51
8	j	352	GLY	N-CA	-6.52	1.36	1.46
1	M	514	SER	CA-CB	6.50	1.62	1.52
1	M	403	TYR	CZ-OH	6.50	1.49	1.37
8	e	281	SER	CA-CB	6.50	1.62	1.52
8	d	375	GLY	CA-C	-6.50	1.41	1.51
8	f	233	SER	CA-CB	6.49	1.62	1.52
5	L	92	GLU	CD-OE2	6.49	1.32	1.25
3	I	372	PHE	CG-CD1	6.48	1.48	1.38
3	K	587	GLU	CD-OE1	6.47	1.32	1.25
2	D	468	SER	CA-CB	6.47	1.62	1.52
8	a	296	ARG	CZ-NH2	6.46	1.41	1.33
8	m	160	ARG	CZ-NH1	6.46	1.41	1.33
8	k	362	ARG	NE-CZ	6.46	1.41	1.33
4	J	217	VAL	CA-CB	-6.45	1.41	1.54
1	G	675	PHE	CE1-CZ	6.45	1.49	1.37
8	c	152	TYR	CG-CD1	6.44	1.47	1.39
2	H	840	PRO	N-CD	-6.43	1.38	1.47
2	H	883	GLU	CD-OE2	6.43	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	246	SER	CA-CB	6.42	1.62	1.52
7	X	661	ARG	CZ-NH1	6.42	1.41	1.33
8	e	362	ARG	CZ-NH2	6.40	1.41	1.33
2	H	310	ARG	CD-NE	6.40	1.57	1.46
8	j	29	HIS	C-N	6.40	1.44	1.33
8	i	20	GLU	CG-CD	6.39	1.61	1.51
2	F	364	ARG	NE-CZ	6.38	1.41	1.33
2	N	468	SER	CA-CB	6.37	1.62	1.52
2	N	605	ARG	CZ-NH2	6.37	1.41	1.33
8	m	284	SER	CA-CB	6.37	1.62	1.52
3	K	633	ARG	CD-NE	6.37	1.57	1.46
3	K	10	SER	CA-CB	6.36	1.62	1.52
8	f	194	ARG	NE-CZ	6.36	1.41	1.33
8	n	86	TYR	CG-CD1	6.36	1.47	1.39
3	K	538	SER	CA-CB	6.36	1.62	1.52
1	A	326	TYR	CG-CD2	6.34	1.47	1.39
2	F	843	ARG	CZ-NH2	6.33	1.41	1.33
8	e	317	TYR	CG-CD1	6.33	1.47	1.39
8	j	86	TYR	CZ-OH	6.33	1.48	1.37
5	L	1576	ARG	CZ-NH1	6.31	1.41	1.33
3	K	120	SER	CA-CB	6.31	1.62	1.52
1	G	736	CYS	CB-SG	6.30	1.93	1.82
2	H	651	PHE	CE1-CZ	6.30	1.49	1.37
3	K	647	ARG	NE-CZ	6.30	1.41	1.33
1	A	852	HIS	CB-CG	6.29	1.61	1.50
1	E	763	ARG	NE-CZ	6.29	1.41	1.33
2	H	428	PHE	CG-CD1	6.29	1.48	1.38
8	l	129	SER	CA-CB	6.29	1.62	1.52
2	B	526	GLU	CD-OE2	6.29	1.32	1.25
8	l	401	ARG	NE-CZ	6.29	1.41	1.33
8	j	414	PHE	CB-CG	6.28	1.62	1.51
5	L	1607	GLU	CD-OE1	6.28	1.32	1.25
3	K	549	SER	CA-CB	6.28	1.62	1.52
1	E	243	ARG	CZ-NH1	6.28	1.41	1.33
8	b	76	SER	CA-CB	6.28	1.62	1.52
3	I	257	PHE	CB-CG	6.27	1.62	1.51
2	D	274	TYR	CD2-CE2	6.27	1.48	1.39
8	l	51	PHE	CG-CD1	6.27	1.48	1.38
2	D	814	SER	CA-CB	6.26	1.62	1.52
8	e	108	PHE	CG-CD1	6.26	1.48	1.38
8	m	426	GLU	CG-CD	6.26	1.61	1.51
8	b	372	ARG	NE-CZ	6.25	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	719	TYR	CE2-CZ	6.25	1.46	1.38
3	I	253	SER	CA-CB	6.25	1.62	1.52
8	c	389	GLU	CD-OE2	6.25	1.32	1.25
8	a	401	ARG	CZ-NH2	6.24	1.41	1.33
2	F	411	ARG	NE-CZ	6.24	1.41	1.33
2	Q	105	ARG	NE-CZ	6.23	1.41	1.33
1	M	386	TYR	CZ-OH	6.23	1.48	1.37
1	M	503	MET	CA-CB	6.23	1.67	1.53
2	F	719	TYR	CB-CG	6.23	1.60	1.51
5	L	87	GLU	CD-OE2	6.22	1.32	1.25
2	D	582	PRO	N-CD	-6.22	1.39	1.47
8	k	4	GLU	CD-OE2	6.22	1.32	1.25
1	E	505	GLU	CD-OE1	6.21	1.32	1.25
5	L	465	ARG	CD-NE	6.20	1.56	1.46
2	N	511	SER	CB-OG	6.20	1.50	1.42
8	m	161	TYR	CG-CD1	6.20	1.47	1.39
1	G	460	ARG	NE-CZ	6.19	1.41	1.33
8	m	297	LEU	CB-CG	6.19	1.70	1.52
2	D	855	GLY	N-CA	6.18	1.55	1.46
8	m	43	GLU	CG-CD	6.18	1.61	1.51
8	b	22	TRP	NE1-CE2	-6.18	1.29	1.37
3	K	606	ARG	NE-CZ	6.17	1.41	1.33
6	P	86	TRP	CG-CD1	6.17	1.45	1.36
8	d	309	ARG	CZ-NH2	6.16	1.41	1.33
8	g	343	ARG	NE-CZ	6.16	1.41	1.33
8	k	351	TRP	NE1-CE2	-6.16	1.29	1.37
6	P	2	GLU	CG-CD	6.16	1.61	1.51
5	L	1376	TYR	CB-CG	6.15	1.60	1.51
8	d	364	SER	CA-CB	6.15	1.62	1.52
2	N	376	ARG	CZ-NH1	6.14	1.41	1.33
1	G	694	TYR	CZ-OH	6.14	1.48	1.37
2	H	874	PHE	CG-CD1	6.14	1.48	1.38
2	D	537	TYR	CZ-OH	6.14	1.48	1.37
2	B	870	GLU	N-CA	-6.14	1.34	1.46
8	d	353	PRO	N-CA	-6.14	1.36	1.47
8	c	434	GLU	CB-CG	6.13	1.63	1.52
8	e	239	SER	CA-CB	6.13	1.62	1.52
8	l	401	ARG	CZ-NH2	6.13	1.41	1.33
2	F	310	ARG	CZ-NH2	6.12	1.41	1.33
4	J	220	TYR	CZ-OH	6.12	1.48	1.37
8	l	47	ARG	CZ-NH2	6.12	1.41	1.33
1	M	642	ARG	NE-CZ	6.11	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	C	559	ARG	NE-CZ	6.11	1.41	1.33
8	n	3	ARG	NE-CZ	6.10	1.41	1.33
1	M	714	SER	CA-CB	6.10	1.62	1.52
8	k	170	SER	CB-OG	6.10	1.50	1.42
8	j	395	TYR	CE1-CZ	6.10	1.46	1.38
1	E	514	SER	CB-OG	-6.09	1.34	1.42
8	h	140	SER	CA-CB	6.09	1.62	1.52
2	F	703	CYS	CB-SG	6.09	1.92	1.82
6	P	156	GLY	CA-C	-6.09	1.42	1.51
8	a	436	HIS	CB-CG	6.08	1.61	1.50
8	c	311	ARG	CZ-NH1	6.08	1.41	1.33
8	n	51	PHE	CG-CD1	6.08	1.47	1.38
1	A	866	PHE	CG-CD2	6.08	1.47	1.38
8	d	160	ARG	CZ-NH1	6.08	1.41	1.33
8	c	124	ARG	CD-NE	6.08	1.56	1.46
1	G	243	ARG	NE-CZ	6.08	1.41	1.33
2	B	335	TYR	CG-CD2	6.07	1.47	1.39
4	J	721	PHE	CG-CD2	6.07	1.47	1.38
8	b	63	ARG	NE-CZ	6.07	1.41	1.33
2	F	397	SER	CA-CB	6.07	1.62	1.52
1	E	278	GLU	CG-CD	6.07	1.61	1.51
5	L	562	GLY	N-CA	6.07	1.55	1.46
1	E	337	LEU	CA-CB	6.07	1.67	1.53
2	N	339	SER	CA-CB	6.06	1.62	1.52
2	T	99	SER	CA-CB	6.06	1.62	1.52
8	f	237	SER	CA-CB	6.06	1.62	1.52
4	J	231	SER	CB-OG	6.06	1.50	1.42
4	J	838	PHE	CG-CD1	6.06	1.47	1.38
1	A	492	ASN	CB-CG	6.05	1.65	1.51
4	J	927	ARG	CD-NE	6.05	1.56	1.46
1	C	253	SER	CA-CB	6.05	1.62	1.52
5	L	1688	ARG	CZ-NH1	6.05	1.41	1.33
8	l	408	PHE	CG-CD1	6.05	1.47	1.38
8	e	89	GLU	CD-OE2	6.04	1.32	1.25
1	M	455	TYR	CG-CD2	6.04	1.47	1.39
8	e	156	ARG	NE-CZ	6.04	1.40	1.33
3	K	87	ARG	CZ-NH1	6.04	1.40	1.33
8	i	418	PHE	CE2-CZ	6.04	1.48	1.37
8	c	296	ARG	CA-CB	6.04	1.67	1.53
2	N	619	ARG	CZ-NH2	6.03	1.40	1.33
2	F	552	TYR	CE2-CZ	6.03	1.46	1.38
2	N	442	TYR	CG-CD1	6.03	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	K	489	SER	CA-CB	6.01	1.61	1.52
8	a	225	PHE	CG-CD2	6.01	1.47	1.38
8	e	82	TYR	CZ-OH	6.01	1.48	1.37
8	j	86	TYR	CB-CG	6.01	1.60	1.51
2	N	659	TYR	CZ-OH	6.01	1.48	1.37
2	D	802	ARG	CD-NE	6.00	1.56	1.46
5	L	1465	TYR	CB-CG	-6.00	1.42	1.51
2	B	843	ARG	NE-CZ	6.00	1.40	1.33
8	e	339	ARG	CZ-NH2	6.00	1.40	1.33
8	b	296	ARG	CD-NE	5.99	1.56	1.46
1	G	859	TYR	CG-CD1	5.99	1.47	1.39
1	A	440	SER	CA-CB	5.98	1.61	1.52
6	P	240	TYR	CZ-OH	5.98	1.48	1.37
9	t	58	ARG	NE-CZ	5.98	1.40	1.33
2	N	792	TYR	CE2-CZ	5.97	1.46	1.38
1	M	682	ARG	NE-CZ	5.97	1.40	1.33
8	h	362	ARG	CD-NE	5.96	1.56	1.46
1	M	694	TYR	CZ-OH	5.96	1.48	1.37
8	d	21	PHE	CG-CD2	5.96	1.47	1.38
2	F	592	TYR	CZ-OH	5.96	1.48	1.37
2	F	680	TRP	NE1-CE2	5.96	1.45	1.37
8	g	245	TYR	CE2-CZ	5.96	1.46	1.38
1	A	619	TYR	CE2-CZ	5.96	1.46	1.38
8	j	348	PHE	CA-CB	5.96	1.67	1.53
8	m	53	TYR	CG-CD2	5.96	1.46	1.39
8	k	401	ARG	CZ-NH2	5.95	1.40	1.33
9	p	28	GLY	CA-C	5.95	1.61	1.51
2	F	641	TYR	CE2-CZ	5.95	1.46	1.38
3	I	338	GLU	CG-CD	5.94	1.60	1.51
3	I	361	TYR	CZ-OH	5.94	1.48	1.37
6	P	234	SER	CA-CB	5.94	1.61	1.52
2	H	724	GLU	CB-CG	5.94	1.63	1.52
1	M	486	ARG	CZ-NH2	5.94	1.40	1.33
7	U	651	GLU	CG-CD	5.93	1.60	1.51
7	W	668	ARG	NE-CZ	5.93	1.40	1.33
5	L	1683	GLU	CB-CG	5.93	1.63	1.52
8	g	372	ARG	CZ-NH2	5.93	1.40	1.33
5	L	405	GLY	N-CA	-5.93	1.37	1.46
5	L	107	SER	CA-CB	5.93	1.61	1.52
1	M	314	ARG	CZ-NH2	5.93	1.40	1.33
1	G	705	TRP	CD1-NE1	-5.93	1.27	1.38
1	G	369	SER	CA-CB	5.93	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	J	745	GLU	CD-OE1	5.92	1.32	1.25
2	D	538	PHE	CG-CD2	5.92	1.47	1.38
1	E	274	ARG	CD-NE	5.91	1.56	1.46
1	C	222	TYR	CD2-CE2	5.91	1.48	1.39
2	F	434	TYR	CZ-OH	5.90	1.47	1.37
2	Q	61	GLU	CB-CG	5.90	1.63	1.52
2	D	365	ARG	CZ-NH1	5.89	1.40	1.33
8	a	389	GLU	CD-OE1	5.89	1.32	1.25
8	a	420	GLU	CG-CD	5.89	1.60	1.51
1	C	396	ARG	NE-CZ	5.89	1.40	1.33
8	i	109	SER	CB-OG	5.88	1.49	1.42
1	E	867	TYR	CB-CG	5.88	1.60	1.51
3	I	360	PHE	CG-CD2	5.88	1.47	1.38
8	l	362	ARG	CD-NE	5.88	1.56	1.46
4	J	228	PHE	CE1-CZ	5.88	1.48	1.37
1	C	274	ARG	CD-NE	5.87	1.56	1.46
3	K	442	ARG	CD-NE	5.87	1.56	1.46
1	A	491	TYR	CE2-CZ	5.87	1.46	1.38
2	F	402	TYR	CE1-CZ	5.87	1.46	1.38
3	I	193	HIS	CB-CG	-5.87	1.39	1.50
1	M	363	PHE	CB-CG	5.87	1.61	1.51
1	G	365	TYR	CG-CD2	5.86	1.46	1.39
8	h	93	LEU	CA-C	-5.86	1.37	1.52
8	n	117	ASP	CA-CB	5.86	1.66	1.53
8	a	28	GLU	CD-OE1	5.86	1.32	1.25
1	M	763	ARG	NE-CZ	5.86	1.40	1.33
3	K	145	SER	CA-CB	5.86	1.61	1.52
2	H	359	SER	N-CA	5.85	1.58	1.46
2	B	720	TYR	CG-CD1	5.85	1.46	1.39
8	c	393	ARG	NE-CZ	5.85	1.40	1.33
8	h	296	ARG	CD-NE	5.85	1.56	1.46
3	I	87	ARG	CD-NE	5.85	1.56	1.46
8	e	273	TYR	CG-CD2	5.84	1.46	1.39
8	h	393	ARG	CZ-NH2	5.84	1.40	1.33
8	a	286	ARG	CD-NE	5.84	1.56	1.46
2	N	574	ARG	CZ-NH2	5.83	1.40	1.33
8	l	34	GLU	CD-OE2	5.83	1.32	1.25
2	B	855	GLY	CA-C	-5.83	1.42	1.51
1	C	211	SER	CA-CB	5.83	1.61	1.52
2	B	835	PHE	CG-CD2	5.83	1.47	1.38
2	D	472	SER	CB-OG	5.83	1.49	1.42
4	J	229	SER	CA-CB	5.83	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	P	69	TYR	CD2-CE2	5.83	1.48	1.39
3	K	166	PRO	N-CD	-5.83	1.39	1.47
2	R	37	ARG	NE-CZ	5.82	1.40	1.33
8	n	217	ARG	CZ-NH2	5.82	1.40	1.33
2	D	255	TYR	CE2-CZ	5.82	1.46	1.38
3	K	650	TYR	CG-CD1	5.82	1.46	1.39
8	m	309	ARG	NE-CZ	5.82	1.40	1.33
8	c	63	ARG	NE-CZ	5.82	1.40	1.33
1	A	517	HIS	CB-CG	5.81	1.60	1.50
2	H	847	ARG	NE-CZ	5.81	1.40	1.33
1	C	535	GLU	CG-CD	5.81	1.60	1.51
8	c	226	SER	CA-CB	5.81	1.61	1.52
1	C	373	GLU	CD-OE2	5.80	1.32	1.25
3	K	618	PHE	CB-CG	5.80	1.61	1.51
1	E	431	TYR	CZ-OH	5.80	1.47	1.37
4	J	492	ARG	CD-NE	5.79	1.56	1.46
1	C	688	PHE	CG-CD1	5.79	1.47	1.38
8	d	341	ARG	CZ-NH1	5.79	1.40	1.33
3	I	267	TYR	CZ-OH	5.79	1.47	1.37
2	B	853	TYR	CE1-CZ	5.79	1.46	1.38
2	D	273	CYS	CB-SG	5.78	1.92	1.82
8	a	129	SER	CB-OG	5.78	1.49	1.42
2	D	713	PHE	CG-CD2	5.77	1.47	1.38
8	f	233	SER	CB-OG	5.77	1.49	1.42
1	C	491	TYR	CB-CG	5.77	1.60	1.51
4	J	316	TYR	CE1-CZ	5.76	1.46	1.38
2	H	831	ARG	NE-CZ	5.76	1.40	1.33
2	T	61	GLU	CG-CD	5.76	1.60	1.51
8	c	248	TYR	CA-CB	5.76	1.66	1.53
8	h	389	GLU	CB-CG	5.76	1.63	1.52
8	i	414	PHE	CG-CD2	5.76	1.47	1.38
8	i	129	SER	CA-CB	5.76	1.61	1.52
8	k	217	ARG	NE-CZ	5.76	1.40	1.33
3	K	530	TYR	CB-CG	5.75	1.60	1.51
8	m	292	ASP	CA-CB	5.75	1.66	1.53
8	h	395	TYR	CG-CD2	5.75	1.46	1.39
1	G	518	TYR	CG-CD2	5.75	1.46	1.39
2	D	792	TYR	CE2-CZ	5.74	1.46	1.38
8	l	2	PRO	N-CD	5.74	1.55	1.47
2	D	654	GLU	CD-OE2	5.74	1.31	1.25
8	a	32	SER	CA-CB	-5.74	1.44	1.52
8	g	295	ARG	CD-NE	5.74	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	i	47	ARG	CZ-NH2	5.74	1.40	1.33
8	l	110	GLN	C-N	5.74	1.43	1.33
1	M	859	TYR	CZ-OH	5.74	1.47	1.37
1	C	724	HIS	CB-CG	5.73	1.60	1.50
2	F	466	ARG	NE-CZ	5.73	1.40	1.33
8	l	420	GLU	CD-OE2	5.73	1.31	1.25
1	A	302	TYR	CE1-CZ	5.73	1.46	1.38
2	F	583	GLU	CG-CD	5.73	1.60	1.51
8	e	226	SER	CA-CB	5.72	1.61	1.52
8	e	435	TYR	CZ-OH	5.72	1.47	1.37
2	F	423	TYR	CB-CG	-5.72	1.43	1.51
8	m	99	GLY	N-CA	-5.72	1.37	1.46
7	W	620	ARG	NE-CZ	5.71	1.40	1.33
1	C	430	ARG	NE-CZ	5.71	1.40	1.33
2	F	778	PHE	CG-CD2	5.71	1.47	1.38
2	B	270	SER	CA-CB	5.71	1.61	1.52
2	H	780	GLN	CG-CD	5.71	1.64	1.51
1	C	461	GLU	CD-OE2	5.71	1.31	1.25
8	e	434	GLU	CD-OE2	5.71	1.31	1.25
8	m	355	SER	CA-CB	5.71	1.61	1.52
8	k	156	ARG	CD-NE	5.70	1.56	1.46
2	F	522	PHE	CG-CD1	5.70	1.47	1.38
8	n	86	TYR	CE2-CZ	5.70	1.46	1.38
1	A	296	ARG	CD-NE	5.70	1.56	1.46
1	G	684	ARG	CZ-NH2	5.69	1.40	1.33
5	L	44	TYR	CZ-OH	5.69	1.47	1.37
8	a	51	PHE	CG-CD2	5.69	1.47	1.38
8	k	82	TYR	CZ-OH	5.68	1.47	1.37
1	G	240	ARG	CD-NE	5.68	1.56	1.46
9	r	42	GLU	CB-CG	5.68	1.62	1.52
8	f	194	ARG	CD-NE	5.68	1.56	1.46
8	m	296	ARG	NE-CZ	5.68	1.40	1.33
8	j	47	ARG	CZ-NH2	5.67	1.40	1.33
8	b	26	CYS	CA-CB	5.67	1.66	1.53
8	e	374	SER	CA-CB	5.67	1.61	1.52
8	j	408	PHE	CG-CD1	5.67	1.47	1.38
2	D	464	SER	CA-CB	5.67	1.61	1.52
1	M	624	PRO	N-CA	-5.67	1.37	1.47
8	h	22	TRP	CE2-CZ2	-5.67	1.30	1.39
8	h	147	SER	CA-CB	5.67	1.61	1.52
5	L	1661	TYR	CE1-CZ	5.66	1.46	1.38
1	E	455	TYR	CZ-OH	5.66	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	e	124	ARG	NE-CZ	5.66	1.40	1.33
2	N	409	TYR	CE1-CZ	5.66	1.46	1.38
2	N	333	GLU	CD-OE1	5.66	1.31	1.25
8	n	20	GLU	N-CA	-5.65	1.35	1.46
2	D	635	ASP	N-CA	-5.65	1.35	1.46
1	E	396	ARG	CZ-NH2	5.65	1.40	1.33
8	j	343	ARG	CZ-NH2	5.65	1.40	1.33
5	L	1503	TYR	CE1-CZ	5.65	1.45	1.38
3	K	304	GLU	CB-CG	5.63	1.62	1.52
7	V	628	GLU	CD-OE2	5.63	1.31	1.25
1	A	709	GLU	CB-CG	5.63	1.62	1.52
1	A	377	TYR	CE1-CZ	5.62	1.45	1.38
1	E	497	VAL	CB-CG1	5.62	1.64	1.52
1	G	616	SER	CA-CB	5.62	1.61	1.52
1	M	487	ILE	N-CA	-5.62	1.35	1.46
7	U	658	GLU	CD-OE1	5.62	1.31	1.25
8	g	390	ARG	NE-CZ	5.62	1.40	1.33
8	f	58	GLU	CD-OE1	5.62	1.31	1.25
1	M	684	ARG	NE-CZ	5.62	1.40	1.33
1	E	248	GLU	CD-OE2	5.62	1.31	1.25
8	c	239	SER	CA-CB	5.61	1.61	1.52
1	G	821	GLU	CG-CD	5.61	1.60	1.51
8	e	53	TYR	CG-CD2	5.61	1.46	1.39
2	F	480	ARG	NE-CZ	5.60	1.40	1.33
1	G	440	SER	CB-OG	5.60	1.49	1.42
8	c	190	LEU	CA-C	-5.60	1.38	1.52
7	X	658	GLU	CG-CD	5.60	1.60	1.51
8	c	72	ARG	CZ-NH2	5.60	1.40	1.33
2	F	503	SER	CB-OG	-5.59	1.34	1.42
1	G	365	TYR	CZ-OH	5.59	1.47	1.37
5	L	1572	TRP	CD2-CE2	5.59	1.48	1.41
1	M	395	TYR	CD2-CE2	5.59	1.47	1.39
8	j	402	GLU	CG-CD	5.59	1.60	1.51
2	F	314	ARG	NE-CZ	5.58	1.40	1.33
8	n	194	ARG	NE-CZ	5.58	1.40	1.33
7	V	647	TYR	CZ-OH	5.58	1.47	1.37
8	i	72	ARG	CZ-NH2	5.58	1.40	1.33
8	m	188	SER	CA-CB	5.58	1.61	1.52
2	B	837	GLU	CD-OE2	5.58	1.31	1.25
8	j	372	ARG	CD-NE	5.58	1.55	1.46
8	l	435	TYR	CG-CD1	5.58	1.46	1.39
1	E	324	TRP	CZ2-CH2	5.58	1.48	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	H	398	ALA	CA-CB	5.57	1.64	1.52
4	J	703	TYR	CZ-OH	5.57	1.47	1.37
8	i	429	GLN	CA-CB	5.57	1.66	1.53
2	H	760	ARG	NE-CZ	5.57	1.40	1.33
2	D	274	TYR	CB-CG	-5.57	1.43	1.51
3	I	28	SER	CA-CB	5.57	1.61	1.52
2	T	49	ARG	CZ-NH1	5.57	1.40	1.33
1	A	370	GLN	CA-CB	5.57	1.66	1.53
8	l	339	ARG	NE-CZ	5.57	1.40	1.33
8	e	272	GLY	CA-C	-5.56	1.43	1.51
3	K	551	ARG	CZ-NH2	5.56	1.40	1.33
2	D	491	PHE	CG-CD2	5.56	1.47	1.38
6	P	60	SER	CA-CB	5.56	1.61	1.52
8	g	152	TYR	CG-CD1	5.56	1.46	1.39
3	K	194	GLY	CA-C	-5.56	1.43	1.51
2	B	323	PHE	CG-CD1	5.55	1.47	1.38
2	N	837	GLU	CG-CD	5.55	1.60	1.51
6	P	288	ASP	CA-CB	5.55	1.66	1.53
4	J	321	PHE	CG-CD1	5.55	1.47	1.38
3	K	36	PRO	C-N	5.55	1.43	1.33
8	i	193	LYS	CA-CB	5.55	1.66	1.53
1	C	460	ARG	NE-CZ	5.55	1.40	1.33
6	P	290	ARG	NE-CZ	5.55	1.40	1.33
8	c	44	GLY	CA-C	-5.55	1.43	1.51
8	k	409	ARG	CZ-NH2	5.55	1.40	1.33
4	J	709	TYR	CZ-OH	5.54	1.47	1.37
3	K	650	TYR	CZ-OH	5.54	1.47	1.37
8	f	343	ARG	CZ-NH1	5.54	1.40	1.33
9	t	28	GLY	N-CA	-5.54	1.37	1.46
8	n	217	ARG	CD-NE	5.54	1.55	1.46
1	C	339	SER	CA-CB	5.54	1.61	1.52
9	p	48	GLU	CB-CG	5.54	1.62	1.52
5	L	1458	ASN	CA-CB	5.53	1.67	1.53
8	e	156	ARG	CZ-NH1	5.53	1.40	1.33
2	D	574	ARG	NE-CZ	5.53	1.40	1.33
8	h	268	PHE	CB-CG	5.53	1.60	1.51
8	k	18	GLY	N-CA	-5.53	1.37	1.46
8	m	237	SER	CA-CB	5.53	1.61	1.52
1	E	298	LEU	C-N	5.52	1.43	1.33
8	m	87	ASN	C-N	5.52	1.44	1.34
6	P	53	TYR	CG-CD1	5.51	1.46	1.39
8	k	369	SER	CA-CB	5.51	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	480	GLU	CG-CD	5.50	1.60	1.51
1	E	269	TYR	CG-CD2	5.50	1.46	1.39
8	d	202	VAL	CA-CB	-5.50	1.43	1.54
8	m	418	PHE	CE1-CZ	5.50	1.47	1.37
8	n	3	ARG	CZ-NH1	5.50	1.40	1.33
2	B	828	GLU	CG-CD	5.50	1.60	1.51
2	S	56	GLU	CD-OE1	5.50	1.31	1.25
8	n	342	GLU	CB-CG	5.50	1.62	1.52
1	G	243	ARG	CZ-NH1	5.50	1.40	1.33
8	c	284	SER	CA-CB	5.50	1.61	1.52
8	c	386	SER	CA-CB	5.50	1.61	1.52
8	j	169	TYR	CE1-CZ	5.50	1.45	1.38
3	I	100	TYR	CZ-OH	5.49	1.47	1.37
8	d	212	ARG	CZ-NH2	5.49	1.40	1.33
5	L	1448	SER	CA-CB	5.49	1.61	1.52
8	b	248	TYR	CD2-CE2	5.49	1.47	1.39
1	E	233	SER	CA-CB	5.49	1.61	1.52
2	F	314	ARG	CZ-NH2	5.48	1.40	1.33
8	l	156	ARG	CZ-NH2	5.48	1.40	1.33
3	I	260	ARG	CZ-NH2	5.48	1.40	1.33
8	d	295	ARG	CZ-NH1	5.48	1.40	1.33
8	k	237	SER	CA-CB	5.48	1.61	1.52
2	R	66	ARG	CZ-NH2	5.48	1.40	1.33
8	e	43	GLU	CD-OE2	5.48	1.31	1.25
8	j	51	PHE	CA-CB	5.48	1.66	1.53
8	j	161	TYR	CZ-OH	5.48	1.47	1.37
1	C	256	LYS	CA-CB	5.48	1.66	1.53
2	F	802	ARG	CD-NE	5.47	1.55	1.46
8	f	222	ASN	C-N	5.47	1.44	1.34
5	L	382	GLN	C-N	5.47	1.42	1.33
3	I	399	SER	CA-CB	5.47	1.61	1.52
8	a	311	ARG	CZ-NH1	5.47	1.40	1.33
8	h	378	MET	CA-CB	5.47	1.66	1.53
6	P	235	SER	CA-CB	5.47	1.61	1.52
8	c	295	ARG	CZ-NH1	5.47	1.40	1.33
8	l	155	GLU	CD-OE2	5.47	1.31	1.25
8	i	186	TYR	CG-CD2	5.47	1.46	1.39
2	B	668	ARG	CZ-NH1	5.47	1.40	1.33
5	L	213	ARG	NE-CZ	5.46	1.40	1.33
8	g	108	PHE	CG-CD1	5.46	1.47	1.38
4	J	283	PHE	CB-CG	-5.46	1.42	1.51
8	g	265	ARG	CZ-NH1	5.46	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	459	TRP	CD2-CE2	5.46	1.48	1.41
8	i	117	ASP	CA-CB	5.46	1.66	1.53
8	c	295	ARG	NE-CZ	5.46	1.40	1.33
2	B	586	ARG	CZ-NH2	5.46	1.40	1.33
2	D	278	GLY	CA-C	-5.45	1.43	1.51
8	f	319	ALA	CA-CB	5.45	1.64	1.52
8	f	425	ARG	CZ-NH1	5.45	1.40	1.33
5	L	1587	GLU	CD-OE1	5.45	1.31	1.25
2	B	734	TRP	NE1-CE2	-5.45	1.30	1.37
5	L	1385	TYR	CE1-CZ	5.44	1.45	1.38
8	c	11	GLY	CA-C	-5.44	1.43	1.51
1	A	361	ARG	NE-CZ	5.44	1.40	1.33
8	c	414	PHE	CA-CB	5.44	1.66	1.53
8	j	194	ARG	CZ-NH1	5.44	1.40	1.33
8	m	161	TYR	CE1-CZ	5.44	1.45	1.38
8	n	226	SER	CA-CB	5.44	1.61	1.52
3	K	258	SER	CB-OG	5.44	1.49	1.42
8	d	338	GLN	CG-CD	5.44	1.63	1.51
1	G	325	PHE	CG-CD1	5.44	1.47	1.38
8	e	60	TYR	CZ-OH	5.43	1.47	1.37
8	i	80	SER	CA-CB	5.43	1.61	1.52
1	E	493	TYR	CE1-CZ	5.43	1.45	1.38
7	W	658	GLU	CG-CD	5.43	1.60	1.51
8	n	361	SER	CA-CB	5.43	1.61	1.52
4	J	466	ARG	CZ-NH2	5.43	1.40	1.33
2	N	878	ARG	NE-CZ	5.43	1.40	1.33
5	L	1457	SER	CB-OG	5.43	1.49	1.42
4	J	999	ARG	CZ-NH1	5.42	1.40	1.33
5	L	410	ARG	CD-NE	5.42	1.55	1.46
2	H	812	ARG	NE-CZ	5.42	1.40	1.33
4	J	209	ARG	CA-CB	5.42	1.65	1.53
9	s	59	ARG	CD-NE	5.42	1.55	1.46
5	L	224	ARG	CD-NE	5.42	1.55	1.46
2	F	654	GLU	CG-CD	5.42	1.60	1.51
2	H	334	TYR	CG-CD2	5.42	1.46	1.39
5	L	1551	GLU	CB-CG	5.42	1.62	1.52
8	f	32	SER	CB-OG	5.42	1.49	1.42
8	j	70	GLU	CD-OE1	5.42	1.31	1.25
1	C	507	GLU	CG-CD	5.41	1.60	1.51
2	D	376	ARG	CZ-NH2	5.41	1.40	1.33
3	I	449	TRP	NE1-CE2	-5.41	1.30	1.37
8	i	169	TYR	CZ-OH	5.41	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	L	120	SER	CB-OG	5.41	1.49	1.42
2	N	251	ARG	CZ-NH2	5.40	1.40	1.33
1	M	287	VAL	CA-CB	-5.40	1.43	1.54
8	c	80	SER	CA-CB	5.40	1.61	1.52
8	d	265	ARG	NE-CZ	5.40	1.40	1.33
1	A	269	TYR	CE1-CZ	5.40	1.45	1.38
3	K	584	GLU	CG-CD	5.40	1.60	1.51
8	h	35	GLY	CA-C	-5.40	1.43	1.51
8	j	273	TYR	CE2-CZ	5.40	1.45	1.38
1	A	763	ARG	CZ-NH2	5.39	1.40	1.33
1	A	392	ARG	NE-CZ	5.39	1.40	1.33
1	C	302	TYR	CE2-CZ	5.39	1.45	1.38
1	M	332	ARG	CD-NE	5.39	1.55	1.46
8	c	109	SER	CB-OG	5.39	1.49	1.42
8	e	388	PHE	CE2-CZ	5.39	1.47	1.37
2	B	316	PHE	CG-CD2	5.39	1.46	1.38
2	N	661	ARG	CA-CB	5.39	1.65	1.53
8	l	311	ARG	CZ-NH2	5.39	1.40	1.33
4	J	835	VAL	CA-CB	-5.38	1.43	1.54
1	M	631	ARG	CZ-NH1	5.38	1.40	1.33
2	D	460	HIS	N-CA	-5.38	1.35	1.46
2	N	674	TYR	CE2-CZ	5.38	1.45	1.38
8	c	374	SER	CB-OG	5.38	1.49	1.42
6	P	337	TYR	CE1-CZ	5.38	1.45	1.38
8	e	366	TYR	CZ-OH	5.38	1.47	1.37
1	A	764	PHE	CG-CD2	5.38	1.46	1.38
8	m	233	SER	CA-CB	5.38	1.61	1.52
1	G	395	TYR	CG-CD1	5.38	1.46	1.39
2	T	66	ARG	CD-NE	5.38	1.55	1.46
8	m	281	SER	CA-CB	5.38	1.61	1.52
1	A	636	ARG	CZ-NH2	5.37	1.40	1.33
2	D	336	ARG	NE-CZ	5.37	1.40	1.33
8	h	299	GLN	N-CA	-5.37	1.35	1.46
8	c	435	TYR	CE2-CZ	5.37	1.45	1.38
8	d	124	ARG	CD-NE	5.37	1.55	1.46
7	U	668	ARG	CZ-NH1	5.37	1.40	1.33
8	l	414	PHE	CE2-CZ	5.37	1.47	1.37
2	R	34	TYR	CE1-CZ	5.37	1.45	1.38
2	R	95	TYR	CD1-CE1	5.36	1.47	1.39
8	g	2	PRO	N-CA	5.36	1.56	1.47
8	i	76	SER	CA-CB	5.36	1.60	1.52
8	k	366	TYR	CZ-OH	5.36	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	709	GLU	CD-OE1	5.36	1.31	1.25
1	M	559	ARG	CD-NE	5.36	1.55	1.46
2	H	719	TYR	CG-CD1	5.36	1.46	1.39
8	b	339	ARG	CZ-NH1	5.36	1.40	1.33
2	N	428	PHE	CG-CD2	5.35	1.46	1.38
8	m	39	GLU	CD-OE1	5.35	1.31	1.25
4	J	749	ASN	CB-CG	5.35	1.63	1.51
8	l	342	GLU	CA-CB	5.35	1.65	1.53
8	n	126	ALA	N-CA	-5.35	1.35	1.46
6	P	147	ARG	CZ-NH2	5.35	1.40	1.33
3	I	91	ARG	CA-CB	5.34	1.65	1.53
2	N	792	TYR	CD2-CE2	-5.34	1.31	1.39
1	G	281	SER	CA-CB	5.34	1.60	1.52
1	C	843	SER	CA-CB	5.34	1.60	1.52
1	E	827	PHE	CG-CD2	5.34	1.46	1.38
8	c	158	ASN	CB-CG	5.34	1.63	1.51
8	j	372	ARG	CZ-NH1	5.34	1.40	1.33
8	m	389	GLU	CG-CD	5.34	1.59	1.51
1	C	821	GLU	CD-OE2	5.34	1.31	1.25
8	k	72	ARG	NE-CZ	5.34	1.40	1.33
1	G	688	PHE	CD2-CE2	-5.34	1.28	1.39
3	I	449	TRP	CA-CB	5.34	1.65	1.53
2	S	85	GLY	CA-C	-5.34	1.43	1.51
8	k	339	ARG	NE-CZ	5.34	1.40	1.33
2	D	797	GLU	CD-OE2	-5.33	1.19	1.25
1	M	827	PHE	CG-CD2	5.33	1.46	1.38
6	P	300	SER	CB-OG	5.33	1.49	1.42
8	k	246	PRO	N-CD	-5.33	1.40	1.47
2	O	51	GLU	CB-CG	5.33	1.62	1.52
9	t	35	SER	CB-OG	5.33	1.49	1.42
2	H	310	ARG	CZ-NH1	5.33	1.40	1.33
5	L	478	CYS	CA-CB	5.33	1.65	1.53
2	T	34	TYR	CE2-CZ	5.33	1.45	1.38
2	H	412	SER	CA-CB	5.33	1.60	1.52
8	i	3	ARG	CZ-NH1	5.33	1.40	1.33
8	l	161	TYR	CG-CD2	5.33	1.46	1.39
3	I	631	SER	CA-CB	5.33	1.60	1.52
8	f	309	ARG	CZ-NH2	5.33	1.40	1.33
8	h	343	ARG	NE-CZ	5.32	1.40	1.33
7	U	656	GLU	CD-OE1	5.32	1.31	1.25
2	H	323	PHE	CG-CD2	5.32	1.46	1.38
9	q	61	SER	CA-CB	5.32	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	838	SER	CA-CB	5.32	1.60	1.52
8	b	112	GLU	CD-OE2	5.31	1.31	1.25
2	D	314	ARG	NE-CZ	5.31	1.40	1.33
2	N	634	TRP	NE1-CE2	-5.31	1.30	1.37
8	i	372	ARG	CZ-NH2	5.31	1.40	1.33
9	p	59	ARG	CD-NE	5.31	1.55	1.46
2	B	801	GLN	CG-CD	5.31	1.63	1.51
8	m	265	ARG	CZ-NH2	5.31	1.40	1.33
8	i	362	ARG	CD-NE	5.31	1.55	1.46
8	l	336	SER	CA-CB	5.31	1.60	1.52
4	J	926	TYR	CE2-CZ	5.31	1.45	1.38
8	c	194	ARG	CZ-NH1	5.31	1.40	1.33
8	i	286	ARG	CD-NE	5.30	1.55	1.46
8	h	341	ARG	CZ-NH2	5.30	1.40	1.33
2	H	734	TRP	CD2-CE2	-5.30	1.34	1.41
8	b	98	GLY	CA-C	-5.30	1.43	1.51
2	N	674	TYR	CZ-OH	5.30	1.46	1.37
8	j	339	ARG	CZ-NH1	5.30	1.40	1.33
3	K	597	SER	CB-OG	5.30	1.49	1.42
3	K	22	ARG	CD-NE	5.30	1.55	1.46
6	P	226	GLU	CG-CD	5.30	1.59	1.51
2	O	67	ARG	CZ-NH1	5.29	1.40	1.33
4	J	385	LYS	CB-CG	5.29	1.66	1.52
6	P	155	SER	CA-CB	5.29	1.60	1.52
8	a	124	ARG	CZ-NH2	5.29	1.40	1.33
8	i	341	ARG	NE-CZ	5.29	1.40	1.33
3	I	515	ARG	NE-CZ	5.29	1.40	1.33
5	L	1694	TYR	CG-CD1	5.29	1.46	1.39
6	P	266	PHE	CG-CD1	5.29	1.46	1.38
1	C	350	PHE	CG-CD1	5.29	1.46	1.38
2	D	255	TYR	CE1-CZ	5.28	1.45	1.38
1	G	856	ASN	CB-CG	5.28	1.63	1.51
2	H	472	SER	CB-OG	5.28	1.49	1.42
8	g	395	TYR	CB-CG	5.28	1.59	1.51
8	l	399	ARG	CD-NE	5.28	1.55	1.46
4	J	696	GLU	CA-CB	5.28	1.65	1.53
8	c	157	LEU	CA-CB	5.28	1.65	1.53
2	N	828	GLU	CG-CD	5.28	1.59	1.51
5	L	1485	TYR	CE2-CZ	5.28	1.45	1.38
2	D	508	VAL	CB-CG1	5.28	1.64	1.52
3	K	54	ARG	CZ-NH2	5.28	1.40	1.33
3	K	592	PHE	CG-CD1	5.28	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	n	309	ARG	NE-CZ	5.28	1.40	1.33
8	n	53	TYR	CE1-CZ	5.27	1.45	1.38
2	O	48	GLU	CD-OE1	5.27	1.31	1.25
7	X	651	GLU	CD-OE2	5.27	1.31	1.25
8	a	116	GLU	CD-OE2	-5.27	1.19	1.25
8	d	283	ALA	CA-CB	5.27	1.63	1.52
8	e	336	SER	CA-CB	5.27	1.60	1.52
2	F	336	ARG	CZ-NH1	5.27	1.39	1.33
9	q	35	SER	CA-CB	5.26	1.60	1.52
8	j	33	PRO	N-CD	-5.26	1.40	1.47
2	H	628	SER	CA-CB	5.26	1.60	1.52
3	I	1	MET	CA-CB	5.26	1.65	1.53
8	k	47	ARG	CZ-NH1	5.26	1.39	1.33
9	s	23	ARG	CZ-NH2	5.26	1.39	1.33
1	E	215	CYS	CB-SG	5.26	1.91	1.82
8	n	28	GLU	CG-CD	5.26	1.59	1.51
8	m	29	HIS	CB-CG	5.26	1.59	1.50
1	C	278	GLU	CA-CB	5.26	1.65	1.53
8	l	160	ARG	NE-CZ	5.25	1.39	1.33
2	F	815	GLU	CD-OE1	5.25	1.31	1.25
3	K	111	PHE	N-CA	-5.25	1.35	1.46
7	V	614	PHE	CG-CD1	5.25	1.46	1.38
8	m	3	ARG	NE-CZ	5.25	1.39	1.33
1	G	615	PHE	CG-CD2	5.25	1.46	1.38
1	M	463	GLY	CA-C	-5.25	1.43	1.51
8	j	328	VAL	N-CA	-5.25	1.35	1.46
1	A	561	SER	CA-CB	5.25	1.60	1.52
1	G	455	TYR	CG-CD1	5.25	1.46	1.39
2	H	517	ASP	CA-CB	5.25	1.65	1.53
4	J	412	PHE	CG-CD2	5.25	1.46	1.38
7	X	614	PHE	CE2-CZ	5.25	1.47	1.37
8	c	38	GLU	CG-CD	5.25	1.59	1.51
3	I	633	ARG	CZ-NH2	5.25	1.39	1.33
8	l	252	ASP	N-CA	-5.25	1.35	1.46
1	E	240	ARG	CZ-NH1	5.25	1.39	1.33
8	d	13	CYS	C-N	5.25	1.42	1.33
8	n	106	SER	CA-CB	5.25	1.60	1.52
2	B	430	TYR	CE1-CZ	5.24	1.45	1.38
3	I	12	TYR	CZ-OH	5.24	1.46	1.37
8	c	408	PHE	CG-CD1	5.24	1.46	1.38
8	h	388	PHE	CE2-CZ	5.24	1.47	1.37
8	k	390	ARG	CZ-NH2	5.24	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	m	422	ASP	N-CA	-5.24	1.35	1.46
1	G	705	TRP	NE1-CE2	5.24	1.44	1.37
1	A	363	PHE	CE1-CZ	5.24	1.47	1.37
2	B	877	PHE	CB-CG	5.24	1.60	1.51
1	E	822	SER	CA-CB	5.24	1.60	1.52
1	G	252	ASP	CB-CG	5.24	1.62	1.51
1	C	747	PHE	CG-CD1	5.24	1.46	1.38
2	N	815	GLU	CD-OE1	5.24	1.31	1.25
8	l	12	GLN	CG-CD	5.24	1.63	1.51
3	I	650	TYR	CZ-OH	5.24	1.46	1.37
1	M	867	TYR	CZ-OH	5.24	1.46	1.37
6	P	28	ARG	NE-CZ	5.24	1.39	1.33
8	b	390	ARG	CD-NE	5.24	1.55	1.46
2	N	543	TYR	CE1-CZ	5.23	1.45	1.38
8	d	22	TRP	CA-CB	5.23	1.65	1.53
8	b	296	ARG	CZ-NH1	5.23	1.39	1.33
8	f	152	TYR	CG-CD1	5.23	1.46	1.39
3	K	206	ARG	NE-CZ	5.23	1.39	1.33
1	A	339	SER	CA-CB	5.23	1.60	1.52
8	h	160	ARG	CD-NE	5.23	1.55	1.46
1	C	427	TRP	CD2-CE2	5.22	1.47	1.41
1	C	281	SER	CA-CB	5.22	1.60	1.52
8	c	435	TYR	CG-CD2	5.22	1.46	1.39
8	g	89	GLU	CG-CD	5.22	1.59	1.51
1	G	641	PHE	CG-CD2	5.21	1.46	1.38
2	H	659	TYR	CB-CG	-5.21	1.43	1.51
1	M	752	SER	CA-CB	5.21	1.60	1.52
1	E	274	ARG	CZ-NH2	5.21	1.39	1.33
3	I	456	TYR	CD2-CE2	5.21	1.47	1.39
4	J	999	ARG	NE-CZ	5.21	1.39	1.33
3	I	278	PHE	CG-CD2	5.21	1.46	1.38
8	h	194	ARG	CD-NE	5.20	1.55	1.46
8	k	160	ARG	NE-CZ	5.20	1.39	1.33
8	m	45	THR	N-CA	-5.20	1.35	1.46
2	T	84	GLN	CA-CB	5.20	1.65	1.53
2	S	105	ARG	CZ-NH2	5.20	1.39	1.33
8	e	63	ARG	CZ-NH2	5.20	1.39	1.33
8	m	155	GLU	CD-OE2	5.20	1.31	1.25
8	n	44	GLY	CA-C	-5.20	1.43	1.51
2	F	409	TYR	CZ-OH	5.20	1.46	1.37
2	F	661	ARG	CD-NE	5.20	1.55	1.46
3	I	179	CYS	CB-SG	-5.20	1.73	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	k	424	SER	CA-CB	5.20	1.60	1.52
8	l	245	TYR	CB-CG	-5.20	1.43	1.51
3	I	394	VAL	CA-C	-5.19	1.39	1.52
9	t	19	LEU	N-CA	-5.19	1.35	1.46
2	B	768	ARG	CD-NE	5.19	1.55	1.46
4	J	809	SER	CA-CB	5.19	1.60	1.52
7	U	666	ARG	CZ-NH2	5.19	1.39	1.33
1	C	829	SER	CB-OG	5.19	1.49	1.42
8	f	425	ARG	CZ-NH2	5.19	1.39	1.33
8	a	244	ARG	CZ-NH2	5.19	1.39	1.33
7	X	668	ARG	NE-CZ	5.18	1.39	1.33
1	E	222	TYR	CE2-CZ	5.18	1.45	1.38
2	N	316	PHE	CG-CD2	5.18	1.46	1.38
2	Q	99	SER	CA-CB	5.18	1.60	1.52
1	G	396	ARG	CD-NE	5.18	1.55	1.46
1	G	863	PHE	CG-CD1	5.18	1.46	1.38
2	N	731	ASP	CB-CG	5.18	1.62	1.51
2	O	68	GLU	CB-CG	5.18	1.61	1.52
8	m	107	GLY	CA-C	-5.18	1.43	1.51
1	A	736	CYS	CB-SG	-5.17	1.73	1.81
1	A	859	TYR	CE2-CZ	5.17	1.45	1.38
8	b	51	PHE	CE1-CZ	5.17	1.47	1.37
8	c	399	ARG	CZ-NH1	5.17	1.39	1.33
2	F	564	TYR	CE2-CZ	5.17	1.45	1.38
2	H	563	ARG	CZ-NH1	5.17	1.39	1.33
5	L	1656	TYR	CD2-CE2	-5.17	1.31	1.39
8	n	86	TYR	CE1-CZ	5.17	1.45	1.38
8	n	174	ASN	CA-CB	5.17	1.66	1.53
8	h	160	ARG	CZ-NH1	5.17	1.39	1.33
8	e	186	TYR	CE1-CZ	5.17	1.45	1.38
1	A	832	SER	CB-OG	5.17	1.49	1.42
7	X	647	TYR	CE2-CZ	5.17	1.45	1.38
8	b	160	ARG	NE-CZ	5.17	1.39	1.33
8	f	426	GLU	CD-OE1	5.17	1.31	1.25
8	i	237	SER	CB-OG	-5.17	1.35	1.42
1	G	636	ARG	CZ-NH2	5.16	1.39	1.33
1	E	314	ARG	CD-NE	5.16	1.55	1.46
8	e	404	PHE	CA-CB	5.16	1.65	1.53
8	m	86	TYR	CG-CD2	5.16	1.45	1.39
1	E	364	GLY	CA-C	-5.16	1.43	1.51
8	f	157	LEU	N-CA	-5.16	1.36	1.46
8	l	60	TYR	CB-CG	-5.16	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	N	359	SER	N-CA	5.16	1.56	1.46
2	N	863	LEU	CA-CB	5.15	1.65	1.53
8	d	186	TYR	CD1-CE1	5.15	1.47	1.39
3	K	62	TYR	CE1-CZ	5.15	1.45	1.38
8	a	435	TYR	CD2-CE2	5.15	1.47	1.39
8	e	366	TYR	CG-CD1	5.15	1.45	1.39
6	P	182	GLY	CA-C	-5.15	1.43	1.51
8	d	160	ARG	NE-CZ	5.15	1.39	1.33
8	j	110	GLN	C-N	5.14	1.42	1.33
8	h	40	PHE	CB-CG	5.14	1.60	1.51
8	l	295	ARG	N-CA	-5.14	1.36	1.46
8	d	358	VAL	CB-CG1	5.14	1.63	1.52
1	C	248	GLU	CD-OE1	5.14	1.31	1.25
5	L	319	ARG	CZ-NH2	5.14	1.39	1.33
8	m	90	ASN	CA-CB	5.14	1.66	1.53
5	L	99	GLU	CD-OE2	5.14	1.31	1.25
5	L	223	SER	CA-CB	5.14	1.60	1.52
8	i	152	TYR	CG-CD2	5.14	1.45	1.39
1	E	403	TYR	CG-CD2	5.13	1.45	1.39
2	F	406	GLY	CA-C	-5.13	1.43	1.51
3	K	190	TRP	CG-CD1	5.13	1.44	1.36
8	e	295	ARG	CZ-NH2	5.13	1.39	1.33
2	D	673	GLU	CD-OE2	5.13	1.31	1.25
4	J	759	GLU	CD-OE1	5.13	1.31	1.25
5	L	1521	ARG	CD-NE	5.13	1.55	1.46
2	T	56	GLU	CD-OE1	5.13	1.31	1.25
8	l	140	SER	CA-CB	5.13	1.60	1.52
8	n	401	ARG	C-N	5.13	1.45	1.34
5	L	7	LEU	N-CA	-5.13	1.36	1.46
1	C	509	VAL	CB-CG2	5.12	1.63	1.52
2	S	25	GLU	CG-CD	5.12	1.59	1.51
8	d	116	GLU	CG-CD	5.12	1.59	1.51
8	f	214	ALA	N-CA	-5.12	1.36	1.46
3	K	606	ARG	CZ-NH2	5.12	1.39	1.33
8	n	70	GLU	CG-CD	5.12	1.59	1.51
2	F	793	ARG	CZ-NH1	5.12	1.39	1.33
8	e	240	THR	N-CA	-5.12	1.36	1.46
8	i	47	ARG	NE-CZ	5.12	1.39	1.33
2	B	543	TYR	CG-CD2	5.11	1.45	1.39
2	F	680	TRP	CD2-CE3	-5.11	1.32	1.40
8	a	307	THR	C-N	5.11	1.42	1.33
8	b	229	ASN	C-N	5.11	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	852	HIS	CG-CD2	5.11	1.44	1.35
3	I	89	PHE	CE1-CZ	5.11	1.47	1.37
8	f	350	PRO	N-CA	-5.11	1.38	1.47
8	n	155	GLU	CG-CD	5.11	1.59	1.51
8	e	244	ARG	CZ-NH2	5.11	1.39	1.33
2	H	805	PHE	CG-CD2	5.11	1.46	1.38
2	H	863	LEU	CA-CB	5.11	1.65	1.53
8	i	115	HIS	CB-CG	-5.11	1.40	1.50
1	E	549	ARG	CZ-NH1	5.10	1.39	1.33
8	f	341	ARG	CZ-NH1	5.10	1.39	1.33
8	l	20	GLU	CD-OE1	-5.10	1.20	1.25
8	d	47	ARG	NE-CZ	5.10	1.39	1.33
8	m	82	TYR	CA-CB	5.10	1.65	1.53
8	n	161	TYR	N-CA	-5.10	1.36	1.46
1	C	859	TYR	CE1-CZ	5.10	1.45	1.38
8	d	89	GLU	CG-CD	5.10	1.59	1.51
8	m	156	ARG	NE-CZ	5.10	1.39	1.33
1	G	645	PHE	CE1-CZ	5.10	1.47	1.37
8	a	131	SER	CA-CB	5.09	1.60	1.52
2	H	553	ASN	CA-C	-5.09	1.39	1.52
2	N	323	PHE	CG-CD2	5.09	1.46	1.38
8	n	245	TYR	CB-CG	-5.09	1.44	1.51
5	L	44	TYR	CB-CG	5.09	1.59	1.51
8	j	355	SER	CA-CB	5.09	1.60	1.52
4	J	683	ARG	CZ-NH2	5.09	1.39	1.33
8	n	406	GLU	CD-OE1	-5.09	1.20	1.25
8	b	326	GLY	CA-C	-5.09	1.43	1.51
8	d	317	TYR	CG-CD2	5.09	1.45	1.39
2	D	359	SER	N-CA	5.08	1.56	1.46
1	C	842	LEU	CA-CB	5.08	1.65	1.53
8	f	401	ARG	NE-CZ	5.08	1.39	1.33
8	n	418	PHE	CG-CD2	5.08	1.46	1.38
1	C	270	SER	CA-CB	5.08	1.60	1.52
2	N	651	PHE	CG-CD1	5.08	1.46	1.38
8	a	126	ALA	N-CA	-5.08	1.36	1.46
7	X	648	SER	CA-CB	5.08	1.60	1.52
3	K	514	TRP	CD2-CE2	5.07	1.47	1.41
5	L	1476	ASP	CB-CG	5.07	1.62	1.51
8	e	72	ARG	CZ-NH1	5.07	1.39	1.33
8	k	399	ARG	NE-CZ	5.07	1.39	1.33
8	b	148	GLY	CA-C	-5.07	1.43	1.51
1	E	684	ARG	CZ-NH2	5.07	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	c	3	ARG	CZ-NH2	5.07	1.39	1.33
8	m	217	ARG	CZ-NH1	5.07	1.39	1.33
8	c	111	GLY	CA-C	-5.07	1.43	1.51
2	F	630	GLY	N-CA	-5.06	1.38	1.46
8	a	308	GLY	N-CA	5.06	1.53	1.46
1	E	225	ILE	C-N	5.06	1.42	1.33
2	N	391	LYS	C-N	5.06	1.42	1.33
1	C	526	PHE	CG-CD2	5.06	1.46	1.38
7	X	645	GLU	CD-OE1	5.06	1.31	1.25
1	A	279	ASN	CB-CG	5.06	1.62	1.51
2	B	719	TYR	CG-CD2	5.06	1.45	1.39
1	E	397	GLY	N-CA	-5.06	1.38	1.46
6	P	69	TYR	CG-CD1	5.06	1.45	1.39
1	A	322	LYS	CA-CB	5.06	1.65	1.53
2	F	615	GLU	CB-CG	5.06	1.61	1.52
1	A	518	TYR	CZ-OH	5.05	1.46	1.37
2	B	295	GLU	CD-OE1	5.05	1.31	1.25
2	B	853	TYR	CD1-CE1	5.05	1.47	1.39
2	N	409	TYR	CG-CD2	5.05	1.45	1.39
2	Q	66	ARG	NE-CZ	5.05	1.39	1.33
8	n	92	TYR	CE1-CZ	5.05	1.45	1.38
1	C	649	HIS	CG-CD2	5.05	1.44	1.35
8	n	119	PHE	CG-CD1	5.05	1.46	1.38
1	A	753	VAL	CB-CG2	5.05	1.63	1.52
3	I	318	PRO	CA-CB	-5.05	1.43	1.53
8	j	194	ARG	CD-NE	5.05	1.55	1.46
1	M	859	TYR	CG-CD1	5.05	1.45	1.39
8	c	156	ARG	CZ-NH2	5.05	1.39	1.33
8	c	362	ARG	CZ-NH1	5.05	1.39	1.33
8	i	22	TRP	NE1-CE2	-5.05	1.30	1.37
8	l	86	TYR	CB-CG	5.05	1.59	1.51
2	D	723	PHE	CE1-CZ	5.05	1.47	1.37
2	H	359	SER	CA-CB	5.05	1.60	1.52
8	h	351	TRP	NE1-CE2	-5.04	1.30	1.37
8	h	401	ARG	CZ-NH1	5.04	1.39	1.33
2	D	708	SER	CA-CB	5.04	1.60	1.52
2	H	434	TYR	CZ-OH	5.04	1.46	1.37
2	H	586	ARG	CZ-NH1	5.04	1.39	1.33
3	K	267	TYR	CG-CD2	5.04	1.45	1.39
2	D	271	GLU	CD-OE2	5.04	1.31	1.25
2	T	66	ARG	NE-CZ	5.04	1.39	1.33
3	K	450	ALA	N-CA	-5.04	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	812	ARG	CZ-NH2	5.04	1.39	1.33
8	g	133	GLU	CB-CG	5.04	1.61	1.52
8	l	12	GLN	CA-CB	5.04	1.65	1.53
2	H	838	SER	CA-CB	5.03	1.60	1.52
8	l	44	GLY	CA-C	-5.03	1.43	1.51
1	A	230	ARG	NE-CZ	5.03	1.39	1.33
1	A	455	TYR	CA-CB	5.03	1.65	1.53
3	I	333	ARG	CZ-NH2	5.03	1.39	1.33
1	M	658	TRP	CD2-CE2	-5.03	1.35	1.41
8	a	39	GLU	CA-CB	5.03	1.65	1.53
6	P	206	ARG	CZ-NH2	5.03	1.39	1.33
3	K	555	SER	CA-CB	5.03	1.60	1.52
2	N	514	SER	CA-CB	5.03	1.60	1.52
2	N	792	TYR	CG-CD2	5.03	1.45	1.39
2	S	61	GLU	CD-OE2	5.03	1.31	1.25
8	e	370	ALA	CA-CB	5.03	1.63	1.52
2	D	869	ASP	CA-CB	5.03	1.65	1.53
8	k	244	ARG	NE-CZ	5.02	1.39	1.33
8	i	414	PHE	CE2-CZ	5.02	1.46	1.37
1	A	430	ARG	NE-CZ	5.02	1.39	1.33
2	B	807	GLU	CD-OE1	5.02	1.31	1.25
3	K	495	TRP	NE1-CE2	5.02	1.44	1.37
8	j	161	TYR	CE1-CZ	5.02	1.45	1.38
8	f	406	GLU	CD-OE2	5.02	1.31	1.25
3	K	637	ILE	CB-CG2	5.01	1.68	1.52
2	N	601	GLU	CD-OE2	5.01	1.31	1.25
8	a	63	ARG	CZ-NH2	5.01	1.39	1.33
1	M	825	ASN	CB-CG	5.01	1.62	1.51
8	h	408	PHE	CE1-CZ	5.01	1.46	1.37
2	N	825	GLU	C-N	5.01	1.45	1.34
8	n	119	PHE	CE1-CZ	5.01	1.46	1.37
8	c	404	PHE	CE2-CZ	5.01	1.46	1.37
2	H	767	SER	CA-CB	5.01	1.60	1.52
3	K	253	SER	CB-OG	5.01	1.48	1.42
8	j	111	GLY	CA-C	-5.01	1.43	1.51
8	m	214	ALA	N-CA	5.01	1.56	1.46
5	L	52	PHE	CG-CD2	5.00	1.46	1.38
6	P	130	PRO	N-CA	-5.00	1.38	1.47
8	d	95	GLU	CD-OE2	-5.00	1.20	1.25
2	H	423	TYR	CG-CD1	5.00	1.45	1.39
7	V	645	GLU	CG-CD	5.00	1.59	1.51
8	k	155	GLU	CB-CG	5.00	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	l	194	ARG	CZ-NH1	5.00	1.39	1.33

All (3317) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	515	ARG	NE-CZ-NH1	-52.78	93.91	120.30
8	j	372	ARG	NE-CZ-NH2	-22.99	108.81	120.30
3	K	515	ARG	NE-CZ-NH2	22.59	131.59	120.30
5	L	1386	TYR	CB-CG-CD1	21.38	133.83	121.00
8	g	425	ARG	NE-CZ-NH1	21.25	130.92	120.30
8	d	265	ARG	NE-CZ-NH2	-20.56	110.02	120.30
1	G	431	TYR	CB-CG-CD2	-20.27	108.84	121.00
8	d	265	ARG	NE-CZ-NH1	20.25	130.43	120.30
1	C	559	ARG	NE-CZ-NH1	20.24	130.42	120.30
8	n	393	ARG	NE-CZ-NH1	20.11	130.36	120.30
8	j	409	ARG	NE-CZ-NH1	19.68	130.14	120.30
8	h	372	ARG	NE-CZ-NH2	-19.28	110.66	120.30
2	D	802	ARG	NE-CZ-NH1	-19.04	110.78	120.30
2	F	812	ARG	NE-CZ-NH1	18.98	129.79	120.30
8	j	343	ARG	NE-CZ-NH2	-18.05	111.27	120.30
3	K	22	ARG	NE-CZ-NH2	-18.05	111.27	120.30
2	N	802	ARG	NE-CZ-NH2	18.00	129.30	120.30
8	j	409	ARG	NE-CZ-NH2	-17.49	111.55	120.30
2	H	457	ARG	NE-CZ-NH1	17.19	128.89	120.30
1	G	642	ARG	NE-CZ-NH1	17.16	128.88	120.30
8	n	372	ARG	NE-CZ-NH2	-17.13	111.74	120.30
8	k	401	ARG	NE-CZ-NH1	16.93	128.77	120.30
2	S	105	ARG	NE-CZ-NH2	-16.54	112.03	120.30
5	L	1543	ARG	NE-CZ-NH1	16.48	128.54	120.30
2	D	574	ARG	NE-CZ-NH1	16.43	128.52	120.30
2	H	605	ARG	NE-CZ-NH1	-16.36	112.12	120.30
8	e	63	ARG	NE-CZ-NH2	-16.32	112.14	120.30
2	H	365	ARG	NE-CZ-NH2	-16.22	112.19	120.30
8	e	409	ARG	NE-CZ-NH1	16.21	128.40	120.30
2	B	574	ARG	NE-CZ-NH1	16.13	128.37	120.30
8	i	286	ARG	NE-CZ-NH2	-15.90	112.35	120.30
2	B	457	ARG	NE-CZ-NH2	-15.90	112.35	120.30
1	E	695	TYR	CB-CG-CD1	15.88	130.53	121.00
8	f	341	ARG	NE-CZ-NH2	15.80	128.20	120.30
8	j	194	ARG	NE-CZ-NH2	-15.78	112.41	120.30
8	m	343	ARG	NE-CZ-NH2	-15.74	112.43	120.30
3	K	44	ARG	NE-CZ-NH2	-15.55	112.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	q	58	ARG	NE-CZ-NH2	-15.47	112.56	120.30
3	I	551	ARG	NE-CZ-NH1	15.46	128.03	120.30
2	F	668	ARG	NE-CZ-NH1	15.22	127.91	120.30
1	G	222	TYR	CB-CG-CD2	-15.21	111.87	121.00
1	C	314	ARG	NE-CZ-NH1	15.18	127.89	120.30
8	i	72	ARG	NE-CZ-NH2	-15.12	112.74	120.30
5	L	1601	PHE	CB-CG-CD2	15.05	131.33	120.80
8	m	388	PHE	CB-CG-CD2	-15.04	110.27	120.80
8	i	425	ARG	NE-CZ-NH2	15.01	127.81	120.30
2	N	812	ARG	NE-CZ-NH1	14.99	127.80	120.30
5	L	224	ARG	NE-CZ-NH2	-14.99	112.80	120.30
8	f	212	ARG	NE-CZ-NH2	-14.91	112.84	120.30
1	E	684	ARG	NE-CZ-NH1	14.82	127.71	120.30
5	L	404	TYR	CB-CG-CD1	-14.80	112.12	121.00
8	l	372	ARG	NE-CZ-NH1	14.76	127.68	120.30
1	C	240	ARG	NE-CZ-NH1	14.75	127.67	120.30
4	J	466	ARG	NE-CZ-NH2	-14.73	112.93	120.30
1	G	296	ARG	NE-CZ-NH1	-14.72	112.94	120.30
8	j	341	ARG	NE-CZ-NH2	-14.66	112.97	120.30
5	L	1548	TYR	CB-CG-CD1	-14.56	112.26	121.00
8	m	72	ARG	NE-CZ-NH2	-14.51	113.05	120.30
1	G	867	TYR	CB-CG-CD2	-14.48	112.31	121.00
8	h	409	ARG	NE-CZ-NH1	14.40	127.50	120.30
2	F	364	ARG	NE-CZ-NH2	-14.35	113.12	120.30
8	d	393	ARG	NE-CZ-NH2	14.31	127.46	120.30
1	A	549	ARG	NE-CZ-NH2	-14.31	113.14	120.30
1	M	243	ARG	NE-CZ-NH2	-14.30	113.15	120.30
3	K	442	ARG	NE-CZ-NH2	-14.27	113.16	120.30
5	L	1676	ARG	NE-CZ-NH2	-14.24	113.18	120.30
1	G	845	TYR	CB-CG-CD1	14.24	129.54	121.00
2	N	802	ARG	NE-CZ-NH1	-14.22	113.19	120.30
8	n	286	ARG	NE-CZ-NH2	-14.21	113.20	120.30
1	C	296	ARG	NE-CZ-NH1	14.21	127.40	120.30
6	P	147	ARG	NE-CZ-NH2	-14.19	113.20	120.30
5	L	410	ARG	NE-CZ-NH2	-14.19	113.21	120.30
4	J	227	ARG	NE-CZ-NH2	-14.16	113.22	120.30
2	N	878	ARG	NE-CZ-NH2	-14.16	113.22	120.30
1	M	684	ARG	NE-CZ-NH2	-14.01	113.29	120.30
8	d	425	ARG	NE-CZ-NH1	14.01	127.31	120.30
8	n	296	ARG	NE-CZ-NH2	14.01	127.30	120.30
1	C	763	ARG	NE-CZ-NH2	-14.00	113.30	120.30
1	E	747	PHE	CB-CG-CD2	-14.00	111.00	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	j	341	ARG	NE-CZ-NH1	13.98	127.29	120.30
8	e	339	ARG	NE-CZ-NH2	-13.98	113.31	120.30
8	n	309	ARG	NE-CZ-NH2	-13.97	113.31	120.30
2	D	878	ARG	NE-CZ-NH1	13.96	127.28	120.30
3	K	169	ARG	NE-CZ-NH1	13.95	127.28	120.30
8	f	72	ARG	NE-CZ-NH1	13.93	127.27	120.30
8	c	217	ARG	NE-CZ-NH1	13.88	127.24	120.30
2	D	466	ARG	NE-CZ-NH2	-13.88	113.36	120.30
2	F	651	PHE	CB-CG-CD2	-13.79	111.15	120.80
8	d	425	ARG	NE-CZ-NH2	-13.75	113.43	120.30
3	K	515	ARG	NH1-CZ-NH2	13.72	134.49	119.40
8	h	3	ARG	NE-CZ-NH1	13.71	127.16	120.30
2	H	390	ARG	NE-CZ-NH1	13.67	127.14	120.30
9	r	23	ARG	NE-CZ-NH1	13.61	127.10	120.30
2	S	90	ARG	NE-CZ-NH1	13.59	127.10	120.30
8	k	160	ARG	NE-CZ-NH2	-13.58	113.51	120.30
8	g	295	ARG	NE-CZ-NH1	13.56	127.08	120.30
8	i	341	ARG	NE-CZ-NH1	13.54	127.07	120.30
8	e	161	TYR	CB-CG-CD2	13.53	129.12	121.00
1	E	636	ARG	NE-CZ-NH2	-13.49	113.56	120.30
2	D	431	ARG	NE-CZ-NH2	-13.49	113.56	120.30
3	I	466	PHE	CB-CG-CD1	-13.40	111.42	120.80
1	G	642	ARG	NE-CZ-NH2	-13.34	113.63	120.30
2	F	409	TYR	CB-CG-CD2	-13.31	113.02	121.00
2	S	37	ARG	NE-CZ-NH2	13.29	126.94	120.30
9	s	59	ARG	NE-CZ-NH2	-13.26	113.67	120.30
8	i	341	ARG	NE-CZ-NH2	-13.21	113.69	120.30
2	F	843	ARG	NE-CZ-NH1	13.20	126.90	120.30
2	H	784	PHE	CB-CG-CD2	-13.20	111.56	120.80
8	j	372	ARG	NE-CZ-NH1	13.20	126.90	120.30
1	M	549	ARG	NE-CZ-NH2	13.19	126.89	120.30
6	P	62	ARG	NE-CZ-NH1	13.17	126.88	120.30
8	m	425	ARG	NE-CZ-NH2	-13.15	113.73	120.30
2	R	70	ASP	CB-CG-OD2	-13.13	106.49	118.30
1	G	302	TYR	CB-CG-CD2	13.12	128.87	121.00
2	H	653	ARG	NE-CZ-NH2	13.11	126.86	120.30
8	e	390	ARG	NE-CZ-NH1	13.11	126.86	120.30
8	c	47	ARG	NE-CZ-NH1	13.09	126.84	120.30
8	j	47	ARG	NE-CZ-NH1	13.09	126.84	120.30
8	l	311	ARG	NE-CZ-NH1	13.08	126.84	120.30
2	B	537	TYR	CB-CG-CD2	13.07	128.84	121.00
8	a	296	ARG	NE-CZ-NH1	12.98	126.79	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	m	388	PHE	CB-CG-CD1	12.96	129.87	120.80
3	K	91	ARG	NE-CZ-NH2	-12.96	113.82	120.30
2	B	457	ARG	NE-CZ-NH1	12.96	126.78	120.30
2	S	64	ARG	NE-CZ-NH2	-12.94	113.83	120.30
2	F	775	ARG	NE-CZ-NH1	12.93	126.76	120.30
8	f	296	ARG	NE-CZ-NH2	-12.91	113.84	120.30
8	j	19	PHE	CB-CG-CD2	-12.90	111.77	120.80
1	G	222	TYR	CB-CG-CD1	12.89	128.74	121.00
8	g	309	ARG	NE-CZ-NH1	12.89	126.75	120.30
8	k	92	TYR	CB-CG-CD2	12.88	128.73	121.00
8	g	194	ARG	NE-CZ-NH1	12.87	126.74	120.30
2	R	67	ARG	NE-CZ-NH2	12.83	126.72	120.30
1	A	431	TYR	CB-CG-CD2	12.83	128.70	121.00
8	g	425	ARG	NE-CZ-NH2	-12.82	113.89	120.30
8	m	339	ARG	NE-CZ-NH1	12.82	126.71	120.30
3	K	267	TYR	CB-CG-CD1	12.80	128.68	121.00
4	J	939	ARG	NE-CZ-NH1	12.80	126.70	120.30
7	W	666	ARG	NE-CZ-NH1	12.78	126.69	120.30
8	f	372	ARG	NE-CZ-NH2	-12.78	113.91	120.30
8	b	286	ARG	NE-CZ-NH1	12.76	126.68	120.30
2	N	623	ARG	NE-CZ-NH1	-12.75	113.92	120.30
8	h	414	PHE	CB-CG-CD2	12.73	129.71	120.80
8	c	286	ARG	NE-CZ-NH2	-12.70	113.95	120.30
1	C	486	ARG	NE-CZ-NH2	-12.70	113.95	120.30
2	T	64	ARG	NE-CZ-NH1	12.69	126.64	120.30
2	B	802	ARG	NE-CZ-NH1	-12.68	113.96	120.30
8	e	341	ARG	NE-CZ-NH1	-12.68	113.96	120.30
3	K	44	ARG	NE-CZ-NH1	12.67	126.64	120.30
8	a	366	TYR	CB-CG-CD1	12.62	128.57	121.00
8	m	286	ARG	NE-CZ-NH2	-12.61	114.00	120.30
2	D	390	ARG	NE-CZ-NH1	12.60	126.60	120.30
8	e	194	ARG	NE-CZ-NH2	-12.58	114.01	120.30
2	N	661	ARG	NE-CZ-NH1	12.51	126.55	120.30
4	J	428	ARG	NE-CZ-NH1	12.50	126.55	120.30
8	g	395	TYR	CB-CG-CD2	-12.49	113.50	121.00
3	I	365	ARG	NE-CZ-NH1	12.47	126.54	120.30
8	b	244	ARG	NE-CZ-NH2	-12.44	114.08	120.30
8	k	435	TYR	CB-CG-CD2	-12.43	113.54	121.00
2	D	563	ARG	NE-CZ-NH2	-12.42	114.09	120.30
8	f	86	TYR	CB-CG-CD1	12.42	128.45	121.00
1	C	571	ASP	CB-CG-OD2	-12.38	107.15	118.30
8	k	292	ASP	CB-CG-OD1	12.38	129.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	793	ARG	NE-CZ-NH2	-12.35	114.13	120.30
1	C	386	TYR	CB-CG-CD2	12.35	128.41	121.00
2	D	314	ARG	NE-CZ-NH1	-12.33	114.14	120.30
4	J	935	ARG	NE-CZ-NH2	12.30	126.45	120.30
2	O	90	ARG	NE-CZ-NH1	12.28	126.44	120.30
8	a	120	ASP	CB-CG-OD1	12.27	129.34	118.30
8	h	362	ARG	NE-CZ-NH1	12.26	126.43	120.30
2	N	480	ARG	NE-CZ-NH1	12.24	126.42	120.30
1	G	747	PHE	CB-CG-CD1	12.23	129.36	120.80
8	c	372	ARG	NE-CZ-NH1	12.21	126.40	120.30
6	P	166	TYR	CB-CG-CD1	-12.19	113.68	121.00
8	c	124	ARG	NE-CZ-NH1	12.19	126.39	120.30
8	n	152	TYR	CB-CG-CD1	-12.18	113.69	121.00
5	L	438	ARG	NE-CZ-NH2	-12.17	114.22	120.30
4	J	591	PHE	CB-CG-CD1	-12.16	112.29	120.80
8	k	194	ARG	NE-CZ-NH1	12.16	126.38	120.30
1	A	763	ARG	NE-CZ-NH1	12.12	126.36	120.30
2	Q	37	ARG	NE-CZ-NH1	12.09	126.34	120.30
9	r	12	ARG	NE-CZ-NH1	12.08	126.34	120.30
8	n	217	ARG	NE-CZ-NH2	-12.03	114.29	120.30
5	L	1543	ARG	NE-CZ-NH2	-12.00	114.30	120.30
7	V	620	ARG	NE-CZ-NH1	11.96	126.28	120.30
1	C	844	MET	CG-SD-CE	-11.96	81.06	100.20
8	l	72	ARG	NE-CZ-NH1	11.94	126.27	120.30
8	c	362	ARG	NE-CZ-NH2	-11.93	114.34	120.30
8	l	339	ARG	NE-CZ-NH2	-11.93	114.34	120.30
4	J	227	ARG	NE-CZ-NH1	11.92	126.26	120.30
8	j	47	ARG	NE-CZ-NH2	-11.92	114.34	120.30
2	F	562	ARG	NE-CZ-NH2	-11.91	114.35	120.30
8	k	435	TYR	CB-CG-CD1	11.90	128.14	121.00
6	P	188	TYR	CB-CG-CD2	11.86	128.12	121.00
3	K	22	ARG	NE-CZ-NH1	11.84	126.22	120.30
9	p	58	ARG	NE-CZ-NH2	-11.81	114.39	120.30
1	C	240	ARG	NE-CZ-NH2	-11.80	114.40	120.30
3	I	55	PHE	CB-CG-CD1	11.79	129.06	120.80
8	a	393	ARG	NE-CZ-NH1	11.79	126.20	120.30
1	M	326	TYR	CB-CG-CD2	11.78	128.07	121.00
8	b	343	ARG	NE-CZ-NH2	-11.78	114.41	120.30
8	f	156	ARG	NE-CZ-NH2	-11.74	114.43	120.30
2	B	251	ARG	NE-CZ-NH2	-11.74	114.43	120.30
8	e	72	ARG	NE-CZ-NH1	11.74	126.17	120.30
8	a	194	ARG	NE-CZ-NH2	-11.74	114.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	l	72	ARG	NE-CZ-NH2	-11.72	114.44	120.30
8	m	372	ARG	NE-CZ-NH2	-11.70	114.45	120.30
3	K	633	ARG	NE-CZ-NH2	-11.68	114.46	120.30
8	b	273	TYR	CB-CG-CD2	-11.68	113.99	121.00
2	N	619	ARG	NE-CZ-NH1	11.65	126.13	120.30
8	c	217	ARG	NE-CZ-NH2	-11.65	114.47	120.30
8	l	339	ARG	NE-CZ-NH1	11.64	126.12	120.30
8	b	393	ARG	NE-CZ-NH2	-11.64	114.48	120.30
8	i	72	ARG	NE-CZ-NH1	11.63	126.11	120.30
7	X	666	ARG	NE-CZ-NH1	-11.62	114.49	120.30
1	A	840	ASP	CB-CG-OD1	11.61	128.75	118.30
8	g	245	TYR	CB-CG-CD1	11.59	127.96	121.00
8	l	309	ARG	NE-CZ-NH2	-11.59	114.50	120.30
8	m	390	ARG	NE-CZ-NH1	-11.59	114.51	120.30
5	L	564	ARG	NE-CZ-NH2	11.58	126.09	120.30
8	m	72	ARG	NE-CZ-NH1	11.58	126.09	120.30
8	b	63	ARG	NE-CZ-NH2	11.56	126.08	120.30
8	f	362	ARG	NE-CZ-NH1	-11.56	114.52	120.30
2	F	860	PHE	CB-CG-CD1	-11.55	112.72	120.80
7	X	615	ARG	NE-CZ-NH2	-11.55	114.53	120.30
4	J	982	PHE	CB-CG-CD2	-11.54	112.72	120.80
8	j	401	ARG	NE-CZ-NH2	-11.54	114.53	120.30
8	j	245	TYR	CB-CG-CD2	11.52	127.91	121.00
1	M	675	PHE	CB-CG-CD2	11.52	128.86	120.80
1	A	559	ARG	NE-CZ-NH1	11.52	126.06	120.30
1	A	431	TYR	CB-CG-CD1	-11.50	114.10	121.00
2	F	885	TYR	CB-CG-CD1	11.46	127.87	121.00
8	l	124	ARG	NE-CZ-NH1	11.43	126.02	120.30
1	A	549	ARG	NE-CZ-NH1	11.40	126.00	120.30
8	g	156	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	G	863	PHE	CB-CG-CD1	11.35	128.74	120.80
4	J	742	ARG	NE-CZ-NH1	11.35	125.97	120.30
1	M	866	PHE	CB-CG-CD2	-11.34	112.86	120.80
9	p	39	ARG	NE-CZ-NH1	11.32	125.96	120.30
8	l	418	PHE	CB-CG-CD1	-11.31	112.88	120.80
2	D	802	ARG	NE-CZ-NH2	11.31	125.96	120.30
8	b	343	ARG	NE-CZ-NH1	11.31	125.95	120.30
8	e	161	TYR	CB-CG-CD1	-11.30	114.22	121.00
8	b	3	ARG	NE-CZ-NH2	-11.30	114.65	120.30
8	j	51	PHE	CB-CG-CD1	11.30	128.71	120.80
3	I	111	PHE	CB-CG-CD2	-11.29	112.90	120.80
2	F	885	TYR	CB-CG-CD2	-11.28	114.23	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	b	399	ARG	NE-CZ-NH2	11.27	125.94	120.30
8	i	393	ARG	NE-CZ-NH1	11.26	125.93	120.30
2	O	66	ARG	NE-CZ-NH1	11.22	125.91	120.30
3	K	271	ARG	NE-CZ-NH2	-11.22	114.69	120.30
3	K	203	PHE	CB-CG-CD2	-11.20	112.96	120.80
1	G	431	TYR	CB-CG-CD1	11.20	127.72	121.00
1	C	361	ARG	NE-CZ-NH2	-11.18	114.71	120.30
4	J	242	TRP	CE2-CD2-CG	-11.17	98.37	107.30
3	I	557	ARG	NE-CZ-NH2	-11.16	114.72	120.30
2	N	808	ARG	NE-CZ-NH1	11.13	125.87	120.30
1	C	860	ARG	NE-CZ-NH1	11.11	125.85	120.30
2	B	623	ARG	NE-CZ-NH2	-11.10	114.75	120.30
8	f	372	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	E	332	ARG	NE-CZ-NH1	-11.09	114.75	120.30
8	a	82	TYR	CB-CG-CD1	-11.09	114.35	121.00
8	h	317	TYR	CB-CG-CD1	-11.08	114.35	121.00
7	U	633	PHE	CB-CG-CD2	-11.03	113.08	120.80
8	l	63	ARG	NE-CZ-NH1	11.03	125.82	120.30
4	J	571	ARG	NE-CZ-NH2	-11.03	114.79	120.30
4	J	503	PHE	CB-CG-CD1	11.00	128.50	120.80
2	B	793	ARG	NE-CZ-NH1	10.97	125.79	120.30
8	h	390	ARG	NE-CZ-NH1	-10.97	114.81	120.30
8	h	286	ARG	NE-CZ-NH1	10.97	125.79	120.30
2	H	457	ARG	NE-CZ-NH2	-10.96	114.82	120.30
1	G	684	ARG	NE-CZ-NH2	-10.95	114.83	120.30
2	B	537	TYR	CB-CG-CD1	-10.94	114.44	121.00
4	J	443	TYR	CB-CG-CD2	-10.94	114.44	121.00
8	k	3	ARG	NE-CZ-NH1	10.93	125.77	120.30
8	b	212	ARG	NE-CZ-NH2	-10.93	114.84	120.30
8	h	92	TYR	CB-CG-CD1	-10.91	114.45	121.00
2	N	480	ARG	NE-CZ-NH2	-10.90	114.85	120.30
2	F	753	PHE	CB-CG-CD1	-10.87	113.19	120.80
8	k	292	ASP	CB-CG-OD2	-10.85	108.54	118.30
2	B	659	TYR	CB-CG-CD2	-10.83	114.50	121.00
2	N	719	TYR	CB-CG-CD1	10.82	127.49	121.00
8	f	135	PHE	CB-CG-CD1	10.82	128.38	120.80
8	n	212	ARG	NE-CZ-NH1	10.82	125.71	120.30
1	G	559	ARG	NE-CZ-NH2	-10.80	114.90	120.30
2	H	641	TYR	CB-CG-CD1	-10.77	114.54	121.00
1	G	845	TYR	CB-CG-CD2	-10.76	114.55	121.00
3	I	515	ARG	NE-CZ-NH2	-10.72	114.94	120.30
3	I	649	ASP	CB-CG-OD2	-10.72	108.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	546	ARG	NE-CZ-NH1	-10.71	114.94	120.30
8	d	399	ARG	NE-CZ-NH2	-10.71	114.95	120.30
3	I	557	ARG	NE-CZ-NH1	10.70	125.65	120.30
3	I	653	TYR	CB-CG-CD1	10.69	127.42	121.00
2	N	316	PHE	CB-CG-CD2	10.69	128.28	120.80
8	d	399	ARG	NE-CZ-NH1	10.69	125.64	120.30
8	g	401	ARG	NE-CZ-NH2	-10.68	114.96	120.30
8	n	19	PHE	CB-CG-CD1	-10.67	113.33	120.80
8	k	172	PHE	CB-CG-CD1	10.66	128.26	120.80
8	b	295	ARG	NE-CZ-NH2	10.66	125.63	120.30
2	T	90	ARG	NE-CZ-NH1	10.66	125.63	120.30
2	D	446	PHE	CB-CG-CD1	-10.65	113.34	120.80
8	d	53	TYR	CB-CG-CD2	-10.63	114.62	121.00
1	G	631	ARG	NE-CZ-NH1	10.62	125.61	120.30
3	I	633	ARG	NE-CZ-NH1	10.62	125.61	120.30
6	P	147	ARG	NE-CZ-NH1	10.61	125.61	120.30
2	Q	79	ARG	NE-CZ-NH2	10.61	125.61	120.30
1	G	332	ARG	NE-CZ-NH2	-10.61	115.00	120.30
1	M	460	ARG	NE-CZ-NH1	10.60	125.60	120.30
4	J	709	TYR	CB-CG-CD1	-10.59	114.64	121.00
5	L	1386	TYR	CB-CG-CD2	-10.57	114.66	121.00
1	A	559	ARG	NE-CZ-NH2	-10.56	115.02	120.30
1	M	642	ARG	NE-CZ-NH2	-10.55	115.02	120.30
8	k	92	TYR	CB-CG-CD1	-10.54	114.67	121.00
8	e	160	ARG	NE-CZ-NH2	-10.54	115.03	120.30
3	K	650	TYR	CB-CG-CD2	-10.53	114.68	121.00
1	A	302	TYR	CB-CG-CD2	10.52	127.31	121.00
2	N	537	TYR	CB-CG-CD2	-10.52	114.69	121.00
8	f	309	ARG	NE-CZ-NH1	10.52	125.56	120.30
2	N	306	TYR	CB-CG-CD2	10.51	127.31	121.00
3	K	267	TYR	CB-CG-CD2	-10.50	114.70	121.00
2	B	423	TYR	CB-CG-CD1	-10.50	114.70	121.00
8	c	388	PHE	CB-CG-CD2	-10.50	113.45	120.80
8	b	244	ARG	NE-CZ-NH1	10.48	125.54	120.30
8	c	19	PHE	CB-CG-CD1	10.48	128.14	120.80
8	i	286	ARG	NE-CZ-NH1	10.44	125.52	120.30
2	F	562	ARG	NE-CZ-NH1	10.43	125.52	120.30
5	L	1685	PHE	CB-CG-CD1	10.43	128.10	120.80
8	m	343	ARG	NE-CZ-NH1	10.43	125.52	120.30
8	d	40	PHE	CB-CG-CD2	-10.42	113.50	120.80
2	B	653	ARG	NE-CZ-NH1	10.42	125.51	120.30
1	E	619	TYR	CB-CG-CD1	10.42	127.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	92	TYR	CB-CG-CD2	10.41	127.25	121.00
2	H	623	ARG	NE-CZ-NH1	10.40	125.50	120.30
2	N	878	ARG	NE-CZ-NH1	10.40	125.50	120.30
2	B	653	ARG	NE-CZ-NH2	-10.40	115.10	120.30
8	m	47	ARG	NE-CZ-NH2	-10.40	115.10	120.30
8	i	194	ARG	NE-CZ-NH2	-10.38	115.11	120.30
2	H	402	TYR	CB-CG-CD2	-10.38	114.77	121.00
8	l	414	PHE	CB-CG-CD2	10.38	128.06	120.80
8	n	309	ARG	NE-CZ-NH1	10.37	125.48	120.30
8	j	304	MET	CG-SD-CE	10.37	116.78	100.20
2	D	572	PHE	CB-CG-CD2	10.35	128.04	120.80
8	l	425	ARG	NE-CZ-NH2	-10.35	115.13	120.30
2	F	251	ARG	NE-CZ-NH2	10.34	125.47	120.30
8	j	395	TYR	CB-CG-CD2	10.32	127.19	121.00
4	J	321	PHE	CB-CG-CD2	10.30	128.01	120.80
8	m	273	TYR	CB-CG-CD1	10.28	127.17	121.00
2	B	768	ARG	NE-CZ-NH1	-10.27	115.17	120.30
1	G	274	ARG	NE-CZ-NH2	-10.26	115.17	120.30
9	s	59	ARG	NE-CZ-NH1	10.23	125.41	120.30
1	C	275	PHE	CB-CG-CD2	10.21	127.95	120.80
3	K	87	ARG	NE-CZ-NH2	10.20	125.40	120.30
1	E	526	PHE	CB-CG-CD2	10.15	127.91	120.80
8	g	317	TYR	CB-CG-CD1	10.13	127.08	121.00
1	M	483	TYR	CB-CG-CD2	-10.13	114.92	121.00
3	I	480	TYR	CB-CG-CD2	-10.12	114.93	121.00
1	A	845	TYR	CB-CG-CD2	-10.11	114.93	121.00
1	G	501	PHE	CB-CG-CD2	10.10	127.87	120.80
8	n	206	ASP	CB-CG-OD2	-10.10	109.21	118.30
1	A	261	ARG	NE-CZ-NH2	-10.10	115.25	120.30
4	J	1002	PHE	CB-CG-CD1	-10.10	113.73	120.80
2	D	480	ARG	NE-CZ-NH2	10.10	125.35	120.30
8	e	362	ARG	NE-CZ-NH2	-10.10	115.25	120.30
2	H	605	ARG	NE-CZ-NH2	10.09	125.35	120.30
2	D	376	ARG	NE-CZ-NH2	-10.09	115.26	120.30
7	X	615	ARG	NE-CZ-NH1	10.09	125.34	120.30
8	d	124	ARG	NE-CZ-NH2	-10.07	115.27	120.30
7	U	671	PHE	CB-CG-CD2	-10.06	113.76	120.80
2	D	473	PHE	CB-CG-CD1	10.06	127.84	120.80
4	J	734	TYR	CB-CG-CD1	-10.03	114.98	121.00
8	i	372	ARG	NE-CZ-NH2	-10.03	115.29	120.30
8	e	317	TYR	CB-CG-CD1	-10.02	114.99	121.00
1	C	282	PHE	CB-CG-CD2	10.00	127.80	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	X	647	TYR	CB-CG-CD1	10.00	127.00	121.00
2	N	430	TYR	CB-CG-CD2	-10.00	115.00	121.00
8	e	390	ARG	NE-CZ-NH2	-10.00	115.30	120.30
1	C	395	TYR	CB-CG-CD1	9.99	127.00	121.00
4	J	365	TYR	CB-CG-CD2	-9.99	115.00	121.00
1	A	361	ARG	NE-CZ-NH2	-9.98	115.31	120.30
8	i	135	PHE	CB-CG-CD1	-9.98	113.81	120.80
8	m	273	TYR	CB-CG-CD2	-9.97	115.02	121.00
8	l	156	ARG	NE-CZ-NH1	9.96	125.28	120.30
8	d	86	TYR	CB-CG-CD1	-9.95	115.03	121.00
9	s	58	ARG	NE-CZ-NH1	9.95	125.28	120.30
1	M	231	TYR	CB-CG-CD1	-9.94	115.03	121.00
8	k	194	ARG	NE-CZ-NH2	-9.94	115.33	120.30
1	M	867	TYR	CB-CG-CD2	-9.92	115.05	121.00
1	A	430	ARG	NE-CZ-NH2	-9.91	115.34	120.30
8	a	212	ARG	NE-CZ-NH1	-9.91	115.34	120.30
6	P	198	TYR	CB-CG-CD1	9.91	126.95	121.00
4	J	899	ARG	NE-CZ-NH2	-9.90	115.35	120.30
2	D	457	ARG	NE-CZ-NH2	9.89	125.24	120.30
8	a	120	ASP	CB-CG-OD2	-9.86	109.42	118.30
8	g	309	ARG	NE-CZ-NH2	-9.86	115.37	120.30
5	L	445	ARG	NE-CZ-NH2	-9.86	115.37	120.30
4	J	571	ARG	NE-CZ-NH1	9.84	125.22	120.30
2	O	90	ARG	NE-CZ-NH2	-9.83	115.39	120.30
8	g	172	PHE	CB-CG-CD2	9.83	127.68	120.80
8	j	245	TYR	CB-CG-CD1	-9.81	115.12	121.00
1	G	326	TYR	CB-CG-CD2	9.81	126.88	121.00
4	J	588	TYR	CB-CG-CD1	-9.80	115.12	121.00
2	B	802	ARG	NE-CZ-NH2	9.80	125.20	120.30
8	c	401	ARG	NE-CZ-NH1	9.78	125.19	120.30
4	J	321	PHE	CB-CG-CD1	-9.78	113.95	120.80
2	B	665	PHE	CB-CG-CD1	-9.78	113.96	120.80
8	e	3	ARG	NE-CZ-NH1	9.77	125.19	120.30
5	L	34	ARG	NE-CZ-NH1	9.77	125.19	120.30
8	d	40	PHE	CB-CG-CD1	9.77	127.64	120.80
8	g	161	TYR	CB-CG-CD2	-9.77	115.14	121.00
2	D	431	ARG	NE-CZ-NH1	9.76	125.18	120.30
1	E	747	PHE	CB-CG-CD1	9.75	127.62	120.80
8	f	366	TYR	CG-CD1-CE1	-9.74	113.51	121.30
1	M	522	ASP	CB-CG-OD1	9.73	127.06	118.30
8	n	206	ASP	CB-CG-OD1	9.73	127.06	118.30
2	D	473	PHE	CB-CG-CD2	-9.73	113.99	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	k	286	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	C	401	ASP	CB-CG-OD2	-9.71	109.56	118.30
1	C	396	ARG	NE-CZ-NH2	-9.70	115.45	120.30
8	n	390	ARG	NE-CZ-NH2	9.70	125.15	120.30
8	b	388	PHE	CB-CG-CD1	9.70	127.59	120.80
5	L	1688	ARG	NE-CZ-NH2	9.69	125.15	120.30
1	M	392	ARG	NE-CZ-NH1	-9.69	115.46	120.30
1	E	284	TYR	CB-CG-CD1	9.69	126.81	121.00
8	a	72	ARG	NE-CZ-NH1	9.67	125.14	120.30
2	B	831	ARG	NE-CZ-NH1	9.67	125.13	120.30
8	i	273	TYR	CB-CG-CD2	-9.66	115.20	121.00
1	E	361	ARG	NE-CZ-NH1	-9.66	115.47	120.30
8	l	341	ARG	NE-CZ-NH1	9.66	125.13	120.30
8	a	135	PHE	CB-CG-CD1	-9.66	114.04	120.80
7	X	647	TYR	CB-CG-CD2	-9.65	115.21	121.00
8	d	152	TYR	CB-CG-CD1	-9.63	115.22	121.00
1	M	549	ARG	NE-CZ-NH1	-9.63	115.49	120.30
1	E	695	TYR	CB-CG-CD2	-9.61	115.23	121.00
9	t	12	ARG	NE-CZ-NH2	-9.61	115.49	120.30
5	L	445	ARG	NE-CZ-NH1	9.59	125.10	120.30
2	F	831	ARG	NE-CZ-NH1	9.59	125.10	120.30
1	C	519	PHE	CB-CG-CD1	9.59	127.51	120.80
4	J	443	TYR	CB-CG-CD1	9.58	126.75	121.00
1	M	460	ARG	NE-CZ-NH2	-9.56	115.52	120.30
2	F	552	TYR	CB-CG-CD1	9.56	126.73	121.00
8	e	295	ARG	NE-CZ-NH2	-9.56	115.52	120.30
1	C	274	ARG	NE-CZ-NH1	9.56	125.08	120.30
8	a	225	PHE	CB-CG-CD2	-9.55	114.11	120.80
8	i	47	ARG	NE-CZ-NH2	-9.55	115.52	120.30
4	J	412	PHE	CB-CG-CD1	-9.55	114.12	120.80
1	A	302	TYR	CB-CG-CD1	-9.54	115.28	121.00
2	R	95	TYR	CB-CG-CD2	-9.54	115.28	121.00
8	h	414	PHE	CB-CG-CD1	-9.54	114.12	120.80
8	h	422	ASP	CB-CG-OD2	9.52	126.87	118.30
8	m	92	TYR	CB-CG-CD1	-9.52	115.29	121.00
2	F	480	ARG	NE-CZ-NH1	9.52	125.06	120.30
6	P	306	TYR	CB-CG-CD2	-9.52	115.29	121.00
4	J	877	ARG	NE-CZ-NH2	-9.51	115.55	120.30
8	i	53	TYR	CB-CG-CD1	-9.51	115.30	121.00
8	n	47	ARG	NE-CZ-NH2	-9.50	115.55	120.30
2	H	753	PHE	CB-CG-CD2	9.50	127.45	120.80
6	P	254	ARG	NE-CZ-NH1	-9.50	115.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	230	ARG	NE-CZ-NH1	9.49	125.05	120.30
5	L	567	ARG	NE-CZ-NH2	-9.48	115.56	120.30
7	X	668	ARG	NE-CZ-NH2	-9.47	115.56	120.30
8	k	388	PHE	CB-CG-CD2	-9.46	114.17	120.80
4	J	326	PHE	CB-CG-CD1	9.45	127.42	120.80
8	d	309	ARG	NE-CZ-NH2	-9.45	115.58	120.30
8	j	92	TYR	CB-CG-CD1	-9.44	115.33	121.00
2	Q	67	ARG	NE-CZ-NH2	-9.44	115.58	120.30
1	E	636	ARG	NE-CZ-NH1	9.43	125.01	120.30
2	N	264	PHE	CB-CG-CD2	9.43	127.40	120.80
8	k	390	ARG	NE-CZ-NH2	-9.43	115.59	120.30
8	a	339	ARG	NE-CZ-NH1	9.42	125.01	120.30
2	N	651	PHE	CB-CG-CD2	9.40	127.38	120.80
8	e	156	ARG	NE-CZ-NH2	-9.40	115.60	120.30
6	P	210	ARG	NE-CZ-NH2	-9.39	115.60	120.30
1	G	570	ASP	CB-CG-OD2	-9.39	109.85	118.30
8	j	86	TYR	CB-CG-CD2	-9.39	115.37	121.00
2	Q	103	ASP	CB-CG-OD1	9.38	126.74	118.30
3	K	313	ARG	NE-CZ-NH2	-9.37	115.62	120.30
8	i	53	TYR	CB-CG-CD2	9.37	126.62	121.00
8	j	152	TYR	CB-CG-CD1	-9.37	115.38	121.00
8	i	425	ARG	NE-CZ-NH1	-9.36	115.62	120.30
3	K	529	TYR	CB-CG-CD2	-9.35	115.39	121.00
2	N	410	MET	CG-SD-CE	-9.34	85.25	100.20
1	E	406	PHE	CB-CG-CD2	-9.34	114.26	120.80
7	V	614	PHE	CB-CG-CD1	-9.34	114.27	120.80
3	K	618	PHE	CB-CG-CD1	9.31	127.32	120.80
5	L	1419	PHE	CB-CG-CD1	-9.31	114.28	120.80
1	G	860	ARG	NE-CZ-NH1	9.31	124.95	120.30
6	P	124	PHE	CB-CG-CD1	9.31	127.32	120.80
1	G	512	LEU	CB-CG-CD1	9.31	126.82	111.00
9	t	39	ARG	NE-CZ-NH1	9.30	124.95	120.30
2	F	434	TYR	CB-CG-CD2	-9.30	115.42	121.00
3	K	206	ARG	NE-CZ-NH1	-9.29	115.66	120.30
8	c	268	PHE	CB-CG-CD1	-9.29	114.30	120.80
2	D	671	ARG	NE-CZ-NH1	9.29	124.94	120.30
8	d	156	ARG	NE-CZ-NH1	9.28	124.94	120.30
2	B	314	ARG	NE-CZ-NH2	9.27	124.94	120.30
2	B	323	PHE	CB-CG-CD2	9.26	127.28	120.80
8	h	399	ARG	NE-CZ-NH1	9.26	124.93	120.30
8	m	169	TYR	CB-CG-CD1	-9.25	115.45	121.00
8	b	124	ARG	NE-CZ-NH1	-9.25	115.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	R	66	ARG	NE-CZ-NH2	-9.25	115.68	120.30
2	B	812	ARG	NE-CZ-NH1	9.24	124.92	120.30
8	b	390	ARG	NE-CZ-NH1	9.23	124.91	120.30
2	H	812	ARG	NE-CZ-NH1	9.22	124.91	120.30
2	H	572	PHE	CB-CG-CD2	-9.22	114.35	120.80
1	A	617	PHE	CB-CG-CD1	9.22	127.25	120.80
2	F	641	TYR	CB-CG-CD1	-9.21	115.48	121.00
8	m	433	ASP	CB-CG-OD2	9.20	126.58	118.30
1	G	827	PHE	CB-CG-CD1	9.20	127.24	120.80
2	H	751	ASP	CB-CG-OD1	9.18	126.56	118.30
2	F	411	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	M	827	PHE	CB-CG-CD1	9.17	127.22	120.80
8	h	372	ARG	NE-CZ-NH1	9.17	124.88	120.30
1	A	728	PHE	CB-CG-CD2	9.16	127.21	120.80
8	c	343	ARG	NE-CZ-NH2	-9.16	115.72	120.30
2	B	277	ASP	CB-CG-OD2	-9.16	110.06	118.30
8	k	265	ARG	NE-CZ-NH2	-9.15	115.72	120.30
8	d	208	THR	CA-CB-CG2	-9.15	99.60	112.40
1	G	728	PHE	CB-CG-CD2	-9.14	114.40	120.80
1	C	275	PHE	CB-CG-CD1	-9.14	114.40	120.80
2	F	564	TYR	CB-CG-CD1	-9.14	115.52	121.00
3	K	91	ARG	NE-CZ-NH1	9.14	124.87	120.30
3	I	320	PHE	CB-CG-CD2	-9.14	114.41	120.80
2	N	537	TYR	CB-CG-CD1	9.14	126.48	121.00
6	P	39	ARG	NE-CZ-NH2	-9.13	115.73	120.30
2	N	430	TYR	CB-CG-CD1	9.13	126.48	121.00
2	D	538	PHE	CB-CG-CD2	9.12	127.18	120.80
2	N	310	ARG	NE-CZ-NH2	-9.11	115.75	120.30
8	f	47	ARG	NE-CZ-NH1	9.11	124.85	120.30
2	D	365	ARG	NE-CZ-NH1	9.11	124.85	120.30
2	N	779	ASP	CB-CG-OD1	9.10	126.49	118.30
2	D	335	TYR	CB-CG-CD1	-9.10	115.54	121.00
1	E	430	ARG	NE-CZ-NH2	-9.10	115.75	120.30
6	P	210	ARG	NE-CZ-NH1	9.09	124.85	120.30
5	L	1656	TYR	CB-CG-CD2	-9.09	115.55	121.00
8	a	124	ARG	NE-CZ-NH1	-9.06	115.77	120.30
4	J	326	PHE	CB-CG-CD2	-9.05	114.47	120.80
2	F	371	PHE	CB-CG-CD1	-9.04	114.47	120.80
3	K	320	PHE	CB-CG-CD2	9.04	127.13	120.80
5	L	1503	TYR	CB-CG-CD2	-9.04	115.58	121.00
5	L	1649	PHE	CB-CG-CD1	-9.04	114.47	120.80
5	L	1465	TYR	CB-CG-CD2	9.04	126.42	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	o	12	ARG	NE-CZ-NH1	9.04	124.82	120.30
3	I	16	ILE	CB-CG1-CD1	9.04	139.20	113.90
8	g	244	ARG	NE-CZ-NH2	-9.04	115.78	120.30
1	M	476	TYR	CB-CG-CD1	-9.03	115.58	121.00
2	R	79	ARG	NE-CZ-NH1	9.02	124.81	120.30
3	I	372	PHE	CB-CG-CD2	9.02	127.11	120.80
1	G	501	PHE	CB-CG-CD1	-9.01	114.49	120.80
9	s	23	ARG	NE-CZ-NH1	9.01	124.81	120.30
8	m	309	ARG	NE-CZ-NH1	9.01	124.80	120.30
8	c	317	TYR	CB-CG-CD2	-9.00	115.60	121.00
8	i	409	ARG	NE-CZ-NH2	-8.98	115.81	120.30
2	D	564	TYR	CB-CG-CD1	8.98	126.39	121.00
2	F	720	TYR	CB-CG-CD2	-8.97	115.62	121.00
8	h	86	TYR	CB-CG-CD2	-8.97	115.62	121.00
1	E	252	ASP	CB-CG-OD2	-8.96	110.24	118.30
8	j	401	ARG	NE-CZ-NH1	8.96	124.78	120.30
5	L	1685	PHE	CB-CG-CD2	-8.94	114.54	120.80
2	H	623	ARG	NE-CZ-NH2	-8.94	115.83	120.30
5	L	1485	TYR	CB-CG-CD1	-8.94	115.64	121.00
8	n	169	TYR	CB-CG-CD1	-8.93	115.64	121.00
2	B	314	ARG	NE-CZ-NH1	-8.93	115.84	120.30
2	F	802	ARG	NE-CZ-NH2	8.92	124.76	120.30
2	Q	49	ARG	NE-CZ-NH1	8.92	124.76	120.30
2	Q	105	ARG	NE-CZ-NH2	-8.91	115.84	120.30
8	a	341	ARG	NE-CZ-NH1	8.91	124.75	120.30
8	j	296	ARG	NE-CZ-NH1	8.90	124.75	120.30
8	n	362	ARG	NE-CZ-NH1	8.89	124.75	120.30
2	D	390	ARG	NE-CZ-NH2	-8.89	115.86	120.30
3	K	184	TYR	CB-CG-CD1	-8.88	115.67	121.00
6	P	198	TYR	CB-CG-CD2	-8.88	115.67	121.00
8	b	286	ARG	NE-CZ-NH2	-8.88	115.86	120.30
8	n	161	TYR	CB-CG-CD1	8.88	126.33	121.00
2	B	430	TYR	CB-CG-CD2	8.87	126.32	121.00
1	E	867	TYR	CZ-CE2-CD2	-8.87	111.82	119.80
3	K	557	ARG	NE-CZ-NH2	-8.87	115.87	120.30
4	J	242	TRP	CG-CD1-NE1	8.87	118.97	110.10
8	c	161	TYR	CB-CG-CD2	8.87	126.32	121.00
8	k	3	ARG	NE-CZ-NH2	-8.86	115.87	120.30
7	V	621	ASP	CB-CG-OD1	8.86	126.27	118.30
1	E	365	TYR	CB-CG-CD2	8.85	126.31	121.00
2	H	751	ASP	CB-CG-OD2	-8.85	110.33	118.30
1	A	403	TYR	CB-CG-CD1	-8.85	115.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	j	265	ARG	NE-CZ-NH1	8.85	124.72	120.30
1	C	652	ARG	NE-CZ-NH1	8.84	124.72	120.30
2	H	264	PHE	CB-CG-CD2	8.84	126.99	120.80
8	m	3	ARG	NE-CZ-NH2	-8.84	115.88	120.30
8	d	311	ARG	NE-CZ-NH1	8.83	124.72	120.30
7	U	671	PHE	CB-CG-CD1	8.81	126.97	120.80
8	i	399	ARG	NE-CZ-NH1	-8.81	115.90	120.30
2	D	661	ARG	NE-CZ-NH2	-8.80	115.90	120.30
2	S	50	ASP	N-CA-CB	8.79	126.43	110.60
2	N	402	TYR	CB-CG-CD2	-8.79	115.73	121.00
2	N	574	ARG	NE-CZ-NH1	8.78	124.69	120.30
2	H	562	ARG	NE-CZ-NH2	-8.78	115.91	120.30
8	h	341	ARG	NE-CZ-NH2	-8.78	115.91	120.30
2	N	586	ARG	NE-CZ-NH1	8.77	124.69	120.30
2	F	592	TYR	CB-CG-CD2	-8.77	115.74	121.00
7	V	666	ARG	NE-CZ-NH1	8.76	124.68	120.30
4	J	703	TYR	CB-CG-CD2	-8.76	115.75	121.00
1	M	675	PHE	CB-CG-CD1	-8.76	114.67	120.80
1	E	646	TYR	CB-CG-CD1	-8.75	115.75	121.00
8	h	86	TYR	CB-CG-CD1	8.75	126.25	121.00
1	G	403	TYR	CZ-CE2-CD2	8.74	127.67	119.80
5	L	224	ARG	NE-CZ-NH1	8.74	124.67	120.30
8	i	124	ARG	NE-CZ-NH1	-8.72	115.94	120.30
8	d	393	ARG	NE-CZ-NH1	-8.72	115.94	120.30
8	b	296	ARG	NE-CZ-NH1	8.72	124.66	120.30
4	J	508	TYR	CB-CG-CD2	8.72	126.23	121.00
1	M	396	ARG	NE-CZ-NH1	8.72	124.66	120.30
2	F	723	PHE	CB-CG-CD2	8.71	126.90	120.80
5	L	1363	MET	CG-SD-CE	-8.71	86.26	100.20
8	g	46	ASP	CB-CG-OD2	8.71	126.14	118.30
2	N	434	TYR	CB-CG-CD1	8.70	126.22	121.00
2	R	64	ARG	NE-CZ-NH2	8.70	124.65	120.30
1	C	860	ARG	NE-CZ-NH2	-8.70	115.95	120.30
1	C	230	ARG	NE-CZ-NH1	8.69	124.65	120.30
3	K	474	TYR	CB-CG-CD2	-8.69	115.78	121.00
4	J	492	ARG	NE-CZ-NH1	8.69	124.64	120.30
2	H	784	PHE	CB-CG-CD1	8.69	126.88	120.80
6	P	228	ALA	N-CA-CB	8.69	122.26	110.10
2	H	586	ARG	NE-CZ-NH1	8.68	124.64	120.30
8	a	51	PHE	CB-CG-CD1	8.68	126.88	120.80
8	j	399	ARG	NE-CZ-NH1	-8.68	115.96	120.30
2	F	431	ARG	NE-CZ-NH1	8.67	124.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	j	296	ARG	NE-CZ-NH2	-8.67	115.97	120.30
2	D	812	ARG	NE-CZ-NH2	-8.66	115.97	120.30
8	e	339	ARG	NE-CZ-NH1	8.65	124.63	120.30
8	h	212	ARG	NE-CZ-NH2	-8.65	115.98	120.30
2	N	749	ALA	N-CA-CB	8.64	122.20	110.10
2	N	563	ARG	NE-CZ-NH2	-8.64	115.98	120.30
4	J	678	PHE	CB-CG-CD2	-8.63	114.76	120.80
8	f	390	ARG	NE-CZ-NH1	-8.63	115.99	120.30
8	g	225	PHE	CB-CG-CD2	-8.61	114.77	120.80
1	G	526	PHE	CB-CG-CD2	8.60	126.82	120.80
1	A	867	TYR	CB-CG-CD2	-8.60	115.84	121.00
4	J	502	ASP	CB-CG-OD1	8.59	126.03	118.30
5	L	410	ARG	NE-CZ-NH1	8.58	124.59	120.30
2	N	605	ARG	NE-CZ-NH1	8.58	124.59	120.30
2	B	430	TYR	CB-CG-CD1	-8.58	115.85	121.00
1	E	230	ARG	NE-CZ-NH1	8.58	124.59	120.30
1	G	747	PHE	CB-CG-CD2	-8.58	114.80	120.80
1	C	730	ASP	CB-CG-OD2	-8.57	110.58	118.30
7	V	615	ARG	NE-CZ-NH2	-8.57	116.02	120.30
8	f	139	HIS	CA-CB-CG	8.57	128.17	113.60
8	c	186	TYR	CB-CG-CD1	-8.57	115.86	121.00
1	M	522	ASP	CB-CG-OD2	-8.56	110.59	118.30
3	I	606	ARG	NE-CZ-NH2	-8.56	116.02	120.30
2	F	653	ARG	NE-CZ-NH1	-8.56	116.02	120.30
1	E	641	PHE	CB-CG-CD2	8.55	126.79	120.80
3	I	313	ARG	NE-CZ-NH2	8.55	124.58	120.30
1	C	296	ARG	NE-CZ-NH2	-8.55	116.03	120.30
1	G	682	ARG	NE-CZ-NH2	-8.53	116.03	120.30
4	J	962	ARG	NE-CZ-NH1	-8.53	116.03	120.30
2	F	314	ARG	NE-CZ-NH2	-8.52	116.04	120.30
1	G	867	TYR	CG-CD2-CE2	-8.52	114.49	121.30
2	H	364	ARG	NE-CZ-NH1	8.51	124.55	120.30
8	c	401	ARG	NE-CZ-NH2	-8.51	116.05	120.30
1	E	837	ASP	CB-CG-OD2	-8.50	110.65	118.30
2	F	847	ARG	NE-CZ-NH2	8.50	124.55	120.30
2	F	723	PHE	CB-CG-CD1	-8.49	114.85	120.80
8	n	186	TYR	CB-CG-CD1	-8.49	115.90	121.00
1	E	526	PHE	CB-CG-CD1	-8.49	114.86	120.80
1	G	455	TYR	CB-CG-CD1	8.48	126.09	121.00
8	n	372	ARG	NE-CZ-NH1	8.48	124.54	120.30
8	m	40	PHE	CB-CG-CD2	-8.48	114.86	120.80
1	C	470	ASP	CB-CG-OD1	8.47	125.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
7	V	620	ARG	NE-CZ-NH2	-8.47	116.06	120.30
8	f	412	ASP	CB-CG-OD2	-8.47	110.67	118.30
1	A	361	ARG	NE-CZ-NH1	8.46	124.53	120.30
5	L	44	TYR	CB-CG-CD2	8.45	126.07	121.00
4	J	410	ARG	NE-CZ-NH1	-8.44	116.08	120.30
1	E	261	ARG	NE-CZ-NH2	-8.44	116.08	120.30
8	i	3	ARG	NE-CZ-NH2	-8.44	116.08	120.30
2	H	316	PHE	CB-CG-CD2	8.44	126.71	120.80
8	c	21	PHE	CB-CG-CD1	-8.44	114.89	120.80
8	l	399	ARG	NE-CZ-NH1	-8.43	116.08	120.30
8	n	47	ARG	NE-CZ-NH1	8.43	124.52	120.30
8	j	124	ARG	NE-CZ-NH2	-8.43	116.09	120.30
2	B	835	PHE	CB-CG-CD1	8.42	126.69	120.80
2	F	659	TYR	CB-CG-CD1	8.41	126.05	121.00
5	L	34	ARG	NE-CZ-NH2	-8.41	116.09	120.30
1	C	684	ARG	NE-CZ-NH2	8.40	124.50	120.30
2	S	19	ARG	NE-CZ-NH1	8.39	124.50	120.30
8	f	339	ARG	NE-CZ-NH1	8.39	124.50	120.30
2	B	251	ARG	NE-CZ-NH1	8.39	124.49	120.30
2	N	831	ARG	NE-CZ-NH1	8.38	124.49	120.30
2	B	571	ASP	CB-CG-OD1	8.37	125.83	118.30
8	m	212	ARG	NE-CZ-NH1	8.37	124.49	120.30
5	L	44	TYR	CB-CG-CD1	-8.37	115.98	121.00
8	a	366	TYR	CB-CG-CD2	-8.37	115.98	121.00
8	d	92	TYR	N-CA-CB	8.36	125.65	110.60
8	e	343	ARG	NE-CZ-NH1	-8.36	116.12	120.30
2	D	720	TYR	CB-CG-CD2	-8.35	115.99	121.00
2	H	498	ASP	CB-CG-OD2	-8.33	110.80	118.30
8	h	3	ARG	NE-CZ-NH2	-8.33	116.13	120.30
2	H	653	ARG	NE-CZ-NH1	-8.33	116.14	120.30
1	E	619	TYR	CB-CG-CD2	-8.32	116.01	121.00
8	i	292	ASP	CB-CG-OD2	-8.32	110.81	118.30
8	b	390	ARG	NE-CZ-NH2	-8.31	116.14	120.30
8	j	435	TYR	CB-CG-CD1	8.31	125.99	121.00
3	K	137	MET	CG-SD-CE	-8.31	86.91	100.20
8	g	194	ARG	NE-CZ-NH2	-8.31	116.15	120.30
8	h	348	PHE	CB-CG-CD1	-8.31	114.98	120.80
8	d	194	ARG	NE-CZ-NH2	-8.30	116.15	120.30
5	L	1548	TYR	CB-CG-CD2	8.30	125.98	121.00
6	P	288	ASP	CB-CG-OD1	-8.30	110.83	118.30
4	J	365	TYR	CB-CG-CD1	8.30	125.98	121.00
2	D	611	PHE	CB-CG-CD2	8.30	126.61	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	623	ARG	NE-CZ-NH2	-8.29	116.15	120.30
2	F	651	PHE	CB-CG-CD1	8.29	126.60	120.80
8	f	268	PHE	CB-CG-CD2	8.29	126.60	120.80
8	l	311	ARG	NE-CZ-NH2	-8.29	116.16	120.30
8	m	92	TYR	CB-CG-CD2	8.28	125.97	121.00
2	F	376	ARG	NE-CZ-NH1	-8.28	116.16	120.30
2	H	847	ARG	NE-CZ-NH1	-8.28	116.16	120.30
2	H	257	PHE	CB-CG-CD1	-8.28	115.01	120.80
1	G	377	TYR	CB-CG-CD2	-8.27	116.04	121.00
8	e	311	ARG	NE-CZ-NH1	-8.27	116.17	120.30
9	o	59	ARG	NE-CZ-NH2	-8.27	116.17	120.30
5	L	74	MET	CG-SD-CE	-8.27	86.97	100.20
9	s	12	ARG	NE-CZ-NH2	8.27	124.44	120.30
2	B	434	TYR	CB-CG-CD1	8.27	125.96	121.00
8	l	217	ARG	NE-CZ-NH2	-8.26	116.17	120.30
1	E	325	PHE	CB-CG-CD2	8.25	126.58	120.80
2	N	264	PHE	CB-CG-CD1	-8.25	115.02	120.80
2	B	605	ARG	NE-CZ-NH2	8.25	124.42	120.30
8	l	366	TYR	CB-CG-CD1	8.25	125.95	121.00
3	I	85	TYR	CB-CG-CD2	8.24	125.95	121.00
6	P	206	ARG	NE-CZ-NH1	8.23	124.42	120.30
8	l	425	ARG	NE-CZ-NH1	8.23	124.42	120.30
2	F	409	TYR	CG-CD1-CE1	-8.23	114.72	121.30
8	j	124	ARG	NE-CZ-NH1	8.23	124.41	120.30
2	H	661	ARG	NE-CZ-NH1	8.22	124.41	120.30
8	h	435	TYR	CB-CG-CD2	-8.22	116.07	121.00
8	e	317	TYR	CG-CD1-CE1	-8.22	114.72	121.30
2	F	572	PHE	CB-CG-CD2	8.21	126.55	120.80
8	i	309	ARG	NE-CZ-NH1	8.21	124.40	120.30
8	l	217	ARG	NE-CZ-NH1	8.21	124.41	120.30
2	B	574	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	M	377	TYR	CB-CG-CD2	8.20	125.92	121.00
2	N	564	TYR	CB-CG-CD2	8.20	125.92	121.00
8	b	265	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	A	235	GLN	CA-CB-CG	8.20	131.43	113.40
7	V	646	ARG	NE-CZ-NH2	-8.19	116.20	120.30
4	J	999	ARG	NE-CZ-NH1	8.19	124.39	120.30
2	H	498	ASP	CB-CG-OD1	8.18	125.67	118.30
8	b	152	TYR	CG-CD1-CE1	-8.18	114.75	121.30
8	b	292	ASP	CB-CG-OD1	-8.18	110.94	118.30
2	N	574	ARG	NE-CZ-NH2	-8.17	116.21	120.30
8	h	286	ARG	NE-CZ-NH2	-8.17	116.22	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	l	268	PHE	CB-CG-CD1	8.17	126.52	120.80
4	J	503	PHE	CB-CG-CD2	-8.16	115.08	120.80
1	M	530	PHE	CB-CG-CD2	-8.15	115.09	120.80
2	S	90	ARG	NE-CZ-NH2	-8.14	116.23	120.30
8	g	52	PHE	CB-CG-CD1	-8.14	115.10	120.80
8	k	265	ARG	NE-CZ-NH1	8.14	124.37	120.30
8	k	362	ARG	NE-CZ-NH2	8.14	124.37	120.30
8	k	418	PHE	CB-CG-CD2	-8.14	115.11	120.80
7	W	661	ARG	NE-CZ-NH1	8.13	124.36	120.30
1	C	289	HIS	CA-CB-CG	8.12	127.41	113.60
8	l	212	ARG	NE-CZ-NH1	8.12	124.36	120.30
3	K	618	PHE	CB-CG-CD2	-8.12	115.11	120.80
2	R	79	ARG	NE-CZ-NH2	-8.12	116.24	120.30
2	F	434	TYR	CG-CD1-CE1	-8.10	114.82	121.30
2	H	885	TYR	CB-CG-CD1	-8.10	116.14	121.00
8	i	295	ARG	NE-CZ-NH1	-8.10	116.25	120.30
1	A	242	SER	N-CA-CB	8.09	122.64	110.50
5	L	506	TYR	CB-CG-CD1	8.09	125.85	121.00
2	F	529	PHE	CB-CG-CD2	-8.09	115.14	120.80
1	G	684	ARG	NE-CZ-NH1	8.09	124.34	120.30
2	N	805	PHE	CB-CG-CD1	-8.08	115.14	120.80
8	k	366	TYR	CB-CG-CD1	-8.07	116.16	121.00
8	e	408	PHE	CB-CG-CD1	-8.07	115.15	120.80
1	C	442	LEU	CB-CG-CD1	8.07	124.71	111.00
8	h	393	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	M	493	TYR	CD1-CE1-CZ	8.05	127.04	119.80
1	C	549	ARG	NE-CZ-NH2	-8.05	116.28	120.30
8	l	372	ARG	NH1-CZ-NH2	-8.04	110.55	119.40
5	L	1691	PHE	CB-CG-CD2	-8.04	115.17	120.80
1	C	658	TRP	CB-CG-CD2	-8.04	116.15	126.60
8	e	295	ARG	NE-CZ-NH1	8.03	124.31	120.30
8	h	362	ARG	NH1-CZ-NH2	-8.03	110.57	119.40
1	G	863	PHE	CB-CG-CD2	-8.02	115.19	120.80
5	L	1376	TYR	CB-CG-CD1	8.01	125.81	121.00
8	i	59	HIS	N-CA-C	-8.01	89.36	111.00
2	N	885	TYR	CB-CG-CD1	-8.01	116.19	121.00
1	G	532	ASP	CB-CG-OD1	8.00	125.50	118.30
3	K	320	PHE	CB-CG-CD1	-8.00	115.20	120.80
2	H	562	ARG	NE-CZ-NH1	8.00	124.30	120.30
8	l	418	PHE	CB-CG-CD2	8.00	126.40	120.80
8	a	51	PHE	CB-CG-CD2	-7.99	115.20	120.80
8	n	393	ARG	NH1-CZ-NH2	-7.99	110.61	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	641	TYR	CG-CD1-CE1	-7.98	114.92	121.30
8	f	362	ARG	NE-CZ-NH2	7.98	124.29	120.30
1	C	619	TYR	CG-CD1-CE1	7.98	127.68	121.30
2	D	880	ASP	CB-CG-OD2	-7.96	111.14	118.30
8	b	295	ARG	NH1-CZ-NH2	-7.96	110.64	119.40
8	e	86	TYR	CB-CG-CD2	-7.96	116.22	121.00
1	M	513	ARG	NE-CZ-NH1	7.95	124.28	120.30
8	n	295	ARG	NE-CZ-NH2	-7.95	116.33	120.30
8	b	425	ARG	NE-CZ-NH1	7.95	124.27	120.30
9	o	31	MET	CG-SD-CE	-7.94	87.49	100.20
2	H	409	TYR	CG-CD2-CE2	-7.94	114.95	121.30
8	n	172	PHE	CB-CG-CD2	7.94	126.36	120.80
3	I	331	ARG	NE-CZ-NH1	7.94	124.27	120.30
2	B	674	TYR	CB-CG-CD2	-7.94	116.24	121.00
1	C	282	PHE	CB-CG-CD1	-7.93	115.25	120.80
1	G	471	ALA	N-CA-CB	7.93	121.21	110.10
2	F	805	PHE	CB-CG-CD1	7.93	126.35	120.80
1	M	608	ALA	N-CA-CB	7.93	121.20	110.10
7	X	666	ARG	NE-CZ-NH2	7.93	124.27	120.30
8	l	348	PHE	CB-CG-CD1	-7.92	115.25	120.80
2	F	376	ARG	NE-CZ-NH2	7.92	124.26	120.30
1	E	396	ARG	NE-CZ-NH2	7.91	124.26	120.30
8	i	329	ASP	CB-CG-OD2	-7.91	111.18	118.30
2	D	274	TYR	CB-CG-CD1	-7.91	116.25	121.00
2	N	463	TYR	CB-CG-CD2	-7.91	116.25	121.00
3	K	557	ARG	NE-CZ-NH1	7.91	124.25	120.30
2	B	428	PHE	CB-CG-CD2	-7.91	115.27	120.80
8	e	245	TYR	CB-CG-CD2	-7.90	116.26	121.00
8	m	217	ARG	NE-CZ-NH1	7.90	124.25	120.30
2	H	335	TYR	CG-CD2-CE2	-7.89	114.98	121.30
8	e	119	PHE	CB-CG-CD1	-7.89	115.27	120.80
1	A	261	ARG	NE-CZ-NH1	7.89	124.25	120.30
8	f	93	LEU	CB-CG-CD2	7.89	124.41	111.00
3	I	365	ARG	NE-CZ-NH2	-7.89	116.36	120.30
8	g	343	ARG	NE-CZ-NH2	-7.88	116.36	120.30
8	h	47	ARG	NE-CZ-NH2	7.88	124.24	120.30
4	J	492	ARG	NE-CZ-NH2	-7.88	116.36	120.30
8	n	169	TYR	CB-CG-CD2	7.88	125.73	121.00
2	F	552	TYR	CG-CD2-CE2	7.88	127.60	121.30
6	P	255	PHE	CB-CG-CD2	-7.88	115.29	120.80
2	N	768	ARG	NE-CZ-NH2	7.87	124.24	120.30
8	h	156	ARG	NE-CZ-NH2	7.87	124.24	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	695	TYR	CB-CG-CD2	-7.87	116.28	121.00
2	Q	74	PHE	CB-CG-CD1	-7.87	115.29	120.80
8	g	372	ARG	NE-CZ-NH2	7.87	124.23	120.30
8	g	60	TYR	CB-CG-CD1	7.86	125.71	121.00
2	N	364	ARG	NE-CZ-NH1	7.85	124.23	120.30
2	B	411	ARG	NE-CZ-NH1	-7.85	116.37	120.30
8	e	72	ARG	NH1-CZ-NH2	-7.85	110.77	119.40
1	A	491	TYR	CB-CG-CD1	-7.85	116.29	121.00
5	L	1376	TYR	CB-CG-CD2	-7.85	116.29	121.00
8	b	19	PHE	CB-CG-CD2	-7.84	115.31	120.80
8	c	296	ARG	NE-CZ-NH2	-7.84	116.38	120.30
8	f	159	ASP	CB-CG-OD1	7.84	125.35	118.30
8	f	393	ARG	NE-CZ-NH2	7.84	124.22	120.30
1	E	493	TYR	CB-CG-CD2	-7.83	116.30	121.00
1	A	230	ARG	NE-CZ-NH2	-7.83	116.39	120.30
8	l	433	ASP	CB-CG-OD2	-7.83	111.26	118.30
8	i	329	ASP	CB-CG-OD1	7.82	125.34	118.30
1	M	679	PHE	CB-CG-CD2	7.81	126.27	120.80
7	U	668	ARG	NE-CZ-NH2	7.81	124.20	120.30
8	m	317	TYR	CG-CD1-CE1	-7.81	115.05	121.30
1	C	757	PHE	CB-CG-CD1	-7.80	115.34	120.80
5	L	1419	PHE	CB-CG-CD2	7.80	126.26	120.80
2	B	873	ARG	NE-CZ-NH2	7.80	124.20	120.30
2	N	562	ARG	NE-CZ-NH1	7.80	124.20	120.30
8	c	68	ASP	CB-CG-OD2	-7.80	111.28	118.30
8	h	401	ARG	NE-CZ-NH2	7.80	124.20	120.30
7	W	633	PHE	CB-CG-CD2	-7.79	115.34	120.80
2	S	19	ARG	NE-CZ-NH2	-7.79	116.40	120.30
7	V	647	TYR	CB-CG-CD1	7.79	125.67	121.00
1	C	274	ARG	NE-CZ-NH2	-7.79	116.41	120.30
1	A	493	TYR	CB-CG-CD1	-7.77	116.34	121.00
1	M	728	PHE	CB-CG-CD2	7.77	126.24	120.80
7	V	613	ASP	CB-CG-OD1	7.77	125.29	118.30
2	B	277	ASP	CB-CG-OD1	7.76	125.29	118.30
2	B	723	PHE	CB-CG-CD2	7.76	126.23	120.80
8	b	273	TYR	CB-CG-CD1	7.76	125.66	121.00
8	f	152	TYR	CB-CG-CD1	-7.76	116.34	121.00
8	j	156	ARG	NE-CZ-NH2	7.76	124.18	120.30
8	g	296	ARG	NE-CZ-NH2	7.76	124.18	120.30
8	h	127	ASP	CB-CG-OD1	-7.75	111.33	118.30
8	i	249	MET	CG-SD-CE	7.75	112.60	100.20
1	M	867	TYR	CB-CG-CD1	7.75	125.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	Q	19	ARG	NE-CZ-NH2	-7.75	116.43	120.30
3	K	529	TYR	CB-CG-CD1	7.74	125.65	121.00
8	e	401	ARG	NE-CZ-NH1	7.74	124.17	120.30
8	k	393	ARG	NE-CZ-NH1	7.74	124.17	120.30
5	L	1427	THR	CA-CB-CG2	-7.73	101.58	112.40
8	e	328	VAL	CA-CB-CG1	7.73	122.50	110.90
1	A	863	PHE	CB-CG-CD2	-7.73	115.39	120.80
2	Q	64	ARG	NE-CZ-NH1	7.73	124.16	120.30
2	B	651	PHE	CB-CG-CD1	7.72	126.21	120.80
2	N	669	ALA	N-CA-CB	7.72	120.92	110.10
2	D	653	ARG	NE-CZ-NH1	7.72	124.16	120.30
2	F	428	PHE	CB-CG-CD2	-7.72	115.40	120.80
1	E	325	PHE	CB-CG-CD1	-7.71	115.40	120.80
8	i	265	ARG	NE-CZ-NH1	7.71	124.16	120.30
8	k	273	TYR	CB-CG-CD1	7.70	125.62	121.00
5	L	444	TYR	CB-CG-CD1	7.70	125.62	121.00
4	J	926	TYR	CB-CG-CD1	-7.69	116.39	121.00
8	a	244	ARG	NE-CZ-NH1	7.69	124.15	120.30
2	F	805	PHE	CB-CG-CD2	-7.68	115.42	120.80
1	G	646	TYR	CB-CG-CD2	7.68	125.61	121.00
8	m	409	ARG	NE-CZ-NH1	-7.68	116.46	120.30
8	n	295	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	H	308	ASP	CB-CG-OD2	7.67	125.21	118.30
2	H	538	PHE	CB-CG-CD1	7.67	126.17	120.80
1	C	570	ASP	CB-CG-OD2	-7.67	111.40	118.30
8	f	341	ARG	NE-CZ-NH1	-7.67	116.46	120.30
7	W	666	ARG	NE-CZ-NH2	-7.67	116.47	120.30
1	A	460	ARG	NE-CZ-NH1	7.67	124.13	120.30
8	n	248	TYR	CB-CG-CD1	7.67	125.60	121.00
2	N	862	VAL	CA-CB-CG2	-7.66	99.40	110.90
8	c	135	PHE	CB-CG-CD1	7.66	126.17	120.80
2	H	522	PHE	CB-CG-CD1	-7.66	115.44	120.80
4	J	501	ARG	NE-CZ-NH1	-7.66	116.47	120.30
1	C	831	PHE	CB-CG-CD2	-7.66	115.44	120.80
1	G	571	ASP	CB-CG-OD1	7.66	125.19	118.30
1	C	460	ARG	NE-CZ-NH2	-7.65	116.48	120.30
3	I	58	PHE	CB-CG-CD1	-7.65	115.45	120.80
8	l	135	PHE	CB-CG-CD2	-7.65	115.45	120.80
3	I	606	ARG	NE-CZ-NH1	7.65	124.12	120.30
2	B	334	TYR	CB-CG-CD2	-7.64	116.41	121.00
7	W	647	TYR	CB-CG-CD2	-7.64	116.41	121.00
4	J	702	MET	CG-SD-CE	-7.64	87.97	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	j	343	ARG	NE-CZ-NH1	7.64	124.12	120.30
8	g	286	ARG	NE-CZ-NH2	-7.63	116.48	120.30
1	E	486	ARG	NE-CZ-NH1	-7.63	116.49	120.30
1	M	428	ASP	CB-CG-OD2	-7.63	111.43	118.30
2	H	546	ASP	CB-CG-OD2	-7.62	111.44	118.30
2	N	719	TYR	CB-CG-CD2	-7.62	116.43	121.00
4	J	764	ARG	NE-CZ-NH2	7.61	124.11	120.30
9	r	12	ARG	NE-CZ-NH2	-7.61	116.50	120.30
8	m	156	ARG	NE-CZ-NH1	7.61	124.10	120.30
8	l	92	TYR	CB-CG-CD1	7.61	125.56	121.00
2	B	334	TYR	CB-CG-CD1	7.60	125.56	121.00
1	E	388	ASP	CB-CG-OD2	-7.60	111.46	118.30
8	n	72	ARG	NE-CZ-NH1	7.60	124.10	120.30
1	C	688	PHE	CB-CG-CD1	7.60	126.12	120.80
8	e	160	ARG	NE-CZ-NH1	7.59	124.10	120.30
8	l	390	ARG	NE-CZ-NH2	-7.59	116.50	120.30
8	k	286	ARG	NE-CZ-NH2	-7.59	116.50	120.30
1	E	403	TYR	CA-CB-CG	-7.59	98.98	113.40
5	L	1609	ALA	N-CA-CB	7.59	120.72	110.10
6	P	169	TYR	CB-CG-CD1	-7.59	116.45	121.00
8	d	263	THR	CA-CB-CG2	7.58	123.02	112.40
8	e	108	PHE	CB-CG-CD1	-7.58	115.49	120.80
6	P	256	ARG	NE-CZ-NH1	-7.58	116.51	120.30
9	q	39	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	E	261	ARG	NE-CZ-NH1	7.58	124.09	120.30
2	N	572	PHE	CB-CG-CD2	7.57	126.10	120.80
2	F	563	ARG	NE-CZ-NH2	-7.57	116.52	120.30
2	B	423	TYR	CG-CD1-CE1	-7.57	115.25	121.30
6	P	199	SER	N-CA-CB	7.57	121.85	110.50
8	j	225	PHE	CB-CG-CD2	-7.57	115.50	120.80
8	c	161	TYR	CB-CG-CD1	-7.56	116.46	121.00
3	I	54	ARG	NE-CZ-NH2	-7.56	116.52	120.30
2	F	792	TYR	CB-CG-CD2	-7.56	116.47	121.00
2	F	529	PHE	CB-CG-CD1	7.55	126.09	120.80
8	j	418	PHE	CB-CG-CD1	-7.55	115.51	120.80
8	b	170	SER	N-CA-CB	7.55	121.82	110.50
8	h	200	ASP	CB-CG-OD2	7.55	125.09	118.30
8	l	104	TRP	CB-CG-CD1	-7.55	117.19	127.00
8	m	19	PHE	CB-CG-CD1	-7.54	115.52	120.80
8	i	409	ARG	NE-CZ-NH1	7.54	124.07	120.30
2	F	592	TYR	CB-CG-CD1	7.54	125.52	121.00
6	P	62	ARG	NE-CZ-NH2	-7.54	116.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	396	PHE	CB-CG-CD2	-7.54	115.52	120.80
1	C	831	PHE	CB-CG-CD1	7.54	126.08	120.80
8	i	217	ARG	NE-CZ-NH1	7.53	124.06	120.30
3	I	320	PHE	CB-CG-CD1	7.53	126.07	120.80
2	N	310	ARG	NE-CZ-NH1	7.53	124.06	120.30
2	D	511	SER	N-CA-CB	7.51	121.77	110.50
1	E	431	TYR	CD1-CE1-CZ	-7.51	113.04	119.80
1	C	682	ARG	NE-CZ-NH2	7.51	124.06	120.30
3	I	200	TYR	CB-CG-CD1	-7.51	116.49	121.00
8	n	396	ASP	CB-CG-OD2	-7.50	111.55	118.30
2	F	364	ARG	NE-CZ-NH1	7.50	124.05	120.30
3	I	55	PHE	CB-CG-CD2	-7.50	115.55	120.80
7	X	633	PHE	CB-CG-CD2	-7.50	115.55	120.80
8	f	268	PHE	CB-CG-CD1	-7.50	115.55	120.80
1	A	831	PHE	CB-CG-CD1	-7.49	115.56	120.80
2	F	445	PHE	CB-CG-CD2	-7.49	115.56	120.80
8	c	310	ASP	CB-CG-OD1	7.49	125.04	118.30
2	F	445	PHE	CB-CG-CD1	7.49	126.04	120.80
8	m	216	ASP	CB-CG-OD2	-7.48	111.56	118.30
3	I	89	PHE	CB-CG-CD1	7.48	126.04	120.80
3	K	170	SER	N-CA-CB	7.48	121.72	110.50
5	L	1400	ARG	NE-CZ-NH1	7.48	124.04	120.30
5	L	573	TYR	CB-CG-CD2	-7.47	116.52	121.00
2	B	385	ASP	CB-CG-OD1	7.47	125.02	118.30
2	Q	34	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	G	455	TYR	CB-CG-CD2	-7.47	116.52	121.00
4	J	710	ARG	NE-CZ-NH2	-7.47	116.57	120.30
2	F	671	ARG	NE-CZ-NH2	-7.46	116.57	120.30
2	B	466	ARG	NE-CZ-NH2	-7.45	116.57	120.30
7	V	614	PHE	CB-CG-CD2	7.45	126.02	120.80
1	A	269	TYR	CB-CG-CD2	-7.45	116.53	121.00
2	D	605	ARG	NE-CZ-NH1	7.45	124.03	120.30
1	A	460	ARG	NE-CZ-NH2	-7.45	116.58	120.30
2	Q	29	ALA	N-CA-CB	7.44	120.52	110.10
8	a	225	PHE	CB-CG-CD1	7.44	126.01	120.80
8	c	135	PHE	CB-CG-CD2	-7.44	115.59	120.80
3	K	478	PHE	CB-CG-CD1	7.44	126.01	120.80
8	l	401	ARG	NE-CZ-NH2	-7.44	116.58	120.30
2	D	865	THR	CA-CB-CG2	-7.44	101.98	112.40
3	K	606	ARG	NE-CZ-NH1	-7.44	116.58	120.30
9	r	58	ARG	NE-CZ-NH2	7.44	124.02	120.30
1	A	867	TYR	CZ-CE2-CD2	-7.43	113.11	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	f	366	TYR	CB-CG-CD1	-7.43	116.54	121.00
8	m	226	SER	N-CA-CB	7.43	121.64	110.50
3	K	650	TYR	CB-CG-CD1	7.43	125.46	121.00
8	m	130	ASP	CB-CG-OD1	7.43	124.98	118.30
1	C	763	ARG	NH1-CZ-NH2	7.42	127.57	119.40
8	c	310	ASP	CB-CG-OD2	-7.42	111.62	118.30
1	C	828	ASP	CB-CG-OD2	-7.42	111.62	118.30
5	L	504	TYR	CB-CG-CD2	-7.42	116.55	121.00
8	a	416	ASP	CB-CG-OD1	7.42	124.98	118.30
8	n	92	TYR	CG-CD2-CE2	7.42	127.23	121.30
8	l	403	ALA	N-CA-CB	7.41	120.48	110.10
1	E	607	LEU	CB-CG-CD1	7.40	123.59	111.00
2	D	364	ARG	NE-CZ-NH1	7.39	124.00	120.30
2	Q	34	TYR	CG-CD1-CE1	-7.39	115.39	121.30
1	E	431	TYR	CG-CD1-CE1	7.39	127.21	121.30
8	k	245	TYR	CB-CG-CD1	-7.39	116.57	121.00
8	c	92	TYR	CZ-CE2-CD2	7.39	126.45	119.80
2	R	70	ASP	CB-CG-OD1	7.39	124.95	118.30
2	N	678	ASP	CB-CG-OD1	7.38	124.95	118.30
8	l	127	ASP	CB-CG-OD2	-7.38	111.65	118.30
4	J	888	PHE	CB-CG-CD1	-7.38	115.64	120.80
8	l	286	ARG	NE-CZ-NH2	-7.38	116.61	120.30
1	M	637	TYR	CB-CG-CD1	7.38	125.42	121.00
2	F	310	ARG	NE-CZ-NH1	7.37	123.99	120.30
8	l	3	ARG	NE-CZ-NH1	7.37	123.98	120.30
2	F	843	ARG	NE-CZ-NH2	-7.37	116.61	120.30
5	L	1576	ARG	NE-CZ-NH1	7.37	123.98	120.30
8	l	95	GLU	N-CA-CB	7.36	123.85	110.60
8	k	53	TYR	CB-CG-CD2	-7.36	116.59	121.00
4	J	982	PHE	CB-CG-CD1	7.35	125.95	120.80
2	D	336	ARG	NE-CZ-NH1	7.35	123.98	120.30
8	c	60	TYR	CB-CG-CD2	-7.35	116.59	121.00
8	j	3	ARG	NE-CZ-NH1	7.35	123.97	120.30
1	G	570	ASP	CB-CG-OD1	7.35	124.91	118.30
2	H	323	PHE	CB-CG-CD2	7.34	125.94	120.80
3	I	515	ARG	NE-CZ-NH1	7.33	123.97	120.30
8	a	265	ARG	NE-CZ-NH2	-7.33	116.64	120.30
8	l	362	ARG	NE-CZ-NH1	-7.33	116.64	120.30
2	N	365	ARG	NE-CZ-NH1	7.33	123.96	120.30
8	c	47	ARG	NE-CZ-NH2	-7.33	116.64	120.30
9	o	58	ARG	NE-CZ-NH1	7.33	123.96	120.30
2	F	831	ARG	NH1-CZ-NH2	-7.33	111.34	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	n	21	PHE	CB-CG-CD2	-7.32	115.67	120.80
2	T	70	ASP	CB-CG-OD2	-7.32	111.71	118.30
2	N	742	ASP	CB-CG-OD2	-7.32	111.71	118.30
8	i	169	TYR	CB-CG-CD1	7.31	125.39	121.00
8	m	104	TRP	CB-CG-CD2	7.31	136.11	126.60
8	f	206	ASP	CB-CG-OD2	-7.31	111.72	118.30
8	b	152	TYR	CB-CG-CD2	-7.31	116.61	121.00
8	n	53	TYR	CB-CG-CD2	7.31	125.39	121.00
2	R	60	LYS	N-CA-CB	7.30	123.73	110.60
8	i	194	ARG	NE-CZ-NH1	7.29	123.95	120.30
8	k	172	PHE	CB-CG-CD2	-7.29	115.70	120.80
1	M	679	PHE	CB-CG-CD1	-7.29	115.70	120.80
8	b	296	ARG	NH1-CZ-NH2	-7.29	111.38	119.40
2	F	257	PHE	CB-CG-CD1	7.29	125.90	120.80
8	f	399	ARG	NE-CZ-NH1	7.29	123.94	120.30
2	B	605	ARG	NE-CZ-NH1	7.29	123.94	120.30
1	M	559	ARG	NE-CZ-NH2	-7.28	116.66	120.30
8	j	295	ARG	NE-CZ-NH1	7.28	123.94	120.30
8	b	53	TYR	CB-CG-CD1	7.28	125.37	121.00
8	d	382	THR	CA-CB-CG2	-7.28	102.21	112.40
1	G	403	TYR	CG-CD2-CE2	-7.27	115.48	121.30
8	g	47	ARG	NE-CZ-NH1	7.27	123.94	120.30
1	A	243	ARG	CD-NE-CZ	7.27	133.77	123.60
3	K	331	ARG	NE-CZ-NH2	7.27	123.93	120.30
8	h	366	TYR	CB-CG-CD2	-7.27	116.64	121.00
2	T	62	PHE	CB-CG-CD2	-7.26	115.72	120.80
8	l	348	PHE	CB-CG-CD2	7.26	125.88	120.80
5	L	469	ARG	NE-CZ-NH1	-7.25	116.67	120.30
2	R	37	ARG	NE-CZ-NH2	-7.25	116.67	120.30
7	V	613	ASP	CB-CG-OD2	-7.25	111.78	118.30
1	G	492	ASN	O-C-N	-7.25	111.10	122.70
3	I	169	ARG	NE-CZ-NH2	-7.25	116.68	120.30
8	g	334	HIS	CA-CB-CG	7.25	125.92	113.60
8	e	3	ARG	NE-CZ-NH2	-7.25	116.68	120.30
5	L	1503	TYR	CB-CG-CD1	7.24	125.34	121.00
2	D	723	PHE	CB-CG-CD2	-7.23	115.74	120.80
3	K	293	MET	CG-SD-CE	-7.23	88.63	100.20
7	W	647	TYR	CB-CG-CD1	7.23	125.34	121.00
1	C	863	PHE	CB-CG-CD2	-7.22	115.75	120.80
2	D	480	ARG	NH1-CZ-NH2	-7.22	111.46	119.40
8	k	156	ARG	NE-CZ-NH2	-7.22	116.69	120.30
1	M	518	TYR	CB-CG-CD1	-7.21	116.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	g	161	TYR	CG-CD2-CE2	-7.21	115.53	121.30
3	I	100	TYR	CB-CG-CD2	7.21	125.33	121.00
9	o	51	SER	N-CA-CB	7.20	121.31	110.50
1	C	401	ASP	CB-CG-OD1	7.20	124.78	118.30
8	i	60	TYR	CG-CD1-CE1	-7.20	115.54	121.30
1	M	641	PHE	CB-CG-CD1	7.20	125.84	120.80
2	D	843	ARG	NE-CZ-NH2	-7.19	116.70	120.30
4	J	274	LEU	CB-CG-CD2	7.19	123.23	111.00
4	J	782	ALA	CB-CA-C	-7.19	99.31	110.10
8	g	341	ARG	NE-CZ-NH2	-7.19	116.70	120.30
2	F	247	THR	CA-CB-CG2	-7.19	102.33	112.40
8	g	19	PHE	CB-CG-CD2	-7.19	115.77	120.80
3	I	627	ARG	NE-CZ-NH1	7.19	123.89	120.30
8	c	136	VAL	CA-CB-CG2	-7.18	100.13	110.90
8	h	341	ARG	NE-CZ-NH1	7.18	123.89	120.30
1	A	393	TRP	CE3-CZ3-CH2	-7.18	113.30	121.20
6	P	221	LEU	CB-CG-CD1	7.17	123.20	111.00
5	L	1465	TYR	CB-CG-CD1	-7.17	116.70	121.00
2	D	491	PHE	CB-CG-CD1	7.17	125.82	120.80
9	t	58	ARG	NE-CZ-NH2	-7.17	116.72	120.30
8	d	217	ARG	NE-CZ-NH1	-7.16	116.72	120.30
3	I	474	TYR	CB-CG-CD2	-7.16	116.70	121.00
1	A	867	TYR	CB-CG-CD1	7.16	125.30	121.00
2	D	740	ALA	N-CA-CB	7.16	120.12	110.10
2	S	50	ASP	CB-CG-OD1	7.16	124.74	118.30
8	e	124	ARG	NE-CZ-NH2	-7.15	116.72	120.30
1	A	840	ASP	CB-CG-OD2	-7.15	111.86	118.30
5	L	1691	PHE	CB-CG-CD1	7.14	125.80	120.80
2	D	564	TYR	CB-CG-CD2	-7.14	116.72	121.00
2	H	411	ARG	NE-CZ-NH1	7.14	123.87	120.30
3	I	85	TYR	CA-CB-CG	-7.13	99.84	113.40
3	I	485	ARG	NE-CZ-NH2	7.13	123.87	120.30
6	P	188	TYR	CB-CG-CD1	-7.13	116.72	121.00
1	G	341	ALA	N-CA-CB	7.13	120.08	110.10
8	b	194	ARG	NE-CZ-NH1	7.13	123.86	120.30
2	N	411	ARG	NE-CZ-NH1	-7.12	116.74	120.30
6	P	169	TYR	CB-CG-CD2	7.12	125.27	121.00
8	c	152	TYR	CB-CG-CD1	-7.12	116.73	121.00
8	j	86	TYR	CB-CG-CD1	7.12	125.27	121.00
1	M	361	ARG	NE-CZ-NH1	7.12	123.86	120.30
1	G	302	TYR	CG-CD2-CE2	7.11	126.99	121.30
5	L	1386	TYR	CG-CD2-CE2	7.11	126.99	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	645	PHE	CB-CG-CD1	7.11	125.78	120.80
2	N	730	TRP	CD1-NE1-CE2	7.11	115.40	109.00
5	L	1688	ARG	NE-CZ-NH1	-7.10	116.75	120.30
1	M	682	ARG	NE-CZ-NH2	-7.10	116.75	120.30
8	h	390	ARG	NE-CZ-NH2	7.10	123.85	120.30
8	l	86	TYR	CB-CG-CD2	-7.10	116.74	121.00
9	t	23	ARG	NE-CZ-NH1	7.10	123.85	120.30
3	K	55	PHE	CB-CG-CD1	7.10	125.77	120.80
4	J	591	PHE	CB-CG-CD2	7.09	125.76	120.80
8	c	409	ARG	NE-CZ-NH2	7.09	123.84	120.30
8	h	351	TRP	CB-CG-CD1	7.09	136.22	127.00
1	E	645	PHE	CB-CG-CD2	-7.09	115.84	120.80
8	l	433	ASP	CB-CG-OD1	7.09	124.68	118.30
8	a	161	TYR	CB-CG-CD1	7.08	125.25	121.00
1	M	228	ASP	CB-CG-OD2	-7.07	111.94	118.30
2	O	52	PHE	CB-CG-CD1	-7.07	115.85	120.80
8	b	399	ARG	NH1-CZ-NH2	-7.07	111.63	119.40
8	m	396	ASP	CB-CG-OD2	-7.07	111.94	118.30
1	C	529	HIS	CA-CB-CG	-7.07	101.59	113.60
2	B	605	ARG	NH1-CZ-NH2	-7.06	111.63	119.40
5	L	1691	PHE	N-CA-CB	7.06	123.31	110.60
1	M	652	ARG	NE-CZ-NH2	-7.06	116.77	120.30
6	P	95	ARG	NE-CZ-NH1	7.06	123.83	120.30
2	T	19	ARG	NE-CZ-NH2	-7.06	116.77	120.30
2	F	740	ALA	N-CA-CB	7.05	119.97	110.10
8	h	419	ASP	CB-CG-OD1	7.05	124.65	118.30
8	i	295	ARG	NE-CZ-NH2	7.05	123.83	120.30
8	h	161	TYR	CG-CD1-CE1	7.05	126.94	121.30
3	K	486	ARG	NE-CZ-NH2	-7.04	116.78	120.30
4	J	295	ASP	CB-CG-OD1	-7.04	111.96	118.30
2	B	789	ASP	CB-CG-OD2	-7.04	111.97	118.30
2	B	874	PHE	CB-CG-CD2	-7.04	115.88	120.80
2	H	793	ARG	NE-CZ-NH2	7.03	123.81	120.30
8	k	393	ARG	NE-CZ-NH2	-7.03	116.78	120.30
1	E	652	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	M	445	VAL	CA-CB-CG2	-7.03	100.36	110.90
8	m	248	TYR	CB-CG-CD1	7.03	125.22	121.00
1	C	641	PHE	CB-CG-CD1	7.02	125.72	120.80
8	f	3	ARG	NE-CZ-NH2	7.02	123.81	120.30
8	l	245	TYR	N-CA-C	-7.02	92.05	111.00
1	A	544	ASP	CB-CG-OD1	7.02	124.61	118.30
2	N	793	ARG	NE-CZ-NH1	7.01	123.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	720	TYR	CB-CG-CD1	7.00	125.20	121.00
2	B	674	TYR	CG-CD2-CE2	-7.00	115.70	121.30
2	N	812	ARG	NE-CZ-NH2	-7.00	116.80	120.30
1	C	491	TYR	N-CA-CB	7.00	123.20	110.60
1	A	617	PHE	CB-CG-CD2	-7.00	115.90	120.80
6	P	81	ASP	CB-CG-OD2	6.99	124.59	118.30
2	H	753	PHE	CB-CG-CD1	-6.98	115.91	120.80
3	I	522	PHE	CB-CG-CD2	-6.98	115.91	120.80
3	K	169	ARG	NH1-CZ-NH2	-6.98	111.72	119.40
2	N	661	ARG	NH1-CZ-NH2	-6.98	111.72	119.40
8	h	200	ASP	CB-CG-OD1	-6.98	112.02	118.30
2	F	862	VAL	CA-CB-CG1	6.98	121.37	110.90
8	a	311	ARG	NE-CZ-NH1	-6.98	116.81	120.30
9	s	23	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	A	483	TYR	CB-CG-CD1	-6.97	116.81	121.00
2	S	70	ASP	CB-CG-OD2	-6.97	112.02	118.30
5	L	1521	ARG	NE-CZ-NH1	6.97	123.79	120.30
1	A	302	TYR	CG-CD2-CE2	6.97	126.88	121.30
2	D	440	ASP	CB-CG-OD2	-6.97	112.03	118.30
2	H	409	TYR	CB-CG-CD1	-6.97	116.82	121.00
4	J	458	PHE	CB-CG-CD1	-6.96	115.92	120.80
4	J	771	ARG	NE-CZ-NH2	6.96	123.78	120.30
8	a	135	PHE	CB-CG-CD2	6.96	125.67	120.80
2	F	623	ARG	NE-CZ-NH1	6.96	123.78	120.30
8	l	287	LYS	N-CA-CB	6.95	123.11	110.60
3	I	650	TYR	CB-CG-CD1	6.95	125.17	121.00
8	g	296	ARG	NE-CZ-NH1	-6.94	116.83	120.30
8	e	92	TYR	CG-CD1-CE1	-6.94	115.75	121.30
3	I	369	PHE	CB-CG-CD2	-6.93	115.95	120.80
2	B	621	ASP	CB-CG-OD1	-6.93	112.06	118.30
1	C	549	ARG	NE-CZ-NH1	6.93	123.77	120.30
2	B	723	PHE	CB-CG-CD1	-6.93	115.95	120.80
8	j	19	PHE	CB-CG-CD1	6.93	125.65	120.80
3	I	58	PHE	CB-CG-CD2	6.93	125.65	120.80
3	I	200	TYR	CG-CD2-CE2	-6.93	115.76	121.30
4	J	714	TYR	CB-CG-CD2	-6.93	116.84	121.00
8	d	130	ASP	CB-CG-OD2	-6.93	112.07	118.30
1	A	493	TYR	CB-CG-CD2	6.92	125.15	121.00
1	C	705	TRP	CE2-CD2-CG	6.92	112.84	107.30
8	i	186	TYR	CB-CG-CD1	-6.92	116.85	121.00
8	n	244	ARG	NE-CZ-NH1	6.92	123.76	120.30
2	H	434	TYR	CB-CG-CD1	6.92	125.15	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	568	PHE	CB-CG-CD2	6.91	125.64	120.80
4	J	935	ARG	NE-CZ-NH1	-6.91	116.85	120.30
2	Q	32	PHE	CB-CG-CD1	-6.91	115.97	120.80
1	C	658	TRP	CB-CG-CD1	6.90	135.97	127.00
8	a	156	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	G	549	ARG	NE-CZ-NH1	6.90	123.75	120.30
1	A	314	ARG	NE-CZ-NH2	-6.90	116.85	120.30
4	J	781	LEU	CB-CG-CD2	6.90	122.73	111.00
8	g	21	PHE	CB-CG-CD1	6.90	125.63	120.80
8	a	248	TYR	CB-CG-CD1	-6.89	116.86	121.00
1	C	642	ARG	NE-CZ-NH2	-6.89	116.85	120.30
3	I	486	ARG	NE-CZ-NH2	-6.89	116.86	120.30
8	l	366	TYR	CB-CG-CD2	-6.89	116.87	121.00
8	h	295	ARG	NE-CZ-NH2	-6.89	116.86	120.30
3	K	480	TYR	CD1-CE1-CZ	6.88	125.99	119.80
1	C	559	ARG	NH1-CZ-NH2	-6.88	111.83	119.40
2	B	869	ASP	CB-CG-OD1	-6.88	112.11	118.30
8	j	93	LEU	N-CA-CB	6.87	124.14	110.40
8	k	183	VAL	CG1-CB-CG2	6.87	121.89	110.90
2	H	755	ASP	CB-CG-OD2	-6.87	112.12	118.30
8	n	63	ARG	NE-CZ-NH2	-6.86	116.87	120.30
8	k	93	LEU	CB-CG-CD1	6.86	122.66	111.00
8	b	295	ARG	NE-CZ-NH1	6.86	123.73	120.30
6	P	8	LEU	CB-CG-CD2	6.85	122.65	111.00
1	C	427	TRP	CD1-CG-CD2	6.85	111.78	106.30
8	c	72	ARG	NE-CZ-NH2	-6.85	116.88	120.30
8	f	152	TYR	CG-CD1-CE1	-6.85	115.82	121.30
1	M	637	TYR	CB-CG-CD2	-6.84	116.89	121.00
8	b	53	TYR	CB-CG-CD2	-6.84	116.89	121.00
1	A	360	ASP	CB-CG-OD1	-6.84	112.14	118.30
2	B	428	PHE	CB-CG-CD1	6.84	125.59	120.80
8	a	433	ASP	CB-CG-OD2	-6.84	112.14	118.30
8	n	296	ARG	NE-CZ-NH1	-6.84	116.88	120.30
8	e	286	ARG	NE-CZ-NH2	6.84	123.72	120.30
4	J	262	THR	C-N-CA	6.83	138.79	121.70
8	g	46	ASP	CB-CG-OD1	-6.83	112.15	118.30
9	r	19	LEU	O-C-N	-6.83	111.77	122.70
2	B	411	ARG	NE-CZ-NH2	6.83	123.72	120.30
1	A	314	ARG	NE-CZ-NH1	6.83	123.71	120.30
3	K	500	GLN	N-CA-CB	6.83	122.89	110.60
8	l	436	HIS	CA-CB-CG	6.83	125.21	113.60
1	E	284	TYR	CD1-CE1-CZ	6.82	125.94	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	645	LEU	CB-CG-CD1	6.82	122.60	111.00
4	J	888	PHE	CB-CG-CD2	6.82	125.57	120.80
1	M	756	MET	CG-SD-CE	-6.82	89.29	100.20
2	B	365	ARG	NE-CZ-NH2	6.82	123.71	120.30
5	L	430	PHE	CB-CG-CD2	-6.82	116.03	120.80
6	P	56	ASP	CB-CG-OD1	-6.81	112.17	118.30
5	L	567	ARG	NE-CZ-NH1	6.81	123.71	120.30
8	f	296	ARG	NE-CZ-NH1	6.81	123.71	120.30
8	g	382	THR	CA-CB-CG2	-6.81	102.86	112.40
1	A	530	PHE	CB-CG-CD2	-6.81	116.03	120.80
2	N	877	PHE	CB-CG-CD2	6.81	125.56	120.80
2	Q	12	LEU	CB-CG-CD2	6.81	122.57	111.00
5	L	1573	CYS	N-CA-CB	6.80	122.85	110.60
6	P	69	TYR	CB-CG-CD1	6.80	125.08	121.00
8	h	186	TYR	CG-CD2-CE2	-6.80	115.86	121.30
1	C	486	ARG	NH1-CZ-NH2	6.80	126.88	119.40
8	f	399	ARG	NE-CZ-NH2	-6.80	116.90	120.30
8	k	265	ARG	N-CA-CB	6.80	122.83	110.60
5	L	474	LEU	CB-CG-CD2	6.79	122.55	111.00
1	C	828	ASP	CB-CG-OD1	6.79	124.41	118.30
2	F	446	PHE	CB-CG-CD2	6.79	125.55	120.80
5	L	1386	TYR	CG-CD1-CE1	6.79	126.73	121.30
8	n	56	ASP	CB-CG-OD2	-6.79	112.19	118.30
2	H	873	ARG	NE-CZ-NH2	6.79	123.69	120.30
1	G	525	ASP	CB-CG-OD1	6.79	124.41	118.30
3	K	254	LEU	CB-CG-CD2	6.79	122.53	111.00
1	G	859	TYR	CB-CG-CD2	-6.78	116.93	121.00
2	N	619	ARG	NE-CZ-NH2	-6.78	116.91	120.30
5	L	1661	TYR	CB-CG-CD1	-6.78	116.93	121.00
2	Q	66	ARG	N-CA-CB	6.78	122.81	110.60
1	E	284	TYR	CG-CD2-CE2	6.78	126.72	121.30
8	f	419	ASP	CB-CG-OD2	-6.78	112.20	118.30
2	N	431	ARG	NE-CZ-NH2	-6.78	116.91	120.30
2	D	725	VAL	CA-CB-CG1	6.78	121.07	110.90
8	e	217	ARG	NE-CZ-NH2	6.78	123.69	120.30
8	f	86	TYR	CB-CG-CD2	-6.78	116.93	121.00
2	N	753	PHE	CB-CG-CD1	6.77	125.54	120.80
8	e	311	ARG	NE-CZ-NH2	6.77	123.69	120.30
6	P	69	TYR	CG-CD2-CE2	6.77	126.71	121.30
8	d	186	TYR	CB-CG-CD2	-6.77	116.94	121.00
8	m	172	PHE	CB-CG-CD2	6.77	125.54	120.80
4	J	207	ASP	CB-CG-OD1	-6.76	112.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	543	TYR	CB-CG-CD2	-6.76	116.94	121.00
8	m	119	PHE	CB-CG-CD2	6.76	125.53	120.80
8	f	273	TYR	CB-CG-CD2	-6.76	116.95	121.00
8	l	92	TYR	CB-CG-CD2	-6.76	116.95	121.00
2	H	365	ARG	NE-CZ-NH1	6.75	123.68	120.30
4	J	501	ARG	NE-CZ-NH2	6.75	123.68	120.30
8	f	412	ASP	CB-CG-OD1	6.75	124.38	118.30
1	C	377	TYR	CG-CD1-CE1	-6.75	115.90	121.30
8	m	117	ASP	CB-CG-OD1	6.75	124.38	118.30
1	G	549	ARG	NH1-CZ-NH2	-6.75	111.98	119.40
2	H	768	ARG	NE-CZ-NH2	6.75	123.67	120.30
8	m	341	ARG	NE-CZ-NH2	-6.75	116.93	120.30
2	D	365	ARG	NE-CZ-NH2	-6.74	116.93	120.30
8	i	408	PHE	CB-CG-CD2	-6.74	116.08	120.80
8	g	291	LEU	CB-CG-CD2	6.74	122.45	111.00
2	H	843	ARG	NE-CZ-NH2	-6.73	116.93	120.30
3	I	501	ARG	NE-CZ-NH1	6.73	123.67	120.30
8	a	391	THR	CA-CB-CG2	-6.73	102.98	112.40
2	H	547	VAL	CA-CB-CG1	6.73	120.99	110.90
3	I	501	ARG	NE-CZ-NH2	-6.73	116.94	120.30
8	k	422	ASP	CB-CG-OD2	6.73	124.35	118.30
1	E	284	TYR	CB-CG-CD2	-6.72	116.97	121.00
8	a	278	THR	CA-CB-CG2	-6.72	102.98	112.40
8	l	124	ARG	NE-CZ-NH2	-6.72	116.94	120.30
8	m	73	VAL	CA-CB-CG1	-6.72	100.81	110.90
1	C	295	MET	CG-SD-CE	-6.72	89.45	100.20
2	N	255	TYR	CZ-CE2-CD2	6.72	125.85	119.80
8	k	285	VAL	CA-CB-CG1	-6.72	100.82	110.90
3	K	560	HIS	CA-CB-CG	6.72	125.02	113.60
8	m	92	TYR	CA-CB-CG	6.72	126.17	113.40
8	m	386	SER	N-CA-CB	6.72	120.58	110.50
2	D	335	TYR	CD1-CG-CD2	6.72	125.29	117.90
5	L	1694	TYR	CB-CG-CD1	6.72	125.03	121.00
8	g	3	ARG	NE-CZ-NH2	6.72	123.66	120.30
8	l	252	ASP	CB-CA-C	-6.72	96.97	110.40
2	H	635	ASP	CB-CG-OD1	6.71	124.34	118.30
2	F	432	TRP	CA-CB-CG	6.71	126.45	113.70
2	B	455	THR	N-CA-C	-6.71	92.89	111.00
1	M	513	ARG	NH1-CZ-NH2	-6.71	112.02	119.40
2	D	661	ARG	NE-CZ-NH1	6.71	123.65	120.30
2	F	719	TYR	CB-CG-CD2	-6.71	116.98	121.00
2	T	91	TRP	CB-CG-CD1	-6.71	118.28	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	f	295	ARG	NE-CZ-NH2	6.70	123.65	120.30
1	G	338	ALA	CB-CA-C	-6.70	100.05	110.10
8	e	408	PHE	CB-CG-CD2	6.70	125.49	120.80
4	J	420	PRO	N-CA-CB	6.70	111.34	103.30
1	G	645	PHE	CB-CG-CD2	-6.70	116.11	120.80
8	c	120	ASP	CB-CG-OD1	6.70	124.33	118.30
9	o	12	ARG	NE-CZ-NH2	-6.70	116.95	120.30
8	i	339	ARG	NE-CZ-NH1	6.69	123.64	120.30
1	M	513	ARG	NE-CZ-NH2	6.68	123.64	120.30
1	G	500	ASP	CB-CG-OD1	6.68	124.31	118.30
1	C	234	VAL	CA-CB-CG2	-6.68	100.88	110.90
2	N	631	ASP	CB-CG-OD2	-6.68	112.29	118.30
2	N	792	TYR	CB-CG-CD1	-6.68	116.99	121.00
4	J	703	TYR	CB-CG-CD1	6.67	125.00	121.00
8	l	399	ARG	NE-CZ-NH2	6.67	123.64	120.30
1	G	427	TRP	CZ3-CH2-CZ2	-6.67	113.59	121.60
5	L	404	TYR	CG-CD1-CE1	-6.67	115.96	121.30
8	g	414	PHE	CB-CG-CD1	6.67	125.47	120.80
1	M	525	ASP	CB-CG-OD1	6.67	124.30	118.30
8	b	159	ASP	CB-CG-OD2	6.67	124.30	118.30
8	i	372	ARG	NE-CZ-NH1	6.67	123.63	120.30
4	J	788	VAL	C-N-CA	6.67	138.37	121.70
2	H	700	LEU	CB-CG-CD1	6.66	122.33	111.00
4	J	360	PHE	CB-CG-CD2	-6.66	116.14	120.80
2	N	623	ARG	NE-CZ-NH2	6.66	123.63	120.30
8	i	244	ARG	NE-CZ-NH1	-6.66	116.97	120.30
8	e	393	ARG	NE-CZ-NH1	6.66	123.63	120.30
1	C	519	PHE	CB-CG-CD2	-6.65	116.14	120.80
8	d	156	ARG	NE-CZ-NH2	-6.65	116.97	120.30
2	H	552	TYR	CB-CG-CD1	-6.65	117.01	121.00
8	h	169	TYR	CG-CD2-CE2	-6.65	115.98	121.30
8	k	317	TYR	CB-CG-CD1	-6.65	117.01	121.00
5	L	1562	TYR	CB-CG-CD1	-6.65	117.01	121.00
8	f	414	PHE	CB-CG-CD2	6.64	125.45	120.80
8	i	92	TYR	CB-CG-CD1	-6.64	117.01	121.00
8	a	348	PHE	CB-CG-CD1	-6.64	116.15	120.80
8	d	86	TYR	CD1-CE1-CZ	6.64	125.78	119.80
1	M	230	ARG	NE-CZ-NH2	-6.64	116.98	120.30
9	q	32	GLU	OE1-CD-OE2	6.64	131.26	123.30
1	C	269	TYR	CG-CD2-CE2	-6.64	115.99	121.30
1	M	848	SER	CB-CA-C	6.64	122.71	110.10
7	X	621	ASP	CB-CG-OD1	6.63	124.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	e	156	ARG	NE-CZ-NH1	6.63	123.62	120.30
9	o	39	ARG	NE-CZ-NH1	-6.63	116.98	120.30
3	I	278	PHE	CB-CG-CD2	6.63	125.44	120.80
3	K	396	PHE	CB-CG-CD1	-6.63	116.16	120.80
5	L	158	PHE	CB-CG-CD2	-6.63	116.16	120.80
2	N	402	TYR	CG-CD1-CE1	-6.63	116.00	121.30
2	B	334	TYR	CD1-CE1-CZ	6.62	125.76	119.80
8	j	123	ASP	CB-CG-OD1	6.62	124.26	118.30
8	m	66	LEU	N-CA-CB	6.62	123.64	110.40
2	F	661	ARG	NE-CZ-NH2	-6.62	116.99	120.30
8	k	22	TRP	CB-CG-CD1	6.62	135.60	127.00
9	s	58	ARG	NE-CZ-NH2	-6.62	116.99	120.30
5	L	1576	ARG	NE-CZ-NH2	-6.62	116.99	120.30
1	A	735	ASP	CB-CG-OD2	-6.62	112.34	118.30
8	f	415	LYS	CA-CB-CG	6.62	127.96	113.40
8	c	206	ASP	CB-CG-OD2	-6.61	112.35	118.30
8	j	215	THR	CA-CB-OG1	6.61	122.88	109.00
1	A	234	VAL	CA-CB-CG2	-6.60	101.00	110.90
2	O	49	ARG	NE-CZ-NH1	6.60	123.60	120.30
8	c	252	ASP	CB-CG-OD2	6.60	124.24	118.30
8	e	70	GLU	N-CA-CB	6.60	122.48	110.60
2	O	9	PRO	N-CA-CB	6.60	111.22	103.30
2	H	335	TYR	CB-CG-CD2	-6.60	117.04	121.00
1	M	303	MET	CG-SD-CE	-6.59	89.65	100.20
8	g	264	PRO	O-C-N	6.59	133.25	122.70
2	T	66	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	E	386	TYR	CB-CG-CD2	-6.59	117.05	121.00
1	E	406	PHE	CB-CG-CD1	6.59	125.42	120.80
9	r	23	ARG	NE-CZ-NH2	-6.59	117.00	120.30
5	L	217	PHE	CB-CG-CD1	6.59	125.41	120.80
7	V	610	THR	CA-CB-CG2	-6.59	103.18	112.40
8	d	86	TYR	CB-CG-CD2	6.59	124.95	121.00
8	i	433	ASP	CB-CG-OD1	6.59	124.23	118.30
8	n	160	ARG	NE-CZ-NH1	6.58	123.59	120.30
3	I	478	PHE	CD1-CE1-CZ	-6.58	112.20	120.10
2	D	261	ASP	CB-CG-OD1	6.58	124.22	118.30
2	D	751	ASP	N-CA-CB	6.58	122.45	110.60
6	P	44	MET	CG-SD-CE	6.58	110.73	100.20
7	U	661	ARG	NE-CZ-NH1	6.58	123.59	120.30
1	E	688	PHE	CB-CG-CD1	6.58	125.40	120.80
5	L	1678	TYR	CB-CG-CD2	6.58	124.94	121.00
8	c	152	TYR	CB-CG-CD2	6.58	124.94	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	g	422	ASP	CB-CG-OD1	6.57	124.22	118.30
2	N	306	TYR	CB-CG-CD1	-6.57	117.06	121.00
2	O	91	TRP	CD1-NE1-CE2	6.57	114.91	109.00
8	j	145	THR	CA-CB-CG2	-6.57	103.20	112.40
3	I	52	TYR	CZ-CE2-CD2	-6.57	113.89	119.80
8	c	395	TYR	CB-CG-CD1	-6.56	117.06	121.00
2	F	619	ARG	NE-CZ-NH2	-6.56	117.02	120.30
8	a	64	ALA	N-CA-CB	6.56	119.28	110.10
9	t	30	ASP	CB-CG-OD1	6.56	124.20	118.30
8	j	395	TYR	CB-CG-CD1	-6.55	117.07	121.00
1	A	527	PHE	CB-CG-CD2	6.55	125.39	120.80
5	L	158	PHE	CB-CG-CD1	6.55	125.39	120.80
8	d	401	ARG	NE-CZ-NH2	-6.55	117.03	120.30
8	h	225	PHE	CB-CG-CD1	6.55	125.39	120.80
8	a	401	ARG	N-CA-CB	6.55	122.39	110.60
8	g	279	ASP	CB-CG-OD1	-6.55	112.41	118.30
8	h	194	ARG	NE-CZ-NH1	6.55	123.57	120.30
2	H	255	TYR	CG-CD1-CE1	-6.55	116.06	121.30
2	S	47	VAL	CA-CB-CG2	-6.55	101.08	110.90
8	h	351	TRP	CB-CG-CD2	-6.55	118.09	126.60
1	M	478	LEU	CB-CG-CD2	6.54	122.13	111.00
1	A	719	ASP	CB-CG-OD1	-6.54	112.41	118.30
2	B	663	PHE	CG-CD1-CE1	6.54	128.00	120.80
2	F	407	ASP	CB-CG-OD1	6.54	124.19	118.30
2	F	574	ARG	NE-CZ-NH1	6.54	123.57	120.30
9	s	34	LEU	CB-CG-CD1	6.54	122.12	111.00
8	d	51	PHE	CB-CG-CD2	-6.53	116.23	120.80
5	L	1676	ARG	NH1-CZ-NH2	6.53	126.58	119.40
1	E	252	ASP	CB-CG-OD1	6.53	124.17	118.30
8	f	304	MET	CG-SD-CE	-6.53	89.76	100.20
8	j	286	ARG	NE-CZ-NH1	-6.53	117.04	120.30
1	C	617	PHE	CB-CG-CD1	-6.52	116.23	120.80
1	G	368	ASP	CB-CG-OD1	-6.52	112.43	118.30
3	I	158	TYR	CG-CD1-CE1	-6.52	116.08	121.30
3	I	551	ARG	NH1-CZ-NH2	-6.52	112.23	119.40
1	C	482	ALA	N-CA-CB	6.52	119.22	110.10
8	c	343	ARG	NE-CZ-NH1	6.52	123.56	120.30
8	f	131	SER	N-CA-CB	6.51	120.27	110.50
3	I	552	ASP	CB-CG-OD1	6.51	124.16	118.30
5	L	1602	ARG	NE-CZ-NH2	-6.51	117.04	120.30
8	c	72	ARG	NE-CZ-NH1	6.51	123.56	120.30
8	c	425	ARG	NE-CZ-NH1	6.51	123.55	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	466	VAL	CA-CB-CG1	-6.50	101.14	110.90
2	B	823	ALA	CB-CA-C	-6.50	100.34	110.10
8	k	343	ARG	NE-CZ-NH2	6.50	123.55	120.30
1	E	243	ARG	NE-CZ-NH1	-6.50	117.05	120.30
2	O	34	TYR	CB-CG-CD2	-6.50	117.10	121.00
3	K	485	ARG	NE-CZ-NH1	6.50	123.55	120.30
8	b	21	PHE	CB-CG-CD1	-6.50	116.25	120.80
5	L	506	TYR	CD1-CE1-CZ	6.50	125.65	119.80
8	a	92	TYR	CB-CG-CD1	-6.50	117.10	121.00
2	D	805	PHE	CB-CG-CD2	6.50	125.35	120.80
5	L	560	TYR	CB-CG-CD2	-6.50	117.10	121.00
8	c	160	ARG	NE-CZ-NH2	-6.50	117.05	120.30
8	h	409	ARG	NH1-CZ-NH2	-6.50	112.25	119.40
2	H	852	PHE	CB-CG-CD1	6.50	125.35	120.80
2	T	74	PHE	CB-CG-CD2	-6.50	116.25	120.80
2	Q	79	ARG	NH1-CZ-NH2	-6.49	112.26	119.40
8	c	27	ALA	N-CA-CB	6.49	119.19	110.10
8	n	286	ARG	NE-CZ-NH1	6.49	123.55	120.30
3	K	604	ASP	CB-CG-OD1	6.49	124.14	118.30
5	L	1494	VAL	CA-CB-CG2	-6.49	101.17	110.90
8	n	60	TYR	CB-CG-CD2	-6.49	117.11	121.00
2	B	347	VAL	CA-CB-CG1	-6.49	101.17	110.90
8	a	72	ARG	NH1-CZ-NH2	-6.49	112.27	119.40
1	A	493	TYR	CG-CD2-CE2	6.49	126.49	121.30
1	G	859	TYR	CD1-CE1-CZ	6.49	125.64	119.80
3	K	325	PHE	CB-CG-CD1	6.49	125.34	120.80
2	N	316	PHE	CB-CG-CD1	-6.49	116.26	120.80
2	N	445	PHE	CG-CD2-CE2	-6.48	113.67	120.80
8	i	293	VAL	CA-CB-CG1	-6.48	101.18	110.90
2	F	831	ARG	NE-CZ-NH2	6.48	123.54	120.30
2	Q	54	VAL	CA-CB-CG1	6.48	120.62	110.90
1	E	618	ASP	CB-CG-OD2	-6.47	112.47	118.30
5	L	518	TYR	CG-CD2-CE2	-6.47	116.12	121.30
1	E	476	TYR	CB-CG-CD2	6.47	124.88	121.00
5	L	233	ASP	N-CA-CB	6.47	122.24	110.60
1	A	728	PHE	CB-CG-CD1	-6.46	116.28	120.80
1	G	513	ARG	NE-CZ-NH1	6.46	123.53	120.30
5	L	1649	PHE	CG-CD2-CE2	-6.46	113.69	120.80
6	P	56	ASP	CB-CG-OD2	6.46	124.12	118.30
2	H	267	MET	CG-SD-CE	6.46	110.54	100.20
7	X	668	ARG	NE-CZ-NH1	6.46	123.53	120.30
2	H	463	TYR	CB-CG-CD2	-6.46	117.12	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	c	372	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	A	388	ASP	CB-CG-OD1	-6.46	112.49	118.30
8	k	135	PHE	CG-CD2-CE2	-6.46	113.70	120.80
8	m	161	TYR	CB-CG-CD2	-6.46	117.13	121.00
8	c	292	ASP	CB-CG-OD1	-6.45	112.49	118.30
8	m	317	TYR	CB-CG-CD1	-6.45	117.13	121.00
1	A	334	MET	CG-SD-CE	-6.45	89.88	100.20
2	D	435	ASP	CB-CG-OD1	-6.45	112.50	118.30
3	K	387	VAL	CG1-CB-CG2	6.45	121.22	110.90
1	M	674	TRP	CB-CG-CD2	-6.45	118.22	126.60
1	M	728	PHE	CB-CG-CD1	-6.45	116.29	120.80
2	B	423	TYR	CD1-CE1-CZ	6.45	125.60	119.80
6	P	53	TYR	CB-CG-CD2	6.44	124.87	121.00
8	n	396	ASP	CB-CG-OD1	6.44	124.10	118.30
1	E	828	ASP	CB-CG-OD1	6.44	124.09	118.30
8	b	309	ARG	NE-CZ-NH1	6.44	123.52	120.30
8	d	92	TYR	CZ-CE2-CD2	-6.44	114.00	119.80
1	M	365	TYR	CB-CG-CD1	6.44	124.86	121.00
8	a	21	PHE	CB-CG-CD1	-6.44	116.30	120.80
8	a	404	PHE	CB-CG-CD2	6.44	125.31	120.80
8	b	56	ASP	CB-CG-OD1	-6.44	112.51	118.30
3	I	627	ARG	NE-CZ-NH2	-6.43	117.08	120.30
3	K	111	PHE	CD1-CE1-CZ	-6.43	112.38	120.10
2	T	62	PHE	CB-CG-CD1	6.43	125.30	120.80
3	K	480	TYR	CG-CD1-CE1	-6.43	116.15	121.30
8	d	161	TYR	CG-CD2-CE2	-6.43	116.15	121.30
8	d	161	TYR	CG-CD1-CE1	-6.43	116.16	121.30
8	j	435	TYR	CB-CG-CD2	-6.43	117.14	121.00
8	m	274	THR	CA-C-O	-6.43	106.60	120.10
8	h	123	ASP	CB-CG-OD1	6.43	124.09	118.30
3	I	203	PHE	CB-CG-CD2	-6.43	116.30	120.80
1	M	860	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	C	867	TYR	CB-CG-CD1	6.42	124.85	121.00
2	H	390	ARG	NE-CZ-NH2	-6.42	117.09	120.30
2	B	247	THR	CA-CB-CG2	-6.42	103.41	112.40
3	I	100	TYR	CB-CG-CD1	-6.42	117.15	121.00
8	a	343	ARG	NE-CZ-NH1	6.42	123.51	120.30
8	e	225	PHE	CB-CG-CD2	-6.42	116.31	120.80
8	m	339	ARG	NE-CZ-NH2	-6.42	117.09	120.30
1	E	641	PHE	CB-CG-CD1	-6.42	116.31	120.80
8	j	92	TYR	CG-CD2-CE2	-6.42	116.17	121.30
2	N	376	ARG	NE-CZ-NH1	6.41	123.51	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	O	79	ARG	NE-CZ-NH2	-6.41	117.09	120.30
1	E	302	TYR	CB-CG-CD1	6.41	124.85	121.00
3	K	604	ASP	CB-CG-OD2	-6.41	112.53	118.30
1	C	245	PHE	CB-CG-CD1	6.41	125.28	120.80
3	I	104	LEU	CB-CG-CD2	6.41	121.89	111.00
1	M	854	MET	CG-SD-CE	-6.41	89.95	100.20
8	e	225	PHE	CB-CG-CD1	6.40	125.28	120.80
8	b	362	ARG	NE-CZ-NH2	-6.40	117.10	120.30
8	n	245	TYR	CB-CG-CD2	6.40	124.84	121.00
2	N	680	TRP	CD1-NE1-CE2	6.40	114.76	109.00
2	Q	37	ARG	NH1-CZ-NH2	-6.40	112.36	119.40
9	q	58	ARG	NE-CZ-NH1	6.40	123.50	120.30
4	J	721	PHE	CB-CG-CD1	6.39	125.28	120.80
8	f	58	GLU	N-CA-CB	6.39	122.10	110.60
2	N	605	ARG	NE-CZ-NH2	-6.39	117.11	120.30
3	I	349	ASP	CB-CG-OD2	-6.39	112.55	118.30
1	A	501	PHE	CG-CD2-CE2	-6.38	113.78	120.80
5	L	1564	ALA	CB-CA-C	-6.38	100.52	110.10
8	h	309	ARG	NE-CZ-NH2	-6.38	117.11	120.30
8	j	160	ARG	NE-CZ-NH1	6.38	123.49	120.30
1	M	222	TYR	CB-CG-CD1	6.38	124.83	121.00
2	D	274	TYR	CG-CD2-CE2	-6.38	116.20	121.30
3	I	89	PHE	CB-CG-CD2	-6.38	116.34	120.80
2	N	306	TYR	CD1-CE1-CZ	6.38	125.54	119.80
8	m	132	LEU	CB-CG-CD2	6.37	121.83	111.00
5	L	68	VAL	CA-CB-CG1	6.37	120.46	110.90
8	c	68	ASP	CB-CG-OD1	6.37	124.03	118.30
3	I	345	VAL	CA-CB-CG1	6.37	120.45	110.90
2	N	650	VAL	CG1-CB-CG2	6.37	121.09	110.90
8	c	21	PHE	CG-CD1-CE1	-6.37	113.80	120.80
8	e	317	TYR	CD1-CE1-CZ	6.37	125.53	119.80
2	H	572	PHE	CB-CG-CD1	6.37	125.26	120.80
8	h	248	TYR	CB-CG-CD2	-6.37	117.18	121.00
2	N	853	TYR	CB-CG-CD1	6.37	124.82	121.00
8	k	53	TYR	CB-CG-CD1	6.37	124.82	121.00
8	b	252	ASP	CB-CG-OD2	-6.36	112.57	118.30
8	m	404	PHE	CB-CG-CD1	6.36	125.25	120.80
4	J	242	TRP	CB-CG-CD1	-6.36	118.73	127.00
3	I	442	ARG	NE-CZ-NH2	6.36	123.48	120.30
1	G	617	PHE	CB-CG-CD1	6.36	125.25	120.80
1	M	493	TYR	CG-CD1-CE1	-6.36	116.22	121.30
8	m	433	ASP	CB-CG-OD1	-6.36	112.58	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	361	TYR	CB-CG-CD2	6.35	124.81	121.00
8	e	290	VAL	CG1-CB-CG2	6.35	121.07	110.90
8	e	412	ASP	N-CA-CB	6.34	122.02	110.60
8	f	127	ASP	CB-CG-OD2	-6.34	112.59	118.30
9	t	30	ASP	CB-CG-OD2	-6.34	112.59	118.30
3	I	460	TRP	C-N-CD	-6.34	106.66	120.60
8	a	404	PHE	CB-CG-CD1	-6.34	116.36	120.80
3	I	563	PHE	CB-CG-CD2	-6.34	116.36	120.80
9	r	62	ASP	CB-CG-OD1	6.34	124.00	118.30
8	n	46	ASP	CB-CG-OD2	6.33	124.00	118.30
2	D	323	PHE	CB-CG-CD1	6.33	125.23	120.80
8	i	202	VAL	CA-CB-CG2	6.33	120.40	110.90
5	L	473	TYR	CZ-CE2-CD2	-6.33	114.10	119.80
1	A	240	ARG	NE-CZ-NH2	-6.33	117.14	120.30
2	D	719	TYR	CA-CB-CG	6.33	125.43	113.40
8	i	283	ALA	N-CA-CB	6.33	118.96	110.10
8	j	311	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	M	684	ARG	NE-CZ-NH1	6.33	123.46	120.30
7	W	636	GLN	N-CA-CB	6.33	121.99	110.60
2	D	705	ILE	O-C-N	6.32	132.82	122.70
3	I	563	PHE	CG-CD2-CE2	-6.32	113.85	120.80
8	i	137	LEU	CB-CG-CD2	6.32	121.75	111.00
8	k	161	TYR	CG-CD2-CE2	-6.32	116.24	121.30
2	F	537	TYR	CB-CG-CD1	-6.32	117.21	121.00
4	J	733	PHE	CB-CG-CD2	-6.32	116.38	120.80
2	N	753	PHE	CB-CG-CD2	-6.32	116.38	120.80
6	P	145	SER	N-CA-CB	-6.32	101.02	110.50
8	i	186	TYR	CG-CD2-CE2	-6.32	116.25	121.30
8	k	343	ARG	NE-CZ-NH1	6.32	123.46	120.30
4	J	939	ARG	NH1-CZ-NH2	-6.31	112.45	119.40
2	N	860	PHE	CB-CG-CD1	-6.31	116.38	120.80
8	c	93	LEU	N-CA-C	-6.31	93.95	111.00
8	f	119	PHE	CB-CG-CD2	-6.31	116.38	120.80
1	E	621	VAL	N-CA-C	-6.31	93.96	111.00
8	n	294	MET	CG-SD-CE	-6.31	90.11	100.20
8	e	60	TYR	CB-CG-CD1	6.31	124.78	121.00
8	i	343	ARG	NE-CZ-NH1	6.31	123.45	120.30
5	L	1630	LEU	CB-CG-CD2	6.30	121.71	111.00
4	J	734	TYR	CB-CG-CD2	6.30	124.78	121.00
8	g	89	GLU	N-CA-CB	6.29	121.93	110.60
8	n	212	ARG	NE-CZ-NH2	-6.29	117.15	120.30
1	E	460	ARG	NE-CZ-NH1	6.29	123.44	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	431	ARG	NE-CZ-NH2	6.29	123.44	120.30
4	J	242	TRP	CG-CD2-CE3	6.29	139.56	133.90
5	L	101	SER	N-CA-CB	6.29	119.93	110.50
7	U	634	HIS	CA-CB-CG	6.29	124.28	113.60
1	C	455	TYR	CG-CD2-CE2	-6.28	116.28	121.30
2	F	686	ASN	N-CA-CB	6.28	121.90	110.60
8	a	409	ARG	NE-CZ-NH2	-6.28	117.16	120.30
7	V	661	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	B	257	PHE	CB-CG-CD1	6.28	125.19	120.80
1	C	324	TRP	CA-CB-CG	6.28	125.62	113.70
2	D	584	LEU	CB-CG-CD2	6.28	121.67	111.00
5	L	1626	PHE	CB-CG-CD2	-6.27	116.41	120.80
7	V	615	ARG	NE-CZ-NH1	6.27	123.44	120.30
8	f	117	ASP	CB-CG-OD1	-6.27	112.66	118.30
2	R	37	ARG	NE-CZ-NH1	6.27	123.43	120.30
1	G	859	TYR	CG-CD1-CE1	-6.26	116.29	121.30
2	B	641	TYR	CB-CG-CD2	-6.26	117.24	121.00
1	G	526	PHE	CD1-CG-CD2	-6.26	110.16	118.30
8	c	53	TYR	CZ-CE2-CD2	-6.26	114.17	119.80
2	F	812	ARG	NH1-CZ-NH2	-6.26	112.52	119.40
8	c	309	ARG	NE-CZ-NH2	-6.26	117.17	120.30
1	G	387	PHE	CB-CG-CD2	-6.25	116.42	120.80
4	J	1002	PHE	CB-CG-CD2	6.25	125.18	120.80
8	b	249	MET	N-CA-C	-6.25	94.11	111.00
1	M	617	PHE	CB-CG-CD1	-6.25	116.42	120.80
8	b	296	ARG	NE-CZ-NH2	6.25	123.42	120.30
8	d	49	ASP	N-CA-CB	6.25	121.85	110.60
2	F	828	GLU	OE1-CD-OE2	6.25	130.80	123.30
2	H	711	VAL	CG1-CB-CG2	-6.25	100.90	110.90
8	n	211	ASN	O-C-N	-6.25	112.70	122.70
8	l	277	THR	CA-CB-CG2	-6.25	103.66	112.40
2	D	257	PHE	CB-CG-CD2	-6.24	116.43	120.80
5	L	1602	ARG	NE-CZ-NH1	6.24	123.42	120.30
1	G	387	PHE	CB-CG-CD1	6.24	125.17	120.80
9	s	14	THR	CA-CB-CG2	-6.24	103.66	112.40
4	J	308	SER	N-CA-C	-6.24	94.16	111.00
8	e	137	LEU	CB-CG-CD1	6.24	121.61	111.00
8	h	425	ARG	NE-CZ-NH2	6.24	123.42	120.30
2	H	254	LEU	CB-CA-C	-6.24	98.35	110.20
2	H	323	PHE	CB-CG-CD1	-6.24	116.43	120.80
8	d	160	ARG	NE-CZ-NH2	-6.24	117.18	120.30
3	K	62	TYR	CB-CG-CD2	6.23	124.74	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	427	TRP	CZ3-CH2-CZ2	-6.23	114.13	121.60
2	H	760	ARG	NE-CZ-NH2	6.23	123.41	120.30
9	s	39	ARG	NE-CZ-NH2	6.23	123.41	120.30
4	J	798	TYR	CB-CG-CD1	-6.22	117.27	121.00
8	b	292	ASP	CB-CG-OD2	6.22	123.90	118.30
2	D	446	PHE	CB-CG-CD2	6.22	125.16	120.80
2	F	644	ASP	CB-CG-OD1	-6.22	112.70	118.30
8	k	282	VAL	CG1-CB-CG2	6.22	120.86	110.90
2	D	306	TYR	CB-CG-CD2	6.22	124.73	121.00
1	A	468	CYS	CB-CA-C	6.21	122.83	110.40
2	B	778	PHE	CB-CG-CD1	6.21	125.15	120.80
1	M	445	VAL	CA-CB-CG1	6.21	120.22	110.90
9	p	39	ARG	NE-CZ-NH2	-6.21	117.19	120.30
8	n	95	GLU	N-CA-CB	6.21	121.78	110.60
1	C	854	MET	CA-CB-CG	6.20	123.84	113.30
1	E	302	TYR	CD1-CE1-CZ	6.20	125.38	119.80
1	E	859	TYR	CZ-CE2-CD2	6.20	125.38	119.80
8	h	217	ARG	NE-CZ-NH2	-6.20	117.20	120.30
8	i	82	TYR	CB-CG-CD2	-6.20	117.28	121.00
5	L	1665	PHE	CB-CG-CD1	-6.20	116.46	120.80
2	N	668	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	D	775	ARG	NE-CZ-NH2	-6.20	117.20	120.30
8	g	152	TYR	CB-CG-CD1	-6.20	117.28	121.00
5	L	369	PHE	CB-CG-CD2	6.19	125.14	120.80
2	N	432	TRP	CG-CD2-CE3	-6.19	128.33	133.90
8	d	86	TYR	CG-CD1-CE1	-6.19	116.35	121.30
8	j	348	PHE	CB-CG-CD2	-6.19	116.47	120.80
8	n	19	PHE	CB-CG-CD2	6.19	125.13	120.80
6	P	106	THR	CA-CB-CG2	-6.18	103.74	112.40
2	H	522	PHE	CB-CG-CD2	6.18	125.13	120.80
6	P	69	TYR	CD1-CE1-CZ	6.18	125.36	119.80
8	d	27	ALA	O-C-N	-6.18	112.81	122.70
8	m	29	HIS	C-N-CA	6.18	135.28	122.30
1	E	324	TRP	CB-CG-CD1	-6.18	118.97	127.00
2	N	875	LEU	CB-CG-CD1	6.18	121.50	111.00
8	h	186	TYR	CZ-CE2-CD2	6.18	125.36	119.80
8	k	294	MET	CG-SD-CE	-6.18	90.32	100.20
2	F	335	TYR	CD1-CE1-CZ	-6.17	114.24	119.80
1	G	275	PHE	CB-CG-CD1	-6.17	116.48	120.80
3	K	654	TYR	CA-CB-CG	-6.17	101.67	113.40
8	j	339	ARG	NE-CZ-NH1	6.17	123.39	120.30
6	P	184	ASP	N-CA-CB	6.17	121.71	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
6	P	372	ARG	NE-CZ-NH2	-6.17	117.21	120.30
8	a	40	PHE	CB-CG-CD1	6.17	125.12	120.80
5	L	10	ASP	CB-CG-OD1	6.17	123.85	118.30
3	K	398	LEU	CB-CG-CD1	6.17	121.48	111.00
1	A	682	ARG	NE-CZ-NH1	6.16	123.38	120.30
1	C	230	ARG	NE-CZ-NH2	-6.16	117.22	120.30
3	I	330	ASP	CB-CG-OD1	-6.16	112.75	118.30
8	h	214	ALA	N-CA-CB	6.16	118.73	110.10
8	k	296	ARG	NE-CZ-NH2	-6.16	117.22	120.30
8	l	225	PHE	CB-CG-CD1	-6.16	116.49	120.80
8	h	60	TYR	CG-CD2-CE2	-6.16	116.37	121.30
8	i	366	TYR	CB-CG-CD2	-6.16	117.30	121.00
2	F	423	TYR	CB-CG-CD2	-6.16	117.31	121.00
2	N	650	VAL	CA-CB-CG2	-6.16	101.66	110.90
8	g	245	TYR	CB-CG-CD2	-6.16	117.30	121.00
8	c	341	ARG	NE-CZ-NH2	-6.16	117.22	120.30
8	k	22	TRP	CG-CD1-NE1	6.15	116.25	110.10
2	B	274	TYR	CG-CD1-CE1	6.15	126.22	121.30
2	N	316	PHE	N-CA-C	-6.15	94.39	111.00
8	h	418	PHE	CB-CG-CD2	6.15	125.10	120.80
8	m	103	ASN	N-CA-C	-6.15	94.40	111.00
4	J	697	CYS	CA-CB-SG	6.15	125.06	114.00
8	a	67	LEU	CB-CG-CD1	6.15	121.45	111.00
8	e	76	SER	N-CA-CB	-6.15	101.28	110.50
2	D	517	ASP	CB-CG-OD2	-6.14	112.77	118.30
2	F	442	TYR	CG-CD1-CE1	6.14	126.22	121.30
1	G	647	CYS	CA-CB-SG	-6.14	102.94	114.00
5	L	1667	PHE	CB-CG-CD1	6.14	125.10	120.80
8	f	388	PHE	CB-CG-CD2	-6.14	116.50	120.80
5	L	1497	ASP	CB-CG-OD2	-6.14	112.77	118.30
2	N	609	ALA	N-CA-CB	6.14	118.70	110.10
8	k	72	ARG	NE-CZ-NH2	-6.14	117.23	120.30
1	G	615	PHE	CB-CG-CD2	-6.14	116.50	120.80
8	e	68	ASP	CB-CG-OD2	-6.13	112.78	118.30
1	A	658	TRP	CB-CG-CD1	-6.13	119.03	127.00
8	g	248	TYR	N-CA-CB	6.13	121.64	110.60
1	G	763	ARG	NE-CZ-NH2	-6.13	117.23	120.30
2	D	262	GLY	N-CA-C	-6.13	97.78	113.10
1	E	324	TRP	CB-CG-CD2	6.13	134.57	126.60
2	H	792	TYR	CB-CG-CD1	-6.13	117.32	121.00
1	M	392	ARG	NE-CZ-NH2	6.13	123.36	120.30
8	k	304	MET	CG-SD-CE	-6.13	90.39	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1688	ARG	CD-NE-CZ	6.12	132.18	123.60
8	b	186	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	E	607	LEU	N-CA-CB	6.12	122.64	110.40
2	H	812	ARG	NE-CZ-NH2	-6.12	117.24	120.30
2	B	764	ASP	CB-CG-OD2	-6.12	112.79	118.30
1	C	744	LEU	CB-CG-CD2	6.12	121.40	111.00
3	I	158	TYR	CG-CD2-CE2	6.12	126.19	121.30
4	J	386	ASP	CB-CG-OD2	-6.12	112.79	118.30
8	l	414	PHE	CB-CG-CD1	-6.12	116.52	120.80
1	C	491	TYR	CG-CD2-CE2	-6.12	116.41	121.30
2	D	539	ASP	CB-CG-OD2	-6.12	112.80	118.30
8	g	343	ARG	NE-CZ-NH1	6.12	123.36	120.30
8	e	48	LYS	O-C-N	6.11	132.48	122.70
1	E	332	ARG	NE-CZ-NH2	6.11	123.36	120.30
8	m	355	SER	N-CA-CB	6.11	119.67	110.50
2	T	66	ARG	N-CA-CB	6.11	121.60	110.60
2	H	878	ARG	O-C-N	-6.11	112.93	122.70
8	j	36	ILE	N-CA-C	-6.11	94.51	111.00
9	t	23	ARG	NE-CZ-NH2	-6.11	117.25	120.30
8	b	288	THR	CA-CB-CG2	-6.11	103.85	112.40
8	k	68	ASP	CB-CG-OD2	-6.11	112.81	118.30
1	M	674	TRP	CB-CG-CD1	6.10	134.93	127.00
2	N	364	ARG	NE-CZ-NH2	-6.10	117.25	120.30
8	g	82	TYR	CB-CG-CD2	-6.10	117.34	121.00
8	j	373	VAL	CG1-CB-CG2	6.10	120.66	110.90
2	D	255	TYR	CB-CG-CD1	-6.10	117.34	121.00
8	m	124	ARG	NE-CZ-NH1	6.10	123.35	120.30
1	A	684	ARG	NE-CZ-NH2	-6.10	117.25	120.30
2	B	522	PHE	CB-CG-CD1	-6.10	116.53	120.80
3	I	572	PHE	CB-CG-CD2	6.10	125.07	120.80
3	I	52	TYR	CG-CD1-CE1	-6.10	116.42	121.30
2	B	367	LEU	CB-CG-CD2	-6.09	100.64	111.00
1	A	261	ARG	CA-CB-CG	6.09	126.80	113.40
8	h	433	ASP	CB-CG-OD1	6.09	123.78	118.30
8	i	292	ASP	CB-CG-OD1	6.09	123.78	118.30
7	X	649	LEU	CB-CG-CD2	-6.08	100.66	111.00
1	A	302	TYR	CG-CD1-CE1	-6.08	116.44	121.30
1	E	387	PHE	CB-CG-CD1	6.08	125.06	120.80
2	F	860	PHE	CB-CG-CD2	6.08	125.06	120.80
5	L	1595	TYR	CG-CD2-CE2	6.08	126.17	121.30
8	k	191	THR	CA-CB-CG2	-6.08	103.89	112.40
8	f	181	VAL	N-CA-C	-6.08	94.58	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	552	TYR	CB-CG-CD2	6.08	124.65	121.00
1	C	243	ARG	NE-CZ-NH1	6.08	123.34	120.30
8	c	317	TYR	CG-CD2-CE2	-6.08	116.44	121.30
2	F	637	PHE	CB-CG-CD2	-6.08	116.55	120.80
3	K	129	PHE	CB-CG-CD1	6.08	125.05	120.80
3	I	468	PRO	O-C-N	6.07	132.42	122.70
8	h	92	TYR	CG-CD1-CE1	-6.07	116.44	121.30
5	L	1662	TYR	CB-CG-CD1	6.07	124.64	121.00
1	C	386	TYR	CB-CG-CD1	-6.07	117.36	121.00
2	H	563	ARG	NE-CZ-NH2	6.07	123.33	120.30
5	L	161	ASP	CB-CG-OD1	6.07	123.76	118.30
5	L	319	ARG	NE-CZ-NH2	-6.07	117.27	120.30
6	P	312	ARG	NE-CZ-NH1	6.07	123.33	120.30
8	f	172	PHE	CD1-CE1-CZ	-6.07	112.82	120.10
2	H	448	ALA	N-CA-CB	6.07	118.59	110.10
5	L	48	PHE	CB-CG-CD1	6.07	125.05	120.80
8	e	333	VAL	CA-CB-CG2	6.07	120.00	110.90
8	l	388	PHE	CB-CG-CD1	6.07	125.05	120.80
8	k	252	ASP	CB-CG-OD2	-6.06	112.84	118.30
8	l	194	ARG	NE-CZ-NH1	6.06	123.33	120.30
2	F	564	TYR	CA-CB-CG	-6.06	101.88	113.40
2	H	719	TYR	CZ-CE2-CD2	6.06	125.26	119.80
1	M	360	ASP	CB-CG-OD2	-6.06	112.84	118.30
2	D	808	ARG	NE-CZ-NH1	6.06	123.33	120.30
8	a	124	ARG	NH1-CZ-NH2	6.06	126.06	119.40
6	P	220	ALA	N-CA-CB	6.06	118.58	110.10
8	f	245	TYR	CA-CB-CG	-6.06	101.89	113.40
2	D	461	ASP	CB-CG-OD1	6.05	123.75	118.30
3	I	466	PHE	CB-CG-CD2	6.05	125.03	120.80
6	P	3	ASP	CB-CG-OD2	6.05	123.75	118.30
2	S	105	ARG	NE-CZ-NH1	6.05	123.33	120.30
8	k	412	ASP	CB-CG-OD1	6.05	123.75	118.30
2	B	847	ARG	NE-CZ-NH1	6.05	123.33	120.30
8	k	187	ASN	CA-CB-CG	6.05	126.71	113.40
6	P	81	ASP	CB-CG-OD1	-6.05	112.86	118.30
8	n	51	PHE	CB-CG-CD1	-6.05	116.57	120.80
1	G	676	ALA	N-CA-CB	6.05	118.56	110.10
3	I	461	PRO	N-CA-C	6.05	127.82	112.10
2	D	482	VAL	CG1-CB-CG2	6.04	120.57	110.90
8	c	3	ARG	NE-CZ-NH2	-6.04	117.28	120.30
1	E	570	ASP	CB-CG-OD2	-6.04	112.86	118.30
8	k	430	GLN	N-CA-CB	6.04	121.48	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	l	401	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	C	688	PHE	CB-CG-CD2	-6.04	116.57	120.80
1	E	867	TYR	CB-CG-CD2	-6.04	117.38	121.00
2	H	652	THR	CA-CB-CG2	-6.04	103.94	112.40
5	L	1529	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	F	672	MET	CG-SD-CE	-6.04	90.54	100.20
3	K	369	PHE	CB-CG-CD1	-6.04	116.57	120.80
8	n	57	ASP	CB-CG-OD2	-6.04	112.87	118.30
8	f	60	TYR	CZ-CE2-CD2	-6.04	114.37	119.80
8	f	270	MET	CG-SD-CE	6.04	109.86	100.20
8	h	160	ARG	NE-CZ-NH2	-6.04	117.28	120.30
8	n	3	ARG	NE-CZ-NH1	-6.04	117.28	120.30
1	M	430	ARG	NE-CZ-NH2	6.03	123.32	120.30
8	g	317	TYR	CB-CG-CD2	-6.03	117.38	121.00
8	n	304	MET	CG-SD-CE	-6.03	90.55	100.20
2	D	468	SER	N-CA-CB	6.03	119.54	110.50
1	E	435	GLN	CG-CD-OE1	-6.03	109.55	121.60
1	G	333	THR	N-CA-CB	6.02	121.74	110.30
5	L	111	ALA	CB-CA-C	-6.02	101.07	110.10
7	W	602	PHE	CB-CG-CD1	-6.02	116.59	120.80
8	m	40	PHE	CB-CA-C	-6.02	98.36	110.40
2	D	251	ARG	CD-NE-CZ	6.01	132.02	123.60
2	N	520	GLU	OE1-CD-OE2	6.01	130.51	123.30
8	b	419	ASP	N-CA-CB	-6.01	99.78	110.60
8	g	82	TYR	CD1-CE1-CZ	6.01	125.21	119.80
8	g	245	TYR	CZ-CE2-CD2	-6.01	114.39	119.80
2	D	405	THR	CA-CB-OG1	6.01	121.62	109.00
8	a	108	PHE	CB-CG-CD1	-6.01	116.59	120.80
1	A	318	LEU	N-CA-CB	6.00	122.41	110.40
4	J	371	PHE	CB-CG-CD1	6.00	125.00	120.80
8	c	245	TYR	CB-CG-CD2	-6.00	117.40	121.00
3	K	331	ARG	O-C-N	-6.00	113.10	122.70
8	n	172	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	G	827	PHE	N-CA-CB	6.00	121.40	110.60
8	m	425	ARG	NE-CZ-NH1	6.00	123.30	120.30
1	E	844	MET	CG-SD-CE	-6.00	90.61	100.20
1	A	631	ARG	NE-CZ-NH1	-5.99	117.30	120.30
1	C	444	LYS	CA-CB-CG	5.99	126.59	113.40
1	C	395	TYR	CG-CD1-CE1	5.99	126.09	121.30
2	D	621	ASP	CB-CG-OD2	-5.99	112.91	118.30
3	I	187	LEU	CB-CG-CD2	5.99	121.18	111.00
3	K	12	TYR	CB-CG-CD1	-5.99	117.41	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	756	MET	CG-SD-CE	-5.99	90.62	100.20
8	b	372	ARG	NE-CZ-NH2	-5.99	117.31	120.30
8	f	279	ASP	CB-CG-OD1	5.99	123.69	118.30
8	h	204	VAL	CG1-CB-CG2	5.99	120.48	110.90
8	i	124	ARG	NE-CZ-NH2	5.98	123.29	120.30
1	M	377	TYR	CB-CG-CD1	-5.98	117.41	121.00
6	P	96	VAL	N-CA-C	-5.98	94.85	111.00
1	C	566	ASP	CB-CG-OD1	-5.98	112.92	118.30
3	K	524	VAL	CA-CB-CG1	-5.98	101.93	110.90
8	h	60	TYR	CB-CG-CD1	-5.98	117.41	121.00
3	I	522	PHE	CB-CG-CD1	5.98	124.98	120.80
2	O	19	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	F	480	ARG	NE-CZ-NH2	-5.98	117.31	120.30
4	J	448	GLU	N-CA-CB	5.98	121.36	110.60
8	h	37	VAL	CA-CB-CG1	-5.98	101.93	110.90
8	h	435	TYR	CB-CG-CD1	5.98	124.59	121.00
1	E	863	PHE	CB-CG-CD1	-5.98	116.62	120.80
3	I	119	ILE	CA-CB-CG1	5.98	122.36	111.00
2	N	805	PHE	CG-CD2-CE2	-5.98	114.23	120.80
1	E	513	ARG	NE-CZ-NH1	5.97	123.29	120.30
4	J	423	THR	N-CA-CB	5.97	121.65	110.30
5	L	404	TYR	CB-CG-CD2	5.97	124.58	121.00
2	B	402	TYR	CB-CG-CD1	5.97	124.58	121.00
2	F	315	ALA	CB-CA-C	-5.97	101.15	110.10
1	C	212	GLN	CB-CA-C	-5.97	98.47	110.40
1	E	527	PHE	CB-CG-CD1	5.97	124.98	120.80
1	M	326	TYR	CG-CD1-CE1	5.97	126.07	121.30
1	A	284	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	G	518	TYR	CB-CG-CD1	-5.96	117.42	121.00
1	A	501	PHE	CB-CG-CD1	-5.96	116.63	120.80
1	A	836	MET	CG-SD-CE	-5.96	90.66	100.20
2	F	430	TYR	CB-CG-CD2	-5.96	117.42	121.00
1	M	236	PRO	N-CA-CB	5.96	110.45	103.30
8	j	303	VAL	CA-CB-CG1	-5.96	101.96	110.90
1	M	282	PHE	CD1-CE1-CZ	5.96	127.25	120.10
8	i	156	ARG	NE-CZ-NH2	5.96	123.28	120.30
8	h	245	TYR	CD1-CE1-CZ	5.96	125.16	119.80
8	k	343	ARG	NH1-CZ-NH2	-5.96	112.85	119.40
1	M	365	TYR	CB-CG-CD2	-5.95	117.43	121.00
8	b	217	ARG	NE-CZ-NH1	-5.95	117.32	120.30
8	g	401	ARG	NE-CZ-NH1	5.95	123.28	120.30
9	t	8	MET	CG-SD-CE	-5.95	90.67	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	472	ARG	NE-CZ-NH2	5.95	123.28	120.30
7	X	621	ASP	CB-CG-OD2	-5.95	112.94	118.30
1	C	525	ASP	N-CA-CB	5.95	121.31	110.60
8	k	160	ARG	NH1-CZ-NH2	5.95	125.94	119.40
1	A	486	ARG	NE-CZ-NH1	5.94	123.27	120.30
2	F	478	GLN	CA-CB-CG	5.94	126.48	113.40
1	E	837	ASP	CB-CG-OD1	5.94	123.65	118.30
3	I	313	ARG	NH1-CZ-NH2	-5.94	112.86	119.40
8	l	248	TYR	CB-CG-CD2	-5.94	117.44	121.00
2	B	442	TYR	CB-CG-CD1	5.94	124.56	121.00
8	d	295	ARG	NE-CZ-NH1	5.94	123.27	120.30
5	L	1478	LEU	CB-CG-CD2	-5.94	100.91	111.00
2	D	335	TYR	CG-CD1-CE1	-5.93	116.55	121.30
1	G	309	LEU	CB-CG-CD2	5.93	121.09	111.00
8	n	100	ALA	C-N-CA	5.93	134.76	122.30
8	n	341	ARG	NE-CZ-NH1	-5.93	117.33	120.30
1	A	658	TRP	CB-CG-CD2	5.93	134.31	126.60
8	a	296	ARG	NH1-CZ-NH2	-5.93	112.87	119.40
8	a	316	CYS	CB-CA-C	-5.93	98.53	110.40
8	n	245	TYR	CG-CD2-CE2	5.93	126.05	121.30
8	f	387	LEU	CB-CG-CD1	5.93	121.08	111.00
1	C	568	PHE	CB-CG-CD1	-5.93	116.65	120.80
1	G	243	ARG	NE-CZ-NH1	5.93	123.26	120.30
1	A	320	LEU	CB-CA-C	-5.92	98.94	110.20
8	c	423	ASN	CB-CG-OD1	-5.92	109.75	121.60
2	F	659	TYR	CB-CG-CD2	-5.92	117.45	121.00
2	H	730	TRP	CD1-NE1-CE2	5.92	114.33	109.00
3	K	512	ILE	CA-CB-CG1	5.92	122.25	111.00
8	f	309	ARG	NE-CZ-NH2	-5.92	117.34	120.30
9	q	37	CYS	CA-CB-SG	-5.92	103.35	114.00
2	B	391	LYS	CA-CB-CG	5.92	126.42	113.40
1	C	571	ASP	CB-CG-OD1	5.92	123.62	118.30
2	D	413	LEU	CB-CG-CD2	5.92	121.06	111.00
1	G	646	TYR	CB-CG-CD1	-5.92	117.45	121.00
6	P	176	LEU	CB-CG-CD1	5.92	121.06	111.00
8	g	248	TYR	N-CA-C	-5.92	95.03	111.00
8	n	123	ASP	CB-CG-OD1	5.92	123.62	118.30
8	f	395	TYR	CB-CG-CD2	5.92	124.55	121.00
8	m	82	TYR	CA-CB-CG	-5.91	102.16	113.40
1	A	430	ARG	NE-CZ-NH1	5.91	123.26	120.30
1	G	847	THR	CA-CB-CG2	-5.91	104.13	112.40
8	k	244	ARG	NE-CZ-NH1	-5.91	117.34	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	l	145	THR	CA-CB-CG2	-5.91	104.12	112.40
3	I	197	LEU	CB-CG-CD1	5.91	121.04	111.00
5	L	1439	SER	N-CA-CB	5.91	119.36	110.50
8	i	160	ARG	NE-CZ-NH1	5.91	123.25	120.30
8	d	270	MET	N-CA-CB	5.91	121.23	110.60
8	l	68	ASP	CB-CG-OD1	5.90	123.61	118.30
2	B	693	MET	CG-SD-CE	-5.90	90.76	100.20
8	j	194	ARG	NH1-CZ-NH2	5.90	125.89	119.40
1	C	314	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	H	689	LEU	CB-CG-CD1	5.90	121.03	111.00
1	M	432	THR	N-CA-CB	5.90	121.50	110.30
8	e	186	TYR	CB-CG-CD1	5.90	124.54	121.00
8	f	67	LEU	N-CA-CB	5.90	122.20	110.40
3	K	13	PRO	C-N-CA	5.90	134.68	122.30
1	A	476	TYR	CB-CG-CD1	-5.89	117.46	121.00
3	I	51	ASP	CB-CG-OD2	-5.89	113.00	118.30
8	e	135	PHE	CB-CG-CD1	-5.89	116.67	120.80
4	J	771	ARG	NE-CZ-NH1	-5.89	117.35	120.30
3	K	100	TYR	CB-CG-CD1	5.89	124.53	121.00
1	C	694	TYR	CB-CG-CD2	5.89	124.53	121.00
8	n	435	TYR	CB-CG-CD2	-5.89	117.47	121.00
5	L	346	VAL	CA-CB-CG1	-5.88	102.07	110.90
5	L	402	ALA	CB-CA-C	-5.88	101.27	110.10
6	P	166	TYR	CG-CD1-CE1	-5.88	116.59	121.30
7	W	671	PHE	CB-CG-CD1	-5.88	116.68	120.80
8	c	360	LEU	CB-CG-CD2	-5.88	101.00	111.00
8	l	206	ASP	CB-CG-OD1	5.88	123.60	118.30
2	B	376	ARG	NE-CZ-NH2	-5.88	117.36	120.30
2	D	376	ARG	NE-CZ-NH1	5.88	123.24	120.30
8	b	156	ARG	NE-CZ-NH1	-5.88	117.36	120.30
1	A	384	ALA	N-CA-CB	5.88	118.33	110.10
8	b	425	ARG	NE-CZ-NH2	-5.88	117.36	120.30
3	I	207	GLN	N-CA-CB	5.88	121.18	110.60
1	M	500	ASP	CB-CG-OD1	5.87	123.59	118.30
1	C	377	TYR	CB-CG-CD1	-5.87	117.48	121.00
2	F	577	MET	CG-SD-CE	5.87	109.59	100.20
2	H	636	VAL	CG1-CB-CG2	5.87	120.30	110.90
8	n	194	ARG	NE-CZ-NH2	-5.87	117.36	120.30
7	V	625	LEU	CB-CG-CD1	5.87	120.98	111.00
1	G	240	ARG	NE-CZ-NH2	-5.87	117.36	120.30
4	J	268	ARG	NE-CZ-NH2	-5.87	117.37	120.30
5	L	1397	GLU	OE1-CD-OE2	-5.87	116.26	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	n	196	THR	CA-CB-CG2	-5.87	104.18	112.40
2	B	431	ARG	NH1-CZ-NH2	-5.87	112.95	119.40
2	H	335	TYR	N-CA-CB	5.87	121.16	110.60
1	E	519	PHE	CB-CG-CD2	-5.87	116.69	120.80
1	G	261	ARG	NE-CZ-NH1	-5.87	117.37	120.30
1	M	549	ARG	N-CA-CB	5.86	121.15	110.60
2	Q	103	ASP	CB-CG-OD2	-5.86	113.02	118.30
8	l	156	ARG	CD-NE-CZ	-5.86	115.39	123.60
2	N	508	VAL	CA-CB-CG1	-5.86	102.11	110.90
1	C	395	TYR	CB-CG-CD2	-5.86	117.49	121.00
2	F	371	PHE	CG-CD2-CE2	-5.86	114.36	120.80
7	X	602	PHE	CB-CG-CD2	-5.86	116.70	120.80
1	E	365	TYR	CG-CD2-CE2	5.86	125.98	121.30
2	F	428	PHE	CB-CG-CD1	5.86	124.90	120.80
3	K	94	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	C	393	TRP	CB-CG-CD1	-5.85	119.39	127.00
2	H	259	GLY	O-C-N	5.85	132.07	122.70
2	F	717	MET	CA-CB-CG	5.85	123.24	113.30
1	G	245	PHE	CB-CG-CD1	5.85	124.89	120.80
8	g	305	VAL	CA-CB-CG1	5.85	119.67	110.90
4	J	755	VAL	CA-CB-CG2	-5.85	102.13	110.90
8	a	94	SER	C-N-CA	5.84	136.31	121.70
4	J	997	VAL	CA-CB-CG2	-5.84	102.14	110.90
5	L	1610	ALA	N-CA-CB	5.84	118.27	110.10
1	C	565	THR	CA-CB-CG2	-5.83	104.23	112.40
3	I	87	ARG	NE-CZ-NH1	5.83	123.22	120.30
8	i	142	ALA	N-CA-CB	5.83	118.27	110.10
8	a	265	ARG	NE-CZ-NH1	5.83	123.22	120.30
1	E	521	MET	CG-SD-CE	-5.83	90.87	100.20
1	A	636	ARG	NE-CZ-NH2	-5.83	117.39	120.30
2	B	473	PHE	N-CA-CB	5.83	121.09	110.60
1	M	431	TYR	CB-CG-CD2	-5.83	117.50	121.00
1	E	342	THR	CA-CB-CG2	-5.83	104.24	112.40
4	J	461	TRP	CH2-CZ2-CE2	5.83	123.22	117.40
2	B	749	ALA	CB-CA-C	-5.82	101.37	110.10
8	j	206	ASP	CB-CG-OD1	-5.82	113.06	118.30
8	b	105	ALA	CB-CA-C	-5.82	101.37	110.10
8	g	265	ARG	N-CA-CB	5.82	121.08	110.60
2	F	589	THR	N-CA-CB	5.82	121.35	110.30
1	M	483	TYR	CG-CD2-CE2	-5.82	116.65	121.30
2	N	251	ARG	NE-CZ-NH2	-5.82	117.39	120.30
3	I	91	ARG	O-C-N	-5.82	113.31	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	517	HIS	CA-CB-CG	5.82	123.49	113.60
8	e	388	PHE	CB-CG-CD1	-5.81	116.73	120.80
5	L	1626	PHE	CB-CG-CD1	5.81	124.87	120.80
2	N	502	ALA	N-CA-CB	5.81	118.24	110.10
3	I	474	TYR	CB-CG-CD1	5.81	124.49	121.00
2	B	662	VAL	CA-CB-CG1	5.81	119.61	110.90
1	C	518	TYR	CA-CB-CG	-5.81	102.36	113.40
5	L	1386	TYR	CD1-CG-CD2	-5.81	111.51	117.90
8	n	159	ASP	CB-CG-OD2	-5.81	113.07	118.30
3	K	203	PHE	CB-CG-CD1	5.81	124.86	120.80
1	A	694	TYR	CG-CD2-CE2	-5.80	116.66	121.30
2	D	831	ARG	NE-CZ-NH1	5.80	123.20	120.30
1	C	508	LEU	CB-CG-CD2	5.80	120.86	111.00
2	F	405	THR	C-N-CA	5.80	134.48	122.30
1	G	360	ASP	CB-CA-C	5.80	122.00	110.40
1	A	619	TYR	CB-CG-CD1	-5.80	117.52	121.00
2	N	778	PHE	CB-CG-CD2	-5.80	116.74	120.80
7	X	623	VAL	CA-CB-CG1	5.80	119.60	110.90
8	l	282	VAL	CG1-CB-CG2	5.80	120.18	110.90
5	L	1505	ARG	NE-CZ-NH2	5.80	123.20	120.30
8	f	169	TYR	CG-CD1-CE1	-5.80	116.66	121.30
8	f	265	ARG	NE-CZ-NH2	5.80	123.20	120.30
2	O	69	ALA	CB-CA-C	-5.79	101.41	110.10
8	b	87	ASN	CB-CA-C	-5.79	98.81	110.40
8	g	106	SER	N-CA-CB	5.79	119.19	110.50
8	a	270	MET	CG-SD-CE	-5.79	90.93	100.20
8	g	292	ASP	CB-CG-OD2	5.79	123.51	118.30
9	t	29	LEU	CB-CG-CD1	5.79	120.85	111.00
8	g	176	ASP	CB-CG-OD1	5.79	123.51	118.30
8	c	186	TYR	CG-CD1-CE1	-5.79	116.67	121.30
8	g	92	TYR	CG-CD1-CE1	-5.79	116.67	121.30
8	m	216	ASP	CB-CG-OD1	5.79	123.51	118.30
4	J	507	THR	CA-CB-CG2	-5.79	104.30	112.40
8	l	367	LEU	CA-C-N	5.79	133.30	117.10
8	a	217	ARG	NE-CZ-NH2	-5.79	117.41	120.30
8	d	395	TYR	CB-CG-CD1	-5.79	117.53	121.00
8	k	311	ARG	NE-CZ-NH1	5.79	123.19	120.30
1	A	763	ARG	NH1-CZ-NH2	-5.78	113.04	119.40
6	P	225	GLN	CA-CB-CG	5.78	126.12	113.40
8	g	21	PHE	CB-CG-CD2	-5.78	116.75	120.80
2	N	843	ARG	NE-CZ-NH1	5.78	123.19	120.30
8	b	161	TYR	CB-CG-CD1	5.78	124.47	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	i	327	GLU	N-CA-CB	5.78	121.00	110.60
1	E	694	TYR	CG-CD2-CE2	-5.78	116.68	121.30
7	W	666	ARG	CB-CA-C	-5.78	98.84	110.40
3	K	486	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	M	483	TYR	CB-CG-CD1	5.78	124.47	121.00
1	M	849	ASP	CB-CG-OD2	-5.77	113.10	118.30
1	C	431	TYR	CB-CG-CD1	5.77	124.46	121.00
2	D	314	ARG	NE-CZ-NH2	5.77	123.19	120.30
2	F	625	LEU	CB-CG-CD2	5.77	120.81	111.00
3	I	331	ARG	NE-CZ-NH2	-5.77	117.41	120.30
5	L	505	LEU	CB-CG-CD1	5.77	120.81	111.00
5	L	1595	TYR	CB-CG-CD1	5.77	124.46	121.00
8	f	108	PHE	CB-CG-CD2	5.77	124.84	120.80
3	I	118	SER	N-CA-CB	5.77	119.15	110.50
8	j	366	TYR	CD1-CE1-CZ	5.77	124.99	119.80
2	B	288	ASP	CB-CG-OD2	-5.77	113.11	118.30
2	H	428	PHE	CB-CG-CD2	5.77	124.84	120.80
2	T	16	LEU	CB-CG-CD1	5.77	120.80	111.00
8	f	86	TYR	CG-CD1-CE1	5.77	125.91	121.30
1	G	866	PHE	CB-CG-CD1	5.76	124.83	120.80
2	N	868	THR	CA-CB-CG2	-5.76	104.33	112.40
8	g	152	TYR	CG-CD1-CE1	-5.76	116.69	121.30
8	l	378	MET	N-CA-C	-5.76	95.44	111.00
8	h	317	TYR	CG-CD1-CE1	-5.76	116.69	121.30
8	b	92	TYR	N-CA-CB	5.76	120.97	110.60
8	j	45	THR	CA-CB-CG2	-5.76	104.33	112.40
8	l	391	THR	CA-CB-CG2	-5.76	104.33	112.40
1	G	751	MET	CA-CB-CG	5.76	123.09	113.30
8	j	366	TYR	CB-CG-CD1	-5.76	117.54	121.00
3	K	486	ARG	NH1-CZ-NH2	5.76	125.73	119.40
8	a	2	PRO	CA-N-CD	-5.76	103.44	111.50
8	i	10	LEU	CA-CB-CG	5.76	128.54	115.30
3	K	158	TYR	CG-CD2-CE2	5.75	125.90	121.30
8	a	124	ARG	CD-NE-CZ	5.75	131.66	123.60
8	d	242	THR	CA-CB-CG2	-5.75	104.34	112.40
2	F	430	TYR	CG-CD1-CE1	-5.75	116.70	121.30
5	L	168	TYR	CB-CG-CD1	-5.75	117.55	121.00
2	T	89	ASN	N-CA-CB	5.75	120.95	110.60
1	E	739	THR	CA-CB-OG1	5.75	121.07	109.00
8	h	161	TYR	CB-CG-CD2	5.75	124.45	121.00
8	h	317	TYR	CD1-CE1-CZ	5.75	124.97	119.80
8	j	328	VAL	CA-CB-CG1	5.75	119.52	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	380	LEU	CB-CG-CD2	5.75	120.77	111.00
1	A	365	TYR	CG-CD2-CE2	-5.74	116.71	121.30
8	a	169	TYR	CB-CG-CD2	-5.74	117.55	121.00
8	h	425	ARG	O-C-N	-5.74	113.51	122.70
8	k	161	TYR	CB-CG-CD2	-5.74	117.55	121.00
8	h	329	ASP	N-CA-C	-5.74	95.50	111.00
2	H	585	VAL	CA-CB-CG1	-5.74	102.29	110.90
5	L	400	GLN	CA-CB-CG	5.74	126.03	113.40
8	h	319	ALA	N-CA-CB	5.74	118.14	110.10
1	G	282	PHE	CG-CD1-CE1	-5.74	114.49	120.80
5	L	522	LEU	CB-CG-CD2	-5.74	101.24	111.00
8	g	51	PHE	CB-CG-CD1	-5.74	116.78	120.80
2	F	442	TYR	CD1-CE1-CZ	-5.74	114.64	119.80
6	P	103	VAL	CA-CB-CG2	-5.74	102.30	110.90
8	c	212	ARG	NE-CZ-NH2	5.74	123.17	120.30
2	N	567	LEU	N-CA-CB	5.73	121.86	110.40
8	m	396	ASP	CB-CG-OD1	5.73	123.46	118.30
4	J	458	PHE	CB-CG-CD2	5.73	124.81	120.80
4	J	988	PHE	CB-CG-CD1	5.73	124.81	120.80
1	M	559	ARG	NE-CZ-NH1	-5.73	117.44	120.30
2	T	90	ARG	NH1-CZ-NH2	-5.73	113.10	119.40
8	f	72	ARG	NH1-CZ-NH2	-5.73	113.10	119.40
2	F	623	ARG	NH1-CZ-NH2	-5.72	113.10	119.40
1	G	325	PHE	CZ-CE2-CD2	-5.72	113.23	120.10
2	H	298	TRP	CD1-CG-CD2	-5.72	101.72	106.30
2	H	851	HIS	N-CA-CB	5.72	120.90	110.60
8	h	161	TYR	CD1-CE1-CZ	-5.72	114.65	119.80
6	P	240	TYR	CB-CG-CD2	-5.72	117.57	121.00
8	i	244	ARG	NE-CZ-NH2	-5.72	117.44	120.30
8	k	135	PHE	CZ-CE2-CD2	5.72	126.97	120.10
1	E	688	PHE	N-CA-CB	5.72	120.90	110.60
3	I	382	THR	CA-CB-OG1	5.72	121.01	109.00
3	I	511	ALA	CB-CA-C	-5.72	101.52	110.10
4	J	466	ARG	NH1-CZ-NH2	5.72	125.69	119.40
8	l	286	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	F	612	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	M	222	TYR	CB-CG-CD2	-5.71	117.57	121.00
8	e	273	TYR	CB-CG-CD1	5.71	124.43	121.00
8	h	170	SER	N-CA-CB	5.71	119.07	110.50
1	G	694	TYR	CG-CD2-CE2	-5.71	116.73	121.30
8	i	56	ASP	CB-CG-OD2	5.71	123.44	118.30
2	D	306	TYR	CB-CG-CD1	-5.71	117.58	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1402	PHE	CB-CG-CD2	-5.71	116.81	120.80
8	g	435	TYR	CB-CG-CD2	-5.71	117.58	121.00
1	G	549	ARG	NE-CZ-NH2	5.71	123.15	120.30
8	k	338	GLN	CA-CB-CG	5.71	125.95	113.40
8	d	115	HIS	CA-CB-CG	5.70	123.30	113.60
8	e	354	ALA	N-CA-CB	-5.70	102.11	110.10
8	c	108	PHE	CB-CG-CD1	-5.70	116.81	120.80
8	e	362	ARG	NH1-CZ-NH2	5.70	125.67	119.40
8	i	433	ASP	N-CA-CB	5.70	120.86	110.60
8	b	169	TYR	CB-CG-CD2	5.70	124.42	121.00
8	i	366	TYR	C-N-CA	5.70	135.95	121.70
1	G	867	TYR	CA-CB-CG	5.70	124.23	113.40
8	e	265	ARG	N-CA-CB	5.70	120.86	110.60
8	l	428	VAL	CA-CB-CG2	-5.70	102.35	110.90
2	N	869	ASP	N-CA-CB	5.70	120.85	110.60
8	a	416	ASP	CB-CG-OD2	-5.70	113.17	118.30
8	d	47	ARG	NE-CZ-NH1	-5.70	117.45	120.30
8	e	252	ASP	N-CA-C	-5.70	95.62	111.00
2	N	431	ARG	N-CA-CB	5.69	120.84	110.60
2	N	543	TYR	CB-CG-CD1	5.69	124.41	121.00
4	J	396	ASP	CB-CG-OD2	-5.69	113.18	118.30
2	N	434	TYR	CB-CG-CD2	-5.69	117.59	121.00
8	e	40	PHE	CB-CG-CD2	5.69	124.78	120.80
2	D	246	GLU	OE1-CD-OE2	-5.69	116.48	123.30
1	G	528	VAL	CA-CB-CG2	-5.69	102.37	110.90
8	d	366	TYR	CZ-CE2-CD2	-5.69	114.68	119.80
4	J	714	TYR	CB-CG-CD1	5.68	124.41	121.00
1	M	699	GLU	OE1-CD-OE2	5.68	130.12	123.30
1	M	253	SER	N-CA-CB	5.68	119.02	110.50
8	l	361	SER	N-CA-CB	5.68	119.02	110.50
3	I	168	VAL	CA-CB-CG1	5.68	119.42	110.90
3	I	449	TRP	CB-CG-CD2	5.68	133.98	126.60
2	T	47	VAL	CA-CB-CG1	-5.68	102.38	110.90
8	f	416	ASP	CB-CG-OD1	-5.68	113.19	118.30
8	n	157	LEU	CB-CA-C	-5.68	99.42	110.20
9	q	30	ASP	C-N-CA	5.68	135.89	121.70
2	S	64	ARG	NE-CZ-NH1	5.67	123.14	120.30
8	c	181	VAL	N-CA-C	-5.67	95.68	111.00
8	h	317	TYR	CB-CG-CD2	5.67	124.40	121.00
8	n	53	TYR	CG-CD1-CE1	5.67	125.84	121.30
1	M	635	THR	N-CA-CB	5.67	121.07	110.30
2	B	255	TYR	CB-CG-CD1	5.67	124.40	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	410	MET	CA-CB-CG	5.67	122.94	113.30
8	b	202	VAL	CA-CB-CG1	5.67	119.40	110.90
2	D	313	ASP	CB-CG-OD1	-5.67	113.20	118.30
5	L	208	PHE	CB-CG-CD2	5.67	124.77	120.80
8	i	22	TRP	CE3-CZ3-CH2	5.67	127.43	121.20
5	L	361	LEU	CB-CG-CD1	5.67	120.63	111.00
1	E	302	TYR	CG-CD2-CE2	5.66	125.83	121.30
2	D	385	ASP	CB-CG-OD1	5.66	123.40	118.30
3	K	161	SER	N-CA-CB	5.66	118.99	110.50
5	L	1524	TRP	CE2-CD2-CG	-5.66	102.77	107.30
4	J	877	ARG	CG-CD-NE	-5.66	99.91	111.80
8	j	366	TYR	CG-CD1-CE1	-5.66	116.77	121.30
2	D	868	THR	CA-CB-CG2	-5.66	104.48	112.40
6	P	120	THR	CA-CB-CG2	5.66	120.32	112.40
8	j	348	PHE	CB-CG-CD1	5.66	124.76	120.80
1	E	284	TYR	CG-CD1-CE1	-5.66	116.78	121.30
8	k	82	TYR	CB-CG-CD1	-5.66	117.61	121.00
8	k	402	GLU	N-CA-CB	5.66	120.78	110.60
2	H	591	LEU	CB-CG-CD2	5.65	120.61	111.00
7	U	669	ALA	CB-CA-C	-5.65	101.62	110.10
8	e	163	LYS	N-CA-C	-5.65	95.73	111.00
8	c	278	THR	CA-CB-CG2	-5.65	104.48	112.40
5	L	506	TYR	CB-CG-CD2	-5.65	117.61	121.00
8	i	24	GLN	CG-CD-OE1	5.65	132.90	121.60
1	G	319	SER	N-CA-CB	5.65	118.97	110.50
8	d	418	PHE	CB-CG-CD2	5.65	124.75	120.80
1	C	518	TYR	CB-CG-CD1	5.65	124.39	121.00
8	a	95	GLU	O-C-N	5.65	131.74	122.70
8	m	202	VAL	CG1-CB-CG2	5.65	119.94	110.90
2	B	385	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	C	576	LEU	CB-CG-CD1	5.65	120.60	111.00
2	D	562	ARG	NE-CZ-NH1	5.64	123.12	120.30
2	N	314	ARG	NE-CZ-NH2	5.64	123.12	120.30
8	d	22	TRP	CD1-NE1-CE2	5.64	114.08	109.00
2	F	778	PHE	CB-CG-CD2	5.64	124.75	120.80
8	j	184	GLN	CA-C-O	-5.64	108.26	120.10
2	H	294	SER	CB-CA-C	-5.64	99.39	110.10
2	B	264	PHE	CB-CG-CD1	-5.63	116.86	120.80
4	J	405	LEU	CB-CG-CD1	5.63	120.58	111.00
3	K	533	VAL	CA-CB-CG1	5.63	119.35	110.90
1	M	282	PHE	CG-CD1-CE1	-5.63	114.60	120.80
8	e	343	ARG	CD-NE-CZ	5.63	131.49	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	k	142	ALA	N-CA-CB	5.63	117.99	110.10
2	H	364	ARG	NE-CZ-NH2	-5.63	117.48	120.30
2	H	434	TYR	CB-CG-CD2	-5.63	117.62	121.00
3	I	111	PHE	CB-CG-CD1	5.63	124.74	120.80
8	f	138	CYS	N-CA-CB	-5.63	100.46	110.60
8	h	412	ASP	N-CA-CB	5.63	120.74	110.60
8	e	176	ASP	CB-CG-OD2	-5.63	113.23	118.30
8	k	131	SER	N-CA-CB	5.63	118.95	110.50
1	M	302	TYR	N-CA-CB	-5.63	100.47	110.60
8	m	209	ALA	N-CA-CB	5.63	117.98	110.10
2	D	518	ALA	CB-CA-C	-5.63	101.66	110.10
3	K	514	TRP	CE3-CZ3-CH2	-5.63	115.01	121.20
8	i	244	ARG	NH1-CZ-NH2	5.63	125.59	119.40
4	J	955	VAL	CG1-CB-CG2	-5.62	101.90	110.90
5	L	1524	TRP	CE2-CD2-CE3	5.62	125.45	118.70
8	m	435	TYR	CG-CD2-CE2	-5.62	116.80	121.30
8	e	19	PHE	CB-CG-CD1	5.62	124.74	120.80
8	k	184	GLN	CA-C-N	5.62	132.84	117.10
2	H	737	VAL	CA-CB-CG1	-5.62	102.47	110.90
8	f	425	ARG	NE-CZ-NH1	5.62	123.11	120.30
8	m	7	THR	CA-CB-CG2	5.62	120.27	112.40
7	X	614	PHE	CB-CG-CD1	5.62	124.73	120.80
1	C	676	ALA	N-CA-CB	5.62	117.97	110.10
1	G	736	CYS	O-C-N	-5.62	113.71	122.70
8	h	52	PHE	CB-CA-C	-5.62	99.17	110.40
8	d	286	ARG	C-N-CA	5.62	135.74	121.70
8	n	60	TYR	CG-CD1-CE1	-5.62	116.81	121.30
1	G	227	VAL	CA-CB-CG1	5.61	119.32	110.90
8	b	342	GLU	OE1-CD-OE2	-5.61	116.57	123.30
8	g	186	TYR	CB-CG-CD1	-5.61	117.63	121.00
9	s	26	ASN	N-CA-CB	5.61	120.70	110.60
8	e	130	ASP	CB-CG-OD2	5.61	123.35	118.30
3	I	633	ARG	NE-CZ-NH2	-5.61	117.50	120.30
1	E	831	PHE	CB-CG-CD1	-5.61	116.88	120.80
2	H	261	ASP	CB-CG-OD2	-5.61	113.25	118.30
2	H	768	ARG	NH1-CZ-NH2	-5.61	113.23	119.40
8	e	51	PHE	CB-CG-CD2	-5.61	116.88	120.80
8	m	131	SER	N-CA-CB	5.61	118.91	110.50
8	a	131	SER	N-CA-CB	5.61	118.91	110.50
2	D	480	ARG	NE-CZ-NH1	5.60	123.10	120.30
2	B	301	ASN	O-C-N	-5.60	113.74	122.70
1	G	302	TYR	CD1-CG-CD2	-5.60	111.74	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	b	52	PHE	CB-CG-CD2	-5.60	116.88	120.80
8	l	294	MET	CG-SD-CE	-5.60	91.24	100.20
1	E	531	MET	CG-SD-CE	-5.60	91.24	100.20
8	g	390	ARG	NE-CZ-NH2	5.60	123.10	120.30
1	C	694	TYR	CB-CG-CD1	-5.60	117.64	121.00
5	L	1437	LEU	CA-CB-CG	5.60	128.18	115.30
8	g	172	PHE	CB-CG-CD1	-5.60	116.88	120.80
2	H	680	TRP	CZ3-CH2-CZ2	-5.60	114.88	121.60
8	g	22	TRP	CA-CB-CG	5.60	124.33	113.70
8	j	388	PHE	CB-CG-CD2	5.60	124.72	120.80
8	f	339	ARG	NE-CZ-NH2	-5.60	117.50	120.30
8	b	422	ASP	CB-CG-OD1	5.59	123.33	118.30
8	a	329	ASP	CB-CG-OD2	-5.59	113.27	118.30
8	g	265	ARG	NE-CZ-NH2	-5.59	117.50	120.30
2	H	431	ARG	N-CA-CB	5.59	120.66	110.60
1	C	368	ASP	CB-CG-OD1	5.59	123.33	118.30
2	D	380	LEU	CB-CG-CD2	5.59	120.50	111.00
1	M	332	ARG	NE-CZ-NH1	5.59	123.09	120.30
7	W	658	GLU	OE1-CD-OE2	5.59	130.01	123.30
8	f	45	THR	N-CA-C	-5.59	95.91	111.00
1	A	698	PHE	CB-CG-CD2	-5.59	116.89	120.80
1	E	452	THR	CA-CB-CG2	5.59	120.22	112.40
8	a	413	ILE	N-CA-C	-5.59	95.92	111.00
8	k	29	HIS	CA-CB-CG	5.59	123.10	113.60
1	G	427	TRP	CH2-CZ2-CE2	5.58	122.98	117.40
3	K	341	TRP	CB-CG-CD2	5.58	133.86	126.60
8	g	51	PHE	CB-CG-CD2	5.58	124.71	120.80
8	k	401	ARG	NH1-CZ-NH2	-5.58	113.26	119.40
8	l	394	GLN	O-C-N	-5.58	113.77	122.70
8	c	296	ARG	NE-CZ-NH1	5.58	123.09	120.30
8	d	160	ARG	NE-CZ-NH1	-5.58	117.51	120.30
8	e	273	TYR	CD1-CG-CD2	-5.58	111.77	117.90
2	D	429	LEU	CB-CG-CD2	5.58	120.48	111.00
1	G	481	GLN	CB-CA-C	-5.58	99.25	110.40
4	J	704	THR	O-C-N	-5.58	113.78	122.70
8	b	139	HIS	CA-CB-CG	5.58	123.08	113.60
2	F	648	ALA	CB-CA-C	-5.57	101.74	110.10
1	G	652	ARG	NE-CZ-NH2	-5.57	117.51	120.30
1	G	867	TYR	CD1-CG-CD2	5.57	124.03	117.90
8	f	366	TYR	CD1-CG-CD2	5.57	124.03	117.90
8	l	401	ARG	NH1-CZ-NH2	5.57	125.53	119.40
1	A	867	TYR	CG-CD2-CE2	5.57	125.75	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	181	VAL	CA-CB-CG2	-5.57	102.55	110.90
8	b	104	TRP	CA-CB-CG	5.57	124.28	113.70
8	e	416	ASP	CB-CG-OD1	-5.57	113.29	118.30
8	h	92	TYR	CZ-CE2-CD2	-5.57	114.79	119.80
8	k	324	ILE	CA-CB-CG1	-5.57	100.42	111.00
1	G	282	PHE	CB-CG-CD1	-5.57	116.90	120.80
2	N	693	MET	CG-SD-CE	5.57	109.11	100.20
8	f	212	ARG	NH1-CZ-NH2	5.57	125.52	119.40
8	l	293	VAL	CG1-CB-CG2	5.57	119.81	110.90
2	B	751	ASP	CB-CG-OD1	5.56	123.31	118.30
8	e	437	ALA	CB-CA-C	-5.56	101.75	110.10
1	E	493	TYR	CD1-CE1-CZ	-5.56	114.79	119.80
2	T	50	ASP	N-CA-C	-5.56	95.98	111.00
8	e	50	VAL	CG1-CB-CG2	5.56	119.80	110.90
2	H	873	ARG	NH1-CZ-NH2	-5.56	113.29	119.40
5	L	573	TYR	CG-CD2-CE2	-5.56	116.86	121.30
8	a	180	HIS	N-CA-C	-5.56	95.99	111.00
8	a	242	THR	CA-CB-CG2	-5.56	104.62	112.40
8	a	414	PHE	CG-CD1-CE1	-5.56	114.69	120.80
9	s	37	CYS	N-CA-CB	5.56	120.60	110.60
2	H	849	LEU	CB-CG-CD1	5.55	120.44	111.00
1	M	456	LEU	CB-CG-CD2	5.55	120.44	111.00
8	f	435	TYR	CB-CG-CD1	5.55	124.33	121.00
8	i	214	ALA	N-CA-CB	5.55	117.87	110.10
1	A	443	GLN	O-C-N	-5.55	113.82	122.70
2	H	564	TYR	CG-CD1-CE1	-5.55	116.86	121.30
4	J	601	HIS	N-CA-CB	5.55	120.58	110.60
8	d	366	TYR	CB-CG-CD2	-5.55	117.67	121.00
8	i	63	ARG	NE-CZ-NH2	5.55	123.07	120.30
8	l	59	HIS	CA-CB-CG	5.54	123.03	113.60
1	M	265	VAL	CA-CB-CG1	5.54	119.22	110.90
2	N	461	ASP	CB-CG-OD1	-5.54	113.31	118.30
2	N	874	PHE	CB-CG-CD2	-5.54	116.92	120.80
4	J	283	PHE	CZ-CE2-CD2	-5.54	113.45	120.10
1	M	404	SER	CB-CA-C	5.54	120.63	110.10
7	U	607	ILE	N-CA-CB	5.54	123.55	110.80
1	G	259	VAL	CA-CB-CG2	-5.54	102.59	110.90
2	H	802	ARG	NE-CZ-NH1	5.54	123.07	120.30
1	M	544	ASP	CB-CG-OD2	-5.54	113.31	118.30
8	f	391	THR	CA-CB-CG2	-5.54	104.65	112.40
1	E	486	ARG	NE-CZ-NH2	5.54	123.07	120.30
2	D	411	ARG	NE-CZ-NH1	5.54	123.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	45	ASP	CB-CG-OD1	5.54	123.28	118.30
2	F	853	TYR	CG-CD1-CE1	5.53	125.73	121.30
1	M	843	SER	CB-CA-C	-5.53	99.59	110.10
8	i	22	TRP	CD1-CG-CD2	-5.53	101.87	106.30
2	H	612	ASP	CA-CB-CG	-5.53	101.23	113.40
1	M	617	PHE	CG-CD2-CE2	-5.53	114.72	120.80
8	c	395	TYR	CD1-CG-CD2	5.53	123.98	117.90
2	B	877	PHE	CG-CD2-CE2	-5.53	114.72	120.80
3	K	115	PRO	N-CA-CB	-5.53	96.52	102.60
7	V	647	TYR	CZ-CE2-CD2	5.53	124.78	119.80
8	d	418	PHE	CB-CG-CD1	-5.53	116.93	120.80
8	k	234	THR	CA-CB-OG1	5.53	120.61	109.00
1	G	308	GLN	N-CA-CB	5.53	120.55	110.60
6	P	187	ASP	CB-CG-OD2	-5.53	113.33	118.30
1	C	293	ALA	CB-CA-C	-5.53	101.81	110.10
2	F	792	TYR	CB-CG-CD1	5.53	124.32	121.00
8	c	292	ASP	CB-CG-OD2	5.53	123.27	118.30
9	t	18	LEU	CB-CG-CD1	5.53	120.39	111.00
8	n	152	TYR	CD1-CG-CD2	5.52	123.98	117.90
2	D	438	LEU	CB-CA-C	-5.52	99.71	110.20
8	c	240	THR	N-CA-C	-5.52	96.09	111.00
8	l	152	TYR	CG-CD2-CE2	-5.52	116.88	121.30
1	G	236	PRO	N-CA-CB	5.52	109.92	103.30
2	H	752	VAL	CA-CB-CG1	5.52	119.18	110.90
1	C	388	ASP	CB-CG-OD2	5.52	123.27	118.30
3	K	260	ARG	N-CA-CB	5.52	120.53	110.60
2	O	36	VAL	CA-CB-CG2	-5.52	102.62	110.90
2	R	74	PHE	CB-CG-CD1	-5.52	116.94	120.80
8	m	86	TYR	CG-CD1-CE1	5.52	125.72	121.30
4	J	999	ARG	N-CA-CB	5.52	120.53	110.60
1	M	455	TYR	CZ-CE2-CD2	5.52	124.77	119.80
2	R	49	ARG	NE-CZ-NH2	-5.52	117.54	120.30
1	C	631	ARG	NE-CZ-NH1	5.51	123.06	120.30
8	a	385	SER	N-CA-CB	5.51	118.77	110.50
8	a	366	TYR	N-CA-C	-5.51	96.12	111.00
8	c	373	VAL	CA-CB-CG1	-5.51	102.63	110.90
8	n	47	ARG	CD-NE-CZ	5.51	131.32	123.60
5	L	68	VAL	CA-CB-CG2	-5.51	102.63	110.90
1	M	831	PHE	CG-CD1-CE1	5.51	126.86	120.80
8	d	225	PHE	CB-CG-CD2	-5.51	116.94	120.80
3	K	7	LEU	N-CA-CB	5.51	121.42	110.40
8	m	104	TRP	CD1-CG-CD2	-5.51	101.89	106.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	782	ALA	N-CA-CB	5.51	117.81	110.10
8	c	401	ARG	C-N-CA	5.51	135.46	121.70
8	d	152	TYR	CB-CG-CD2	5.51	124.30	121.00
8	f	160	ARG	NE-CZ-NH1	5.51	123.05	120.30
2	F	270	SER	N-CA-CB	5.50	118.76	110.50
3	K	649	ASP	O-C-N	-5.50	113.89	122.70
2	Q	28	VAL	CA-CB-CG2	5.50	119.16	110.90
8	f	161	TYR	CD1-CE1-CZ	-5.50	114.84	119.80
2	F	680	TRP	CB-CG-CD2	-5.50	119.45	126.60
8	k	247	GLY	O-C-N	5.50	131.50	122.70
1	A	715	ALA	N-CA-CB	5.50	117.80	110.10
1	M	847	THR	CA-CB-CG2	-5.50	104.70	112.40
1	M	722	LEU	CB-CG-CD2	5.50	120.35	111.00
2	D	273	CYS	C-N-CA	5.50	135.45	121.70
8	h	433	ASP	CB-CG-OD2	-5.50	113.35	118.30
2	B	875	LEU	CB-CG-CD2	5.50	120.34	111.00
2	H	444	GLU	CA-CB-CG	5.50	125.49	113.40
5	L	1670	VAL	CA-CB-CG2	-5.50	102.66	110.90
1	C	368	ASP	CB-CG-OD2	-5.49	113.36	118.30
2	F	538	PHE	CB-CG-CD1	-5.49	116.95	120.80
4	J	392	ALA	N-CA-CB	5.49	117.79	110.10
3	K	522	PHE	CB-CG-CD1	5.49	124.65	120.80
4	J	252	LEU	N-CA-CB	5.49	121.38	110.40
1	M	861	LEU	CA-CB-CG	5.49	127.93	115.30
1	E	631	ARG	NE-CZ-NH1	5.49	123.05	120.30
1	C	704	THR	CA-CB-CG2	5.49	120.08	112.40
1	C	637	TYR	CB-CG-CD1	-5.49	117.71	121.00
2	F	334	TYR	CB-CG-CD2	-5.49	117.71	121.00
8	l	82	TYR	CB-CG-CD2	5.48	124.29	121.00
1	G	302	TYR	CG-CD1-CE1	5.48	125.69	121.30
2	H	471	PRO	N-CA-CB	5.48	109.88	103.30
5	L	1601	PHE	CB-CG-CD1	-5.48	116.96	120.80
8	f	135	PHE	CB-CG-CD2	-5.48	116.96	120.80
2	D	261	ASP	CB-CG-OD2	-5.48	113.37	118.30
1	E	530	PHE	CB-CG-CD1	5.48	124.64	120.80
2	F	512	ALA	N-CA-CB	5.48	117.77	110.10
4	J	776	PHE	CB-CG-CD1	-5.48	116.96	120.80
1	G	243	ARG	N-CA-CB	5.48	120.46	110.60
8	b	217	ARG	NE-CZ-NH2	5.48	123.04	120.30
1	G	370	GLN	CB-CA-C	-5.48	99.44	110.40
1	M	759	ASN	N-CA-CB	5.48	120.46	110.60
6	P	186	THR	CA-CB-CG2	-5.48	104.73	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	e	296	ARG	NE-CZ-NH1	5.48	123.04	120.30
8	f	22	TRP	CH2-CZ2-CE2	-5.48	111.92	117.40
8	g	258	ALA	CB-CA-C	-5.48	101.88	110.10
8	h	437	ALA	N-CA-CB	5.48	117.77	110.10
8	k	199	ALA	N-CA-CB	5.48	117.77	110.10
8	k	395	TYR	CB-CG-CD1	-5.47	117.72	121.00
3	K	626	PHE	CB-CG-CD1	-5.47	116.97	120.80
2	N	269	ASN	N-CA-C	-5.47	96.22	111.00
8	c	247	GLY	N-CA-C	-5.47	99.42	113.10
8	h	199	ALA	N-CA-CB	5.47	117.76	110.10
1	E	399	ILE	N-CA-C	-5.47	96.23	111.00
2	H	499	GLN	CA-CB-CG	5.47	125.44	113.40
8	b	206	ASP	CB-CG-OD2	-5.47	113.38	118.30
5	L	535	PHE	CB-CG-CD2	5.47	124.63	120.80
1	M	694	TYR	CG-CD1-CE1	-5.47	116.92	121.30
8	j	180	HIS	N-CA-C	-5.47	96.24	111.00
4	J	375	LEU	CB-CG-CD1	5.47	120.29	111.00
8	m	100	ALA	C-N-CA	5.47	133.78	122.30
8	n	245	TYR	CD1-CG-CD2	-5.47	111.89	117.90
2	B	315	ALA	N-CA-CB	5.46	117.75	110.10
1	G	365	TYR	CB-CG-CD2	5.46	124.28	121.00
2	H	264	PHE	CB-CG-CD1	-5.46	116.97	120.80
8	h	65	VAL	CG1-CB-CG2	5.46	119.64	110.90
4	J	472	VAL	CA-CB-CG1	5.46	119.09	110.90
3	K	390	HIS	CA-CB-CG	5.46	122.88	113.60
5	L	392	ASP	CB-CG-OD1	-5.46	113.39	118.30
2	B	699	VAL	CA-CB-CG2	-5.46	102.71	110.90
6	P	53	TYR	CD1-CG-CD2	-5.46	111.90	117.90
8	d	408	PHE	CB-CG-CD2	5.46	124.62	120.80
8	j	68	ASP	CB-CG-OD1	-5.46	113.39	118.30
8	m	296	ARG	NE-CZ-NH2	-5.46	117.57	120.30
3	K	649	ASP	CA-CB-CG	5.46	125.40	113.40
8	g	348	PHE	CA-CB-CG	-5.45	100.81	113.90
2	D	805	PHE	CB-CG-CD1	-5.45	116.98	120.80
8	a	2	PRO	N-CD-CG	5.45	111.38	103.20
8	c	181	VAL	CB-CA-C	5.45	121.75	111.40
8	k	112	GLU	N-CA-CB	5.45	120.41	110.60
8	k	277	THR	N-CA-CB	5.45	120.65	110.30
6	P	342	GLY	C-N-CA	5.45	133.74	122.30
2	F	674	TYR	CZ-CE2-CD2	5.45	124.70	119.80
3	I	417	THR	CA-CB-CG2	-5.45	104.78	112.40
8	i	44	GLY	O-C-N	-5.45	113.99	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	D	513	GLU	OE1-CD-OE2	5.44	129.83	123.30
2	F	874	PHE	CB-CG-CD1	-5.44	116.99	120.80
2	H	692	GLY	N-CA-C	-5.44	99.49	113.10
3	I	647	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	M	560	MET	CG-SD-CE	-5.44	91.49	100.20
2	N	808	ARG	CD-NE-CZ	-5.44	115.98	123.60
1	A	432	THR	N-CA-C	-5.44	96.31	111.00
1	C	532	ASP	CB-CG-OD2	-5.44	113.40	118.30
8	g	391	THR	CA-CB-CG2	-5.44	104.78	112.40
3	I	167	PRO	N-CA-CB	5.44	109.83	103.30
2	R	99	SER	N-CA-CB	5.44	118.66	110.50
8	e	161	TYR	CD1-CE1-CZ	-5.44	114.91	119.80
8	i	226	SER	N-CA-CB	5.44	118.66	110.50
8	i	273	TYR	CB-CG-CD1	5.44	124.26	121.00
8	n	135	PHE	N-CA-C	-5.44	96.32	111.00
2	H	680	TRP	CH2-CZ2-CE2	5.44	122.84	117.40
9	o	59	ARG	NE-CZ-NH1	5.44	123.02	120.30
3	I	110	GLU	OE1-CD-OE2	5.43	129.82	123.30
7	V	666	ARG	NE-CZ-NH2	-5.43	117.58	120.30
8	e	245	TYR	CG-CD1-CE1	-5.43	116.95	121.30
8	f	169	TYR	CD1-CE1-CZ	5.43	124.69	119.80
1	G	284	TYR	CB-CG-CD1	5.43	124.26	121.00
5	L	375	LEU	CB-CA-C	-5.43	99.88	110.20
8	d	190	LEU	CB-CA-C	-5.43	99.88	110.20
8	i	161	TYR	CZ-CE2-CD2	5.43	124.69	119.80
1	A	403	TYR	N-CA-CB	5.43	120.37	110.60
8	c	399	ARG	CA-CB-CG	5.43	125.34	113.40
8	g	169	TYR	CB-CA-C	-5.43	99.54	110.40
8	h	26	CYS	CA-CB-SG	5.43	123.77	114.00
8	i	362	ARG	NE-CZ-NH1	-5.43	117.58	120.30
8	e	63	ARG	NH1-CZ-NH2	5.43	125.37	119.40
2	H	730	TRP	NE1-CE2-CD2	-5.42	101.88	107.30
2	Q	57	LYS	CB-CA-C	5.42	121.25	110.40
8	b	92	TYR	CB-CG-CD2	-5.42	117.75	121.00
8	n	104	TRP	CE3-CZ3-CH2	-5.42	115.23	121.20
2	D	319	VAL	CA-CB-CG2	-5.42	102.77	110.90
2	H	274	TYR	CG-CD1-CE1	-5.42	116.96	121.30
2	F	310	ARG	CB-CG-CD	5.42	125.69	111.60
4	J	437	TYR	CB-CG-CD2	-5.42	117.75	121.00
8	e	399	ARG	NE-CZ-NH2	-5.42	117.59	120.30
2	F	791	LEU	O-C-N	5.42	131.37	122.70
1	G	564	ASN	O-C-N	-5.42	114.03	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	860	ARG	NH1-CZ-NH2	-5.42	113.44	119.40
8	l	347	ASN	CB-CG-OD1	-5.42	110.76	121.60
2	F	511	SER	N-CA-CB	5.42	118.63	110.50
2	H	528	ALA	O-C-N	-5.42	114.03	122.70
4	J	461	TRP	CD2-CE2-CZ2	-5.42	115.80	122.30
1	M	375	CYS	N-CA-CB	5.42	120.35	110.60
8	c	19	PHE	CG-CD1-CE1	5.41	126.76	120.80
8	n	161	TYR	CB-CG-CD2	-5.41	117.75	121.00
2	B	471	PRO	N-CD-CG	5.41	111.32	103.20
3	I	495	TRP	CA-CB-CG	5.41	123.98	113.70
8	l	234	THR	CA-CB-CG2	-5.41	104.82	112.40
1	G	393	TRP	CZ3-CH2-CZ2	-5.41	115.11	121.60
1	G	841	LYS	CA-CB-CG	5.41	125.31	113.40
2	H	719	TYR	CB-CG-CD2	-5.41	117.75	121.00
8	b	3	ARG	NH1-CZ-NH2	5.41	125.35	119.40
8	b	232	VAL	CA-CB-CG2	-5.41	102.78	110.90
8	k	81	PRO	N-CA-CB	5.41	109.79	103.30
8	n	386	SER	O-C-N	-5.41	114.04	122.70
1	A	701	MET	CA-CB-CG	5.41	122.49	113.30
4	J	508	TYR	CB-CG-CD1	-5.41	117.75	121.00
2	N	734	TRP	CB-CG-CD1	-5.41	119.97	127.00
8	e	281	SER	N-CA-CB	5.41	118.61	110.50
8	n	236	MET	CG-SD-CE	5.41	108.86	100.20
2	D	586	ARG	NE-CZ-NH1	-5.41	117.60	120.30
1	C	646	TYR	CG-CD2-CE2	-5.41	116.98	121.30
1	E	606	GLU	OE1-CD-OE2	5.41	129.79	123.30
8	h	19	PHE	CB-CG-CD2	-5.41	117.02	120.80
2	B	473	PHE	CB-CG-CD1	-5.40	117.02	120.80
8	c	152	TYR	CG-CD1-CE1	-5.40	116.98	121.30
3	I	101	ARG	NE-CZ-NH2	-5.40	117.60	120.30
3	K	156	THR	CA-CB-CG2	-5.40	104.84	112.40
2	T	74	PHE	CB-CG-CD1	5.40	124.58	120.80
8	b	108	PHE	CG-CD1-CE1	5.40	126.74	120.80
8	d	351	TRP	CE2-CD2-CG	-5.40	102.98	107.30
8	e	435	TYR	CB-CG-CD1	-5.40	117.76	121.00
8	h	362	ARG	NE-CZ-NH2	5.40	123.00	120.30
8	n	290	VAL	CB-CA-C	5.40	121.67	111.40
3	I	260	ARG	NE-CZ-NH2	-5.40	117.60	120.30
2	H	877	PHE	N-CA-CB	5.40	120.32	110.60
3	K	556	ILE	CB-CA-C	-5.40	100.80	111.60
2	N	860	PHE	CD1-CG-CD2	5.40	125.32	118.30
8	c	265	ARG	NE-CZ-NH1	5.40	123.00	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	160	ARG	NE-CZ-NH1	5.39	123.00	120.30
1	C	222	TYR	CD1-CE1-CZ	5.39	124.65	119.80
1	C	396	ARG	NH1-CZ-NH2	5.39	125.33	119.40
2	D	656	MET	CG-SD-CE	-5.39	91.57	100.20
8	a	106	SER	O-C-N	-5.39	114.03	123.20
1	C	864	ASN	CB-CA-C	-5.39	99.62	110.40
2	S	37	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
8	n	317	TYR	CB-CG-CD1	5.39	124.23	121.00
1	E	621	VAL	CG1-CB-CG2	5.39	119.52	110.90
2	D	713	PHE	O-C-N	-5.39	114.08	122.70
3	I	353	GLN	O-C-N	-5.39	114.08	122.70
1	M	318	LEU	N-CA-CB	5.38	121.17	110.40
2	B	880	ASP	CB-CG-OD1	5.38	123.14	118.30
1	C	640	LEU	CB-CG-CD1	5.38	120.15	111.00
8	h	104	TRP	CA-CB-CG	5.38	123.93	113.70
1	E	275	PHE	CB-CG-CD1	5.38	124.57	120.80
1	E	370	GLN	CA-CB-CG	5.38	125.24	113.40
1	A	284	TYR	CG-CD2-CE2	-5.38	117.00	121.30
2	N	631	ASP	C-N-CA	5.38	135.15	121.70
8	g	395	TYR	CD1-CG-CD2	5.38	123.82	117.90
8	h	123	ASP	CB-CG-OD2	-5.38	113.46	118.30
8	h	169	TYR	CZ-CE2-CD2	5.38	124.64	119.80
8	l	404	PHE	CG-CD1-CE1	-5.38	114.88	120.80
2	F	564	TYR	CB-CG-CD2	5.38	124.23	121.00
8	g	268	PHE	CB-CG-CD1	-5.38	117.04	120.80
8	j	362	ARG	N-CA-CB	5.38	120.28	110.60
2	H	873	ARG	NE-CZ-NH1	5.38	122.99	120.30
8	h	245	TYR	CG-CD1-CE1	-5.38	117.00	121.30
1	E	867	TYR	CB-CG-CD1	5.37	124.22	121.00
1	A	441	PHE	CB-CG-CD1	5.37	124.56	120.80
2	H	659	TYR	CB-CG-CD2	-5.37	117.78	121.00
3	K	553	PHE	CB-CG-CD1	-5.37	117.04	120.80
8	l	305	VAL	N-CA-C	-5.37	96.50	111.00
2	N	409	TYR	CZ-CE2-CD2	-5.37	114.97	119.80
1	G	363	PHE	CB-CG-CD2	-5.37	117.04	120.80
2	H	693	MET	CG-SD-CE	-5.37	91.61	100.20
6	P	25	ASP	CB-CG-OD2	-5.37	113.47	118.30
8	n	433	ASP	CB-CG-OD1	5.37	123.13	118.30
1	G	719	ASP	CB-CG-OD2	-5.36	113.47	118.30
2	H	274	TYR	CZ-CE2-CD2	-5.36	114.97	119.80
1	M	243	ARG	NH1-CZ-NH2	5.36	125.30	119.40
8	m	247	GLY	N-CA-C	-5.36	99.69	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	F	768	ARG	NE-CZ-NH1	5.36	122.98	120.30
2	H	842	MET	CG-SD-CE	-5.36	91.62	100.20
1	M	360	ASP	CB-CG-OD1	5.36	123.12	118.30
8	m	354	ALA	N-CA-CB	5.36	117.61	110.10
2	D	634	TRP	CE2-CD2-CG	-5.36	103.01	107.30
6	P	312	ARG	NE-CZ-NH2	-5.36	117.62	120.30
8	h	135	PHE	CD1-CE1-CZ	-5.36	113.67	120.10
8	m	366	TYR	CB-CG-CD1	5.36	124.22	121.00
1	G	531	MET	CA-CB-CG	5.36	122.41	113.30
5	L	552	PHE	N-CA-C	-5.36	96.53	111.00
8	e	412	ASP	CA-CB-CG	5.36	125.19	113.40
8	n	46	ASP	CB-CG-OD1	-5.36	113.48	118.30
2	F	752	VAL	CA-CB-CG1	5.35	118.93	110.90
1	C	455	TYR	CZ-CE2-CD2	5.35	124.62	119.80
2	F	700	LEU	CB-CG-CD1	5.35	120.10	111.00
8	n	60	TYR	CD1-CG-CD2	5.35	123.79	117.90
1	E	859	TYR	CG-CD1-CE1	-5.35	117.02	121.30
1	M	699	GLU	CG-CD-OE1	-5.35	107.60	118.30
2	B	749	ALA	N-CA-CB	5.35	117.59	110.10
1	G	219	ASP	CB-CG-OD1	-5.35	113.49	118.30
8	b	297	LEU	CB-CG-CD2	5.35	120.09	111.00
2	B	737	VAL	CA-CB-CG1	-5.35	102.88	110.90
2	B	538	PHE	CG-CD2-CE2	5.34	126.68	120.80
1	E	573	LYS	N-CA-CB	5.34	120.22	110.60
8	d	388	PHE	CB-CG-CD2	-5.34	117.06	120.80
8	f	130	ASP	CB-CG-OD1	5.34	123.11	118.30
8	i	212	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	E	867	TYR	CG-CD2-CE2	5.34	125.57	121.30
6	P	356	TRP	CH2-CZ2-CE2	-5.34	112.06	117.40
8	f	172	PHE	CG-CD1-CE1	5.34	126.67	120.80
1	G	476	TYR	CG-CD2-CE2	5.34	125.57	121.30
8	c	199	ALA	CB-CA-C	-5.34	102.09	110.10
8	l	305	VAL	C-N-CA	5.34	135.05	121.70
8	b	124	ARG	NH1-CZ-NH2	5.34	125.27	119.40
1	E	847	THR	CA-CB-CG2	-5.34	104.93	112.40
4	J	776	PHE	N-CA-CB	5.34	120.21	110.60
2	N	520	GLU	N-CA-CB	5.34	120.21	110.60
8	a	212	ARG	NE-CZ-NH2	5.34	122.97	120.30
2	D	663	PHE	CB-CG-CD1	5.33	124.53	120.80
1	M	682	ARG	NE-CZ-NH1	5.33	122.97	120.30
2	B	443	HIS	CA-CB-CG	-5.33	104.54	113.60
1	C	636	ARG	NE-CZ-NH1	5.33	122.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	430	ARG	N-CA-CB	5.33	120.19	110.60
8	k	92	TYR	CZ-CE2-CD2	5.33	124.60	119.80
8	n	245	TYR	CB-CA-C	-5.33	99.74	110.40
5	L	532	TYR	CB-CG-CD2	-5.33	117.80	121.00
8	b	393	ARG	NE-CZ-NH1	5.33	122.96	120.30
8	l	252	ASP	CB-CG-OD2	-5.33	113.50	118.30
2	N	341	LEU	CB-CG-CD1	5.33	120.06	111.00
2	D	663	PHE	CG-CD2-CE2	5.33	126.66	120.80
1	E	563	ALA	N-CA-CB	5.33	117.56	110.10
4	J	839	ASN	N-CA-CB	-5.32	101.02	110.60
3	K	341	TRP	CB-CG-CD1	-5.32	120.08	127.00
1	M	265	VAL	CG1-CB-CG2	-5.32	102.38	110.90
8	f	101	GLY	N-CA-C	-5.32	99.79	113.10
8	k	372	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	E	730	ASP	CB-CG-OD2	-5.32	113.51	118.30
2	N	859	GLN	CG-CD-OE1	-5.32	110.96	121.60
8	d	194	ARG	NH1-CZ-NH2	5.32	125.25	119.40
2	H	467	LYS	CB-CA-C	5.32	121.04	110.40
4	J	900	ILE	CA-CB-CG1	5.32	121.11	111.00
1	G	675	PHE	CB-CG-CD2	5.32	124.52	120.80
3	K	545	GLN	CA-CB-CG	5.32	125.09	113.40
8	h	343	ARG	NE-CZ-NH2	5.32	122.96	120.30
9	t	12	ARG	NE-CZ-NH1	5.32	122.96	120.30
8	b	40	PHE	CB-CG-CD2	5.31	124.52	120.80
8	e	395	TYR	CB-CG-CD1	-5.31	117.81	121.00
4	J	420	PRO	CA-C-O	-5.31	107.45	120.20
3	K	120	SER	N-CA-CB	5.31	118.47	110.50
8	d	55	ALA	O-C-N	-5.31	114.20	122.70
1	G	705	TRP	CB-CG-CD2	5.31	133.50	126.60
2	H	531	THR	O-C-N	-5.31	114.20	122.70
8	k	176	ASP	CB-CG-OD2	-5.31	113.52	118.30
8	a	60	TYR	CB-CG-CD2	-5.31	117.81	121.00
8	f	333	VAL	CG1-CB-CG2	-5.31	102.40	110.90
8	l	40	PHE	CB-CG-CD2	-5.31	117.08	120.80
3	K	260	ARG	NE-CZ-NH1	-5.31	117.65	120.30
2	R	19	ARG	NE-CZ-NH1	5.31	122.95	120.30
1	E	230	ARG	NE-CZ-NH2	-5.30	117.65	120.30
8	j	190	LEU	N-CA-CB	5.30	121.01	110.40
1	G	526	PHE	CG-CD1-CE1	5.30	126.63	120.80
2	F	274	TYR	CG-CD1-CE1	-5.30	117.06	121.30
8	j	117	ASP	CA-CB-CG	5.30	125.06	113.40
2	F	453	VAL	CG1-CB-CG2	5.30	119.38	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	H	298	TRP	CB-CG-CD2	5.30	133.49	126.60
2	H	421	VAL	CA-CB-CG1	5.30	118.85	110.90
2	N	648	ALA	CB-CA-C	5.30	118.05	110.10
8	k	100	ALA	CA-C-N	5.30	126.80	116.20
1	G	227	VAL	CA-CB-CG2	-5.30	102.95	110.90
1	M	739	THR	C-N-CA	5.30	134.94	121.70
3	I	35	HIS	CA-CB-CG	-5.30	104.60	113.60
2	N	713	PHE	CD1-CE1-CZ	5.30	126.45	120.10
8	c	119	PHE	CZ-CE2-CD2	-5.30	113.74	120.10
8	h	328	VAL	CA-CB-CG2	5.30	118.84	110.90
2	F	812	ARG	NE-CZ-NH2	-5.29	117.65	120.30
3	I	260	ARG	NE-CZ-NH1	5.29	122.95	120.30
1	M	615	PHE	CB-CG-CD1	-5.29	117.10	120.80
2	T	79	ARG	NE-CZ-NH2	5.29	122.95	120.30
8	a	205	LEU	N-CA-C	-5.29	96.71	111.00
8	e	271	THR	N-CA-CB	5.29	120.36	110.30
8	g	120	ASP	CB-CG-OD1	-5.29	113.54	118.30
8	i	169	TYR	CG-CD1-CE1	5.29	125.53	121.30
8	i	282	VAL	CA-CB-CG1	-5.29	102.96	110.90
8	n	176	ASP	N-CA-CB	5.29	120.12	110.60
5	L	1469	VAL	N-CA-C	-5.29	96.72	111.00
2	Q	77	LEU	CB-CG-CD1	5.29	119.99	111.00
2	F	708	SER	N-CA-CB	5.29	118.43	110.50
1	G	244	SER	N-CA-CB	5.29	118.43	110.50
4	J	588	TYR	CB-CG-CD2	5.29	124.17	121.00
8	a	194	ARG	NE-CZ-NH1	5.29	122.94	120.30
8	d	243	LEU	CB-CG-CD2	-5.29	102.01	111.00
1	C	234	VAL	O-C-N	-5.29	114.24	122.70
2	H	851	HIS	CB-CA-C	-5.29	99.83	110.40
2	D	298	TRP	CD1-NE1-CE2	5.28	113.76	109.00
6	P	192	ILE	CA-CB-CG2	-5.28	100.33	110.90
8	n	248	TYR	CB-CG-CD2	-5.28	117.83	121.00
1	C	617	PHE	CB-CG-CD2	5.28	124.50	120.80
1	C	641	PHE	O-C-N	-5.28	114.25	122.70
1	G	379	THR	CA-CB-CG2	5.28	119.79	112.40
5	L	1601	PHE	CG-CD1-CE1	5.28	126.61	120.80
8	f	124	ARG	CA-CB-CG	5.28	125.02	113.40
8	i	283	ALA	CB-CA-C	-5.28	102.18	110.10
8	k	225	PHE	CB-CG-CD1	5.28	124.50	120.80
8	l	362	ARG	NH1-CZ-NH2	5.28	125.21	119.40
1	M	702	GLU	O-C-N	-5.28	111.07	121.10
2	N	871	SER	N-CA-CB	5.28	118.42	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	482	PHE	CB-CG-CD2	-5.28	117.11	120.80
2	N	520	GLU	C-N-CA	5.28	134.90	121.70
6	P	335	ARG	NE-CZ-NH1	5.28	122.94	120.30
6	P	254	ARG	NE-CZ-NH2	5.28	122.94	120.30
8	g	72	ARG	NE-CZ-NH1	5.28	122.94	120.30
8	f	123	ASP	CB-CG-OD1	5.27	123.05	118.30
2	Q	105	ARG	NE-CZ-NH1	-5.27	117.66	120.30
2	R	67	ARG	NE-CZ-NH1	-5.27	117.66	120.30
2	F	802	ARG	NE-CZ-NH1	-5.27	117.67	120.30
5	L	551	GLU	C-N-CA	5.27	134.88	121.70
8	c	59	HIS	N-CA-CB	5.27	120.09	110.60
8	i	22	TRP	CZ3-CH2-CZ2	-5.27	115.28	121.60
2	F	824	GLU	OE1-CD-OE2	5.27	129.62	123.30
6	P	337	TYR	CA-CB-CG	-5.27	103.39	113.40
8	e	425	ARG	NE-CZ-NH2	-5.27	117.67	120.30
2	F	491	PHE	N-CA-CB	5.27	120.08	110.60
3	K	108	GLU	OE1-CD-OE2	5.27	129.62	123.30
8	k	367	LEU	CA-C-N	5.27	131.85	117.10
2	H	336	ARG	NE-CZ-NH1	-5.26	117.67	120.30
3	K	203	PHE	CG-CD1-CE1	-5.26	115.01	120.80
1	M	695	TYR	CZ-CE2-CD2	5.26	124.54	119.80
2	N	512	ALA	N-CA-CB	5.26	117.47	110.10
8	a	277	THR	CA-CB-CG2	-5.26	105.03	112.40
2	D	812	ARG	NE-CZ-NH1	5.26	122.93	120.30
1	E	722	LEU	CB-CG-CD1	5.26	119.94	111.00
1	E	851	GLU	O-C-N	-5.26	114.28	122.70
8	g	52	PHE	CB-CG-CD2	5.26	124.48	120.80
8	l	366	TYR	CD1-CE1-CZ	5.26	124.53	119.80
8	n	337	LEU	CB-CG-CD2	5.26	119.94	111.00
4	J	569	LYS	N-CA-CB	5.26	120.07	110.60
5	L	384	VAL	C-N-CA	5.26	134.85	121.70
8	c	265	ARG	NE-CZ-NH2	-5.26	117.67	120.30
8	f	418	PHE	CB-CG-CD2	5.26	124.48	120.80
8	n	186	TYR	CG-CD1-CE1	-5.26	117.09	121.30
1	E	562	THR	N-CA-CB	5.26	120.29	110.30
2	B	604	VAL	C-N-CA	5.26	134.84	121.70
2	D	534	ASP	CA-CB-CG	5.26	124.97	113.40
5	L	1618	SER	O-C-N	-5.26	114.29	122.70
1	M	626	SER	O-C-N	5.26	131.11	122.70
8	e	178	MET	N-CA-CB	5.26	120.06	110.60
8	k	251	ASN	O-C-N	-5.26	114.29	122.70
4	J	678	PHE	CB-CG-CD1	5.25	124.48	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	1371	MET	O-C-N	5.25	131.11	122.70
2	T	50	ASP	CB-CG-OD1	5.25	123.03	118.30
2	D	695	GLU	CG-CD-OE1	-5.25	107.80	118.30
6	P	334	GLU	CA-CB-CG	5.25	124.96	113.40
8	i	425	ARG	CA-CB-CG	5.25	124.96	113.40
1	M	840	ASP	CB-CG-OD2	-5.25	113.57	118.30
8	i	22	TRP	CH2-CZ2-CE2	5.25	122.65	117.40
8	k	248	TYR	CG-CD2-CE2	5.25	125.50	121.30
1	A	525	ASP	CB-CG-OD2	-5.25	113.58	118.30
2	D	780	GLN	CA-CB-CG	5.25	124.95	113.40
1	M	406	PHE	CB-CG-CD2	-5.25	117.12	120.80
1	A	218	GLU	OE1-CD-OE2	-5.25	117.00	123.30
1	C	691	ASN	OD1-CG-ND2	5.25	133.97	121.90
1	G	296	ARG	NE-CZ-NH2	5.25	122.92	120.30
2	H	255	TYR	CB-CG-CD2	-5.25	117.85	121.00
2	H	438	LEU	N-CA-CB	5.25	120.90	110.40
3	I	291	VAL	CG1-CB-CG2	-5.25	102.51	110.90
8	l	21	PHE	O-C-N	5.25	131.09	122.70
1	G	619	TYR	CB-CG-CD1	-5.25	117.85	121.00
5	L	444	TYR	CB-CG-CD2	-5.25	117.85	121.00
2	N	710	MET	CG-SD-CE	-5.25	91.81	100.20
8	f	418	PHE	CB-CG-CD1	-5.25	117.13	120.80
2	H	537	TYR	CG-CD1-CE1	-5.24	117.11	121.30
7	U	648	SER	N-CA-CB	5.24	118.36	110.50
8	b	305	VAL	N-CA-C	-5.24	96.85	111.00
8	e	86	TYR	CB-CG-CD1	5.24	124.14	121.00
1	A	644	MET	CB-CA-C	-5.24	99.92	110.40
4	J	359	ALA	N-CA-CB	5.24	117.44	110.10
3	K	480	TYR	CG-CD2-CE2	-5.24	117.11	121.30
1	M	325	PHE	CG-CD1-CE1	5.24	126.56	120.80
1	M	500	ASP	O-C-N	5.24	131.09	122.70
1	G	831	PHE	CB-CG-CD2	-5.24	117.13	120.80
2	N	778	PHE	CG-CD1-CE1	-5.24	115.04	120.80
8	j	329	ASP	CB-CG-OD2	-5.24	113.59	118.30
1	E	501	PHE	CB-CG-CD1	5.24	124.47	120.80
2	S	70	ASP	N-CA-CB	5.24	120.03	110.60
8	g	40	PHE	N-CA-CB	5.24	120.03	110.60
2	B	686	ASN	O-C-N	5.24	131.08	122.70
1	E	688	PHE	CG-CD2-CE2	5.24	126.56	120.80
3	I	91	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	N	307	THR	CA-CB-CG2	-5.24	105.07	112.40
8	i	21	PHE	CD1-CE1-CZ	-5.24	113.82	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	g	295	ARG	NE-CZ-NH2	-5.23	117.68	120.30
5	L	1503	TYR	CG-CD2-CE2	-5.23	117.11	121.30
1	M	549	ARG	CB-CA-C	-5.23	99.94	110.40
8	c	356	ILE	N-CA-CB	5.23	122.83	110.80
8	f	244	ARG	NE-CZ-NH1	5.23	122.92	120.30
8	i	309	ARG	NE-CZ-NH2	-5.23	117.68	120.30
2	D	323	PHE	CB-CG-CD2	-5.23	117.14	120.80
8	c	241	THR	CA-CB-CG2	-5.23	105.08	112.40
8	h	138	CYS	N-CA-CB	-5.23	101.18	110.60
8	m	317	TYR	CD1-CE1-CZ	5.23	124.51	119.80
2	F	334	TYR	CB-CG-CD1	5.23	124.14	121.00
5	L	1433	ASN	CA-C-O	-5.23	109.12	120.10
5	L	1491	LEU	N-CA-CB	5.23	120.85	110.40
2	D	276	VAL	CA-CB-CG1	-5.23	103.06	110.90
1	G	705	TRP	CB-CG-CD1	-5.23	120.21	127.00
3	I	293	MET	CG-SD-CE	-5.23	91.84	100.20
8	a	189	LEU	CB-CG-CD1	5.23	119.88	111.00
8	c	136	VAL	CG1-CB-CG2	5.23	119.26	110.90
2	B	473	PHE	CG-CD1-CE1	-5.22	115.05	120.80
1	G	322	LYS	CD-CE-NZ	5.22	123.72	111.70
3	K	418	ILE	CA-CB-CG1	5.22	120.93	111.00
5	L	579	GLU	N-CA-CB	5.22	120.00	110.60
8	i	242	THR	CA-CB-CG2	-5.22	105.09	112.40
8	k	295	ARG	NE-CZ-NH2	-5.22	117.69	120.30
8	l	344	LYS	N-CA-CB	5.22	120.01	110.60
3	I	206	ARG	NE-CZ-NH1	5.22	122.91	120.30
8	d	296	ARG	NE-CZ-NH1	-5.22	117.69	120.30
2	H	779	ASP	CB-CG-OD2	-5.22	113.60	118.30
8	l	435	TYR	CB-CG-CD1	5.22	124.13	121.00
2	B	318	LEU	C-N-CA	5.22	134.74	121.70
8	f	366	TYR	CD1-CE1-CZ	5.22	124.50	119.80
1	A	641	PHE	CB-CG-CD2	5.22	124.45	120.80
3	I	271	ARG	CG-CD-NE	-5.22	100.84	111.80
4	J	924	ILE	CA-CB-CG2	-5.22	100.47	110.90
8	a	220	ILE	CA-CB-CG2	-5.22	100.47	110.90
8	e	92	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	C	621	VAL	O-C-N	-5.21	114.36	122.70
3	K	451	ALA	O-C-N	-5.21	114.36	122.70
6	P	177	ARG	NE-CZ-NH1	-5.21	117.69	120.30
2	Q	91	TRP	CH2-CZ2-CE2	5.21	122.61	117.40
8	a	225	PHE	O-C-N	5.21	131.04	122.70
8	j	60	TYR	CB-CG-CD1	-5.21	117.87	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	671	SER	N-CA-CB	-5.21	102.68	110.50
4	J	473	ASP	CB-CG-OD1	-5.21	113.61	118.30
2	D	659	TYR	CB-CG-CD2	-5.21	117.87	121.00
8	d	409	ARG	NE-CZ-NH1	-5.21	117.69	120.30
8	k	408	PHE	CB-CG-CD2	-5.21	117.15	120.80
8	n	194	ARG	CD-NE-CZ	5.21	130.90	123.60
8	a	362	ARG	NE-CZ-NH1	-5.21	117.70	120.30
8	c	40	PHE	CB-CG-CD1	-5.21	117.15	120.80
8	h	299	GLN	N-CA-CB	5.21	119.98	110.60
2	H	719	TYR	CG-CD2-CE2	-5.21	117.14	121.30
5	L	314	VAL	CG1-CB-CG2	-5.21	102.57	110.90
1	M	481	GLN	N-CA-CB	5.21	119.97	110.60
8	e	247	GLY	N-CA-C	-5.21	100.09	113.10
1	E	674	TRP	CD1-NE1-CE2	-5.20	104.32	109.00
8	c	358	VAL	N-CA-C	-5.20	96.95	111.00
8	m	2	PRO	N-CD-CG	5.20	111.01	103.20
1	A	326	TYR	CG-CD2-CE2	-5.20	117.14	121.30
1	G	323	LEU	CB-CG-CD2	5.20	119.84	111.00
1	G	445	VAL	CA-CB-CG1	-5.20	103.10	110.90
1	M	538	LEU	CB-CG-CD2	5.20	119.84	111.00
2	H	665	PHE	CB-CG-CD1	5.20	124.44	120.80
3	K	561	ASP	CB-CG-OD1	-5.20	113.62	118.30
2	N	653	ARG	NE-CZ-NH1	-5.20	117.70	120.30
6	P	11	ASP	CB-CG-OD1	-5.20	113.62	118.30
8	a	252	ASP	CB-CG-OD1	5.20	122.98	118.30
8	e	52	PHE	N-CA-CB	5.20	119.96	110.60
8	k	41	ALA	N-CA-CB	5.20	117.38	110.10
2	F	335	TYR	CB-CG-CD2	5.20	124.12	121.00
4	J	999	ARG	NE-CZ-NH2	-5.20	117.70	120.30
5	L	1613	MET	CG-SD-CE	-5.20	91.89	100.20
8	m	60	TYR	CA-CB-CG	-5.19	103.53	113.40
3	I	323	VAL	CA-CB-CG2	-5.19	103.11	110.90
2	S	70	ASP	CB-CG-OD1	5.19	122.97	118.30
8	b	388	PHE	CB-CG-CD2	-5.19	117.17	120.80
8	f	3	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
8	m	82	TYR	CD1-CE1-CZ	5.19	124.47	119.80
4	J	282	ILE	CA-CB-CG2	-5.19	100.52	110.90
8	k	372	ARG	NE-CZ-NH2	-5.19	117.70	120.30
8	i	266	LEU	N-CA-C	-5.19	96.99	111.00
8	j	194	ARG	CG-CD-NE	-5.19	100.90	111.80
1	A	518	TYR	CZ-CE2-CD2	-5.19	115.13	119.80
8	e	263	THR	N-CA-CB	5.19	120.16	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	837	ASP	O-C-N	-5.19	114.40	122.70
8	k	413	ILE	N-CA-C	-5.19	97.00	111.00
2	F	874	PHE	CG-CD1-CE1	-5.18	115.10	120.80
1	G	238	VAL	CA-CB-CG1	-5.18	103.12	110.90
2	N	376	ARG	NE-CZ-NH2	-5.18	117.71	120.30
8	e	244	ARG	NE-CZ-NH2	5.18	122.89	120.30
8	f	104	TRP	CB-CG-CD1	-5.18	120.26	127.00
2	H	671	ARG	NE-CZ-NH1	5.18	122.89	120.30
6	P	101	HIS	O-C-N	-5.18	111.25	121.10
8	a	118	ILE	CA-CB-CG1	5.18	120.85	111.00
8	h	194	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
8	j	219	HIS	N-CA-CB	5.18	119.93	110.60
8	n	160	ARG	NE-CZ-NH2	-5.18	117.71	120.30
8	n	421	LEU	CB-CG-CD2	5.18	119.81	111.00
3	K	330	ASP	CB-CG-OD1	5.18	122.96	118.30
1	G	284	TYR	CB-CG-CD2	-5.18	117.89	121.00
2	H	327	LEU	CB-CA-C	-5.18	100.36	110.20
2	N	870	GLU	N-CA-CB	5.18	119.92	110.60
6	P	164	PRO	N-CA-CB	5.18	109.52	103.30
8	g	252	ASP	N-CA-CB	5.18	119.92	110.60
3	I	22	ARG	CA-CB-CG	5.17	124.78	113.40
8	n	412	ASP	CB-CG-OD2	5.17	122.96	118.30
1	A	634	LEU	CB-CG-CD2	-5.17	102.21	111.00
1	E	684	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
2	F	498	ASP	N-CA-C	-5.17	97.03	111.00
2	B	822	ALA	C-N-CA	5.17	134.63	121.70
2	H	402	TYR	CG-CD1-CE1	-5.17	117.16	121.30
2	T	22	GLY	N-CA-C	-5.17	100.17	113.10
8	j	56	ASP	O-C-N	5.17	130.97	122.70
2	B	423	TYR	CB-CG-CD2	5.17	124.10	121.00
1	C	213	GLU	OE1-CD-OE2	5.17	129.50	123.30
1	G	672	ALA	N-CA-CB	5.17	117.34	110.10
1	G	834	HIS	CB-CG-ND1	5.17	136.12	123.20
2	D	421	VAL	CA-CB-CG1	5.17	118.65	110.90
2	N	314	ARG	N-CA-CB	5.17	119.90	110.60
8	n	176	ASP	CB-CA-C	-5.17	100.07	110.40
2	D	537	TYR	CB-CG-CD2	-5.16	117.90	121.00
3	K	474	TYR	CA-CB-CG	5.16	123.21	113.40
2	N	463	TYR	CG-CD1-CE1	-5.16	117.17	121.30
8	a	92	TYR	CB-CG-CD2	5.16	124.10	121.00
1	E	328	GLN	O-C-N	-5.16	111.29	121.10
8	k	353	PRO	N-CD-CG	5.16	110.94	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	677	THR	CA-CB-CG2	-5.16	105.17	112.40
2	D	574	ARG	NE-CZ-NH2	-5.16	117.72	120.30
2	F	270	SER	N-CA-C	-5.16	97.06	111.00
3	I	12	TYR	CD1-CE1-CZ	5.16	124.44	119.80
8	g	133	GLU	CA-CB-CG	5.16	124.75	113.40
8	j	317	TYR	CB-CG-CD1	-5.16	117.90	121.00
6	P	372	ARG	CD-NE-CZ	5.16	130.82	123.60
8	d	345	LEU	CB-CG-CD2	5.16	119.77	111.00
8	m	296	ARG	NE-CZ-NH1	-5.16	117.72	120.30
9	s	48	GLU	CA-CB-CG	5.16	124.75	113.40
1	E	866	PHE	CB-CG-CD1	-5.16	117.19	120.80
4	J	970	TRP	CH2-CZ2-CE2	-5.16	112.24	117.40
8	m	119	PHE	CB-CG-CD1	-5.16	117.19	120.80
6	P	219	VAL	CA-CB-CG2	-5.16	103.17	110.90
8	i	22	TRP	CG-CD2-CE3	-5.16	129.26	133.90
1	E	519	PHE	CB-CG-CD1	5.15	124.41	120.80
2	H	306	TYR	CB-CG-CD2	-5.15	117.91	121.00
2	N	706	LEU	CB-CG-CD2	5.15	119.76	111.00
8	l	285	VAL	CA-CB-CG1	-5.15	103.17	110.90
1	A	477	THR	CA-CB-CG2	-5.15	105.19	112.40
2	F	370	THR	CA-CB-CG2	5.15	119.61	112.40
7	X	617	ALA	N-CA-CB	5.15	117.31	110.10
8	h	22	TRP	N-CA-CB	5.15	119.87	110.60
1	G	844	MET	CG-SD-CE	-5.15	91.96	100.20
1	A	625	LEU	CA-C-O	5.15	130.91	120.10
2	D	705	ILE	CA-C-N	-5.15	105.88	117.20
8	f	196	THR	CA-CB-CG2	-5.15	105.19	112.40
8	j	388	PHE	CG-CD2-CE2	5.15	126.46	120.80
1	A	570	ASP	CB-CG-OD2	5.14	122.93	118.30
3	K	330	ASP	CB-CG-OD2	-5.14	113.67	118.30
5	L	1601	PHE	CD1-CG-CD2	-5.14	111.61	118.30
7	X	668	ARG	N-CA-CB	5.14	119.86	110.60
8	e	72	ARG	NE-CZ-NH2	5.14	122.87	120.30
8	g	159	ASP	CB-CG-OD1	5.14	122.93	118.30
8	h	388	PHE	CB-CG-CD2	5.14	124.40	120.80
8	m	93	LEU	O-C-N	5.14	130.93	122.70
8	n	104	TRP	CG-CD2-CE3	5.14	138.53	133.90
1	A	441	PHE	CD1-CE1-CZ	-5.14	113.93	120.10
2	B	450	ASP	CB-CG-OD1	-5.14	113.67	118.30
2	D	574	ARG	NH1-CZ-NH2	-5.14	113.74	119.40
1	E	369	SER	N-CA-CB	5.14	118.22	110.50
1	E	543	ASP	CB-CG-OD1	5.14	122.93	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	L	313	TYR	CB-CG-CD2	-5.14	117.91	121.00
8	b	198	ASN	N-CA-CB	5.14	119.86	110.60
8	k	52	PHE	CB-CG-CD2	-5.14	117.20	120.80
1	C	320	LEU	CB-CG-CD2	5.14	119.74	111.00
8	l	351	TRP	CE3-CZ3-CH2	-5.14	115.54	121.20
3	K	611	LEU	CA-CB-CG	5.14	127.12	115.30
5	L	503	SER	CB-CA-C	-5.14	100.34	110.10
8	a	178	MET	CG-SD-CE	-5.14	91.98	100.20
8	k	212	ARG	NE-CZ-NH2	5.14	122.87	120.30
2	O	95	TYR	CB-CG-CD2	5.14	124.08	121.00
1	C	740	ASN	CB-CA-C	-5.14	100.13	110.40
8	d	278	THR	CA-CB-CG2	-5.14	105.21	112.40
8	e	409	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
8	j	346	ALA	CB-CA-C	-5.14	102.40	110.10
8	n	102	ASN	N-CA-CB	5.14	119.85	110.60
1	E	441	PHE	C-N-CA	5.13	134.54	121.70
1	G	326	TYR	CB-CG-CD1	-5.13	117.92	121.00
8	a	82	TYR	CG-CD1-CE1	-5.13	117.19	121.30
8	b	223	PRO	N-CA-CB	5.13	109.46	103.30
2	D	610	GLN	CA-CB-CG	5.13	124.69	113.40
2	D	822	ALA	N-CA-CB	5.13	117.29	110.10
4	J	747	TRP	CA-CB-CG	5.13	123.45	113.70
6	P	246	GLN	O-C-N	-5.13	114.49	122.70
8	f	269	LEU	CB-CA-C	-5.13	100.45	110.20
2	H	296	LEU	CB-CG-CD2	-5.13	102.28	111.00
8	e	92	TYR	CD1-CG-CD2	5.13	123.54	117.90
2	H	541	SER	N-CA-CB	-5.13	102.81	110.50
2	N	499	GLN	N-CA-C	-5.13	97.15	111.00
8	m	292	ASP	CB-CG-OD2	5.13	122.92	118.30
2	H	589	THR	CA-CB-CG2	-5.13	105.22	112.40
3	I	608	ALA	CB-CA-C	-5.13	102.41	110.10
4	J	295	ASP	N-CA-CB	5.13	119.83	110.60
2	O	52	PHE	CB-CG-CD2	5.13	124.39	120.80
2	R	64	ARG	N-CA-CB	5.13	119.83	110.60
8	c	399	ARG	NE-CZ-NH2	-5.13	117.74	120.30
8	i	177	GLU	O-C-N	5.13	130.91	122.70
1	C	559	ARG	NE-CZ-NH2	-5.13	117.74	120.30
2	N	586	ARG	CG-CD-NE	-5.13	101.03	111.80
1	C	460	ARG	NE-CZ-NH1	5.12	122.86	120.30
8	f	98	GLY	C-N-CA	5.12	133.06	122.30
2	H	319	VAL	CB-CA-C	-5.12	101.67	111.40
3	I	460	TRP	CE2-CD2-CG	-5.12	103.20	107.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	S	67	ARG	N-CA-C	-5.12	97.17	111.00
8	c	149	LEU	CB-CG-CD1	5.12	119.71	111.00
8	c	351	TRP	CA-CB-CG	5.12	123.44	113.70
8	f	370	ALA	N-CA-CB	5.12	117.27	110.10
2	D	821	THR	O-C-N	5.12	130.89	122.70
5	L	1661	TYR	CG-CD1-CE1	-5.12	117.20	121.30
6	P	164	PRO	N-CA-C	-5.12	98.78	112.10
8	a	287	LYS	CA-CB-CG	5.12	124.67	113.40
8	g	244	ARG	NE-CZ-NH1	5.12	122.86	120.30
1	C	392	ARG	NE-CZ-NH2	-5.12	117.74	120.30
8	l	252	ASP	N-CA-CB	5.12	119.81	110.60
2	B	778	PHE	N-CA-CB	5.12	119.81	110.60
2	D	529	PHE	CG-CD2-CE2	5.12	126.43	120.80
5	L	455	LEU	CB-CG-CD2	5.12	119.70	111.00
8	n	119	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	C	847	THR	CA-CB-CG2	-5.12	105.24	112.40
6	P	242	LEU	N-CA-C	-5.12	97.18	111.00
8	a	204	VAL	CA-CB-CG2	5.12	118.58	110.90
8	e	422	ASP	CB-CG-OD1	5.12	122.91	118.30
8	l	310	ASP	CB-CG-OD2	5.12	122.91	118.30
1	E	646	TYR	CG-CD2-CE2	-5.12	117.21	121.30
5	L	1413	SER	N-CA-CB	5.12	118.17	110.50
2	O	49	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
6	P	248	ILE	N-CA-C	-5.12	97.19	111.00
8	d	63	ARG	NE-CZ-NH1	-5.12	117.74	120.30
9	r	48	GLU	OE1-CD-OE2	5.12	129.44	123.30
1	A	562	THR	CA-CB-CG2	-5.11	105.24	112.40
2	B	434	TYR	CG-CD1-CE1	5.11	125.39	121.30
2	D	539	ASP	CB-CG-OD1	5.11	122.90	118.30
3	I	467	THR	CA-CB-CG2	-5.11	105.24	112.40
6	P	69	TYR	CD1-CG-CD2	-5.11	112.28	117.90
8	i	433	ASP	CB-CG-OD2	-5.11	113.70	118.30
8	l	414	PHE	CB-CA-C	-5.11	100.17	110.40
2	H	619	ARG	NE-CZ-NH2	-5.11	117.74	120.30
8	c	100	ALA	N-CA-CB	5.11	117.26	110.10
8	m	372	ARG	NH1-CZ-NH2	5.11	125.02	119.40
2	D	703	CYS	CA-CB-SG	5.11	123.20	114.00
1	G	488	GLU	CG-CD-OE2	-5.11	108.08	118.30
2	N	621	ASP	C-N-CA	5.11	134.47	121.70
8	k	81	PRO	O-C-N	5.11	130.88	122.70
4	J	487	GLU	N-CA-CB	5.11	119.79	110.60
3	K	336	VAL	CA-CB-CG1	5.11	118.56	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	877	PHE	CB-CG-CD1	-5.11	117.22	120.80
1	G	672	ALA	CB-CA-C	-5.11	102.44	110.10
4	J	834	ASP	CB-CG-OD2	5.11	122.89	118.30
8	b	60	TYR	CG-CD2-CE2	-5.11	117.22	121.30
1	E	501	PHE	CB-CG-CD2	-5.10	117.23	120.80
3	I	480	TYR	CB-CG-CD1	5.10	124.06	121.00
2	N	740	ALA	N-CA-CB	5.10	117.25	110.10
8	i	432	ILE	O-C-N	-5.10	114.53	122.70
1	A	375	CYS	N-CA-CB	5.10	119.78	110.60
2	F	865	THR	N-CA-CB	5.10	120.00	110.30
8	j	263	THR	N-CA-C	-5.10	97.22	111.00
9	p	23	ARG	NE-CZ-NH1	-5.10	117.75	120.30
1	C	406	PHE	CB-CG-CD2	5.10	124.37	120.80
2	N	255	TYR	CG-CD2-CE2	-5.10	117.22	121.30
2	R	52	PHE	CB-CG-CD1	-5.10	117.23	120.80
8	j	399	ARG	NE-CZ-NH2	5.10	122.85	120.30
8	k	248	TYR	CB-CG-CD1	5.10	124.06	121.00
1	C	483	TYR	CB-CG-CD2	5.10	124.06	121.00
2	F	600	LEU	CB-CG-CD1	5.10	119.66	111.00
8	a	411	GLU	C-N-CA	5.10	134.44	121.70
8	c	412	ASP	CB-CG-OD1	5.10	122.89	118.30
8	l	273	TYR	CB-CG-CD2	5.10	124.06	121.00
8	e	310	ASP	CB-CG-OD2	-5.10	113.71	118.30
8	l	395	TYR	O-C-N	-5.10	114.55	122.70
2	D	744	ASP	N-CA-CB	5.09	119.77	110.60
2	H	730	TRP	CE2-CD2-CG	5.09	111.38	107.30
8	k	127	ASP	CB-CG-OD1	5.09	122.89	118.30
8	n	217	ARG	NE-CZ-NH1	5.09	122.85	120.30
3	K	317	GLN	N-CA-C	-5.09	97.25	111.00
5	L	208	PHE	CG-CD1-CE1	5.09	126.40	120.80
8	d	108	PHE	CB-CG-CD1	5.09	124.36	120.80
5	L	1530	THR	C-N-CA	5.09	134.43	121.70
8	e	305	VAL	CA-CB-CG2	-5.09	103.26	110.90
8	g	268	PHE	CD1-CE1-CZ	-5.09	113.99	120.10
2	D	605	ARG	NH1-CZ-NH2	-5.09	113.80	119.40
2	N	844	SER	N-CA-CB	5.09	118.13	110.50
1	A	536	GLU	C-N-CA	5.09	134.42	121.70
8	c	300	PRO	N-CA-CB	5.09	109.41	103.30
8	d	250	ASN	N-CA-CB	5.09	119.76	110.60
8	d	92	TYR	CG-CD1-CE1	-5.09	117.23	121.30
1	C	646	TYR	CB-CG-CD2	-5.08	117.95	121.00
1	C	753	VAL	CA-CB-CG1	5.08	118.53	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	J	943	SER	N-CA-CB	5.08	118.12	110.50
3	K	54	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	O	33	GLN	N-CA-CB	5.08	119.75	110.60
2	O	50	ASP	CB-CG-OD2	-5.08	113.72	118.30
2	R	61	GLU	N-CA-CB	5.08	119.75	110.60
8	b	100	ALA	C-N-CA	5.08	132.98	122.30
1	G	269	TYR	CB-CG-CD1	-5.08	117.95	121.00
4	J	475	TRP	CD1-CG-CD2	5.08	110.36	106.30
8	d	311	ARG	NE-CZ-NH2	-5.08	117.76	120.30
8	g	380	ASN	N-CA-CB	5.08	119.75	110.60
4	J	912	VAL	CA-CB-CG2	-5.08	103.28	110.90
8	n	320	ILE	CA-CB-CG1	5.08	120.65	111.00
2	B	877	PHE	CD1-CG-CD2	5.08	124.90	118.30
1	E	755	VAL	CA-CB-CG2	-5.08	103.28	110.90
2	F	348	GLU	OE1-CD-OE2	5.08	129.39	123.30
2	F	439	GLU	N-CA-CB	5.08	119.74	110.60
3	I	507	ASN	O-C-N	-5.08	114.58	122.70
1	M	231	TYR	CG-CD1-CE1	-5.08	117.24	121.30
9	q	55	LYS	CA-CB-CG	5.08	124.57	113.40
1	A	695	TYR	CG-CD2-CE2	5.08	125.36	121.30
2	F	563	ARG	NH1-CZ-NH2	5.08	124.98	119.40
8	c	186	TYR	CD1-CE1-CZ	5.08	124.37	119.80
8	e	265	ARG	N-CA-C	-5.08	97.30	111.00
8	e	359	ALA	N-CA-CB	5.08	117.21	110.10
3	I	466	PHE	CG-CD1-CE1	-5.07	115.22	120.80
1	M	845	TYR	CB-CG-CD2	-5.07	117.95	121.00
8	k	212	ARG	CD-NE-CZ	-5.07	116.50	123.60
8	m	63	ARG	CG-CD-NE	-5.07	101.14	111.80
3	K	450	ALA	N-CA-CB	5.07	117.20	110.10
3	I	273	ALA	N-CA-CB	5.07	117.20	110.10
2	N	423	TYR	CG-CD2-CE2	-5.07	117.24	121.30
8	b	63	ARG	NE-CZ-NH1	-5.07	117.77	120.30
8	g	161	TYR	N-CA-C	-5.07	97.31	111.00
1	A	719	ASP	O-C-N	-5.07	114.59	122.70
8	j	212	ARG	NE-CZ-NH2	-5.07	117.77	120.30
8	n	104	TRP	CE2-CD2-CG	-5.07	103.24	107.30
2	N	608	ASN	N-CA-CB	5.07	119.72	110.60
8	c	404	PHE	CB-CG-CD1	-5.07	117.25	120.80
8	e	186	TYR	CA-CB-CG	-5.07	103.77	113.40
8	n	212	ARG	CA-CB-CG	5.07	124.55	113.40
1	G	490	ALA	N-CA-CB	5.07	117.19	110.10
4	J	354	PHE	CG-CD1-CE1	-5.07	115.23	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	52	TYR	CB-CG-CD1	5.07	124.04	121.00
8	g	199	ALA	N-CA-CB	5.07	117.19	110.10
8	g	244	ARG	N-CA-CB	5.07	119.72	110.60
1	E	714	SER	N-CA-CB	-5.06	102.90	110.50
1	G	566	ASP	CA-C-N	5.06	131.28	117.10
5	L	438	ARG	NE-CZ-NH1	5.06	122.83	120.30
5	L	1665	PHE	CB-CG-CD2	5.06	124.34	120.80
1	A	360	ASP	CB-CG-OD2	5.06	122.86	118.30
8	m	372	ARG	CG-CD-NE	-5.06	101.17	111.80
3	I	650	TYR	CB-CG-CD2	-5.06	117.96	121.00
3	I	511	ALA	N-CA-CB	5.06	117.18	110.10
8	h	113	LYS	N-CA-CB	5.06	119.71	110.60
8	k	85	LEU	CB-CG-CD1	5.06	119.60	111.00
2	H	874	PHE	O-C-N	-5.06	114.61	122.70
5	L	575	LEU	CB-CG-CD2	5.06	119.60	111.00
2	N	264	PHE	CA-CB-CG	-5.06	101.76	113.90
8	k	258	ALA	CB-CA-C	-5.06	102.52	110.10
3	K	466	PHE	CB-CG-CD1	-5.06	117.26	120.80
5	L	537	TYR	CB-CG-CD2	-5.06	117.97	121.00
8	a	273	TYR	CZ-CE2-CD2	-5.06	115.25	119.80
8	e	341	ARG	NH1-CZ-NH2	5.06	124.96	119.40
8	j	386	SER	N-CA-CB	5.06	118.08	110.50
2	H	457	ARG	CD-NE-CZ	-5.05	116.52	123.60
4	J	709	TYR	CB-CG-CD2	5.05	124.03	121.00
2	R	19	ARG	NE-CZ-NH2	5.05	122.83	120.30
2	H	316	PHE	CG-CD2-CE2	5.05	126.36	120.80
8	c	156	ARG	NE-CZ-NH2	-5.05	117.77	120.30
2	F	644	ASP	CB-CG-OD2	5.05	122.84	118.30
6	P	42	GLY	N-CA-C	-5.05	100.48	113.10
1	E	646	TYR	CD1-CG-CD2	5.05	123.45	117.90
1	G	689	VAL	CA-CB-CG2	-5.05	103.33	110.90
8	f	153	LEU	CB-CG-CD2	5.05	119.58	111.00
3	I	625	LEU	CB-CG-CD2	-5.05	102.42	111.00
3	K	453	GLY	N-CA-C	-5.05	100.48	113.10
2	T	101	SER	N-CA-CB	5.05	118.07	110.50
9	s	13	GLU	N-CA-CB	-5.05	101.52	110.60
1	M	227	VAL	N-CA-C	-5.04	97.38	111.00
7	U	633	PHE	CG-CD1-CE1	-5.04	115.25	120.80
8	g	225	PHE	CZ-CE2-CD2	5.04	126.15	120.10
8	l	140	SER	O-C-N	-5.04	114.63	122.70
2	B	310	ARG	NE-CZ-NH2	-5.04	117.78	120.30
5	L	1605	LEU	C-N-CA	5.04	134.31	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	k	206	ASP	CB-CG-OD2	-5.04	113.76	118.30
2	N	854	GLN	N-CA-CB	5.04	119.67	110.60
8	d	92	TYR	CB-CG-CD2	-5.04	117.98	121.00
2	T	44	ALA	N-CA-CB	5.04	117.16	110.10
8	k	22	TRP	CD1-CG-CD2	-5.04	102.27	106.30
2	D	411	ARG	NH1-CZ-NH2	-5.04	113.86	119.40
3	I	414	LEU	O-C-N	5.04	130.76	122.70
4	J	239	SER	N-CA-CB	5.04	118.06	110.50
5	L	1422	LEU	N-CA-CB	5.04	120.48	110.40
7	V	650	ASN	N-CA-C	-5.04	97.40	111.00
8	a	316	CYS	N-CA-CB	5.04	119.67	110.60
8	c	92	TYR	CG-CD2-CE2	-5.04	117.27	121.30
2	H	660	LEU	CB-CG-CD1	5.04	119.56	111.00
3	I	341	TRP	CB-CG-CD2	5.04	133.15	126.60
2	B	459	TRP	CE3-CZ3-CH2	5.04	126.74	121.20
2	B	826	ASP	CB-CG-OD1	-5.04	113.77	118.30
2	F	285	SER	N-CA-CB	5.04	118.05	110.50
2	H	474	MET	N-CA-CB	5.04	119.66	110.60
4	J	1011	SER	O-C-N	-5.04	114.64	122.70
8	e	113	LYS	CA-CB-CG	5.04	124.48	113.40
8	n	270	MET	CA-CB-CG	5.04	121.86	113.30
5	L	338	ALA	CB-CA-C	-5.03	102.55	110.10
1	M	646	TYR	CZ-CE2-CD2	5.03	124.33	119.80
8	i	293	VAL	CG1-CB-CG2	5.03	118.95	110.90
8	l	104	TRP	CB-CG-CD2	5.03	133.14	126.60
1	E	549	ARG	CB-CG-CD	5.03	124.68	111.60
2	N	473	PHE	CB-CG-CD1	-5.03	117.28	120.80
2	O	62	PHE	CB-CG-CD2	5.03	124.32	120.80
8	b	348	PHE	N-CA-CB	5.03	119.65	110.60
8	c	360	LEU	CB-CA-C	5.03	119.76	110.20
8	f	346	ALA	N-CA-CB	5.03	117.14	110.10
1	A	680	THR	CA-CB-OG1	5.03	119.56	109.00
4	J	765	TYR	CB-CG-CD2	5.03	124.02	121.00
3	K	537	GLU	N-CA-CB	5.03	119.65	110.60
5	L	221	VAL	CG1-CB-CG2	-5.03	102.86	110.90
8	n	10	LEU	CB-CA-C	-5.03	100.65	110.20
2	H	455	THR	CA-CB-CG2	-5.03	105.36	112.40
2	R	19	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
8	f	286	ARG	NE-CZ-NH1	-5.03	117.79	120.30
8	i	186	TYR	CZ-CE2-CD2	5.02	124.32	119.80
8	k	310	ASP	CA-CB-CG	5.02	124.45	113.40
4	J	961	ASP	CB-CG-OD1	5.02	122.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	M	867	TYR	CD1-CE1-CZ	-5.02	115.28	119.80
8	i	348	PHE	N-CA-CB	5.02	119.64	110.60
5	L	404	TYR	CZ-CE2-CD2	-5.02	115.28	119.80
8	b	265	ARG	CD-NE-CZ	5.02	130.63	123.60
8	n	366	TYR	CZ-CE2-CD2	5.02	124.32	119.80
3	K	641	LEU	CB-CG-CD2	-5.02	102.47	111.00
3	K	200	TYR	CB-CG-CD2	-5.02	117.99	121.00
1	A	245	PHE	CB-CG-CD1	5.02	124.31	120.80
1	M	231	TYR	CB-CG-CD2	5.02	124.01	121.00
1	M	428	ASP	CB-CG-OD1	5.02	122.81	118.30
2	F	416	HIS	N-CA-CB	5.01	119.63	110.60
2	H	440	ASP	CB-CG-OD2	5.01	122.81	118.30
8	k	372	ARG	CB-CA-C	-5.01	100.37	110.40
8	n	152	TYR	CG-CD2-CE2	-5.01	117.29	121.30
2	B	852	PHE	CB-CG-CD2	-5.01	117.29	120.80
8	e	22	TRP	CD1-CG-CD2	5.01	110.31	106.30
2	D	466	ARG	NH1-CZ-NH2	5.01	124.91	119.40
2	H	776	ALA	N-CA-CB	5.01	117.11	110.10
2	N	590	THR	CA-CB-CG2	5.01	119.42	112.40
8	f	226	SER	N-CA-CB	5.01	118.02	110.50
8	k	412	ASP	CB-CG-OD2	-5.01	113.79	118.30
1	E	395	TYR	CG-CD1-CE1	5.01	125.31	121.30
2	F	875	LEU	CB-CG-CD2	5.01	119.52	111.00
2	N	867	SER	N-CA-CB	5.01	118.02	110.50
8	f	412	ASP	N-CA-CB	5.01	119.62	110.60
5	L	1436	VAL	CA-CB-CG2	5.01	118.41	110.90
2	N	713	PHE	CB-CG-CD1	-5.01	117.29	120.80
8	f	49	ASP	CB-CG-OD1	5.01	122.81	118.30
1	A	674	TRP	CA-CB-CG	5.01	123.21	113.70
1	C	574	ILE	CA-C-N	-5.01	106.19	117.20
5	L	587	PHE	CB-CG-CD2	-5.01	117.30	120.80
7	U	609	GLU	OE1-CD-OE2	-5.01	117.29	123.30
8	c	82	TYR	CB-CG-CD1	5.01	124.00	121.00
8	j	329	ASP	CB-CG-OD1	5.01	122.81	118.30
5	L	1540	VAL	CA-CB-CG2	-5.00	103.39	110.90
8	c	418	PHE	CB-CG-CD1	5.00	124.30	120.80
1	C	619	TYR	CZ-CE2-CD2	5.00	124.30	119.80
5	L	403	GLU	CA-CB-CG	5.00	124.41	113.40
2	N	362	THR	O-C-N	-5.00	114.69	122.70
8	l	216	ASP	CB-CG-OD1	-5.00	113.80	118.30
4	J	420	PRO	CA-C-N	5.00	131.10	117.10
2	N	446	PHE	CB-CG-CD2	-5.00	117.30	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	a	38	GLU	N-CA-C	-5.00	97.49	111.00
8	h	401	ARG	NE-CZ-NH1	-5.00	117.80	120.30
8	l	82	TYR	CA-CB-CG	-5.00	103.90	113.40
8	m	166	VAL	CG1-CB-CG2	5.00	118.90	110.90

There are no chirality outliers.

All (473) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	240	ARG	Sidechain
1	A	326	TYR	Sidechain
1	A	361	ARG	Sidechain
1	A	377	TYR	Sidechain
1	A	386	TYR	Sidechain
1	A	392	ARG	Sidechain
1	A	406	PHE	Sidechain
1	A	431	TYR	Sidechain
1	A	460	ARG	Sidechain
1	A	493	TYR	Sidechain
1	A	549	ARG	Sidechain
1	A	559	ARG	Sidechain
1	A	617	PHE	Sidechain
1	A	646	TYR	Sidechain
1	A	747	PHE	Sidechain
1	A	845	TYR	Sidechain
1	A	859	TYR	Sidechain
2	B	271	GLU	Peptide
2	B	300	HIS	Sidechain
2	B	311	SER	Peptide
2	B	314	ARG	Sidechain
2	B	336	ARG	Sidechain
2	B	434	TYR	Sidechain
2	B	442	TYR	Sidechain
2	B	463	TYR	Sidechain
2	B	473	PHE	Sidechain
2	B	480	ARG	Sidechain
2	B	522	PHE	Sidechain
2	B	563	ARG	Sidechain
2	B	564	TYR	Sidechain
2	B	586	ARG	Sidechain
2	B	592	TYR	Sidechain
2	B	619	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	B	653	ARG	Sidechain
2	B	674	TYR	Sidechain
2	B	792	TYR	Sidechain
2	B	831	ARG	Sidechain
2	B	843	ARG	Sidechain
2	B	853	TYR	Sidechain
2	B	860	PHE	Sidechain
2	B	873	ARG	Sidechain
1	C	222	TYR	Sidechain
1	C	231	TYR	Sidechain
1	C	361	ARG	Sidechain
1	C	386	TYR	Sidechain
1	C	395	TYR	Sidechain
1	C	403	TYR	Sidechain
1	C	472	LYS	Peptide
1	C	480	GLU	Peptide
1	C	491	TYR	Sidechain
1	C	513	ARG	Sidechain
1	C	518	TYR	Sidechain
1	C	519	PHE	Sidechain
1	C	529	HIS	Sidechain
1	C	646	TYR	Sidechain
1	C	652	ARG	Sidechain
1	C	675	PHE	Sidechain
1	C	694	TYR	Sidechain
1	C	724	HIS	Sidechain
1	C	764	PHE	Sidechain
1	C	859	TYR	Sidechain
2	D	255	TYR	Sidechain
2	D	266	LYS	Peptide
2	D	313	ASP	Peptide
2	D	390	ARG	Sidechain
2	D	411	ARG	Sidechain
2	D	430	TYR	Sidechain
2	D	562	ARG	Sidechain
2	D	663	PHE	Sidechain
2	D	668	ARG	Sidechain
2	D	750	HIS	Sidechain
2	D	812	ARG	Sidechain
2	D	873	ARG	Sidechain
1	E	282	PHE	Peptide
1	E	296	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	E	314	ARG	Sidechain
1	E	395	TYR	Sidechain
1	E	396	ARG	Sidechain
1	E	431	TYR	Sidechain,Peptide
1	E	432	THR	Peptide
1	E	433	ILE	Peptide
1	E	460	ARG	Sidechain
1	E	515	ILE	Peptide
1	E	520	LEU	Peptide
1	E	526	PHE	Sidechain
1	E	649	HIS	Sidechain
1	E	684	ARG	Sidechain
1	E	694	TYR	Sidechain
1	E	714	SER	Peptide
2	F	251	ARG	Sidechain
2	F	274	TYR	Sidechain
2	F	313	ASP	Peptide
2	F	314	ARG	Sidechain
2	F	323	PHE	Sidechain
2	F	328	HIS	Sidechain
2	F	364	ARG	Sidechain
2	F	411	ARG	Sidechain
2	F	463	TYR	Sidechain
2	F	574	ARG	Sidechain
2	F	592	TYR	Sidechain
2	F	659	TYR	Sidechain
2	F	719	TYR	Sidechain
2	F	720	TYR	Sidechain
2	F	762	LEU	Peptide
2	F	802	ARG	Sidechain
2	F	843	ARG	Sidechain
2	F	853	TYR	Sidechain
2	F	885	TYR	Sidechain
1	G	222	TYR	Sidechain
1	G	231	TYR	Sidechain
1	G	240	ARG	Sidechain
1	G	282	PHE	Sidechain
1	G	289	HIS	Sidechain
1	G	326	TYR	Sidechain
1	G	348	GLU	Peptide
1	G	365	TYR	Sidechain
1	G	403	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	G	431	TYR	Sidechain
1	G	441	PHE	Sidechain
1	G	476	TYR	Sidechain
1	G	559	ARG	Sidechain
1	G	631	ARG	Sidechain
1	G	645	PHE	Sidechain
1	G	698	PHE	Sidechain
1	G	763	ARG	Sidechain
1	G	867	TYR	Sidechain
2	H	255	TYR	Sidechain
2	H	271	GLU	Peptide
2	H	274	TYR	Sidechain
2	H	313	ASP	Peptide
2	H	314	ARG	Sidechain
2	H	335	TYR	Sidechain
2	H	364	ARG	Sidechain
2	H	423	TYR	Sidechain
2	H	442	TYR	Sidechain
2	H	445	PHE	Sidechain
2	H	463	TYR	Sidechain
2	H	473	PHE	Sidechain
2	H	522	PHE	Peptide
2	H	537	TYR	Sidechain
2	H	562	ARG	Sidechain
2	H	563	ARG	Sidechain
2	H	592	TYR	Sidechain
2	H	594	HIS	Sidechain
2	H	641	TYR	Sidechain
2	H	674	TYR	Sidechain
2	H	719	TYR	Sidechain
2	H	720	TYR	Sidechain
2	H	760	ARG	Sidechain
2	H	792	TYR	Sidechain
2	H	831	ARG	Sidechain
2	H	860	PHE	Sidechain
2	H	878	ARG	Sidechain
3	I	111	PHE	Sidechain
3	I	12	TYR	Sidechain
3	I	169	ARG	Sidechain
3	I	180	HIS	Sidechain
3	I	184	TYR	Sidechain
3	I	200	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	I	260	ARG	Sidechain
3	I	267	TYR	Sidechain
3	I	460	TRP	Peptide
3	I	52	TYR	Sidechain
3	I	529	TYR	Sidechain
3	I	530	TYR	Sidechain
3	I	55	PHE	Sidechain
3	I	560	HIS	Sidechain
3	I	572	PHE	Peptide
3	I	576	LYS	Peptide
4	J	209	ARG	Sidechain
4	J	220	TYR	Sidechain
4	J	226	PRO	Peptide
4	J	253	TYR	Sidechain
4	J	307	ARG	Mainchain,Peptide
4	J	424	ARG	Peptide
4	J	437	TYR	Sidechain
4	J	468	TYR	Sidechain
4	J	503	PHE	Sidechain
4	J	591	PHE	Sidechain
4	J	687	TYR	Sidechain
4	J	703	TYR	Sidechain
4	J	719	ARG	Sidechain
4	J	816	TYR	Sidechain
4	J	877	ARG	Sidechain
4	J	899	ARG	Sidechain
4	J	902	HIS	Sidechain
4	J	927	ARG	Sidechain
4	J	935	ARG	Sidechain
4	J	982	PHE	Sidechain
3	K	124	TYR	Sidechain
3	K	169	ARG	Sidechain
3	K	184	TYR	Sidechain
3	K	278	PHE	Sidechain
3	K	361	TYR	Sidechain
3	K	396	PHE	Sidechain
3	K	442	ARG	Sidechain
3	K	456	TYR	Sidechain
3	K	460	TRP	Mainchain,Peptide
3	K	466	PHE	Sidechain
3	K	515	ARG	Sidechain
3	K	52	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	K	529	TYR	Sidechain
3	K	530	TYR	Sidechain
3	K	557	ARG	Sidechain
3	K	572	PHE	Peptide
3	K	62	TYR	Sidechain
3	K	647	ARG	Sidechain
5	L	1385	TYR	Sidechain
5	L	1406	GLU	Peptide
5	L	1447	TYR	Sidechain
5	L	1465	TYR	Sidechain
5	L	1503	TYR	Sidechain
5	L	1533	VAL	Peptide
5	L	1539	SER	Peptide
5	L	1540	VAL	Peptide
5	L	1582	VAL	Peptide
5	L	1589	TYR	Sidechain
5	L	1595	TYR	Sidechain
5	L	161	ASP	Sidechain
5	L	1626	PHE	Sidechain
5	L	1662	TYR	Sidechain
5	L	1673	LEU	Peptide
5	L	1674	VAL	Peptide
5	L	326	TYR	Sidechain
5	L	347	LEU	Peptide
5	L	385	TYR	Sidechain,Peptide
5	L	404	TYR	Sidechain
5	L	410	ARG	Sidechain
5	L	413	HIS	Sidechain
5	L	504	TYR	Sidechain
5	L	512	ASN	Peptide
5	L	513	SER	Peptide
5	L	537	TYR	Sidechain
5	L	560	TYR	Sidechain
5	L	582	ASP	Peptide
5	L	585	PRO	Peptide
5	L	97	TYR	Sidechain
1	M	222	TYR	Sidechain
1	M	240	ARG	Sidechain
1	M	302	TYR	Sidechain
1	M	361	ARG	Sidechain
1	M	371	ALA	Peptide
1	M	377	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	M	386	TYR	Sidechain
1	M	406	PHE	Sidechain
1	M	428	ASP	Peptide
1	M	455	TYR	Sidechain
1	M	470	ASP	Peptide
1	M	473	GLU	Peptide
1	M	479	LYS	Peptide
1	M	493	TYR	Sidechain
1	M	501	PHE	Sidechain
1	M	695	TYR	Sidechain
1	M	827	PHE	Sidechain
1	M	831	PHE	Sidechain
1	M	859	TYR	Sidechain
2	N	251	ARG	Sidechain
2	N	306	TYR	Sidechain
2	N	335	TYR	Sidechain
2	N	364	ARG	Sidechain
2	N	376	ARG	Sidechain
2	N	386	HIS	Sidechain
2	N	430	TYR	Sidechain
2	N	431	ARG	Sidechain
2	N	442	TYR	Sidechain
2	N	463	TYR	Sidechain
2	N	466	ARG	Sidechain
2	N	543	TYR	Sidechain
2	N	552	TYR	Sidechain
2	N	592	TYR	Sidechain
2	N	653	ARG	Sidechain
2	N	712	HIS	Sidechain
2	N	784	PHE	Sidechain
2	N	792	TYR	Sidechain
2	N	802	ARG	Sidechain
2	N	839	ILE	Peptide
2	N	878	ARG	Sidechain
2	N	884	HIS	Sidechain
2	N	885	TYR	Sidechain
2	O	64	ARG	Sidechain
2	O	67	ARG	Sidechain
6	P	188	TYR	Sidechain
6	P	198	TYR	Sidechain
6	P	206	ARG	Sidechain
6	P	218	TYR	Sidechain

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Mol	Chain	Res	Type	Group
6	P	290	ARG	Sidechain
6	P	306	TYR	Sidechain
6	P	335	ARG	Sidechain
6	P	362	TYR	Sidechain
2	Q	114	PHE	Sidechain
2	Q	34	TYR	Sidechain
2	Q	37	ARG	Sidechain
2	Q	64	ARG	Sidechain
2	Q	79	ARG	Sidechain
2	R	19	ARG	Sidechain
2	R	34	TYR	Sidechain
2	R	95	TYR	Sidechain
2	S	34	TYR	Sidechain
2	S	67	ARG	Sidechain
2	S	78	HIS	Sidechain
2	T	79	ARG	Sidechain
7	U	620	ARG	Sidechain
7	V	661	ARG	Sidechain
7	V	668	ARG	Sidechain
7	W	620	ARG	Sidechain
7	X	633	PHE	Sidechain
7	X	661	ARG	Sidechain
7	X	666	ARG	Sidechain
8	a	124	ARG	Sidechain
8	a	161	TYR	Sidechain
8	a	194	ARG	Sidechain
8	a	21	PHE	Sidechain
8	a	217	ARG	Sidechain
8	a	219	HIS	Sidechain
8	a	245	TYR	Sidechain
8	a	273	TYR	Sidechain
8	a	343	ARG	Sidechain
8	a	348	PHE	Sidechain
8	a	47	ARG	Sidechain
8	a	53	TYR	Sidechain
8	b	194	ARG	Sidechain
8	b	217	ARG	Sidechain
8	b	245	TYR	Sidechain
8	b	248	TYR	Sidechain
8	b	29	HIS	Sidechain
8	b	295	ARG	Sidechain
8	b	315	HIS	Sidechain

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Mol	Chain	Res	Type	Group
8	b	341	ARG	Sidechain
8	b	362	ARG	Sidechain
8	b	51	PHE	Sidechain
8	b	72	ARG	Sidechain
8	b	82	TYR	Sidechain
8	b	92	TYR	Sidechain
8	c	124	ARG	Sidechain
8	c	152	TYR	Sidechain
8	c	160	ARG	Sidechain
8	c	186	TYR	Sidechain
8	c	248	TYR	Sidechain
8	c	265	ARG	Sidechain
8	c	362	ARG	Sidechain
8	c	393	ARG	Sidechain
8	c	401	ARG	Sidechain
8	c	82	TYR	Sidechain
8	d	273	TYR	Sidechain
8	d	317	TYR	Sidechain
8	d	341	ARG	Sidechain
8	d	343	ARG	Sidechain
8	d	362	ARG	Sidechain
8	d	372	ARG	Sidechain
8	d	390	ARG	Sidechain
8	d	395	TYR	Sidechain
8	d	60	TYR	Sidechain
8	e	217	ARG	Sidechain
8	e	244	ARG	Sidechain
8	e	317	TYR	Sidechain
8	e	399	ARG	Sidechain
8	e	401	ARG	Sidechain
8	e	418	PHE	Sidechain
8	e	425	ARG	Sidechain
8	e	47	ARG	Sidechain
8	e	53	TYR	Sidechain
8	e	60	TYR	Sidechain
8	e	72	ARG	Sidechain
8	e	82	TYR	Sidechain
8	e	96	HIS	Sidechain
8	f	135	PHE	Sidechain
8	f	186	TYR	Sidechain
8	f	245	TYR	Sidechain
8	f	273	TYR	Sidechain

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Mol	Chain	Res	Type	Group
8	f	309	ARG	Sidechain
8	f	311	ARG	Sidechain
8	f	315	HIS	Sidechain
8	f	395	TYR	Sidechain
8	f	404	PHE	Sidechain
8	f	47	ARG	Sidechain
8	f	82	TYR	Sidechain
8	f	92	TYR	Sidechain
8	g	152	TYR	Sidechain
8	g	161	TYR	Sidechain
8	g	273	TYR	Sidechain
8	g	339	ARG	Sidechain
8	g	343	ARG	Sidechain
8	g	348	PHE	Sidechain
8	g	362	ARG	Sidechain
8	g	388	PHE	Sidechain
8	g	395	TYR	Sidechain
8	g	53	TYR	Sidechain
8	g	60	TYR	Sidechain
8	g	82	TYR	Sidechain
8	h	160	ARG	Sidechain
8	h	161	TYR	Sidechain
8	h	180	HIS	Sidechain
8	h	248	TYR	Sidechain
8	h	339	ARG	Sidechain
8	h	343	ARG	Sidechain
8	h	393	ARG	Sidechain
8	h	409	ARG	Sidechain
8	h	436	HIS	Sidechain
8	h	47	ARG	Sidechain
8	h	52	PHE	Sidechain
8	h	60	TYR	Sidechain
8	h	92	TYR	Sidechain
8	i	248	TYR	Sidechain
8	i	273	TYR	Sidechain
8	i	309	ARG	Sidechain
8	i	339	ARG	Sidechain
8	i	366	TYR	Sidechain
8	i	401	ARG	Sidechain
8	i	92	TYR	Sidechain
8	j	124	ARG	Sidechain
8	j	139	HIS	Sidechain

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Mol	Chain	Res	Type	Group
8	j	161	TYR	Sidechain
8	j	180	HIS	Sidechain
8	j	267	HIS	Sidechain
8	j	286	ARG	Sidechain
8	j	315	HIS	Sidechain
8	j	339	ARG	Sidechain
8	j	348	PHE	Sidechain
8	j	362	ARG	Sidechain
8	j	60	TYR	Sidechain
8	j	63	ARG	Sidechain
8	j	82	TYR	Sidechain
8	j	86	TYR	Sidechain
8	j	92	TYR	Sidechain
8	k	156	ARG	Sidechain
8	k	265	ARG	Sidechain
8	k	286	ARG	Sidechain
8	k	3	ARG	Sidechain
8	k	317	TYR	Sidechain
8	k	334	HIS	Sidechain
8	k	366	TYR	Sidechain
8	k	388	PHE	Sidechain
8	k	393	ARG	Sidechain
8	k	408	PHE	Sidechain
8	k	53	TYR	Sidechain
8	k	72	ARG	Sidechain
8	k	92	TYR	Sidechain
8	l	139	HIS	Sidechain
8	l	152	TYR	Sidechain
8	l	161	TYR	Sidechain
8	l	21	PHE	Sidechain
8	l	217	ARG	Sidechain
8	l	244	ARG	Sidechain
8	l	339	ARG	Sidechain
8	l	425	ARG	Sidechain
8	l	47	ARG	Sidechain
8	l	82	TYR	Sidechain
8	m	139	HIS	Sidechain
8	m	161	TYR	Sidechain
8	m	169	TYR	Sidechain
8	m	212	ARG	Sidechain
8	m	296	ARG	Sidechain
8	m	311	ARG	Sidechain

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Mol	Chain	Res	Type	Group
8	m	317	TYR	Sidechain
8	m	334	HIS	Sidechain
8	m	390	ARG	Sidechain
8	m	399	ARG	Sidechain
8	m	401	ARG	Sidechain
8	m	408	PHE	Sidechain
8	m	86	TYR	Sidechain
8	m	92	TYR	Sidechain
8	n	317	TYR	Sidechain
8	n	343	ARG	Sidechain
8	n	348	PHE	Sidechain
8	n	362	ARG	Sidechain
8	n	395	TYR	Sidechain
8	n	418	PHE	Sidechain
8	n	82	TYR	Sidechain
8	n	86	TYR	Sidechain

5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

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	543/896 (61%)	510 (94%)	21 (4%)	12 (2%)	5	29
1	C	543/896 (61%)	506 (93%)	26 (5%)	11 (2%)	6	32
1	E	541/896 (60%)	500 (92%)	27 (5%)	14 (3%)	4	26
1	G	543/896 (61%)	515 (95%)	18 (3%)	10 (2%)	7	34
1	M	541/896 (60%)	492 (91%)	35 (6%)	14 (3%)	4	26
2	B	619/906 (68%)	565 (91%)	34 (6%)	20 (3%)	3	21

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	D	619/906 (68%)	562 (91%)	41 (7%)	16 (3%)	4	26
2	F	619/906 (68%)	568 (92%)	38 (6%)	13 (2%)	5	30
2	H	619/906 (68%)	572 (92%)	36 (6%)	11 (2%)	7	34
2	N	619/906 (68%)	569 (92%)	33 (5%)	17 (3%)	4	26
2	O	91/906 (10%)	87 (96%)	3 (3%)	1 (1%)	12	46
2	Q	107/906 (12%)	98 (92%)	5 (5%)	4 (4%)	2	20
2	R	96/906 (11%)	88 (92%)	7 (7%)	1 (1%)	13	48
2	S	107/906 (12%)	97 (91%)	8 (8%)	2 (2%)	6	33
2	T	91/906 (10%)	84 (92%)	5 (6%)	2 (2%)	5	29
3	I	563/666 (84%)	512 (91%)	35 (6%)	16 (3%)	4	24
3	K	563/666 (84%)	517 (92%)	35 (6%)	11 (2%)	6	32
4	J	624/1019 (61%)	571 (92%)	41 (7%)	12 (2%)	6	33
5	L	762/1698 (45%)	682 (90%)	53 (7%)	27 (4%)	3	20
6	P	369/375 (98%)	336 (91%)	26 (7%)	7 (2%)	6	33
7	U	73/671 (11%)	73 (100%)	0	0	100	100
7	V	73/671 (11%)	73 (100%)	0	0	100	100
7	W	73/671 (11%)	71 (97%)	1 (1%)	1 (1%)	9	40
7	X	73/671 (11%)	71 (97%)	2 (3%)	0	100	100
8	a	434/451 (96%)	370 (85%)	47 (11%)	17 (4%)	2	19
8	b	434/451 (96%)	368 (85%)	50 (12%)	16 (4%)	2	20
8	c	434/451 (96%)	364 (84%)	47 (11%)	23 (5%)	1	16
8	d	434/451 (96%)	364 (84%)	53 (12%)	17 (4%)	2	19
8	e	434/451 (96%)	364 (84%)	49 (11%)	21 (5%)	2	17
8	f	434/451 (96%)	376 (87%)	37 (8%)	21 (5%)	2	17
8	g	434/451 (96%)	371 (86%)	41 (9%)	22 (5%)	1	16
8	h	434/451 (96%)	377 (87%)	41 (9%)	16 (4%)	2	20
8	i	434/451 (96%)	365 (84%)	49 (11%)	20 (5%)	2	17
8	j	434/451 (96%)	375 (86%)	41 (9%)	18 (4%)	2	18
8	k	434/451 (96%)	370 (85%)	47 (11%)	17 (4%)	2	19
8	l	434/451 (96%)	366 (84%)	44 (10%)	24 (6%)	1	15
8	m	434/451 (96%)	368 (85%)	45 (10%)	21 (5%)	2	17

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
8	n	434/451 (96%)	375 (86%)	43 (10%)	16 (4%)	2	20
9	o	50/72 (69%)	49 (98%)	1 (2%)	0	100	100
9	p	54/72 (75%)	54 (100%)	0	0	100	100
9	q	54/72 (75%)	53 (98%)	1 (2%)	0	100	100
9	r	57/72 (79%)	54 (95%)	1 (2%)	2 (4%)	3	20
9	s	57/72 (79%)	55 (96%)	2 (4%)	0	100	100
9	t	56/72 (78%)	53 (95%)	3 (5%)	0	100	100
All	All	15875/27394 (58%)	14210 (90%)	1172 (7%)	493 (3%)	5	22

All (493) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	B	318	LEU
2	B	468	SER
2	B	496	CYS
2	B	522	PHE
1	C	317	LEU
1	C	471	ALA
1	C	473	GLU
1	C	476	TYR
2	D	280	VAL
2	D	314	ARG
2	D	468	SER
2	D	742	ASP
1	E	432	THR
1	E	439	PRO
1	E	740	ASN
1	E	848	SER
2	F	314	ARG
2	F	764	ASP
2	F	867	SER
1	G	465	ASP
1	G	562	THR
1	G	849	ASP
1	G	850	CYS
2	H	314	ARG
2	H	316	PHE
3	I	461	PRO
3	I	575	LEU
3	I	603	LEU

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Mol	Chain	Res	Type
3	I	636	GLN
4	J	252	LEU
4	J	263	GLU
4	J	673	VAL
3	K	638	ASN
5	L	513	SER
5	L	552	PHE
5	L	557	ASN
5	L	566	LYS
5	L	1454	SER
5	L	1492	ASN
5	L	1530	THR
5	L	1584	ASN
5	L	1610	ALA
1	M	430	ARG
1	M	480	GLU
2	N	521	LEU
2	N	609	ALA
2	N	870	GLU
6	P	244	ASP
8	a	47	ARG
8	a	57	ASP
8	a	178	MET
8	a	226	SER
8	a	243	LEU
8	a	301	LYS
8	a	351	TRP
8	b	56	ASP
8	b	328	VAL
8	c	50	VAL
8	c	102	ASN
8	c	226	SER
8	c	248	TYR
8	c	265	ARG
8	c	267	HIS
8	d	181	VAL
8	d	412	ASP
8	e	126	ALA
8	e	263	THR
8	e	287	LYS
8	e	412	ASP
8	f	266	LEU

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Mol	Chain	Res	Type
8	f	267	HIS
8	g	34	GLU
8	g	50	VAL
8	g	265	ARG
8	g	331	THR
8	h	121	ILE
8	h	266	LEU
8	h	370	ALA
8	i	50	VAL
8	i	121	ILE
8	i	266	LEU
8	i	331	THR
8	i	370	ALA
8	j	226	SER
8	k	131	SER
8	k	263	THR
8	k	265	ARG
8	k	369	SER
8	k	436	HIS
8	l	95	GLU
8	l	222	ASN
8	l	226	SER
8	l	267	HIS
8	l	301	LYS
8	l	366	TYR
8	l	370	ALA
8	m	50	VAL
8	m	131	SER
8	m	226	SER
8	m	266	LEU
8	n	50	VAL
8	n	92	TYR
8	n	102	ASN
8	n	266	LEU
1	A	241	GLN
1	A	849	ASP
2	B	312	LEU
2	B	319	VAL
2	B	469	MET
2	B	867	SER
1	C	465	ASP
1	C	673	LYS

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Mol	Chain	Res	Type
2	D	274	TYR
2	D	282	VAL
2	D	502	ALA
2	D	868	THR
2	D	869	ASP
1	E	433	ILE
1	E	521	MET
1	E	544	ASP
2	F	644	ASP
1	G	442	LEU
1	G	471	ALA
2	H	269	ASN
2	H	391	LYS
2	H	452	VAL
2	H	468	SER
2	H	631	ASP
3	I	254	LEU
3	I	412	PRO
4	J	448	GLU
4	J	484	PRO
4	J	490	ILE
4	J	767	ASP
4	J	789	HIS
4	J	939	ARG
3	K	195	LEU
3	K	298	SER
3	K	445	PRO
3	K	636	GLN
5	L	105	GLN
5	L	223	SER
5	L	1426	GLN
5	L	1471	THR
5	L	1606	THR
1	M	229	GLY
1	M	435	GLN
1	M	481	GLN
1	M	568	PHE
2	N	312	LEU
2	N	502	ALA
2	N	871	SER
2	O	48	GLU
6	P	95	ARG

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Mol	Chain	Res	Type
2	Q	26	ALA
8	a	131	SER
8	b	83	ALA
8	b	121	ILE
8	b	248	TYR
8	b	266	LEU
8	c	131	SER
8	c	328	VAL
8	d	50	VAL
8	d	197	GLN
8	d	226	SER
8	d	267	HIS
8	d	310	ASP
8	d	328	VAL
8	e	56	ASP
8	e	95	GLU
8	e	102	ASN
8	e	162	PRO
8	e	197	GLN
8	e	265	ARG
8	f	50	VAL
8	f	89	GLU
8	f	287	LYS
8	f	371	HIS
8	f	406	GLU
8	f	417	ASN
8	g	57	ASP
8	g	89	GLU
8	g	102	ASN
8	g	302	ASN
8	g	371	HIS
8	h	50	VAL
8	h	226	SER
8	h	328	VAL
8	i	226	SER
8	i	369	SER
8	j	267	HIS
8	j	328	VAL
8	j	370	ALA
8	k	50	VAL
8	k	121	ILE
8	k	126	ALA

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Mol	Chain	Res	Type
8	k	284	SER
8	k	302	ASN
8	l	50	VAL
8	l	102	ASN
8	l	121	ILE
8	l	265	ARG
8	l	328	VAL
8	l	371	HIS
8	m	89	GLU
8	m	197	GLN
8	m	287	LYS
8	m	366	TYR
8	n	263	THR
8	n	267	HIS
8	n	292	ASP
8	n	301	LYS
8	n	350	PRO
1	A	314	ARG
1	A	367	GLY
1	A	468	CYS
1	A	480	GLU
1	A	482	ALA
2	B	271	GLU
2	B	277	ASP
2	B	471	PRO
2	B	502	ALA
2	B	526	GLU
2	B	565	LEU
2	B	609	ALA
1	C	228	ASP
1	C	850	CYS
2	D	268	CYS
2	D	467	LYS
1	E	397	GLY
1	E	442	LEU
1	E	716	SER
2	F	272	ASN
2	F	462	LYS
1	G	472	LYS
3	I	115	PRO
3	I	363	LEU
3	I	446	THR

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Mol	Chain	Res	Type
3	I	451	ALA
3	K	163	GLY
3	K	254	LEU
5	L	586	VAL
5	L	1449	LEU
5	L	1585	LEU
5	L	1605	LEU
5	L	1673	LEU
1	M	474	ILE
2	N	271	GLU
2	N	765	SER
2	N	869	ASP
6	P	15	GLY
6	P	201	THR
6	P	222	ASP
6	P	236	LEU
2	Q	24	GLY
2	R	50	ASP
2	S	47	VAL
2	T	88	LYS
8	a	89	GLU
8	a	244	ARG
8	a	266	LEU
8	b	57	ASP
8	b	197	GLN
8	b	282	VAL
8	c	57	ASP
8	c	244	ARG
8	c	302	ASN
8	c	371	HIS
8	d	62	PRO
8	d	127	ASP
8	d	313	THR
8	e	34	GLU
8	e	121	ILE
8	e	179	SER
8	e	267	HIS
8	e	292	ASP
8	e	350	PRO
8	e	371	HIS
8	f	302	ASN
8	g	197	GLN

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Mol	Chain	Res	Type
8	g	328	VAL
8	g	366	TYR
8	g	406	GLU
8	h	34	GLU
8	h	162	PRO
8	h	301	LYS
8	i	59	HIS
8	i	127	ASP
8	i	406	GLU
8	j	262	PRO
8	j	266	LEU
8	k	267	HIS
8	k	406	GLU
8	m	102	ASN
8	m	248	TYR
8	m	292	ASP
8	m	350	PRO
8	n	197	GLN
9	r	45	ILE
1	A	442	LEU
2	B	407	ASP
2	B	607	THR
2	B	765	SER
1	C	468	CYS
1	C	715	ALA
2	D	609	ALA
1	E	562	THR
1	E	741	PRO
2	F	311	SER
2	F	501	PRO
2	F	502	ALA
1	G	286	GLN
1	G	464	HIS
2	H	459	TRP
3	I	165	LEU
3	I	349	ASP
3	I	638	ASN
4	J	417	ALA
3	K	115	PRO
5	L	607	LEU
5	L	1540	VAL
5	L	1679	GLN

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Mol	Chain	Res	Type
1	M	432	THR
1	M	438	ILE
1	M	471	ALA
2	N	272	ASN
2	N	407	ASP
2	N	610	GLN
2	N	840	PRO
6	P	352	PHE
2	Q	87	LEU
7	W	649	LEU
8	a	267	HIS
8	a	366	TYR
8	b	95	GLU
8	b	217	ARG
8	b	287	LYS
8	b	366	TYR
8	c	241	THR
8	c	287	LYS
8	d	406	GLU
8	e	53	TYR
8	e	302	ASN
8	e	406	GLU
8	f	226	SER
8	f	370	ALA
8	g	219	HIS
8	g	248	TYR
8	g	267	HIS
8	g	329	ASP
8	g	402	GLU
8	h	103	ASN
8	h	417	ASN
8	i	56	ASP
8	i	178	MET
8	i	350	PRO
8	j	34	GLU
8	j	49	ASP
8	j	51	PHE
8	j	354	ALA
8	j	368	PRO
8	j	406	GLU
8	k	331	THR
8	l	344	LYS

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Mol	Chain	Res	Type
8	m	243	LEU
8	m	369	SER
8	n	89	GLU
8	n	162	PRO
8	n	302	ASN
8	n	371	HIS
1	A	242	SER
1	A	428	ASP
2	B	466	ARG
2	D	407	ASP
2	D	738	LEU
2	D	873	ARG
1	E	237	LEU
2	F	407	ASP
1	G	429	GLN
2	H	272	ASN
2	H	407	ASP
2	H	610	GLN
3	I	348	SER
4	J	840	GLU
3	K	165	LEU
3	K	316	GLN
3	K	349	ASP
5	L	1535	GLN
5	L	1575	PHE
5	L	1609	ALA
1	M	404	SER
1	M	496	LYS
2	N	443	HIS
2	N	499	GLN
2	N	614	PRO
2	S	50	ASP
2	T	45	PRO
8	a	283	ALA
8	a	329	ASP
8	a	331	THR
8	a	350	PRO
8	b	302	ASN
8	c	34	GLU
8	c	47	ARG
8	c	95	GLU
8	c	113	LYS

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Mol	Chain	Res	Type
8	c	197	GLN
8	c	330	PRO
8	c	406	GLU
8	d	262	PRO
8	d	265	ARG
8	d	370	ALA
8	f	95	GLU
8	f	121	ILE
8	f	248	TYR
8	f	288	THR
8	g	94	SER
8	g	226	SER
8	h	47	ARG
8	h	287	LYS
8	i	89	GLU
8	i	264	PRO
8	i	287	LYS
8	i	301	LYS
8	j	369	SER
8	k	287	LYS
8	k	301	LYS
8	k	370	ALA
8	k	414	PHE
8	l	34	GLU
8	l	127	ASP
8	l	200	ASP
8	l	287	LYS
8	l	302	ASN
8	l	331	THR
8	l	365	PRO
8	m	94	SER
8	m	103	ASN
8	m	219	HIS
8	m	267	HIS
8	n	103	ASN
9	r	26	ASN
1	A	231	TYR
2	B	261	ASP
2	D	261	ASP
2	F	316	PHE
2	F	439	GLU
4	J	446	VAL

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Mol	Chain	Res	Type
5	L	1582	VAL
1	M	240	ARG
1	M	740	ASN
2	N	629	PRO
8	b	408	PHE
8	c	329	ASP
8	d	330	PRO
8	f	197	GLN
8	h	3	ARG
8	h	262	PRO
8	i	62	PRO
8	i	328	VAL
8	j	178	MET
8	j	248	TYR
8	j	287	LYS
8	j	329	ASP
8	m	328	VAL
8	n	287	LYS
1	C	466	VAL
3	I	602	PRO
8	f	262	PRO
8	f	329	ASP
8	f	350	PRO
8	f	365	PRO
8	g	181	VAL
8	m	275	PRO
1	E	402	PRO
8	b	329	ASP
8	e	223	PRO
8	g	350	PRO
5	L	585	PRO
2	Q	47	VAL
8	l	262	PRO
1	A	439	PRO
3	I	318	PRO
8	c	262	PRO
8	d	223	PRO
8	h	81	PRO
8	i	88	PRO
8	j	300	PRO
8	l	88	PRO
8	m	368	PRO

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Mol	Chain	Res	Type
2	F	453	VAL
8	f	328	VAL
8	l	353	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	507/824 (62%)	486 (96%)	21 (4%)	26	48
1	C	507/824 (62%)	488 (96%)	19 (4%)	29	50
1	E	506/824 (61%)	476 (94%)	30 (6%)	16	38
1	G	507/824 (62%)	484 (96%)	23 (4%)	23	45
1	M	505/824 (61%)	487 (96%)	18 (4%)	30	51
2	B	561/798 (70%)	530 (94%)	31 (6%)	18	40
2	D	561/798 (70%)	538 (96%)	23 (4%)	26	48
2	F	561/798 (70%)	531 (95%)	30 (5%)	19	41
2	H	561/798 (70%)	527 (94%)	34 (6%)	15	37
2	N	561/798 (70%)	539 (96%)	22 (4%)	27	49
2	O	82/798 (10%)	79 (96%)	3 (4%)	29	50
2	Q	96/798 (12%)	95 (99%)	1 (1%)	73	81
2	R	87/798 (11%)	85 (98%)	2 (2%)	45	64
2	S	96/798 (12%)	89 (93%)	7 (7%)	11	31
2	T	82/798 (10%)	78 (95%)	4 (5%)	21	42
3	I	518/595 (87%)	490 (95%)	28 (5%)	18	40
3	K	518/595 (87%)	492 (95%)	26 (5%)	20	42
4	J	587/933 (63%)	562 (96%)	25 (4%)	25	47
5	L	709/1539 (46%)	678 (96%)	31 (4%)	24	46
6	P	314/318 (99%)	303 (96%)	11 (4%)	31	52
7	U	72/598 (12%)	70 (97%)	2 (3%)	38	58

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	V	72/598 (12%)	70 (97%)	2 (3%)	38	58
7	W	72/598 (12%)	66 (92%)	6 (8%)	9	28
7	X	72/598 (12%)	69 (96%)	3 (4%)	25	47
8	a	387/400 (97%)	375 (97%)	12 (3%)	35	55
8	b	387/400 (97%)	368 (95%)	19 (5%)	21	42
8	c	387/400 (97%)	365 (94%)	22 (6%)	17	39
8	d	387/400 (97%)	369 (95%)	18 (5%)	22	44
8	e	387/400 (97%)	367 (95%)	20 (5%)	19	41
8	f	387/400 (97%)	365 (94%)	22 (6%)	17	39
8	g	387/400 (97%)	364 (94%)	23 (6%)	16	38
8	h	387/400 (97%)	370 (96%)	17 (4%)	24	46
8	i	387/400 (97%)	368 (95%)	19 (5%)	21	42
8	j	387/400 (97%)	371 (96%)	16 (4%)	26	48
8	k	387/400 (97%)	367 (95%)	20 (5%)	19	41
8	l	387/400 (97%)	376 (97%)	11 (3%)	38	58
8	m	387/400 (97%)	376 (97%)	11 (3%)	38	58
8	n	387/400 (97%)	371 (96%)	16 (4%)	26	48
9	o	48/62 (77%)	47 (98%)	1 (2%)	48	67
9	p	51/62 (82%)	51 (100%)	0	100	100
9	q	51/62 (82%)	50 (98%)	1 (2%)	50	68
9	r	54/62 (87%)	53 (98%)	1 (2%)	52	69
9	s	53/62 (86%)	52 (98%)	1 (2%)	52	69
9	t	53/62 (86%)	52 (98%)	1 (2%)	52	69
All	All	14442/24444 (59%)	13789 (96%)	653 (4%)	26	45

All (653) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	241	GLN
1	A	249	GLN
1	A	305	LEU
1	A	330	THR
1	A	360	ASP
1	A	445	VAL

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Mol	Chain	Res	Type
1	A	499	LEU
1	A	523	GLN
1	A	535	GLU
1	A	562	THR
1	A	564	ASN
1	A	566	ASP
1	A	653	LEU
1	A	675	PHE
1	A	693	GLN
1	A	714	SER
1	A	729	LEU
1	A	838	LEU
1	A	854	MET
1	A	855	ILE
1	A	861	LEU
2	B	256	VAL
2	B	258	GLN
2	B	314	ARG
2	B	318	LEU
2	B	337	LEU
2	B	345	LEU
2	B	347	VAL
2	B	426	LEU
2	B	431	ARG
2	B	435	ASP
2	B	458	LEU
2	B	471	PRO
2	B	475	THR
2	B	514	SER
2	B	532	LYS
2	B	542	LYS
2	B	545	LEU
2	B	561	MET
2	B	580	LEU
2	B	589	THR
2	B	610	GLN
2	B	614	PRO
2	B	620	LEU
2	B	624	LEU
2	B	626	GLU
2	B	654	GLU
2	B	708	SER

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Mol	Chain	Res	Type
2	B	717	MET
2	B	732	GLU
2	B	736	LYS
2	B	784	PHE
1	C	223	ILE
1	C	248	GLU
1	C	261	ARG
1	C	318	LEU
1	C	320	LEU
1	C	321	GLN
1	C	372	GLN
1	C	379	THR
1	C	390	LEU
1	C	444	LYS
1	C	467	THR
1	C	540	LYS
1	C	609	LEU
1	C	612	LEU
1	C	657	VAL
1	C	659	ILE
1	C	704	THR
1	C	835	LEU
1	C	857	ILE
2	D	293	LEU
2	D	337	LEU
2	D	346	GLN
2	D	366	LEU
2	D	426	LEU
2	D	431	ARG
2	D	444	GLU
2	D	458	LEU
2	D	480	ARG
2	D	500	THR
2	D	514	SER
2	D	522	PHE
2	D	532	LYS
2	D	580	LEU
2	D	592	TYR
2	D	595	ASN
2	D	602	THR
2	D	610	GLN
2	D	649	THR

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Mol	Chain	Res	Type
2	D	650	VAL
2	D	700	LEU
2	D	738	LEU
2	D	753	PHE
1	E	230	ARG
1	E	233	SER
1	E	237	LEU
1	E	278	GLU
1	E	317	LEU
1	E	374	LEU
1	E	380	LYS
1	E	396	ARG
1	E	428	ASP
1	E	432	THR
1	E	452	THR
1	E	456	LEU
1	E	488	GLU
1	E	498	LEU
1	E	534	THR
1	E	539	LYS
1	E	548	THR
1	E	565	THR
1	E	607	LEU
1	E	609	LEU
1	E	613	GLU
1	E	635	THR
1	E	640	LEU
1	E	703	PRO
1	E	728	PHE
1	E	739	THR
1	E	744	LEU
1	E	846	SER
1	E	847	THR
1	E	866	PHE
2	F	266	LYS
2	F	288	ASP
2	F	289	ILE
2	F	296	LEU
2	F	370	THR
2	F	431	ARG
2	F	441	THR
2	F	442	TYR

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Mol	Chain	Res	Type
2	F	444	GLU
2	F	478	GLN
2	F	555	LEU
2	F	565	LEU
2	F	575	HIS
2	F	580	LEU
2	F	591	LEU
2	F	618	LYS
2	F	626	GLU
2	F	655	CYS
2	F	656	MET
2	F	662	VAL
2	F	700	LEU
2	F	738	LEU
2	F	743	LEU
2	F	744	ASP
2	F	780	GLN
2	F	791	LEU
2	F	796	LEU
2	F	847	ARG
2	F	854	GLN
2	F	860	PHE
1	G	227	VAL
1	G	243	ARG
1	G	298	LEU
1	G	317	LEU
1	G	318	LEU
1	G	321	GLN
1	G	323	LEU
1	G	332	ARG
1	G	360	ASP
1	G	370	GLN
1	G	379	THR
1	G	391	GLU
1	G	442	LEU
1	G	480	GLU
1	G	514	SER
1	G	526	PHE
1	G	575	GLU
1	G	635	THR
1	G	711	ASN
1	G	728	PHE

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Mol	Chain	Res	Type
1	G	841	LYS
1	G	863	PHE
1	G	867	TYR
2	H	272	ASN
2	H	286	LEU
2	H	287	LYS
2	H	314	ARG
2	H	429	LEU
2	H	431	ARG
2	H	444	GLU
2	H	449	SER
2	H	455	THR
2	H	467	LYS
2	H	475	THR
2	H	491	PHE
2	H	516	LYS
2	H	529	PHE
2	H	555	LEU
2	H	561	MET
2	H	567	LEU
2	H	593	GLN
2	H	595	ASN
2	H	614	PRO
2	H	662	VAL
2	H	686	ASN
2	H	690	LEU
2	H	709	GLU
2	H	736	LYS
2	H	744	ASP
2	H	761	CYS
2	H	780	GLN
2	H	797	GLU
2	H	803	LEU
2	H	849	LEU
2	H	864	LEU
2	H	866	THR
2	H	872	LEU
3	I	1	MET
3	I	20	ASN
3	I	39	THR
3	I	137	MET
3	I	142	GLN

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Mol	Chain	Res	Type
3	I	155	GLU
3	I	187	LEU
3	I	203	PHE
3	I	285	MET
3	I	300	LEU
3	I	311	LEU
3	I	316	GLN
3	I	336	VAL
3	I	350	LEU
3	I	354	LEU
3	I	370	GLN
3	I	415	ASN
3	I	446	THR
3	I	452	LEU
3	I	488	GLN
3	I	494	CYS
3	I	533	VAL
3	I	536	LEU
3	I	545	GLN
3	I	573	ILE
3	I	588	LEU
3	I	633	ARG
3	I	638	ASN
4	J	220	TYR
4	J	222	THR
4	J	238	LEU
4	J	272	TRP
4	J	274	LEU
4	J	284	GLN
4	J	299	THR
4	J	398	LEU
4	J	431	HIS
4	J	481	LEU
4	J	486	LYS
4	J	492	ARG
4	J	503	PHE
4	J	679	GLU
4	J	705	LEU
4	J	718	MET
4	J	733	PHE
4	J	791	LEU
4	J	843	ASN

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Mol	Chain	Res	Type
4	J	899	ARG
4	J	921	LEU
4	J	927	ARG
4	J	946	LYS
4	J	950	MET
4	J	951	LYS
3	K	55	PHE
3	K	117	LEU
3	K	124	TYR
3	K	156	THR
3	K	180	HIS
3	K	187	LEU
3	K	197	LEU
3	K	203	PHE
3	K	254	LEU
3	K	285	MET
3	K	300	LEU
3	K	319	LEU
3	K	338	GLU
3	K	350	LEU
3	K	351	LEU
3	K	355	LYS
3	K	446	THR
3	K	457	LYS
3	K	459	GLN
3	K	460	TRP
3	K	461	PRO
3	K	514	TRP
3	K	583	ASN
3	K	599	ASN
3	K	600	LEU
3	K	650	TYR
5	L	31	SER
5	L	217	PHE
5	L	326	TYR
5	L	360	VAL
5	L	393	ASN
5	L	399	THR
5	L	409	THR
5	L	474	LEU
5	L	516	GLU
5	L	549	CYS

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Mol	Chain	Res	Type
5	L	566	LYS
5	L	567	ARG
5	L	575	LEU
5	L	577	SER
5	L	598	CYS
5	L	607	LEU
5	L	1375	VAL
5	L	1392	MET
5	L	1422	LEU
5	L	1471	THR
5	L	1473	THR
5	L	1492	ASN
5	L	1496	THR
5	L	1514	LYS
5	L	1542	TYR
5	L	1544	GLN
5	L	1576	ARG
5	L	1586	GLU
5	L	1616	ILE
5	L	1623	ILE
5	L	1628	LEU
1	M	263	LEU
1	M	429	GLN
1	M	432	THR
1	M	445	VAL
1	M	449	ILE
1	M	475	THR
1	M	478	LEU
1	M	508	LEU
1	M	526	PHE
1	M	536	GLU
1	M	541	PRO
1	M	609	LEU
1	M	637	TYR
1	M	717	ASN
1	M	728	PHE
1	M	823	THR
1	M	825	ASN
1	M	854	MET
2	N	267	MET
2	N	280	VAL
2	N	306	TYR

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Mol	Chain	Res	Type
2	N	321	GLN
2	N	346	GLN
2	N	403	THR
2	N	410	MET
2	N	458	LEU
2	N	492	LEU
2	N	521	LEU
2	N	555	LEU
2	N	565	LEU
2	N	575	HIS
2	N	580	LEU
2	N	591	LEU
2	N	597	THR
2	N	634	TRP
2	N	655	CYS
2	N	661	ARG
2	N	760	ARG
2	N	841	LYS
2	N	879	LEU
2	O	19	ARG
2	O	61	GLU
2	O	96	LEU
6	P	17	CYS
6	P	66	THR
6	P	96	VAL
6	P	105	LEU
6	P	132	MET
6	P	210	ARG
6	P	213	LYS
6	P	275	HIS
6	P	278	THR
6	P	287	VAL
6	P	334	GLU
2	Q	67	ARG
2	R	14	GLN
2	R	66	ARG
2	S	18	CYS
2	S	50	ASP
2	S	66	ARG
2	S	90	ARG
2	S	96	LEU
2	S	100	LEU

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Mol	Chain	Res	Type
2	S	111	THR
2	T	47	VAL
2	T	53	LEU
2	T	88	LYS
2	T	100	LEU
7	U	606	MET
7	U	642	MET
7	V	655	SER
7	V	666	ARG
7	W	604	LYS
7	W	628	GLU
7	W	632	GLN
7	W	641	GLN
7	W	659	LYS
7	W	671	PHE
7	X	641	GLN
7	X	650	ASN
7	X	657	ILE
8	a	39	GLU
8	a	46	ASP
8	a	166	VAL
8	a	190	LEU
8	a	242	THR
8	a	264	PRO
8	a	277	THR
8	a	304	MET
8	a	348	PHE
8	a	358	VAL
8	a	417	ASN
8	a	425	ARG
8	b	2	PRO
8	b	39	GLU
8	b	42	THR
8	b	50	VAL
8	b	51	PHE
8	b	84	ASN
8	b	115	HIS
8	b	197	GLN
8	b	210	LEU
8	b	212	ARG
8	b	213	ILE
8	b	225	PHE

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Mol	Chain	Res	Type
8	b	251	ASN
8	b	331	THR
8	b	341	ARG
8	b	371	HIS
8	b	381	HIS
8	b	384	ILE
8	b	412	ASP
8	c	2	PRO
8	c	34	GLU
8	c	67	LEU
8	c	89	GLU
8	c	93	LEU
8	c	184	GLN
8	c	210	LEU
8	c	213	ILE
8	c	234	THR
8	c	240	THR
8	c	241	THR
8	c	278	THR
8	c	288	THR
8	c	294	MET
8	c	334	HIS
8	c	360	LEU
8	c	380	ASN
8	c	381	HIS
8	c	391	THR
8	c	399	ARG
8	c	417	ASN
8	c	423	ASN
8	d	2	PRO
8	d	34	GLU
8	d	43	GLU
8	d	71	PRO
8	d	86	TYR
8	d	92	TYR
8	d	96	HIS
8	d	102	ASN
8	d	263	THR
8	d	265	ARG
8	d	274	THR
8	d	301	LYS
8	d	305	VAL

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Mol	Chain	Res	Type
8	d	330	PRO
8	d	360	LEU
8	d	371	HIS
8	d	415	LYS
8	d	425	ARG
8	e	5	ILE
8	e	12	GLN
8	e	34	GLU
8	e	39	GLU
8	e	50	VAL
8	e	78	LEU
8	e	89	GLU
8	e	136	VAL
8	e	137	LEU
8	e	190	LEU
8	e	192	LEU
8	e	210	LEU
8	e	213	ILE
8	e	223	PRO
8	e	263	THR
8	e	306	SER
8	e	362	ARG
8	e	407	GLN
8	e	415	LYS
8	e	422	ASP
8	f	17	ILE
8	f	45	THR
8	f	49	ASP
8	f	69	LEU
8	f	74	ILE
8	f	80	SER
8	f	89	GLU
8	f	92	TYR
8	f	110	GLN
8	f	139	HIS
8	f	197	GLN
8	f	205	LEU
8	f	212	ARG
8	f	259	SER
8	f	277	THR
8	f	362	ARG
8	f	380	ASN

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Mol	Chain	Res	Type
8	f	381	HIS
8	f	391	THR
8	f	415	LYS
8	f	417	ASN
8	f	425	ARG
8	g	15	ASN
8	g	34	GLU
8	g	89	GLU
8	g	102	ASN
8	g	168	THR
8	g	223	PRO
8	g	240	THR
8	g	248	TYR
8	g	250	ASN
8	g	251	ASN
8	g	263	THR
8	g	288	THR
8	g	334	HIS
8	g	335	LYS
8	g	363	LYS
8	g	372	ARG
8	g	381	HIS
8	g	399	ARG
8	g	412	ASP
8	g	417	ASN
8	g	419	ASP
8	g	425	ARG
8	g	435	TYR
8	h	10	LEU
8	h	34	GLU
8	h	37	VAL
8	h	61	ILE
8	h	171	VAL
8	h	187	ASN
8	h	210	LEU
8	h	271	THR
8	h	277	THR
8	h	289	THR
8	h	302	ASN
8	h	303	VAL
8	h	306	SER
8	h	318	ILE

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Mol	Chain	Res	Type
8	h	360	LEU
8	h	381	HIS
8	h	425	ARG
8	i	34	GLU
8	i	45	THR
8	i	65	VAL
8	i	67	LEU
8	i	79	ASN
8	i	84	ASN
8	i	125	GLU
8	i	149	LEU
8	i	240	THR
8	i	265	ARG
8	i	325	GLN
8	i	333	VAL
8	i	334	HIS
8	i	362	ARG
8	i	372	ARG
8	i	378	MET
8	i	399	ARG
8	i	417	ASN
8	i	425	ARG
8	j	5	ILE
8	j	39	GLU
8	j	48	LYS
8	j	51	PHE
8	j	78	LEU
8	j	174	ASN
8	j	204	VAL
8	j	208	THR
8	j	227	GLN
8	j	243	LEU
8	j	271	THR
8	j	362	ARG
8	j	372	ARG
8	j	381	HIS
8	j	412	ASP
8	j	425	ARG
8	k	2	PRO
8	k	29	HIS
8	k	34	GLU
8	k	51	PHE

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Mol	Chain	Res	Type
8	k	92	TYR
8	k	158	ASN
8	k	163	LYS
8	k	178	MET
8	k	204	VAL
8	k	220	ILE
8	k	245	TYR
8	k	248	TYR
8	k	268	PHE
8	k	302	ASN
8	k	303	VAL
8	k	320	ILE
8	k	337	LEU
8	k	360	LEU
8	k	415	LYS
8	k	425	ARG
8	l	39	GLU
8	l	59	HIS
8	l	62	PRO
8	l	74	ILE
8	l	113	LYS
8	l	184	GLN
8	l	288	THR
8	l	318	ILE
8	l	339	ARG
8	l	353	PRO
8	l	365	PRO
8	m	39	GLU
8	m	69	LEU
8	m	89	GLU
8	m	96	HIS
8	m	196	THR
8	m	242	THR
8	m	277	THR
8	m	292	ASP
8	m	362	ARG
8	m	381	HIS
8	m	425	ARG
8	n	48	LYS
8	n	84	ASN
8	n	164	LYS
8	n	166	VAL

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Mol	Chain	Res	Type
8	n	184	GLN
8	n	241	THR
8	n	246	PRO
8	n	248	TYR
8	n	251	ASN
8	n	267	HIS
8	n	277	THR
8	n	289	THR
8	n	335	LYS
8	n	412	ASP
8	n	415	LYS
8	n	417	ASN
9	o	26	ASN
9	q	31	MET
9	r	55	LYS
9	s	39	ARG
9	t	18	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (206) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	286	GLN
1	A	691	ASN
1	A	724	HIS
1	A	731	ASN
2	B	258	GLN
2	B	300	HIS
2	B	328	HIS
2	B	416	HIS
2	B	553	ASN
2	B	683	HIS
2	B	718	GLN
2	B	882	ASN
1	C	311	HIS
1	C	345	ASN
1	C	457	ASN
1	C	464	HIS
1	C	517	HIS
1	C	529	HIS
1	C	564	ASN
1	C	690	GLN
1	C	864	ASN

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Mol	Chain	Res	Type
2	D	497	HIS
2	D	499	GLN
2	D	595	ASN
2	D	610	GLN
2	D	683	HIS
2	D	704	HIS
2	D	716	GLN
2	D	750	HIS
2	D	851	HIS
2	D	858	GLN
1	E	279	ASN
1	E	289	HIS
1	E	321	GLN
1	E	345	ASN
1	E	411	HIS
1	E	630	ASN
1	E	661	ASN
1	E	687	ASN
1	E	706	HIS
1	E	724	HIS
2	F	460	HIS
2	F	551	ASN
2	F	683	HIS
2	F	788	GLN
2	F	854	GLN
1	G	241	GLN
1	G	311	HIS
1	G	359	HIS
1	G	517	HIS
1	G	564	ASN
1	G	691	ASN
2	H	493	HIS
2	H	569	GLN
2	H	788	GLN
2	H	833	GLN
2	H	882	ASN
3	I	29	GLN
3	I	116	HIS
3	I	152	GLN
3	I	353	GLN
3	I	545	GLN
3	I	638	ASN

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Mol	Chain	Res	Type
3	I	651	ASN
4	J	425	ASN
4	J	431	HIS
4	J	754	ASN
4	J	910	HIS
3	K	61	GLN
3	K	82	HIS
3	K	207	GLN
3	K	256	GLN
3	K	475	ASN
3	K	560	HIS
3	K	598	GLN
3	K	621	GLN
5	L	50	HIS
5	L	70	ASN
5	L	393	ASN
5	L	1492	ASN
5	L	1554	HIS
5	L	1566	GLN
5	L	1597	ASN
5	L	1617	HIS
1	M	241	GLN
1	M	315	GLN
1	M	359	HIS
1	M	643	HIS
1	M	649	HIS
1	M	687	ASN
1	M	740	ASN
1	M	834	HIS
1	M	852	HIS
2	N	490	ASN
2	N	608	ASN
2	N	664	ASN
2	N	683	HIS
2	N	701	HIS
2	N	704	HIS
2	N	715	HIS
2	N	716	GLN
2	N	845	GLN
6	P	40	HIS
6	P	161	HIS
6	P	263	GLN

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Mol	Chain	Res	Type
6	P	296	ASN
2	Q	84	GLN
2	Q	89	ASN
7	U	599	GLN
7	V	619	HIS
7	V	626	GLN
7	V	632	GLN
7	W	601	ASN
7	W	624	ASN
7	W	641	GLN
7	W	664	ASN
7	X	650	ASN
8	a	9	GLN
8	a	59	HIS
8	a	184	GLN
8	a	371	HIS
8	a	381	HIS
8	a	417	ASN
8	b	9	GLN
8	b	29	HIS
8	b	75	HIS
8	b	79	ASN
8	b	219	HIS
8	b	315	HIS
8	b	436	HIS
8	c	9	GLN
8	c	15	ASN
8	c	87	ASN
8	c	115	HIS
8	c	197	GLN
8	c	219	HIS
8	c	315	HIS
8	c	338	GLN
8	d	102	ASN
8	d	197	GLN
8	e	103	ASN
8	e	334	HIS
8	e	394	GLN
8	e	429	GLN
8	f	251	ASN
8	f	312	GLN
8	f	338	GLN

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Mol	Chain	Res	Type
8	f	380	ASN
8	f	436	HIS
8	g	15	ASN
8	g	184	GLN
8	g	312	GLN
8	g	436	HIS
8	h	29	HIS
8	h	75	HIS
8	h	103	ASN
8	h	115	HIS
8	h	187	ASN
8	h	198	ASN
8	h	229	ASN
8	h	322	ASN
8	h	325	GLN
8	h	381	HIS
8	i	15	ASN
8	i	96	HIS
8	i	184	GLN
8	i	417	ASN
8	j	103	ASN
8	j	174	ASN
8	j	227	GLN
8	j	325	GLN
8	j	383	ASN
8	j	436	HIS
8	k	59	HIS
8	k	87	ASN
8	k	250	ASN
8	k	302	ASN
8	k	371	HIS
8	k	381	HIS
8	k	407	GLN
8	l	12	GLN
8	l	15	ASN
8	l	24	GLN
8	l	110	GLN
8	l	158	ASN
8	l	197	GLN
8	l	198	ASN
8	l	347	ASN
8	m	54	GLN

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Mol	Chain	Res	Type
8	m	59	HIS
8	m	96	HIS
8	m	174	ASN
8	m	312	GLN
8	m	325	GLN
8	m	334	HIS
8	m	371	HIS
8	m	380	ASN
8	n	16	GLN
8	n	90	ASN
8	n	222	ASN
8	n	250	ASN
8	n	325	GLN
8	n	338	GLN
9	o	26	ASN
9	q	26	ASN
9	s	26	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 oligosaccharides in this entry.

5.6 Ligand geometry [i](#)

There are no ligands in this entry.

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues ⓘ

There are no chain breaks in this entry.

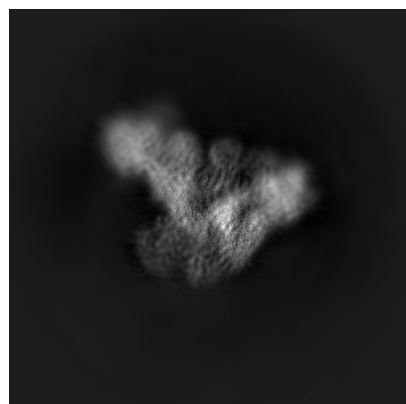
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-52730. These allow visual inspection of the internal detail of the map and identification of artifacts.

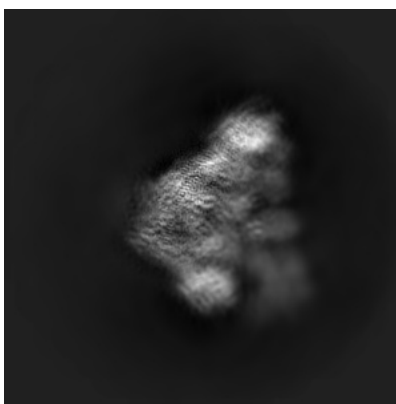
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections [i](#)

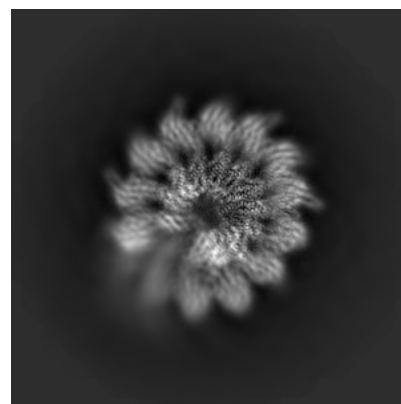
6.1.1 Primary map



X

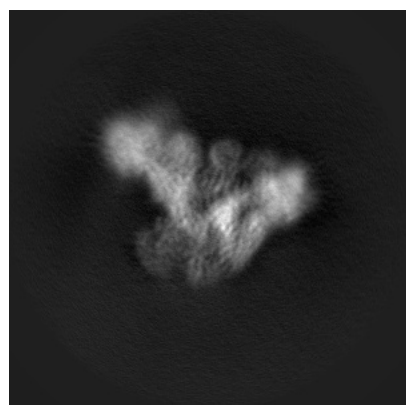


Y

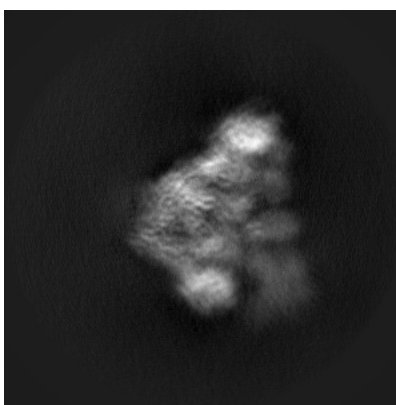


Z

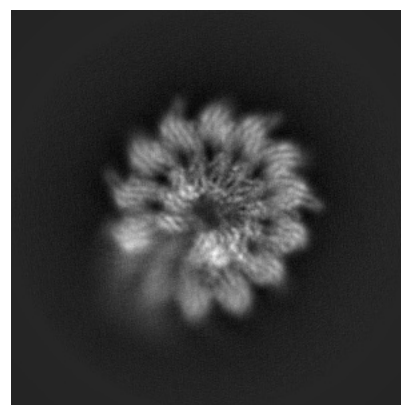
6.1.2 Raw map



X



Y

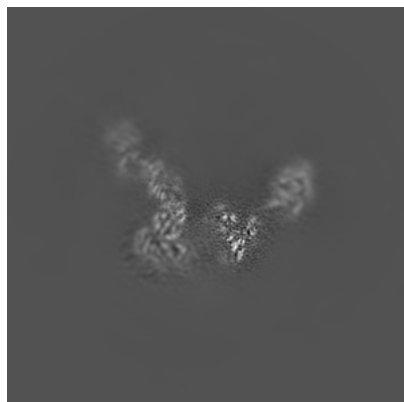


Z

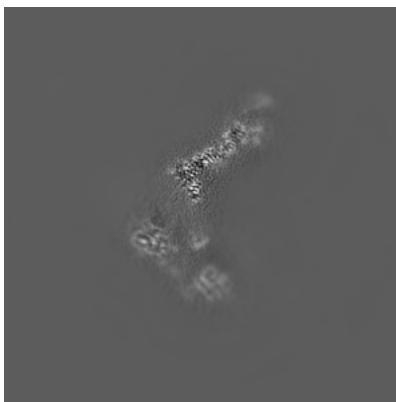
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

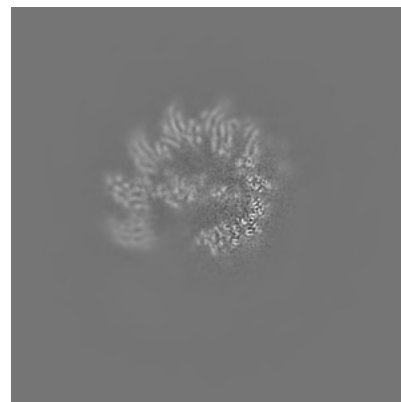
6.2.1 Primary map



X Index: 192



Y Index: 192

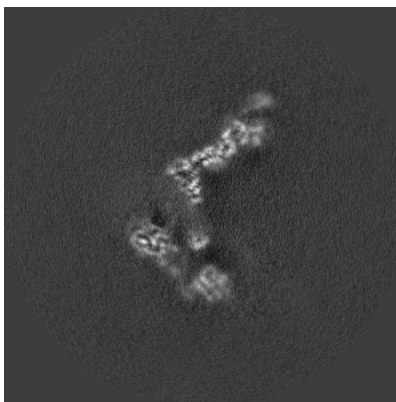


Z Index: 192

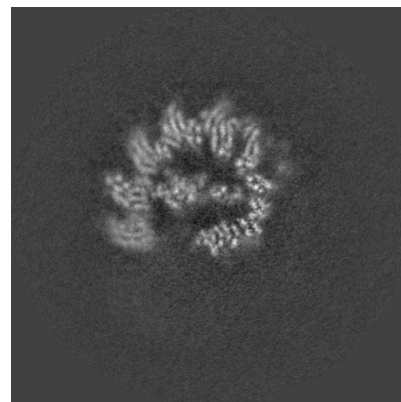
6.2.2 Raw map



X Index: 192



Y Index: 192

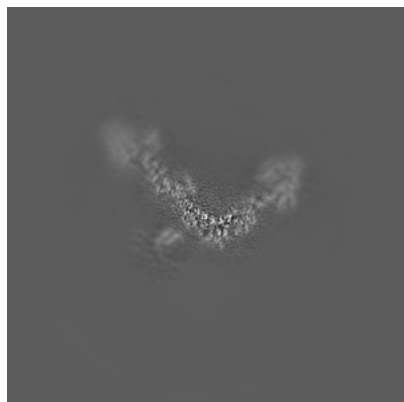


Z Index: 192

The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

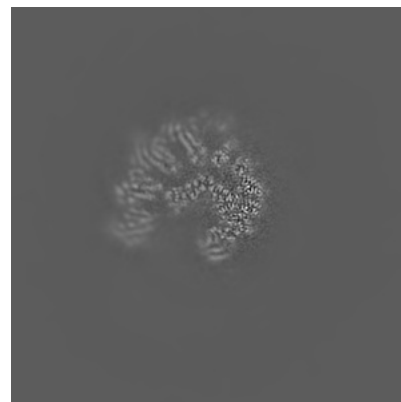
6.3.1 Primary map



X Index: 225

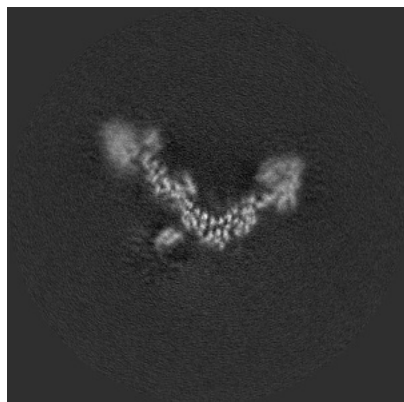


Y Index: 212

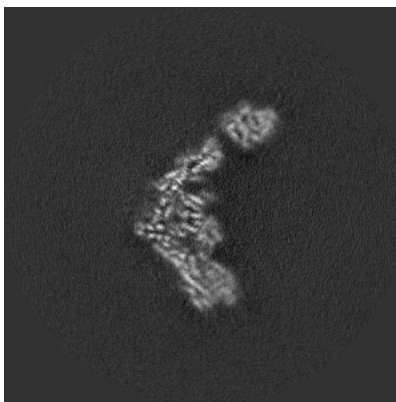


Z Index: 181

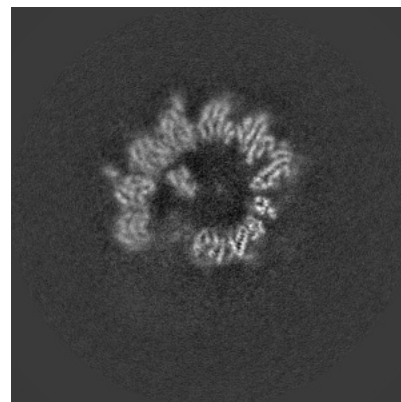
6.3.2 Raw map



X Index: 225



Y Index: 211

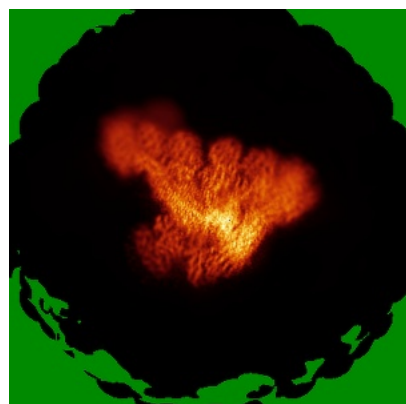


Z Index: 203

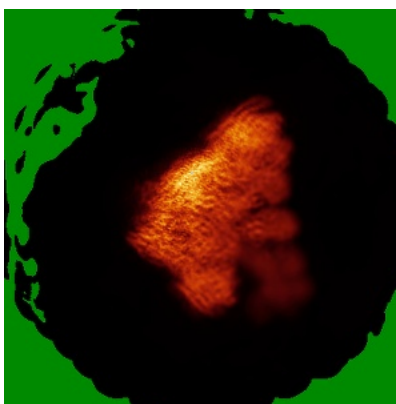
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) [i](#)

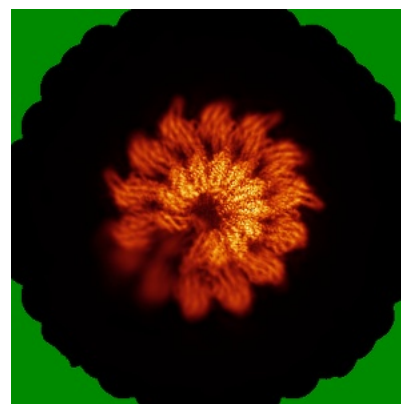
6.4.1 Primary map



X

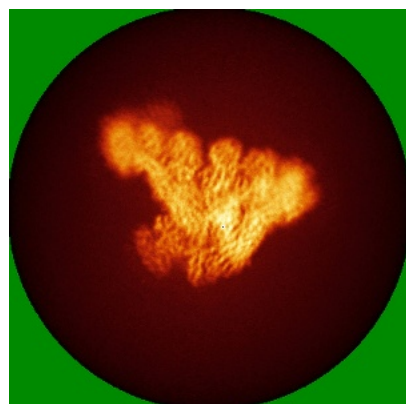


Y

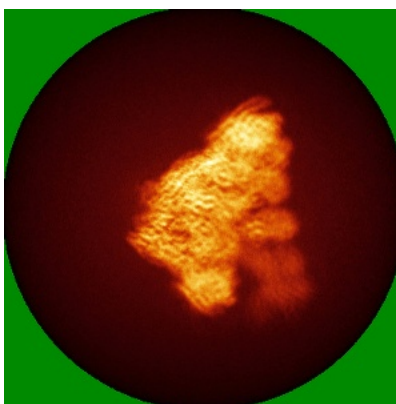


Z

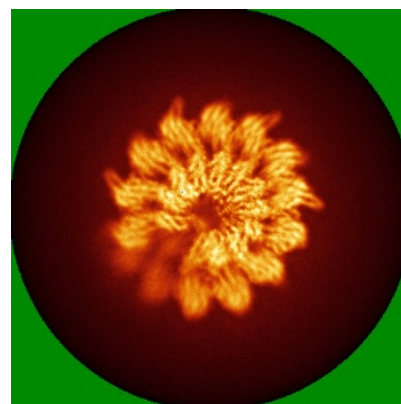
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

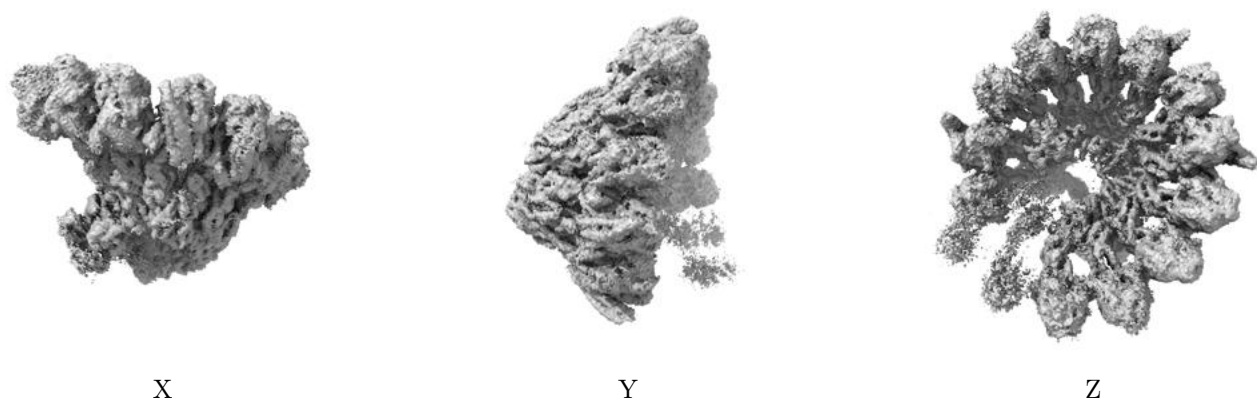
6.5 Orthogonal surface views [i](#)

6.5.1 Primary map



The images above show the 3D surface view of the map at the recommended contour level 0.0217. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

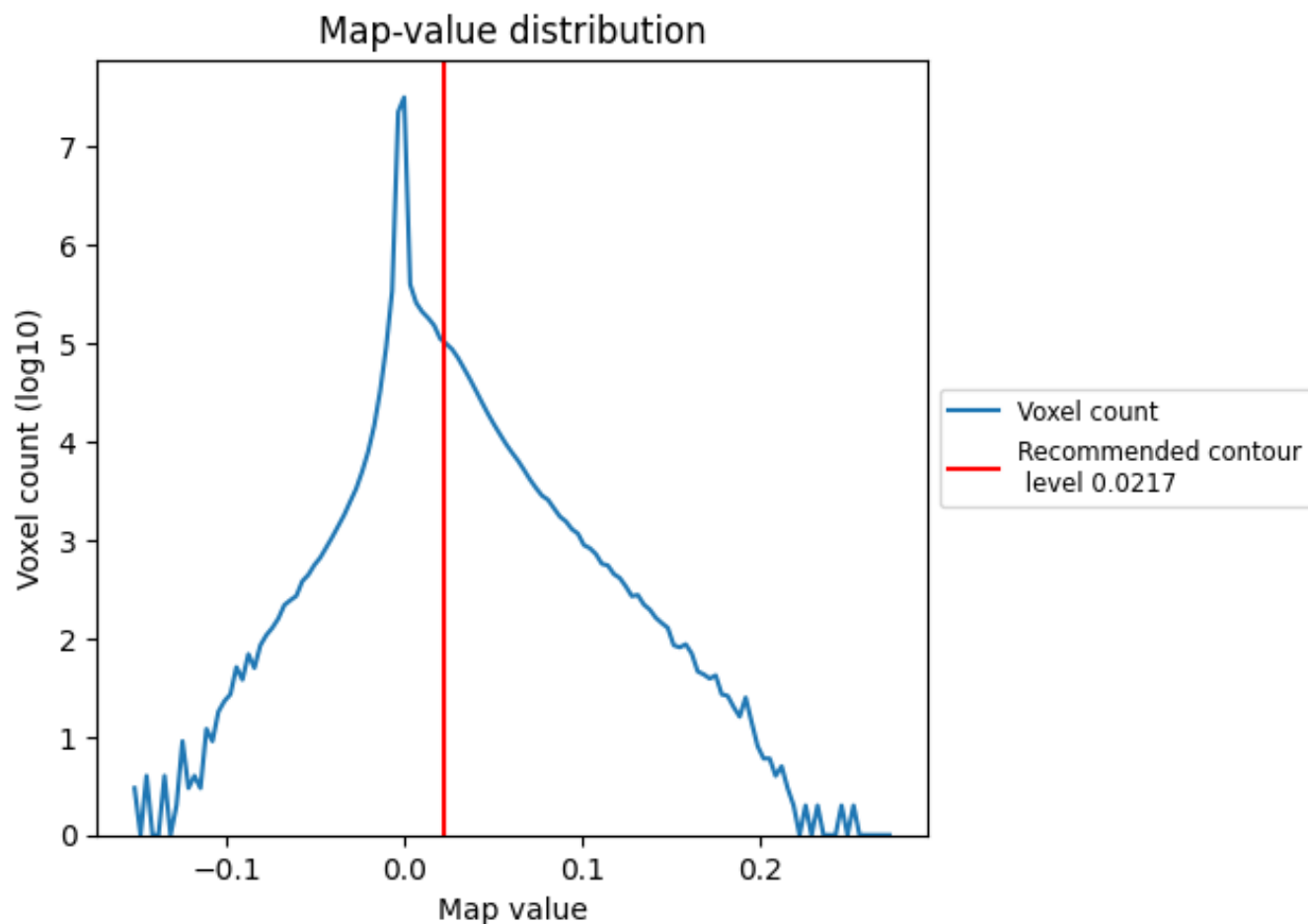
6.6 Mask visualisation [i](#)

This section was not generated. No masks/segmentation were deposited.

7 Map analysis [i](#)

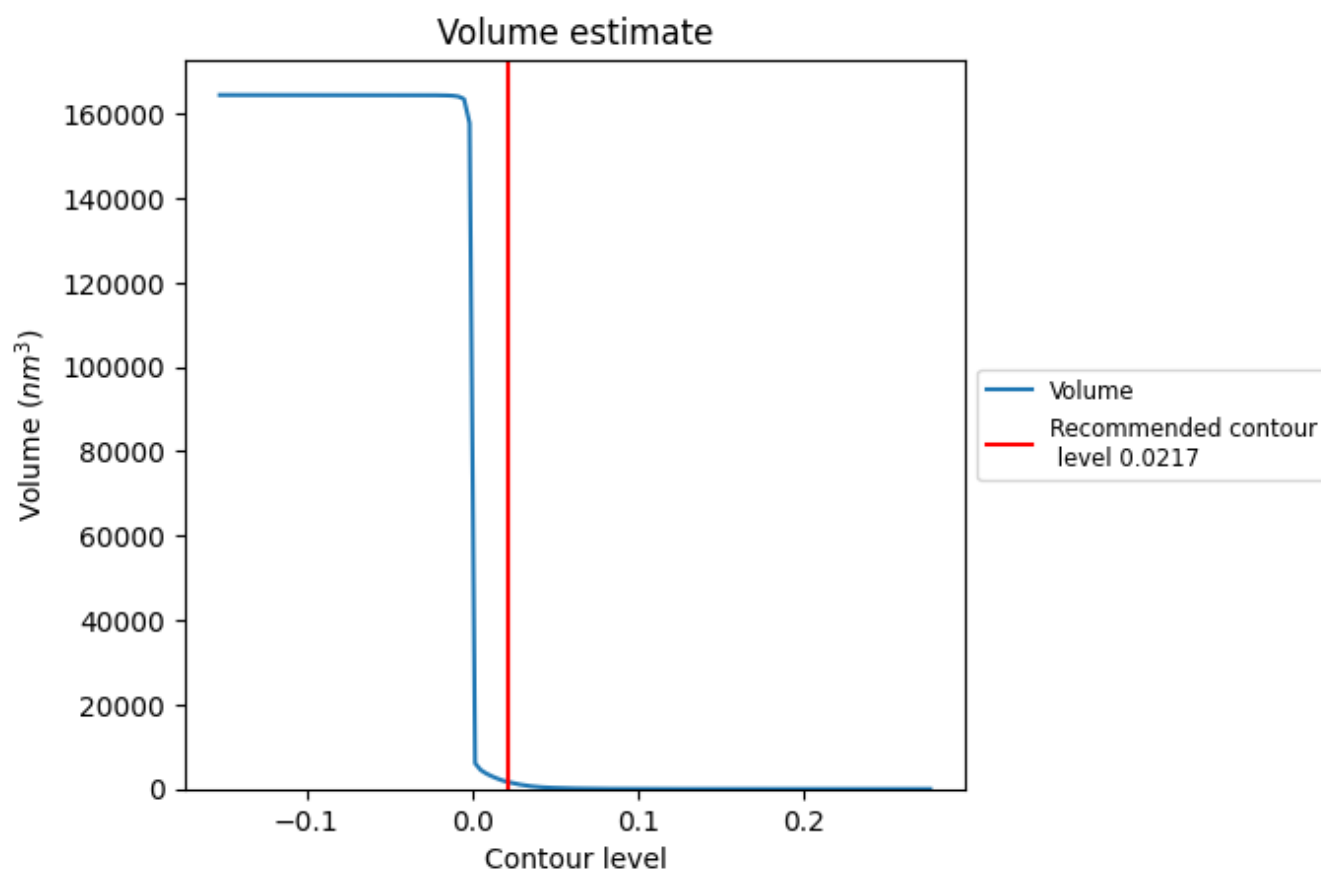
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

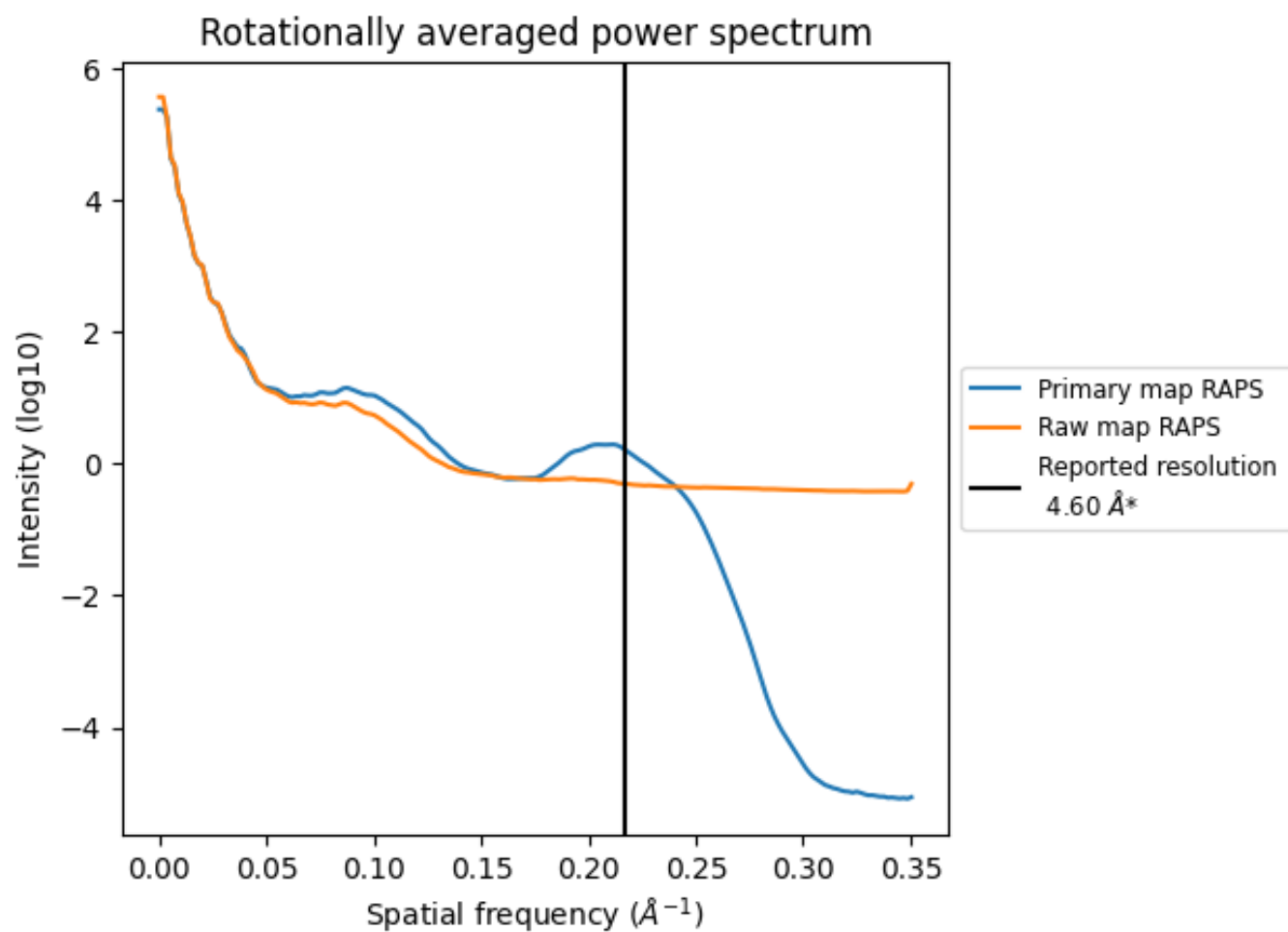
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 1642 nm^3 ; this corresponds to an approximate mass of 1483 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum ⓘ

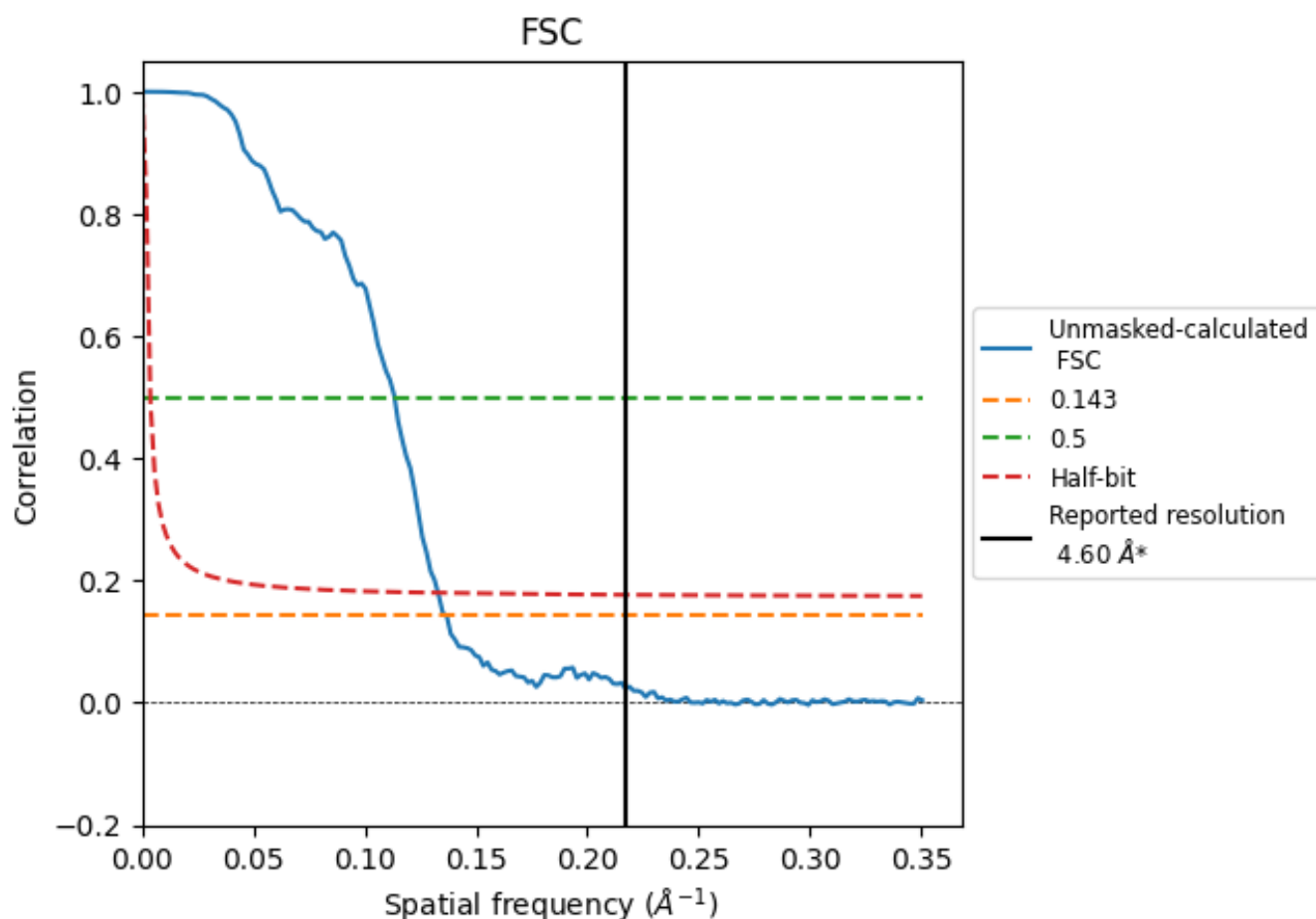


*Reported resolution corresponds to spatial frequency of 0.217 Å⁻¹

8 Fourier-Shell correlation [i](#)

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC [i](#)



*Reported resolution corresponds to spatial frequency of 0.217 \AA^{-1}

8.2 Resolution estimates [i](#)

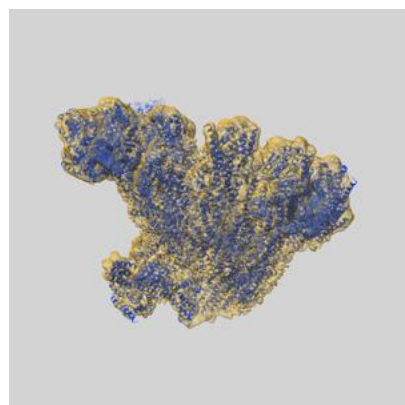
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.60	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	7.34	8.83	7.52

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 7.34 differs from the reported value 4.6 by more than 10 %

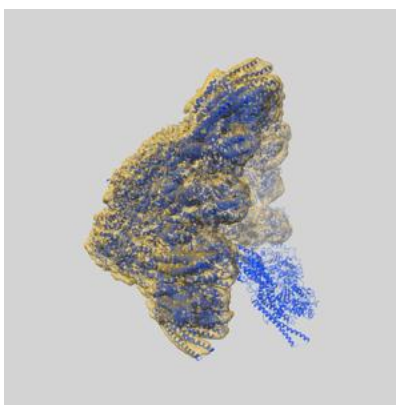
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-52730 and PDB model 9I8N. Per-residue inclusion information can be found in section 3 on page 9.

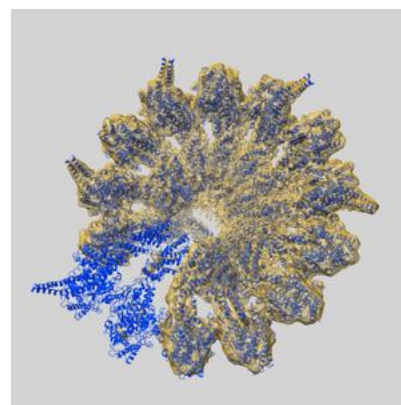
9.1 Map-model overlay [i](#)



X



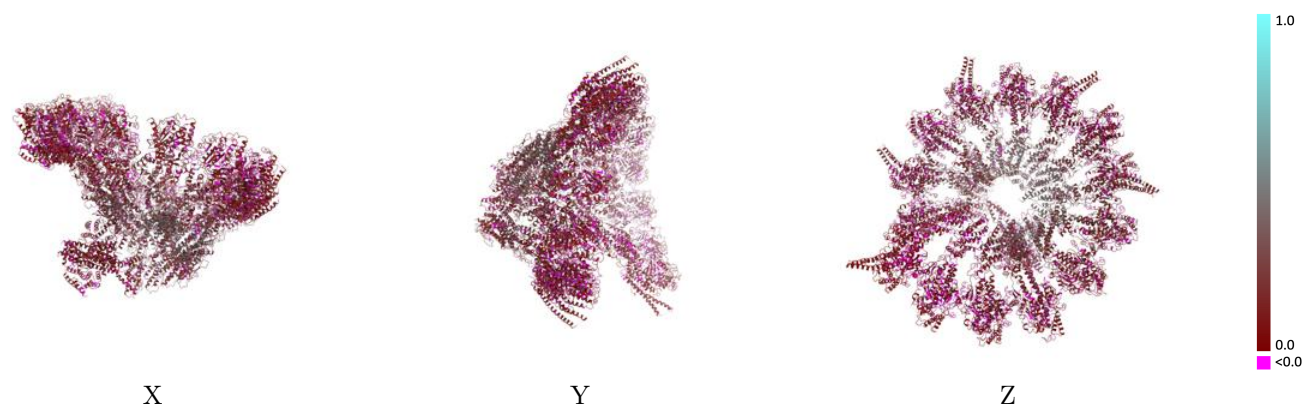
Y



Z

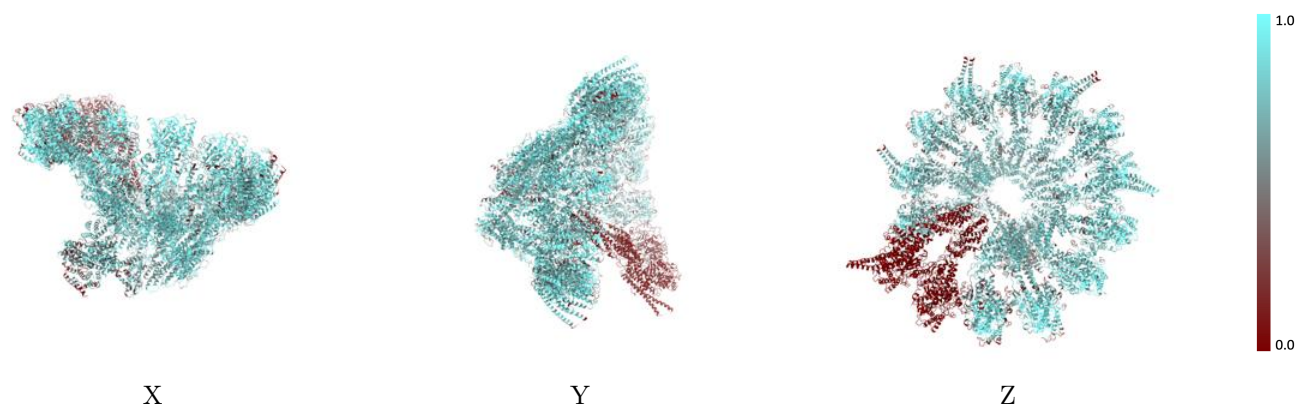
The images above show the 3D surface view of the map at the recommended contour level 0.0217 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



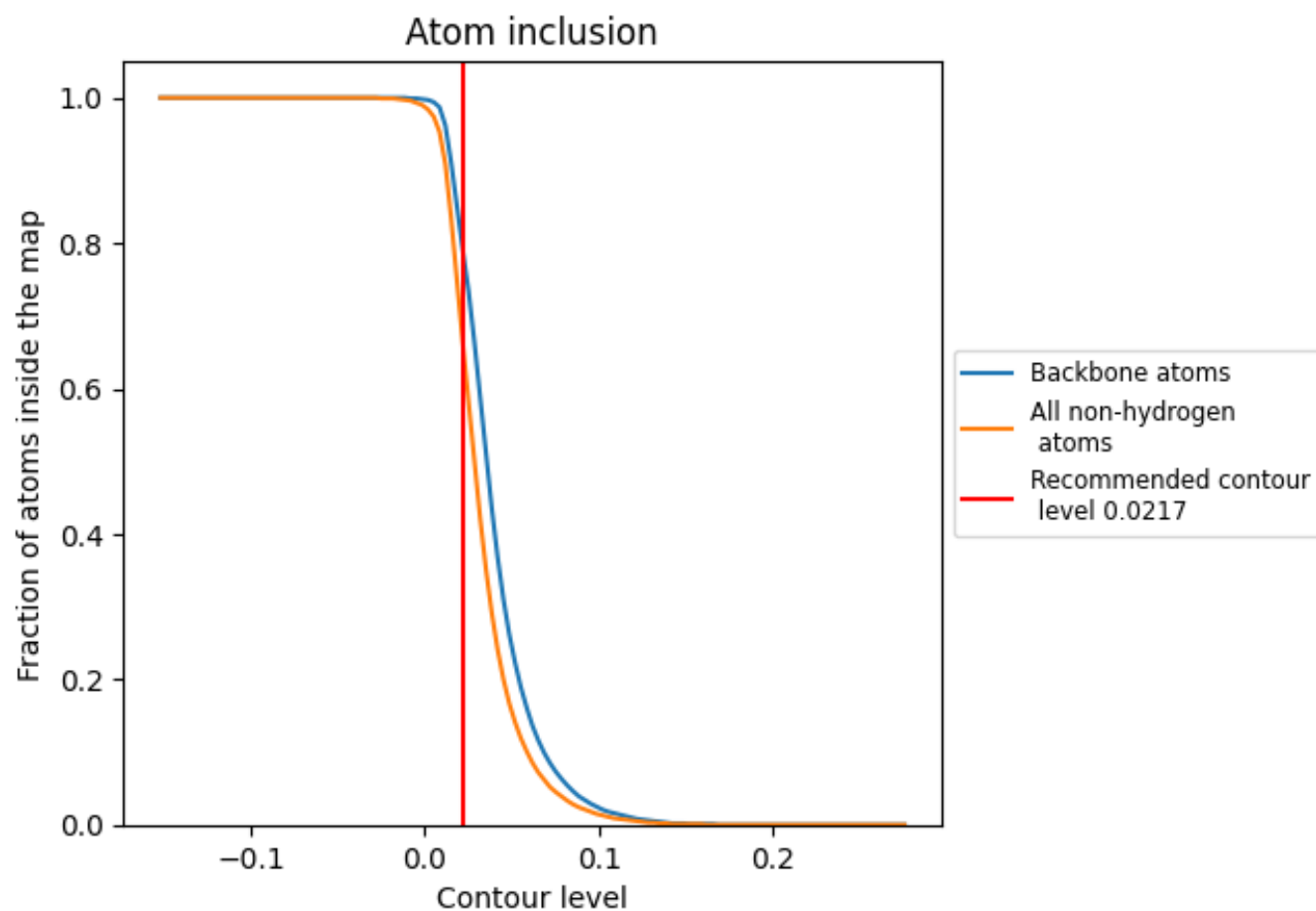
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0217).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 79% of all backbone atoms, 67% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ





















The table lists the average atom inclusion at the recommended contour level (0.0217) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6660	 0.1430
A	 0.7740	 0.1290
B	 0.7540	 0.1560
C	 0.7870	 0.1650
D	 0.7590	 0.1680
E	 0.8060	 0.1940
F	 0.7670	 0.1810
G	 0.8140	 0.2150
H	 0.8140	 0.2320
I	 0.8130	 0.2260
J	 0.7910	 0.1900
K	 0.7840	 0.1600
L	 0.7370	 0.1550
M	 0.0290	 0.0880
N	 0.0000	 0.0740
O	 0.8520	 0.3430
P	 0.7540	 0.2000
Q	 0.5180	 0.1330
R	 0.6590	 0.1460
S	 0.7170	 0.1400
T	 0.4200	 0.1080
U	 0.6280	 0.1310
V	 0.5880	 0.1160
W	 0.5800	 0.1340
X	 0.5700	 0.1220
a	 0.7340	 0.0960
b	 0.7730	 0.1170
c	 0.7230	 0.0790
d	 0.7610	 0.1110
e	 0.7380	 0.0950
f	 0.7420	 0.0980
g	 0.7940	 0.1220
h	 0.8270	 0.1600
i	 0.8150	 0.1450
j	 0.8150	 0.1260



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Chain	Atom inclusion	Q-score
k	 0.7680	 0.0960
l	 0.6540	 0.0830
m	 0.0050	 0.0440
n	 0.0000	 0.0440
o	 0.8400	 0.3530
p	 0.8430	 0.3180
q	 0.4740	 0.1220
r	 0.7050	 0.1580
s	 0.7480	 0.1700
t	 0.5090	 0.1410