



## Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 07:14 am GMT

PDB ID : 6HED  
EMDB ID : EMD-0216  
Title : PAN-proteasome in state 5  
Authors : Majumder, P.; Rudack, T.; Beck, F.; Baumeister, W.  
Deposited on : 2018-08-20  
Resolution : 6.95 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](mailto: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>.

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

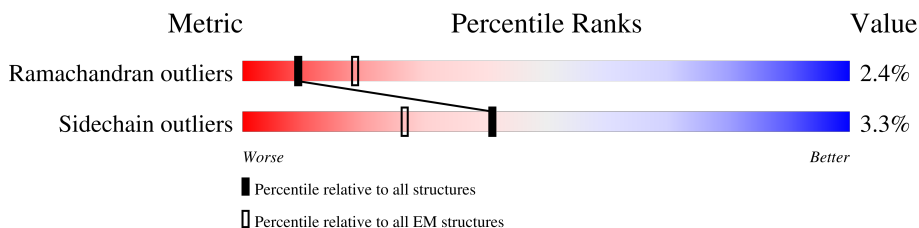
EMDB validation analysis : 0.0.1.dev43  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
MapQ : 1.9.9  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.31.2

# 1 Overall quality at a glance i

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

The reported resolution of this entry is 6.95 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	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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	242	7% (red), 80% (green), 17% (yellow), 0% (orange), 0% (grey)
1	B	242	6% (red), 75% (green), 19% (yellow), 0% (orange), 0% (grey)
1	C	242	7% (red), 74% (green), 23% (yellow), 0% (orange), 0% (grey)
1	D	242	9% (red), 77% (green), 20% (yellow), 0% (orange), 0% (grey)
1	E	242	7% (red), 76% (green), 20% (yellow), 0% (orange), 0% (grey)
1	F	242	7% (red), 76% (green), 22% (yellow), 0% (orange), 0% (grey)
1	G	242	7% (red), 75% (green), 21% (yellow), 0% (orange), 0% (grey)
1	a	242	9% (red), 72% (green), 23% (yellow), 0% (orange), 0% (grey)
1	b	242	10% (red), 76% (green), 19% (yellow), 0% (orange), 0% (grey)

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Mol	Chain	Length	Quality of chain
1	c	242	12% 74% 20% ..
1	d	242	11% 75% 19% 5% .
1	e	242	10% 72% 23% ..
1	f	242	11% 74% 22% ..
1	g	242	9% 78% 18% ..
2	1	202	20% 74% 23% .
2	2	202	18% 74% 21% ..
2	3	202	14% 78% 19% .
2	4	202	14% 77% 20% .
2	5	202	19% 67% 29% .
2	6	202	20% 73% 23% .
2	7	202	20% 76% 21% .
2	h	202	19% 71% 24% .
2	i	202	20% 75% 22% .
2	j	202	24% 74% 24% .
2	k	202	21% 73% 21% 5% .
2	l	202	19% 78% 17% 5% .
2	m	202	24% 79% 19% ..
2	n	202	18% 74% 21% 5% .
3	H	390	29% 72% 24% .
3	I	390	26% 71% 26% .
3	J	390	33% 76% 20% .
3	K	390	31% 71% 26% .
3	L	390	32% 74% 22% .
3	M	390	28% 73% 22% ..

## 2 Entry composition i

There are 6 unique types of molecules in this entry. The entry contains 66909 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 Proteasome subunit alpha.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	242	1907	1211	321	368	7	0	0
1	a	237	1866	1186	315	359	6	0	0
1	B	242	1907	1211	321	368	7	0	0
1	b	237	1866	1186	315	359	6	0	0
1	C	242	1907	1211	321	368	7	0	0
1	c	237	1866	1186	315	359	6	0	0
1	D	242	1907	1211	321	368	7	0	0
1	d	237	1866	1186	315	359	6	0	0
1	E	242	1907	1211	321	368	7	0	0
1	e	237	1866	1186	315	359	6	0	0
1	F	242	1907	1211	321	368	7	0	0
1	f	237	1866	1186	315	359	6	0	0
1	G	242	1907	1211	321	368	7	0	0
1	g	237	1866	1186	315	359	6	0	0

- Molecule 2 is a protein called Proteasome subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	202	1553	982	260	305	6	0	0

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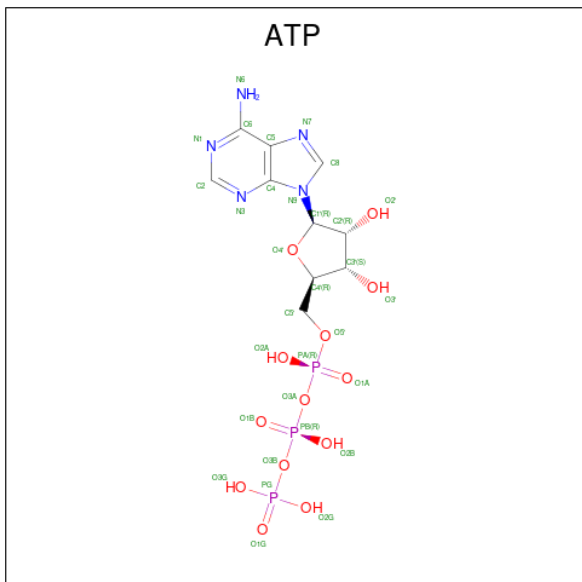
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Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	h	202	Total 1553	C 982	N 260	O 305	S 6	0	0
2	2	202	Total 1553	C 982	N 260	O 305	S 6	0	0
2	i	202	Total 1553	C 982	N 260	O 305	S 6	0	0
2	3	202	Total 1553	C 982	N 260	O 305	S 6	0	0
2	j	202	Total 1553	C 982	N 260	O 305	S 6	0	0
2	4	202	Total 1553	C 982	N 260	O 305	S 6	0	0
2	k	202	Total 1553	C 982	N 260	O 305	S 6	0	0
2	5	202	Total 1553	C 982	N 260	O 305	S 6	0	0
2	l	202	Total 1553	C 982	N 260	O 305	S 6	0	0
2	6	202	Total 1553	C 982	N 260	O 305	S 6	0	0
2	m	202	Total 1553	C 982	N 260	O 305	S 6	0	0
2	7	202	Total 1553	C 982	N 260	O 305	S 6	0	0
2	n	202	Total 1553	C 982	N 260	O 305	S 6	0	0

- Molecule 3 is a protein called Proteasome-activating nucleotidase.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	H	390	Total 3100	C 1974	N 535	O 583	S 8	0	0
3	I	390	Total 3100	C 1974	N 535	O 583	S 8	0	0
3	K	390	Total 3100	C 1974	N 535	O 583	S 8	0	0
3	L	390	Total 3100	C 1974	N 535	O 583	S 8	0	0
3	M	390	Total 3100	C 1974	N 535	O 583	S 8	0	0
3	J	390	Total 3100	C 1974	N 535	O 583	S 8	0	0

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula:  $C_{10}H_{16}N_5O_{13}P_3$ ).

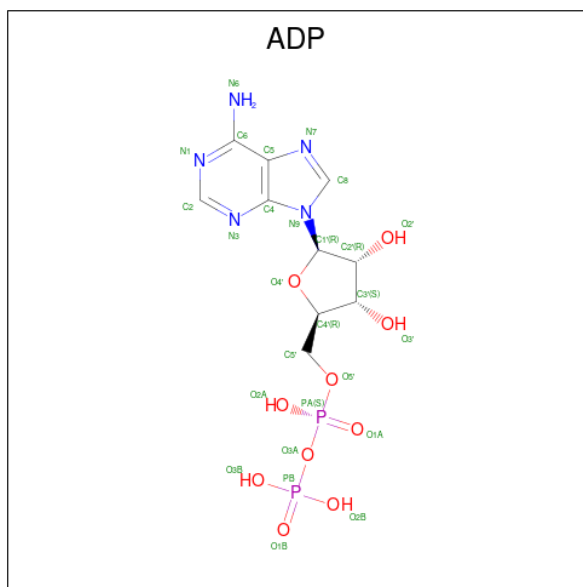


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
4	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
4	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 5 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
			Total	Mg	
5	H	1	Total	Mg	0
			1	1	
5	I	1	Total	Mg	0
			1	1	
5	K	1	Total	Mg	0
			1	1	
5	L	1	Total	Mg	0
			1	1	
5	M	1	Total	Mg	0
			1	1	

- Molecule 6 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula:  $C_{10}H_{15}N_5O_{10}P_2$ ).

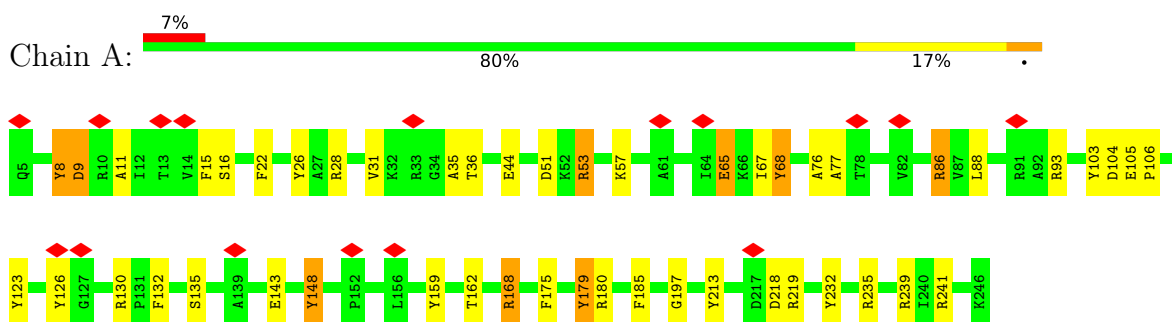


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
6	I	1	27	10	5	10	2	0

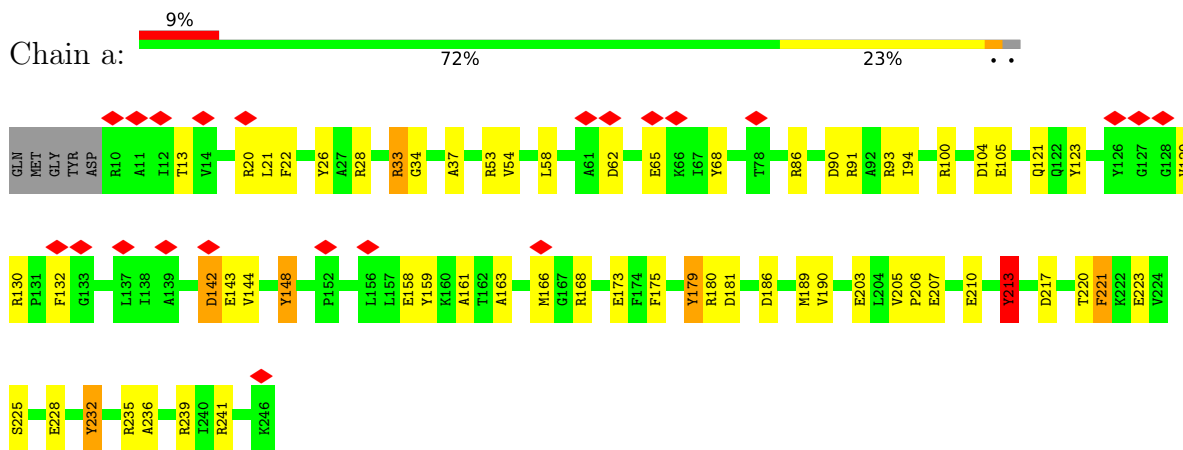
### 3 Residue-property plots

These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

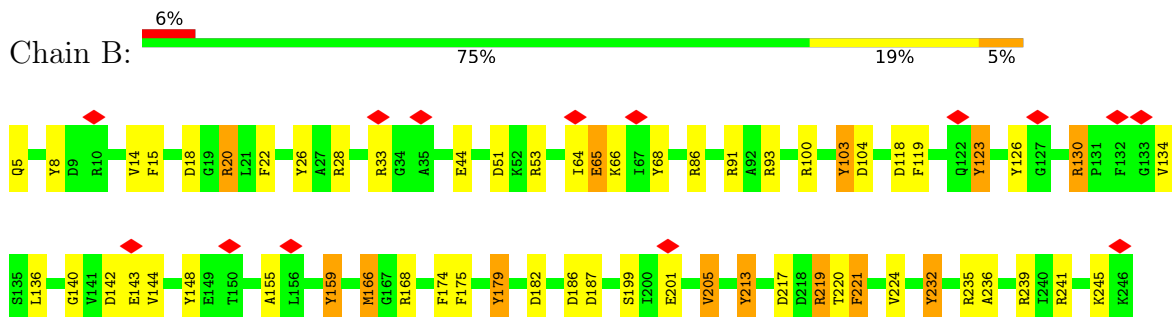
- Molecule 1: Proteasome subunit alpha



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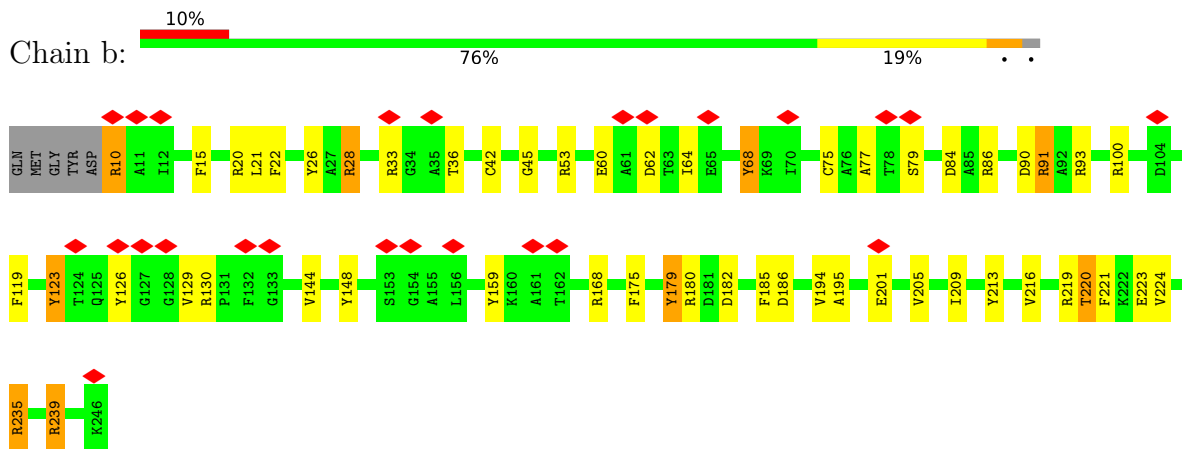


- Molecule 1: Proteasome subunit alpha

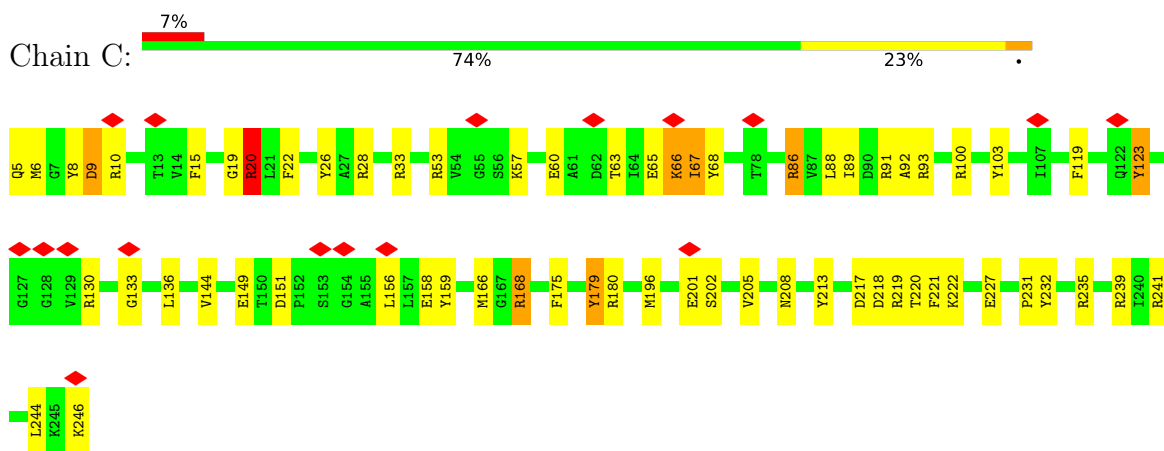




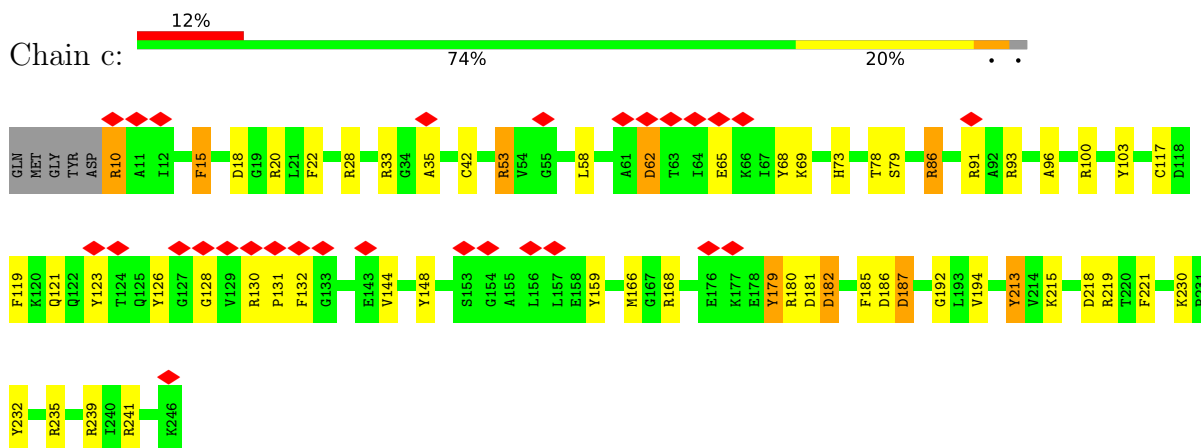
• Molecule 1: Proteasome subunit alpha



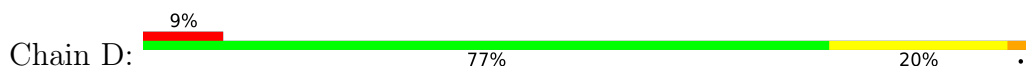
• Molecule 1: Proteasome subunit alpha

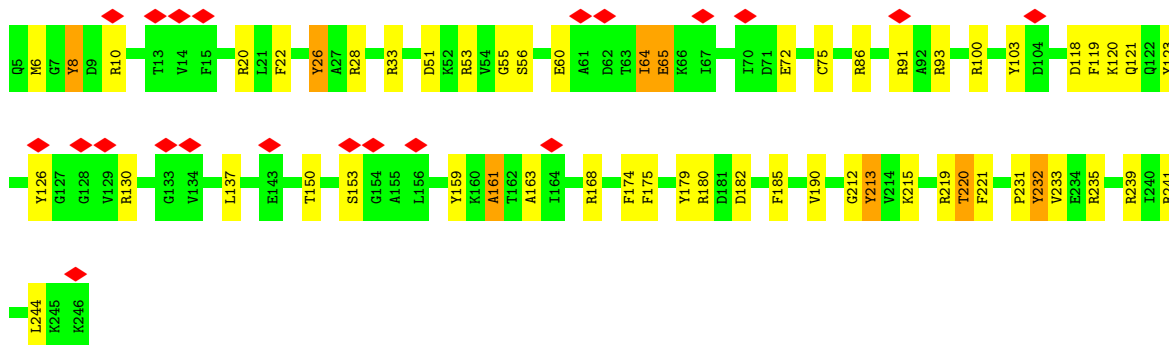


• Molecule 1: Proteasome subunit alpha

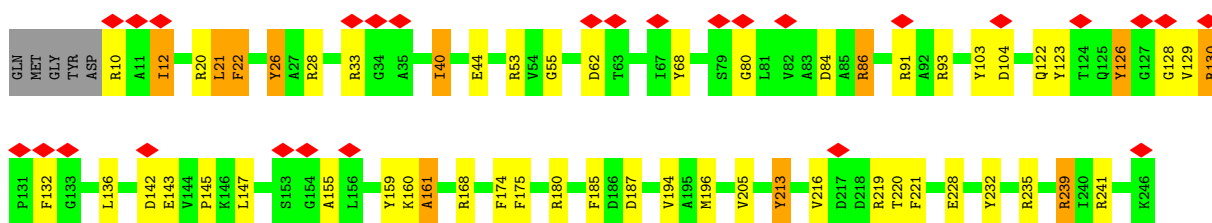
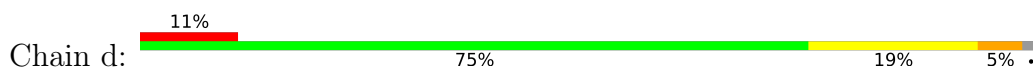


• Molecule 1: Proteasome subunit alpha

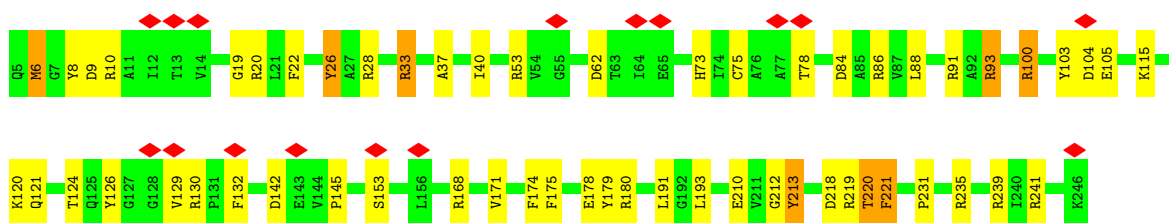
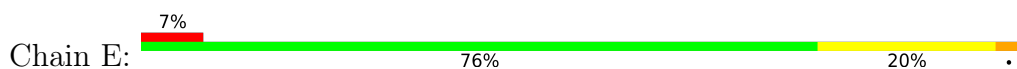




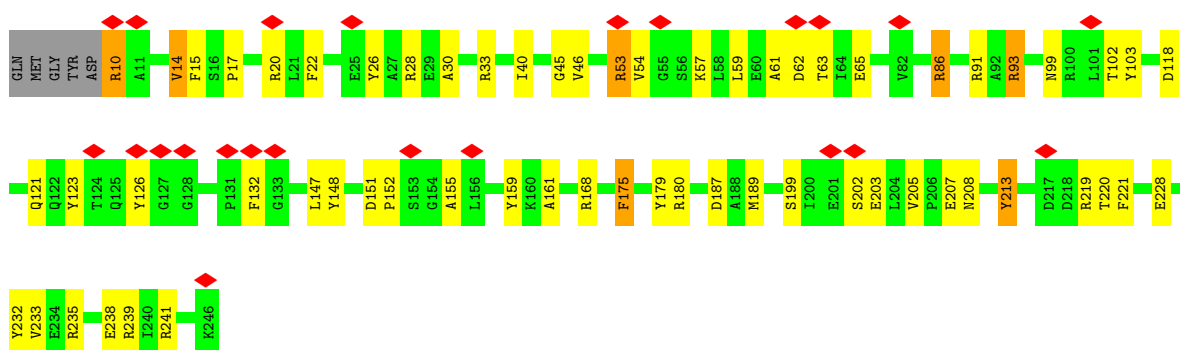
• Molecule 1: Proteasome subunit alpha



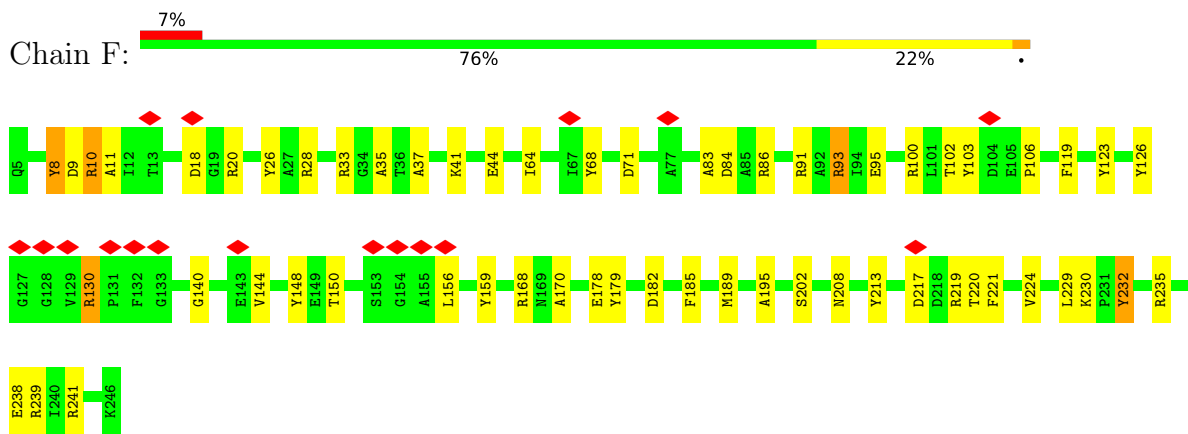
• Molecule 1: Proteasome subunit alpha



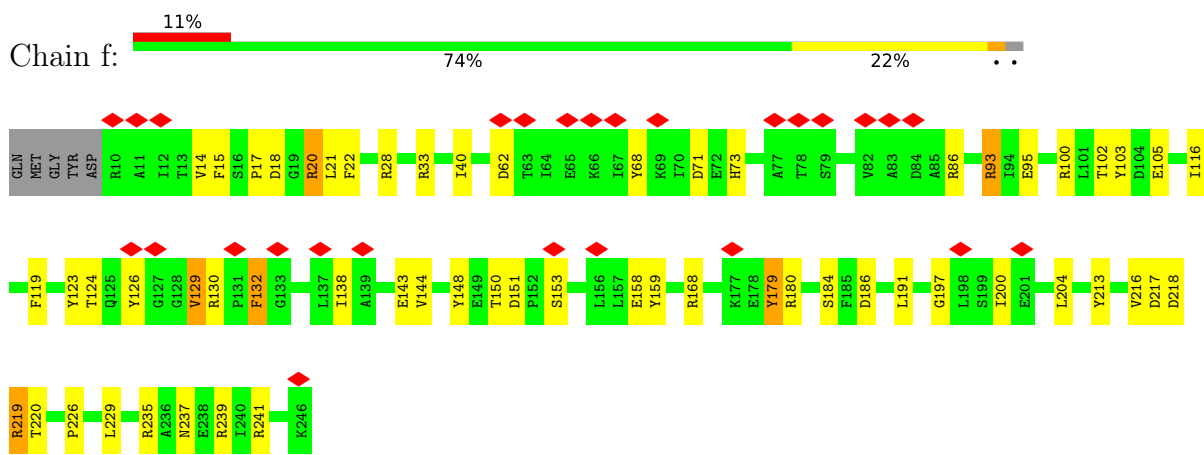
• Molecule 1: Proteasome subunit alpha



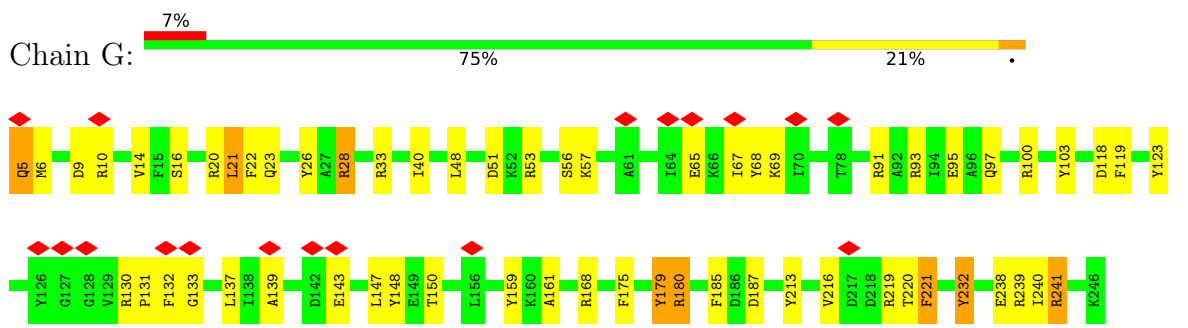
• Molecule 1: Proteasome subunit alpha



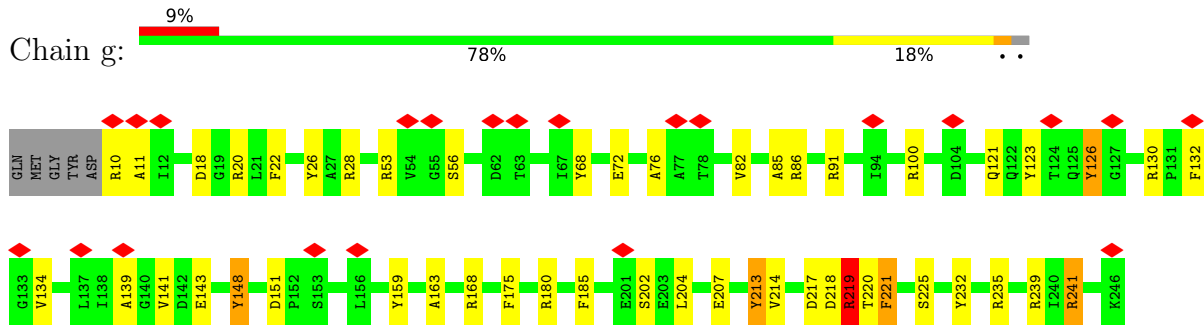
• Molecule 1: Proteasome subunit alpha



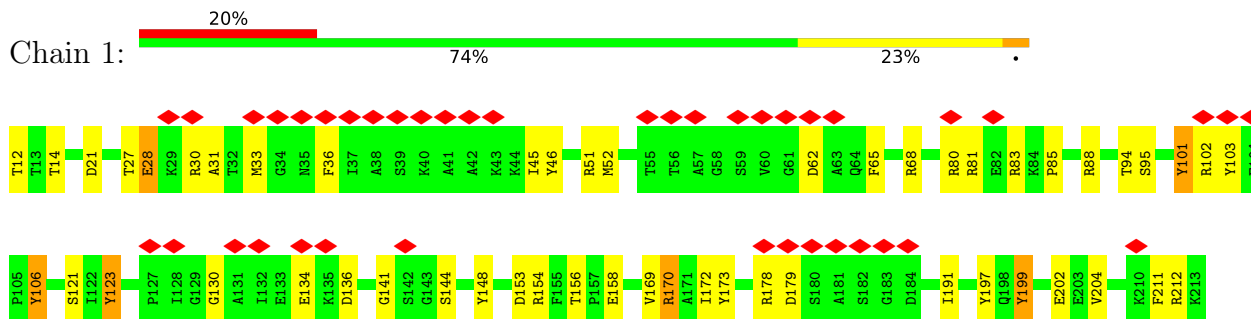
• Molecule 1: Proteasome subunit alpha



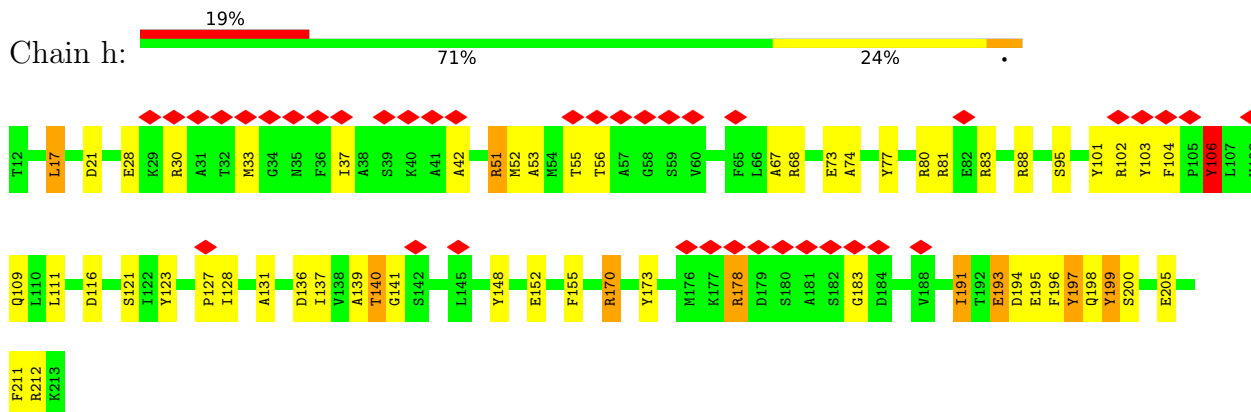
• Molecule 1: Proteasome subunit alpha



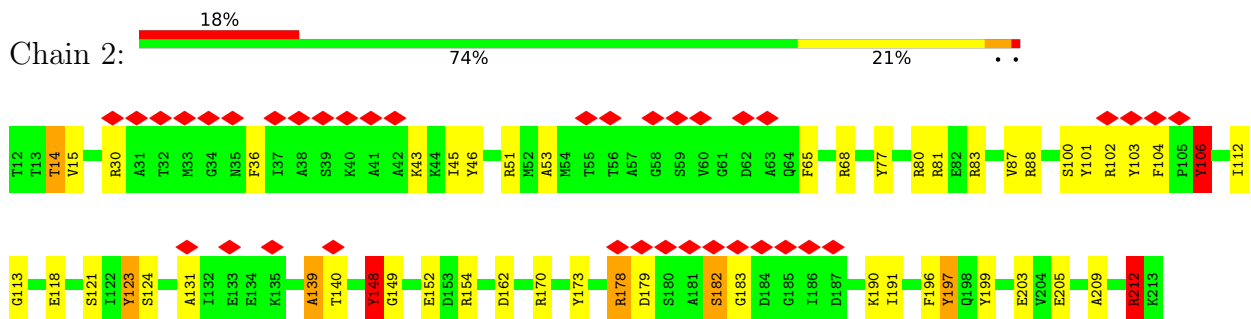
• Molecule 2: Proteasome subunit beta



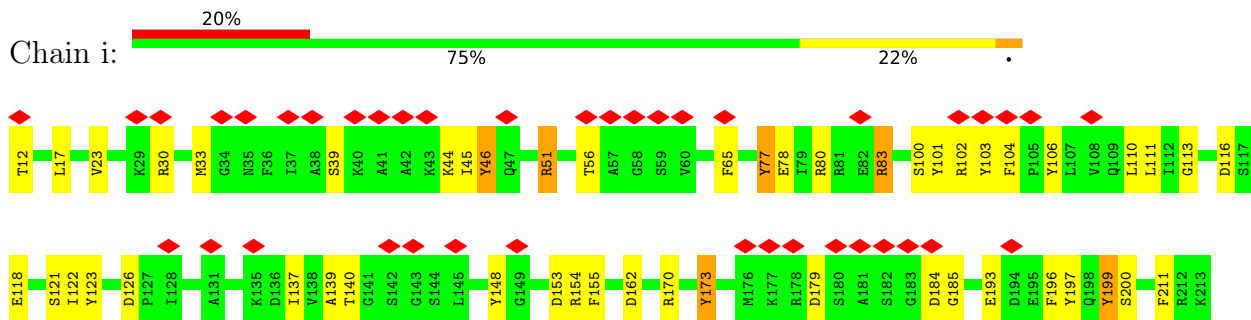
• Molecule 2: Proteasome subunit beta



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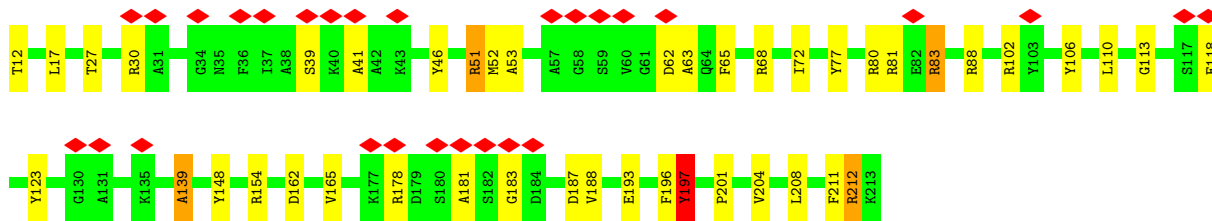


• Molecule 2: Proteasome subunit beta

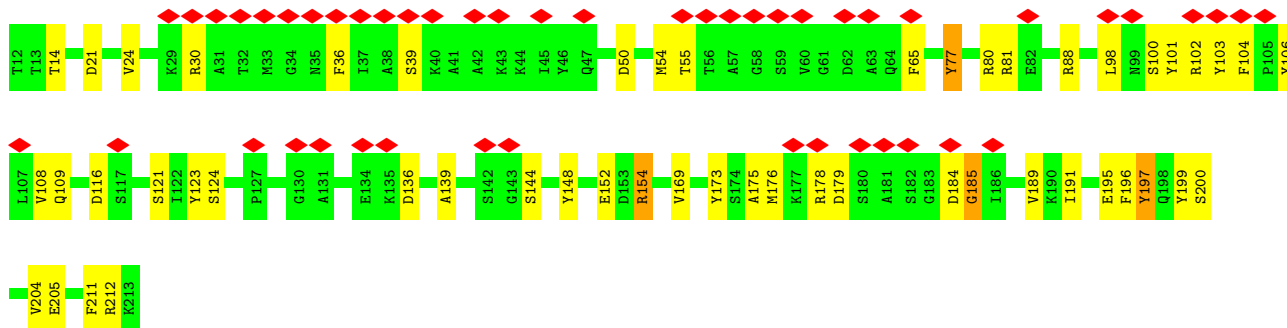
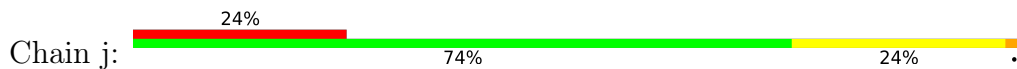


• Molecule 2: Proteasome subunit beta

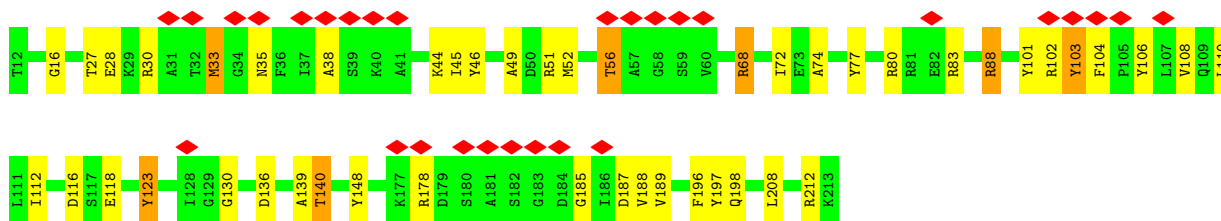
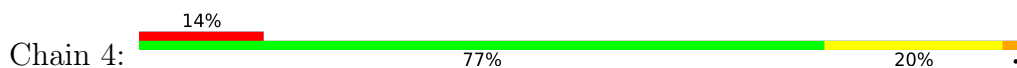




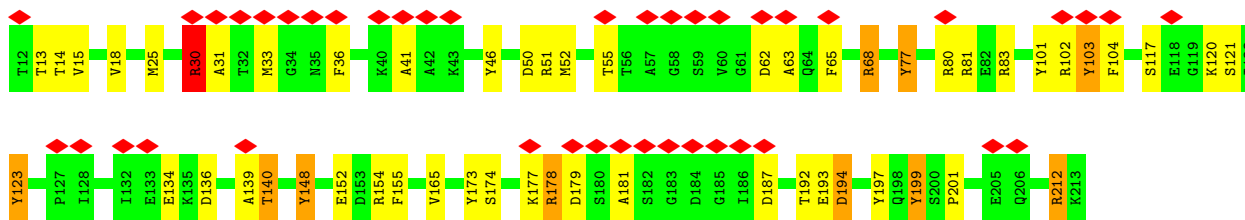
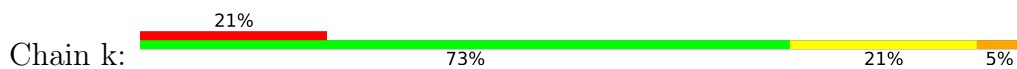
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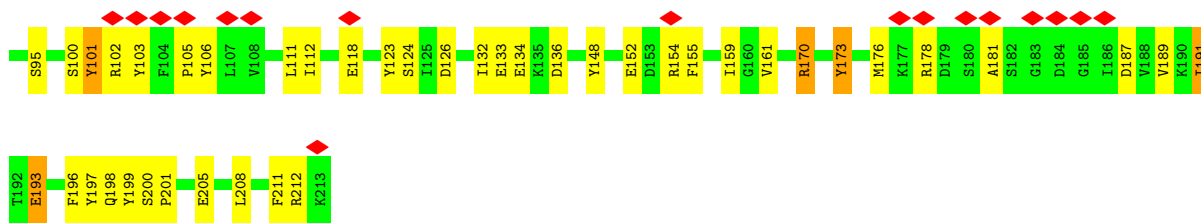


• Molecule 2: Proteasome subunit beta

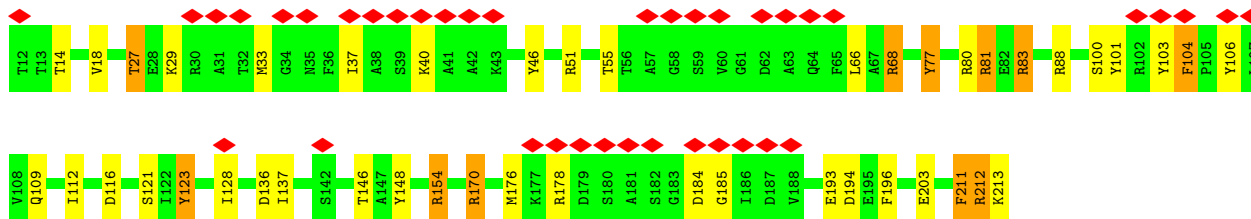
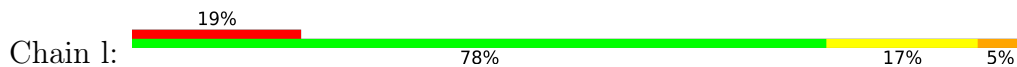


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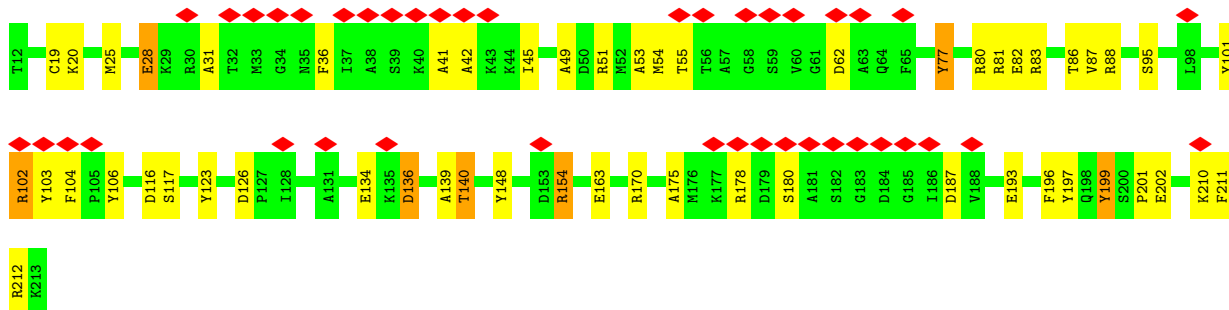
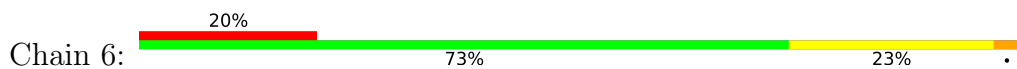




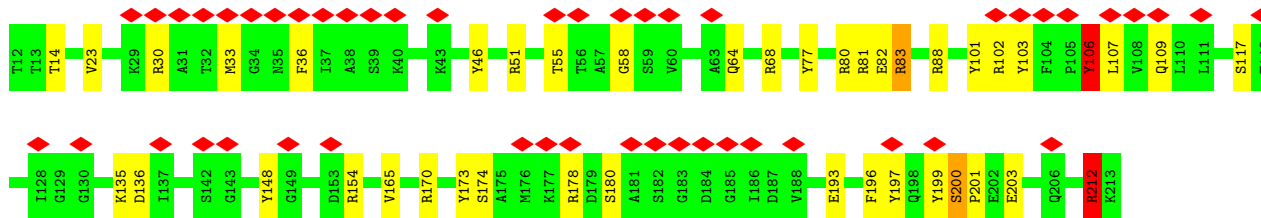
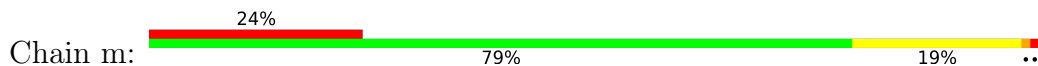
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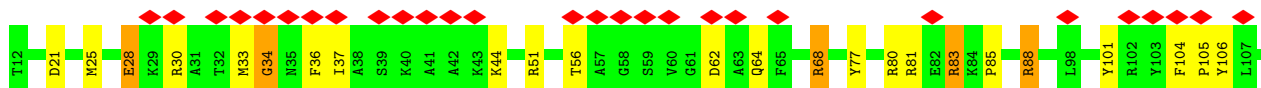
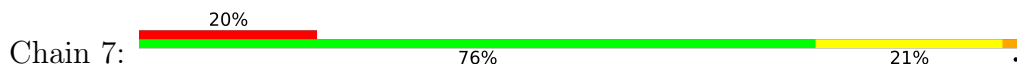
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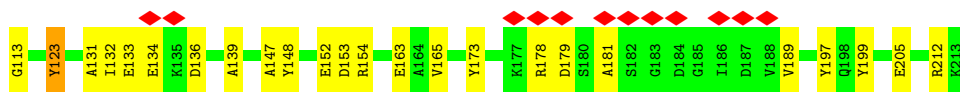


• Molecule 2: Proteasome subunit beta

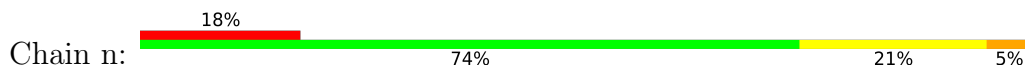


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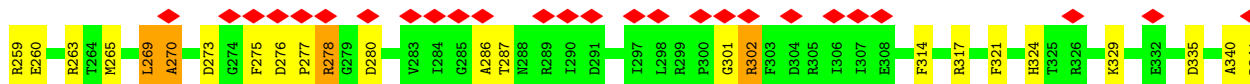
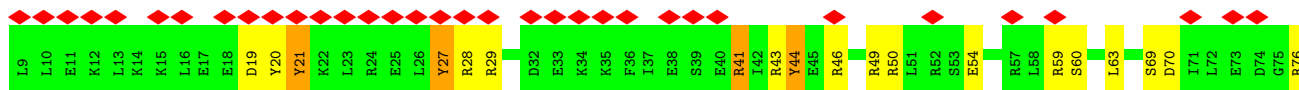




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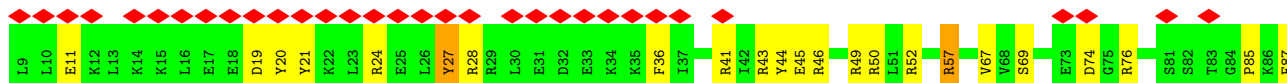
• Molecule 3: Proteasome-activating nucleotidase

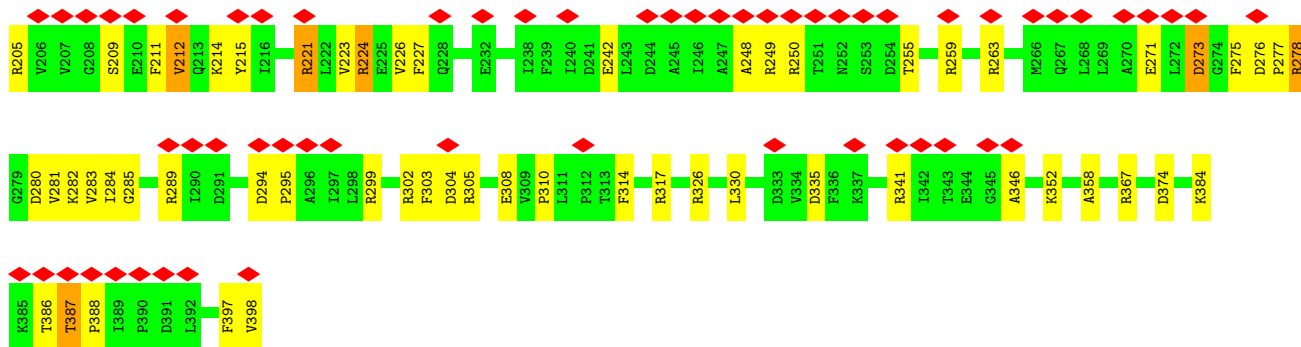


• Molecule 3: Proteasome-activating nucleotidase

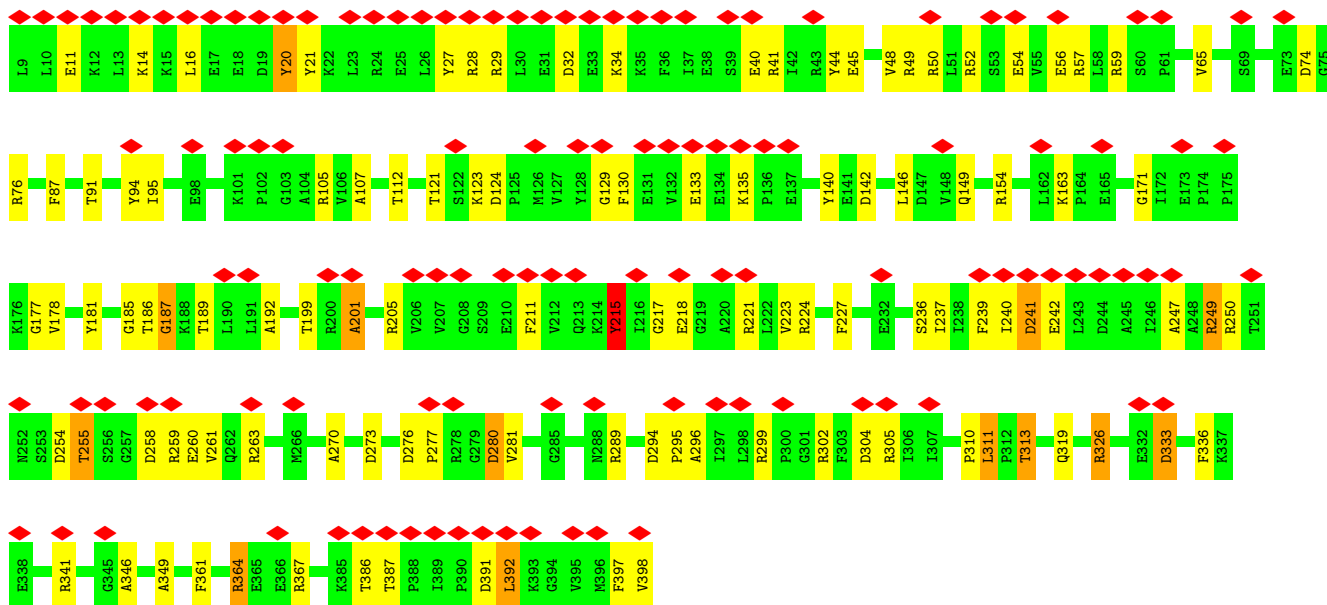


• Molecule 3: Proteasome-activating nucleotidase

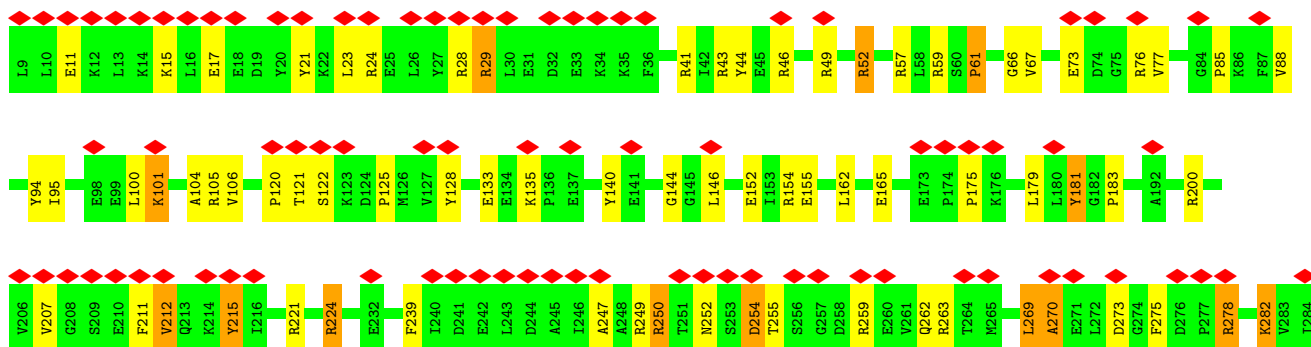
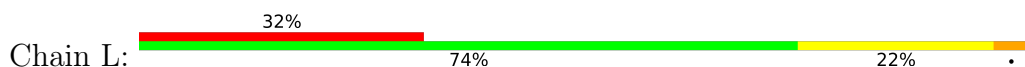




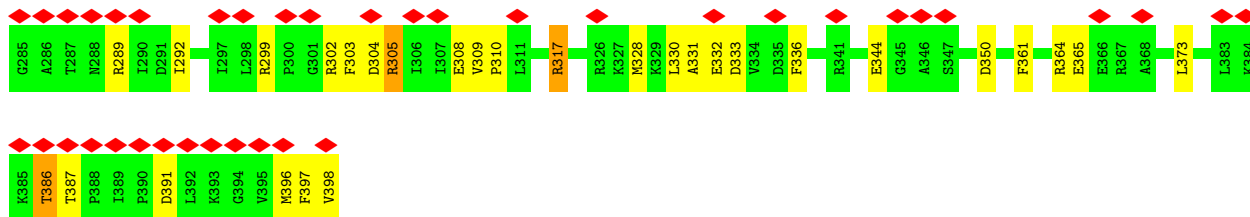
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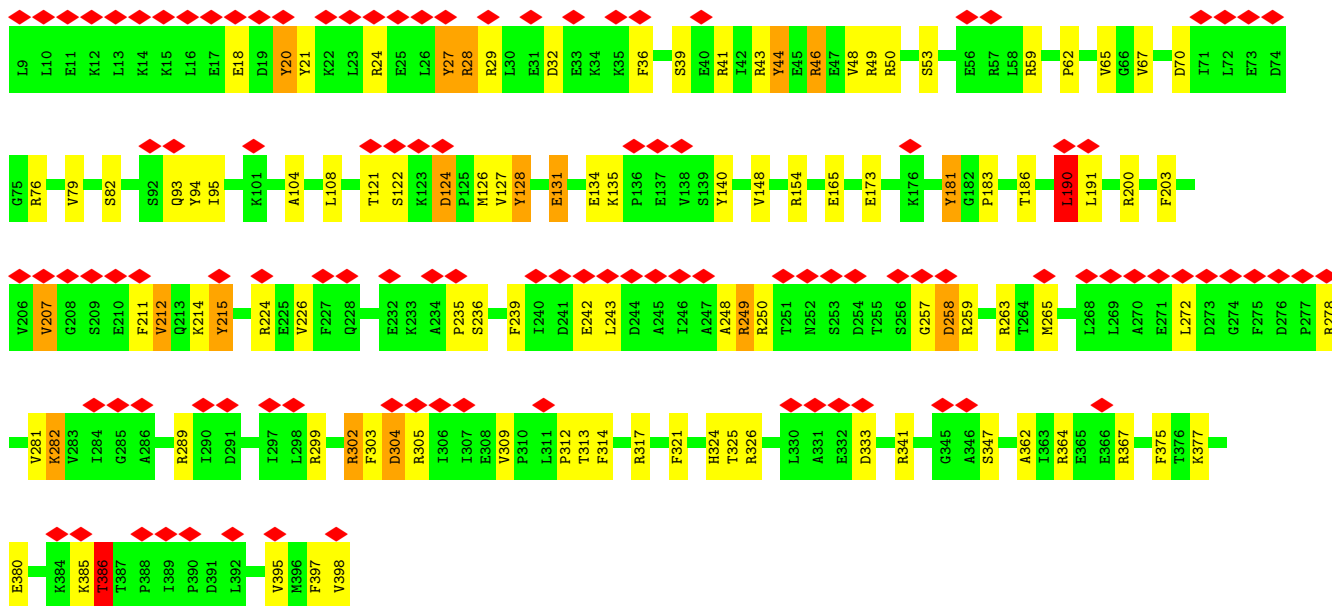
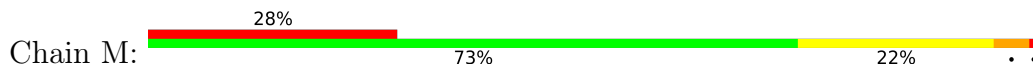
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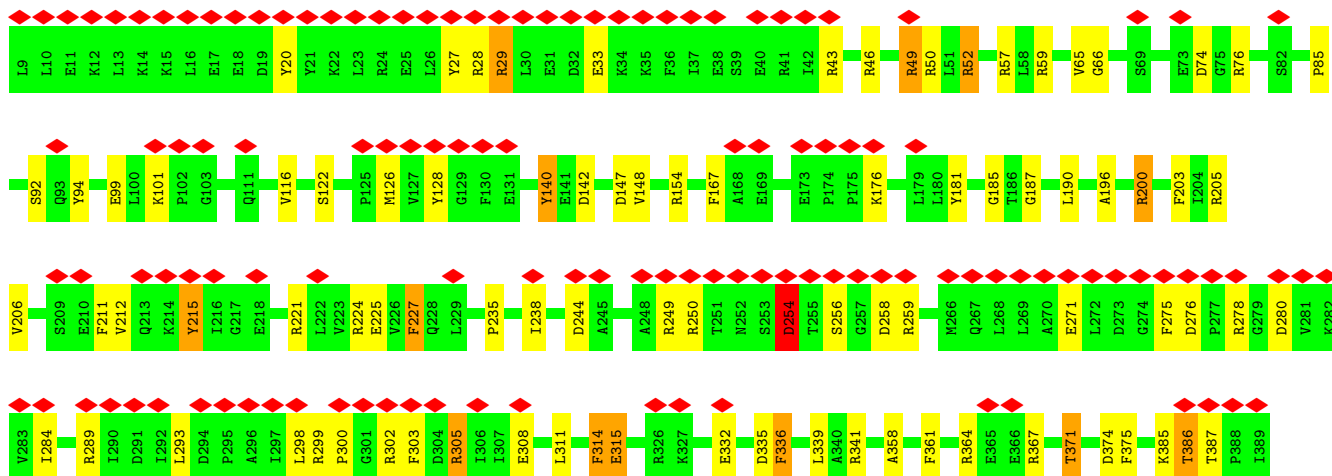
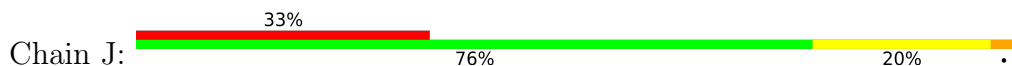


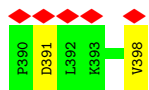


• Molecule 3: Proteasome-activating nucleotidase



• Molecule 3: Proteasome-activating nucleotidase





## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	30758	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ( $e^-/\text{\AA}^2$ )	30	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.051	Depositor
Minimum map value	-0.038	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.001	Depositor
Recommended contour level	0.0068	Depositor
Map size (Å)	514.56, 514.56, 514.56	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.34, 1.34, 1.34	Depositor

## 5 Model quality i

### 5.1 Standard geometry i

Bond lengths and bond angles in the following residue types are not validated in this section: ATP, ADP, MG

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	1.74	13/1934 (0.7%)	1.95	45/2605 (1.7%)
1	B	1.75	24/1934 (1.2%)	2.03	59/2605 (2.3%)
1	C	1.78	22/1934 (1.1%)	1.90	45/2605 (1.7%)
1	D	1.78	21/1934 (1.1%)	2.07	56/2605 (2.1%)
1	E	1.71	13/1934 (0.7%)	2.09	59/2605 (2.3%)
1	F	1.79	31/1934 (1.6%)	1.98	45/2605 (1.7%)
1	G	1.70	11/1934 (0.6%)	1.98	54/2605 (2.1%)
1	a	1.76	21/1892 (1.1%)	1.99	49/2549 (1.9%)
1	b	1.72	21/1892 (1.1%)	1.98	48/2549 (1.9%)
1	c	1.74	22/1892 (1.2%)	1.93	48/2549 (1.9%)
1	d	1.74	16/1892 (0.8%)	1.98	48/2549 (1.9%)
1	e	1.80	17/1892 (0.9%)	1.98	48/2549 (1.9%)
1	f	1.73	16/1892 (0.8%)	1.98	51/2549 (2.0%)
1	g	1.78	18/1892 (1.0%)	1.91	43/2549 (1.7%)
2	1	1.75	21/1573 (1.3%)	2.05	50/2121 (2.4%)
2	2	1.75	21/1573 (1.3%)	1.96	45/2121 (2.1%)
2	3	1.75	18/1573 (1.1%)	1.92	35/2121 (1.7%)
2	4	1.72	12/1573 (0.8%)	1.98	41/2121 (1.9%)
2	5	3.30	23/1573 (1.5%)	2.26	58/2121 (2.7%)
2	6	1.75	19/1573 (1.2%)	2.03	45/2121 (2.1%)
2	7	1.68	12/1573 (0.8%)	2.04	48/2121 (2.3%)
2	h	1.74	24/1573 (1.5%)	1.96	46/2121 (2.2%)
2	i	1.77	14/1573 (0.9%)	1.96	34/2121 (1.6%)
2	j	1.78	16/1573 (1.0%)	1.97	41/2121 (1.9%)
2	k	1.75	15/1573 (1.0%)	1.97	53/2121 (2.5%)
2	l	3.35	19/1573 (1.2%)	2.30	39/2121 (1.8%)
2	m	1.77	20/1573 (1.3%)	2.00	36/2121 (1.7%)
2	n	1.76	14/1573 (0.9%)	1.98	45/2121 (2.1%)
3	H	1.83	42/3146 (1.3%)	1.95	82/4240 (1.9%)
3	I	1.77	42/3146 (1.3%)	2.04	95/4240 (2.2%)
3	J	1.78	33/3146 (1.0%)	1.89	58/4240 (1.4%)
3	K	1.76	37/3146 (1.2%)	2.00	83/4240 (2.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
3	L	1.78	38/3146 (1.2%)	1.93	72/4240 (1.7%)
3	M	1.75	33/3146 (1.0%)	1.98	83/4240 (2.0%)
All	All	1.86	739/67680 (1.1%)	1.99	1787/91212 (2.0%)

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	10
1	B	0	11
1	C	0	10
1	D	0	7
1	E	0	7
1	F	0	9
1	G	0	11
1	a	0	8
1	b	0	10
1	c	0	9
1	d	0	8
1	e	0	8
1	f	0	10
1	g	0	6
2	1	0	8
2	2	0	7
2	3	0	5
2	4	0	6
2	5	0	7
2	6	0	4
2	7	0	7
2	h	0	6
2	i	0	9
2	j	0	4
2	k	0	11
2	l	0	10
2	m	0	4
2	n	0	8
3	H	0	18
3	I	0	12
3	J	0	16
3	K	0	18

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	17
3	M	0	20
All	All	0	321

All (739) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	170	ARG	CZ-NH1	61.42	2.12	1.33
2	5	170	ARG	CZ-NH1	60.13	2.11	1.33
2	l	211	PHE	CG-CD2	48.98	2.12	1.38
2	l	211	PHE	CG-CD1	47.67	2.10	1.38
2	5	211	PHE	CG-CD1	45.47	2.06	1.38
2	5	211	PHE	CG-CD2	44.17	2.05	1.38
2	l	211	PHE	CE1-CZ	37.48	2.08	1.37
2	5	211	PHE	CE1-CZ	37.31	2.08	1.37
2	5	211	PHE	CE2-CZ	33.61	2.01	1.37
2	5	211	PHE	CD2-CE2	32.45	2.04	1.39
2	l	211	PHE	CD2-CE2	31.67	2.02	1.39
2	5	211	PHE	CD1-CE1	31.58	2.02	1.39
2	l	211	PHE	CE2-CZ	31.53	1.97	1.37
2	l	211	PHE	CD1-CE1	30.00	1.99	1.39
3	J	398	VAL	C-O	-12.08	1.00	1.23
3	I	398	VAL	C-O	-12.06	1.00	1.23
3	L	398	VAL	C-O	-12.06	1.00	1.23
3	M	398	VAL	C-O	-12.06	1.00	1.23
3	H	398	VAL	C-OXT	-12.05	1.00	1.23
3	I	398	VAL	C-OXT	-12.05	1.00	1.23
3	L	398	VAL	C-OXT	-12.04	1.00	1.23
3	M	398	VAL	C-OXT	-12.05	1.00	1.23
3	K	398	VAL	C-OXT	-12.03	1.00	1.23
3	H	398	VAL	C-O	-12.03	1.00	1.23
3	K	398	VAL	C-O	-12.03	1.00	1.23
3	J	398	VAL	C-OXT	-12.03	1.00	1.23
1	g	225	SER	CA-CB	9.48	1.67	1.52
2	5	178	ARG	NE-CZ	9.38	1.45	1.33
1	A	123	TYR	CG-CD2	9.10	1.50	1.39
3	H	341	ARG	NE-CZ	8.78	1.44	1.33
3	H	105	ARG	NE-CZ	8.73	1.44	1.33
3	I	299	ARG	NE-CZ	8.50	1.44	1.33
2	n	148	TYR	CE2-CZ	8.34	1.49	1.38
1	b	20	ARG	NE-CZ	8.10	1.43	1.33
2	m	81	ARG	CZ-NH2	8.04	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	46	ARG	CZ-NH1	8.03	1.43	1.33
3	H	128	TYR	CG-CD2	7.90	1.49	1.39
3	H	301	GLY	CA-C	-7.89	1.39	1.51
2	n	81	ARG	NE-CZ	7.87	1.43	1.33
1	F	168	ARG	CD-NE	7.85	1.59	1.46
2	j	100	SER	CA-CB	7.79	1.64	1.52
3	M	82	SER	CA-CB	7.77	1.64	1.52
1	D	168	ARG	CZ-NH1	7.77	1.43	1.33
2	k	178	ARG	CZ-NH2	7.72	1.43	1.33
1	G	91	ARG	NE-CZ	7.67	1.43	1.33
2	l	51	ARG	NE-CZ	7.64	1.43	1.33
3	H	174	PRO	N-CD	-7.64	1.37	1.47
3	I	49	ARG	NE-CZ	7.62	1.43	1.33
2	5	193	GLU	CG-CD	7.61	1.63	1.51
3	M	28	ARG	CZ-NH1	7.56	1.42	1.33
3	K	310	PRO	N-CD	-7.55	1.37	1.47
1	F	10	ARG	CZ-NH1	7.54	1.42	1.33
2	h	80	ARG	CZ-NH2	7.54	1.42	1.33
3	H	92	SER	CA-CB	7.52	1.64	1.52
1	E	153	SER	CA-CB	7.50	1.64	1.52
3	H	139	SER	CA-CB	7.48	1.64	1.52
1	g	20	ARG	CZ-NH1	7.45	1.42	1.33
2	5	212	ARG	CD-NE	7.44	1.59	1.46
1	G	179	TYR	CE2-CZ	7.43	1.48	1.38
1	B	15	PHE	CG-CD1	7.42	1.49	1.38
3	H	46	ARG	NE-CZ	7.39	1.42	1.33
2	1	178	ARG	NE-CZ	7.36	1.42	1.33
3	L	308	GLU	CB-CG	7.33	1.66	1.52
1	f	130	ARG	CD-NE	7.31	1.58	1.46
2	i	83	ARG	CD-NE	7.30	1.58	1.46
3	M	50	ARG	CZ-NH2	7.24	1.42	1.33
1	C	53	ARG	CZ-NH2	7.18	1.42	1.33
2	l	81	ARG	CZ-NH1	7.18	1.42	1.33
3	J	315	GLU	CD-OE2	7.17	1.33	1.25
1	d	53	ARG	CD-NE	7.15	1.58	1.46
1	F	20	ARG	NE-CZ	7.13	1.42	1.33
3	H	260	GLU	CG-CD	7.12	1.62	1.51
1	d	128	GLY	CA-C	-7.11	1.40	1.51
3	M	39	SER	CA-CB	7.11	1.63	1.52
3	H	340	ALA	N-CA	-7.08	1.32	1.46
1	a	213	TYR	CG-CD2	7.08	1.48	1.39
1	e	159	TYR	CG-CD2	7.08	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	g	148	TYR	CB-CG	-7.08	1.41	1.51
3	L	278	ARG	NE-CZ	7.04	1.42	1.33
2	h	193	GLU	CG-CD	7.01	1.62	1.51
2	1	88	ARG	CD-NE	7.00	1.58	1.46
2	h	88	ARG	NE-CZ	7.00	1.42	1.33
3	H	367	ARG	CZ-NH1	6.94	1.42	1.33
1	g	185	PHE	CB-CG	-6.92	1.39	1.51
3	J	200	ARG	CZ-NH2	6.92	1.42	1.33
1	E	10	ARG	NE-CZ	6.91	1.42	1.33
3	K	289	ARG	CD-NE	6.91	1.58	1.46
3	I	209	SER	CA-CB	6.91	1.63	1.52
1	B	213	TYR	CE1-CZ	6.87	1.47	1.38
1	C	149	GLU	CD-OE1	6.87	1.33	1.25
1	d	123	TYR	CG-CD1	6.87	1.48	1.39
1	a	26	TYR	CG-CD1	6.86	1.48	1.39
1	F	130	ARG	CZ-NH1	6.86	1.42	1.33
3	M	21	TYR	CG-CD1	6.85	1.48	1.39
1	B	91	ARG	NE-CZ	6.84	1.42	1.33
2	h	197	TYR	CE1-CZ	6.81	1.47	1.38
2	3	68	ARG	NE-CZ	6.80	1.41	1.33
2	l	154	ARG	CZ-NH2	6.79	1.41	1.33
1	E	239	ARG	CZ-NH2	6.75	1.41	1.33
1	d	232	TYR	CB-CG	-6.75	1.41	1.51
2	1	134	GLU	CD-OE2	6.75	1.33	1.25
2	k	46	TYR	CG-CD1	6.75	1.48	1.39
1	c	28	ARG	CZ-NH1	6.75	1.41	1.33
2	1	28	GLU	CG-CD	6.75	1.62	1.51
3	K	29	ARG	CZ-NH2	6.73	1.41	1.33
2	i	77	TYR	CG-CD2	6.71	1.47	1.39
1	d	168	ARG	CZ-NH2	6.70	1.41	1.33
1	c	103	TYR	CE2-CZ	6.67	1.47	1.38
2	2	124	SER	CA-CB	6.67	1.62	1.52
3	J	142	ASP	CB-CG	6.67	1.65	1.51
3	M	326	ARG	CZ-NH2	6.67	1.41	1.33
1	E	235	ARG	NE-CZ	6.66	1.41	1.33
1	A	168	ARG	CZ-NH1	6.66	1.41	1.33
3	M	29	ARG	NE-CZ	6.66	1.41	1.33
2	k	68	ARG	CZ-NH1	6.65	1.41	1.33
1	G	93	ARG	CZ-NH2	6.65	1.41	1.33
1	f	28	ARG	NE-CZ	6.64	1.41	1.33
3	K	289	ARG	NE-CZ	6.63	1.41	1.33
2	3	113	GLY	CA-C	-6.63	1.41	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	L	144	GLY	CA-C	-6.63	1.41	1.51
2	5	123	TYR	CG-CD1	6.62	1.47	1.39
1	B	219	ARG	CZ-NH1	6.62	1.41	1.33
3	J	28	ARG	CZ-NH1	6.61	1.41	1.33
1	c	130	ARG	CZ-NH1	6.59	1.41	1.33
1	a	207	GLU	CB-CG	6.59	1.64	1.52
1	C	33	ARG	CD-NE	6.58	1.57	1.46
3	H	60	SER	CA-CB	6.58	1.62	1.52
3	L	263	ARG	NE-CZ	6.56	1.41	1.33
1	f	68	TYR	CE1-CZ	6.54	1.47	1.38
3	M	43	ARG	NE-CZ	6.54	1.41	1.33
3	H	82	SER	CA-CB	6.54	1.62	1.52
1	c	185	PHE	CG-CD2	6.53	1.48	1.38
2	3	30	ARG	CZ-NH1	6.53	1.41	1.33
2	h	73	GLU	CD-OE1	6.52	1.32	1.25
3	H	242	GLU	CB-CG	6.52	1.64	1.52
1	F	10	ARG	CD-NE	6.52	1.57	1.46
3	H	263	ARG	CD-NE	6.51	1.57	1.46
3	H	278	ARG	CZ-NH2	6.51	1.41	1.33
3	J	49	ARG	CZ-NH2	6.49	1.41	1.33
1	d	28	ARG	CZ-NH1	6.48	1.41	1.33
1	g	86	ARG	CZ-NH2	6.48	1.41	1.33
3	M	20	TYR	CG-CD2	6.48	1.47	1.39
1	b	239	ARG	CZ-NH1	6.48	1.41	1.33
1	A	197	GLY	CA-C	-6.46	1.41	1.51
3	I	44	TYR	CE2-CZ	6.46	1.47	1.38
2	3	201	PRO	N-CD	-6.45	1.38	1.47
3	J	364	ARG	CD-NE	6.45	1.57	1.46
3	K	221	ARG	NE-CZ	6.44	1.41	1.33
2	j	102	ARG	NE-CZ	6.44	1.41	1.33
2	l	88	ARG	NE-CZ	6.44	1.41	1.33
1	C	201	GLU	CD-OE2	6.43	1.32	1.25
3	J	224	ARG	NE-CZ	6.42	1.41	1.33
2	m	117	SER	CB-OG	6.42	1.50	1.42
1	c	192	GLY	N-CA	6.42	1.55	1.46
1	B	53	ARG	CZ-NH1	6.41	1.41	1.33
2	6	102	ARG	CD-NE	6.41	1.57	1.46
2	3	81	ARG	CZ-NH1	6.41	1.41	1.33
1	d	228	GLU	CG-CD	6.41	1.61	1.51
3	K	11	GLU	CD-OE1	6.41	1.32	1.25
2	4	212	ARG	CD-NE	6.40	1.57	1.46
2	m	148	TYR	CE2-CZ	6.40	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	65	PHE	CG-CD2	6.40	1.48	1.38
1	F	119	PHE	CG-CD1	6.40	1.48	1.38
1	E	26	TYR	CE2-CZ	6.39	1.46	1.38
1	e	241	ARG	CZ-NH1	6.38	1.41	1.33
3	I	57	ARG	CZ-NH2	6.37	1.41	1.33
3	H	169	GLU	CD-OE2	6.36	1.32	1.25
1	a	236	ALA	CA-CB	6.36	1.65	1.52
1	f	22	PHE	CG-CD1	6.36	1.48	1.38
2	k	174	SER	CA-CB	6.36	1.62	1.52
2	n	183	GLY	CA-C	-6.36	1.41	1.51
2	m	197	TYR	CD1-CE1	6.35	1.48	1.39
1	c	168	ARG	NE-CZ	6.34	1.41	1.33
1	E	219	ARG	CZ-NH2	6.33	1.41	1.33
2	7	80	ARG	CZ-NH2	6.33	1.41	1.33
2	6	148	TYR	CG-CD2	6.33	1.47	1.39
3	L	200	ARG	CD-NE	6.32	1.57	1.46
1	e	203	GLU	CD-OE2	6.32	1.32	1.25
2	m	58	GLY	CA-C	-6.32	1.41	1.51
1	G	180	ARG	CZ-NH2	6.31	1.41	1.33
3	H	50	ARG	NE-CZ	6.30	1.41	1.33
2	n	51	ARG	CZ-NH1	6.30	1.41	1.33
1	F	168	ARG	NE-CZ	6.29	1.41	1.33
2	j	80	ARG	CZ-NH1	6.29	1.41	1.33
1	F	93	ARG	CZ-NH1	6.29	1.41	1.33
1	e	219	ARG	CZ-NH2	6.28	1.41	1.33
2	j	124	SER	CA-CB	-6.28	1.43	1.52
2	3	212	ARG	CZ-NH1	6.28	1.41	1.33
2	m	88	ARG	NE-CZ	6.27	1.41	1.33
3	L	49	ARG	CZ-NH1	6.26	1.41	1.33
3	I	45	GLU	CD-OE2	6.26	1.32	1.25
1	e	232	TYR	CB-CG	-6.26	1.42	1.51
3	L	305	ARG	CZ-NH1	6.23	1.41	1.33
1	a	241	ARG	CD-NE	6.22	1.57	1.46
1	D	8	TYR	CB-CG	-6.21	1.42	1.51
2	h	141	GLY	N-CA	-6.20	1.36	1.46
1	f	191	LEU	C-N	6.20	1.44	1.33
3	J	187	GLY	N-CA	-6.20	1.36	1.46
1	a	143	GLU	CD-OE2	6.19	1.32	1.25
1	F	18	ASP	C-N	6.19	1.44	1.33
2	4	30	ARG	NE-CZ	6.19	1.41	1.33
3	M	259	ARG	CD-NE	6.19	1.56	1.46
1	D	26	TYR	CB-CG	6.19	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	i	12	THR	N-CA	6.19	1.58	1.46
3	L	46	ARG	NE-CZ	6.18	1.41	1.33
1	e	20	ARG	CZ-NH2	6.17	1.41	1.33
2	h	83	ARG	CZ-NH1	6.16	1.41	1.33
2	4	185	GLY	N-CA	-6.16	1.36	1.46
1	g	91	ARG	CD-NE	6.15	1.56	1.46
3	H	128	TYR	CE2-CZ	6.15	1.46	1.38
3	J	66	GLY	N-CA	-6.15	1.36	1.46
1	f	103	TYR	CG-CD1	6.14	1.47	1.39
1	F	232	TYR	CE2-CZ	6.14	1.46	1.38
2	1	212	ARG	NE-CZ	6.14	1.41	1.33
3	K	185	GLY	N-CA	-6.13	1.36	1.46
3	L	140	TYR	CZ-OH	6.13	1.48	1.37
1	d	86	ARG	CZ-NH1	6.13	1.41	1.33
3	K	305	ARG	CD-NE	6.12	1.56	1.46
1	b	186	ASP	CA-CB	6.12	1.67	1.53
1	E	8	TYR	CG-CD1	6.12	1.47	1.39
1	b	60	GLU	CG-CD	6.12	1.61	1.51
2	i	199	TYR	CE2-CZ	6.12	1.46	1.38
3	H	224	ARG	CD-NE	6.11	1.56	1.46
1	b	10	ARG	CZ-NH1	6.11	1.41	1.33
1	c	42	CYS	CA-CB	6.09	1.67	1.53
2	n	68	ARG	CD-NE	6.09	1.56	1.46
3	L	24	ARG	CD-NE	6.09	1.56	1.46
1	B	148	TYR	CG-CD1	6.09	1.47	1.39
2	1	130	GLY	N-CA	-6.08	1.36	1.46
2	i	102	ARG	CD-NE	6.08	1.56	1.46
3	M	46	ARG	CD-NE	6.07	1.56	1.46
1	B	179	TYR	CE1-CZ	6.07	1.46	1.38
2	i	83	ARG	CZ-NH1	6.06	1.41	1.33
2	i	170	ARG	CZ-NH2	6.06	1.41	1.33
1	A	168	ARG	NE-CZ	6.05	1.41	1.33
2	n	101	TYR	CE2-CZ	6.05	1.46	1.38
1	b	86	ARG	NE-CZ	6.05	1.41	1.33
1	D	239	ARG	CD-NE	6.05	1.56	1.46
2	6	81	ARG	NE-CZ	6.05	1.41	1.33
1	g	20	ARG	CZ-NH2	6.04	1.41	1.33
2	6	51	ARG	CZ-NH1	6.04	1.41	1.33
3	H	205	ARG	CZ-NH1	6.04	1.41	1.33
3	I	326	ARG	NE-CZ	6.03	1.40	1.33
3	H	278	ARG	CD-NE	6.03	1.56	1.46
2	j	173	TYR	CG-CD2	6.02	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	21	TYR	CE1-CZ	6.02	1.46	1.38
2	k	81	ARG	NE-CZ	6.02	1.40	1.33
2	1	173	TYR	CE1-CZ	6.01	1.46	1.38
3	J	293	LEU	CA-C	-6.01	1.37	1.52
3	I	250	ARG	CD-NE	6.01	1.56	1.46
1	a	94	ILE	C-N	6.01	1.47	1.34
3	L	317	ARG	CZ-NH1	6.01	1.40	1.33
2	6	199	TYR	CE2-CZ	6.00	1.46	1.38
3	I	171	GLY	N-CA	-6.00	1.37	1.46
2	7	68	ARG	NE-CZ	6.00	1.40	1.33
1	e	207	GLU	CD-OE2	-6.00	1.19	1.25
2	3	154	ARG	NE-CZ	6.00	1.40	1.33
1	e	180	ARG	CZ-NH1	6.00	1.40	1.33
2	5	106	TYR	CE2-CZ	6.00	1.46	1.38
3	M	224	ARG	CZ-NH2	6.00	1.40	1.33
2	n	199	TYR	CG-CD1	6.00	1.47	1.39
1	A	180	ARG	CZ-NH2	5.99	1.40	1.33
3	L	128	TYR	CZ-OH	5.99	1.48	1.37
1	F	100	ARG	CZ-NH1	5.98	1.40	1.33
2	k	30	ARG	NE-CZ	5.97	1.40	1.33
3	L	59	ARG	CZ-NH2	5.97	1.40	1.33
2	7	34	GLY	CA-C	-5.97	1.42	1.51
1	B	86	ARG	CZ-NH2	5.96	1.40	1.33
3	I	249	ARG	CZ-NH1	5.96	1.40	1.33
3	H	43	ARG	NE-CZ	5.96	1.40	1.33
1	B	28	ARG	CZ-NH2	5.96	1.40	1.33
1	g	207	GLU	CD-OE1	5.95	1.32	1.25
1	f	226	PRO	N-CA	5.95	1.57	1.47
2	j	81	ARG	NE-CZ	5.94	1.40	1.33
2	5	200	SER	CA-CB	5.94	1.61	1.52
2	m	199	TYR	CE2-CZ	5.93	1.46	1.38
3	M	278	ARG	CZ-NH2	5.93	1.40	1.33
2	1	106	TYR	CG-CD1	5.92	1.46	1.39
3	L	364	ARG	CZ-NH1	5.92	1.40	1.33
1	B	239	ARG	NE-CZ	5.92	1.40	1.33
2	2	170	ARG	NE-CZ	5.92	1.40	1.33
3	L	28	ARG	CZ-NH2	5.92	1.40	1.33
3	J	99	GLU	CD-OE2	5.92	1.32	1.25
1	a	239	ARG	CZ-NH2	5.91	1.40	1.33
1	D	153	SER	CA-CB	5.91	1.61	1.52
3	L	299	ARG	NE-CZ	5.90	1.40	1.33
1	b	126	TYR	CB-CG	-5.90	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	e	53	ARG	CZ-NH2	5.90	1.40	1.33
1	d	130	ARG	CD-NE	5.89	1.56	1.46
3	H	29	ARG	NE-CZ	5.89	1.40	1.33
3	I	305	ARG	CZ-NH2	5.88	1.40	1.33
1	D	130	ARG	CD-NE	5.87	1.56	1.46
3	H	263	ARG	CZ-NH1	5.87	1.40	1.33
2	m	106	TYR	CD1-CE1	5.86	1.48	1.39
3	J	33	GLU	CD-OE1	5.86	1.32	1.25
1	F	35	ALA	CA-CB	5.85	1.64	1.52
1	g	202	SER	CA-CB	5.85	1.61	1.52
1	C	100	ARG	CZ-NH1	5.85	1.40	1.33
1	E	239	ARG	NE-CZ	5.85	1.40	1.33
2	n	83	ARG	CD-NE	5.85	1.56	1.46
1	F	28	ARG	NE-CZ	5.84	1.40	1.33
2	2	183	GLY	CA-C	5.84	1.61	1.51
2	j	197	TYR	CE2-CZ	5.84	1.46	1.38
2	4	123	TYR	CE1-CZ	5.84	1.46	1.38
1	G	20	ARG	NE-CZ	5.83	1.40	1.33
2	i	123	TYR	CG-CD2	5.83	1.46	1.39
2	3	88	ARG	CZ-NH2	5.83	1.40	1.33
1	B	20	ARG	NE-CZ	5.82	1.40	1.33
3	J	278	ARG	CZ-NH1	5.82	1.40	1.33
2	k	197	TYR	CE1-CZ	5.82	1.46	1.38
3	J	341	ARG	NE-CZ	5.82	1.40	1.33
1	c	235	ARG	NE-CZ	5.82	1.40	1.33
1	D	179	TYR	CE2-CZ	5.82	1.46	1.38
2	m	154	ARG	CD-NE	5.82	1.56	1.46
3	H	124	ASP	CA-CB	5.81	1.66	1.53
3	L	133	GLU	CG-CD	5.81	1.60	1.51
2	j	102	ARG	CZ-NH1	5.80	1.40	1.33
1	b	26	TYR	CG-CD1	5.80	1.46	1.39
1	D	65	GLU	CD-OE2	5.80	1.32	1.25
2	2	149	GLY	N-CA	-5.79	1.37	1.46
3	J	57	ARG	CD-NE	5.78	1.56	1.46
1	D	20	ARG	CZ-NH2	5.77	1.40	1.33
3	L	105	ARG	CZ-NH1	5.77	1.40	1.33
3	M	326	ARG	CD-NE	5.77	1.56	1.46
1	D	239	ARG	NE-CZ	5.77	1.40	1.33
1	a	228	GLU	CB-CG	5.77	1.63	1.52
1	g	207	GLU	CB-CG	5.76	1.63	1.52
3	J	29	ARG	CD-NE	5.76	1.56	1.46
2	k	15	VAL	CB-CG1	5.76	1.65	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	68	ARG	CD-NE	5.76	1.56	1.46
2	1	148	TYR	CG-CD2	5.76	1.46	1.39
1	d	33	ARG	NE-CZ	5.75	1.40	1.33
2	2	148	TYR	CG-CD2	5.75	1.46	1.39
3	H	44	TYR	CZ-OH	5.75	1.47	1.37
1	d	44	GLU	CB-CG	5.75	1.63	1.52
2	7	113	GLY	N-CA	-5.75	1.37	1.46
2	3	30	ARG	CZ-NH2	5.75	1.40	1.33
2	3	183	GLY	CA-C	-5.75	1.42	1.51
1	G	239	ARG	CZ-NH2	5.74	1.40	1.33
1	F	241	ARG	NE-CZ	5.74	1.40	1.33
3	M	367	ARG	CZ-NH2	5.74	1.40	1.33
1	a	223	GLU	CD-OE1	5.74	1.31	1.25
2	m	36	PHE	CE2-CZ	5.73	1.48	1.37
2	2	173	TYR	CD2-CE2	5.73	1.48	1.39
1	B	26	TYR	CZ-OH	5.72	1.47	1.37
2	2	152	GLU	CD-OE1	5.71	1.31	1.25
1	f	153	SER	CA-CB	5.71	1.61	1.52
1	G	133	GLY	CA-C	-5.71	1.42	1.51
2	4	80	ARG	NE-CZ	5.71	1.40	1.33
3	M	41	ARG	CZ-NH2	5.71	1.40	1.33
2	l	104	PHE	CG-CD2	5.71	1.47	1.38
1	D	86	ARG	CZ-NH2	5.71	1.40	1.33
2	2	113	GLY	N-CA	-5.70	1.37	1.46
1	e	103	TYR	CE1-CZ	5.70	1.46	1.38
1	B	241	ARG	CZ-NH2	5.69	1.40	1.33
2	6	197	TYR	CG-CD1	5.69	1.46	1.39
3	J	225	GLU	CD-OE2	5.69	1.31	1.25
2	6	163	GLU	CB-CG	5.69	1.62	1.52
3	K	227	PHE	CE1-CZ	5.69	1.48	1.37
2	6	178	ARG	CD-NE	5.69	1.56	1.46
1	e	45	GLY	CA-C	-5.68	1.42	1.51
2	k	152	GLU	CG-CD	5.68	1.60	1.51
2	m	77	TYR	CE1-CZ	5.68	1.46	1.38
1	C	119	PHE	CG-CD1	5.68	1.47	1.38
2	2	212	ARG	NE-CZ	5.68	1.40	1.33
1	f	33	ARG	NE-CZ	5.67	1.40	1.33
2	6	170	ARG	CZ-NH1	5.67	1.40	1.33
3	I	69	SER	CA-CB	5.67	1.61	1.52
1	c	79	SER	C-N	5.67	1.43	1.33
2	l	212	ARG	NE-CZ	5.66	1.40	1.33
3	K	289	ARG	CZ-NH2	5.66	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	69	LYS	N-CA	-5.65	1.35	1.46
3	I	52	ARG	CZ-NH2	5.65	1.40	1.33
2	6	154	ARG	CZ-NH2	5.65	1.40	1.33
1	c	131	PRO	N-CD	-5.65	1.40	1.47
3	L	105	ARG	CD-NE	5.65	1.56	1.46
1	a	241	ARG	N-CA	-5.64	1.35	1.46
1	c	103	TYR	CE1-CZ	5.64	1.45	1.38
3	L	365	GLU	CG-CD	5.63	1.60	1.51
1	d	33	ARG	C-N	5.63	1.43	1.33
2	n	173	TYR	CZ-OH	5.63	1.47	1.37
1	B	201	GLU	CG-CD	5.62	1.60	1.51
3	I	367	ARG	CZ-NH2	5.62	1.40	1.33
1	a	91	ARG	CZ-NH2	5.62	1.40	1.33
1	c	42	CYS	CB-SG	5.62	1.91	1.82
1	F	126	TYR	CZ-OH	5.62	1.47	1.37
3	L	41	ARG	CZ-NH1	5.61	1.40	1.33
3	K	49	ARG	NE-CZ	5.61	1.40	1.33
3	K	28	ARG	CZ-NH2	5.61	1.40	1.33
1	f	180	ARG	CZ-NH2	5.61	1.40	1.33
1	D	93	ARG	CZ-NH2	5.61	1.40	1.33
2	h	28	GLU	CD-OE1	5.61	1.31	1.25
3	I	28	ARG	CZ-NH2	5.61	1.40	1.33
2	2	88	ARG	CZ-NH2	5.60	1.40	1.33
1	B	213	TYR	CE2-CZ	5.60	1.45	1.38
3	I	127	VAL	CB-CG1	5.59	1.64	1.52
3	L	73	GLU	CD-OE1	5.59	1.31	1.25
2	2	83	ARG	CZ-NH1	5.58	1.40	1.33
1	C	168	ARG	NE-CZ	5.58	1.40	1.33
3	M	148	VAL	CB-CG2	5.58	1.64	1.52
3	L	46	ARG	CD-NE	5.57	1.55	1.46
1	F	202	SER	CA-CB	5.57	1.61	1.52
2	7	197	TYR	CZ-OH	5.57	1.47	1.37
3	M	302	ARG	CZ-NH2	5.57	1.40	1.33
2	6	83	ARG	NE-CZ	5.56	1.40	1.33
2	1	95	SER	CA-CB	5.56	1.61	1.52
2	n	56	THR	N-CA	-5.56	1.35	1.46
2	i	30	ARG	CZ-NH2	5.56	1.40	1.33
3	M	302	ARG	NE-CZ	5.56	1.40	1.33
1	D	8	TYR	CE2-CZ	5.55	1.45	1.38
2	6	180	SER	CA-CB	5.55	1.61	1.52
1	f	235	ARG	NE-CZ	5.54	1.40	1.33
1	G	95	GLU	CG-CD	5.54	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	44	GLU	CG-CD	5.54	1.60	1.51
1	C	123	TYR	CD1-CE1	5.54	1.47	1.39
3	L	305	ARG	CZ-NH2	5.54	1.40	1.33
3	K	21	TYR	CG-CD1	5.53	1.46	1.39
2	1	158	GLU	CD-OE2	5.53	1.31	1.25
2	3	211	PHE	CG-CD2	5.53	1.47	1.38
1	g	159	TYR	CB-CG	-5.53	1.43	1.51
2	h	199	TYR	CG-CD2	5.53	1.46	1.39
3	K	54	GLU	CB-CG	5.53	1.62	1.52
3	J	176	LYS	C-N	5.53	1.43	1.33
1	A	235	ARG	NE-CZ	5.52	1.40	1.33
2	6	28	GLU	CD-OE1	5.52	1.31	1.25
3	H	265	MET	CA-CB	5.52	1.66	1.53
3	H	21	TYR	CE1-CZ	5.52	1.45	1.38
2	5	178	ARG	CZ-NH2	5.51	1.40	1.33
1	b	75	CYS	CB-SG	5.51	1.91	1.82
1	b	223	GLU	CB-CG	5.51	1.62	1.52
1	C	202	SER	CA-CB	5.51	1.61	1.52
2	m	46	TYR	CG-CD1	5.51	1.46	1.39
3	L	361	PHE	CG-CD2	5.50	1.47	1.38
2	5	33	MET	CA-CB	5.50	1.66	1.53
2	m	82	GLU	CG-CD	5.50	1.60	1.51
2	m	102	ARG	CZ-NH1	5.50	1.40	1.33
3	H	211	PHE	CG-CD1	5.50	1.47	1.38
2	k	123	TYR	CB-CG	-5.50	1.43	1.51
1	A	103	TYR	CZ-OH	5.50	1.47	1.37
1	B	123	TYR	CG-CD1	5.50	1.46	1.39
1	B	126	TYR	CG-CD1	5.49	1.46	1.39
2	1	106	TYR	CB-CG	-5.49	1.43	1.51
2	l	203	GLU	CB-CG	5.49	1.62	1.52
1	a	123	TYR	CZ-OH	5.49	1.47	1.37
2	h	68	ARG	CD-NE	5.49	1.55	1.46
2	5	88	ARG	NE-CZ	5.49	1.40	1.33
2	7	36	PHE	CG-CD2	5.49	1.47	1.38
3	K	59	ARG	NE-CZ	5.49	1.40	1.33
2	n	197	TYR	CD2-CE2	5.48	1.47	1.39
1	C	149	GLU	CA-CB	5.48	1.66	1.53
2	7	83	ARG	CZ-NH2	5.48	1.40	1.33
1	F	126	TYR	CE2-CZ	5.48	1.45	1.38
1	F	232	TYR	CG-CD1	5.47	1.46	1.39
1	g	241	ARG	NE-CZ	5.47	1.40	1.33
3	I	92	SER	CA-CB	5.47	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	b	28	ARG	NE-CZ	5.47	1.40	1.33
2	4	102	ARG	CZ-NH2	5.46	1.40	1.33
3	M	21	TYR	CZ-OH	5.46	1.47	1.37
1	D	212	GLY	CA-C	-5.46	1.43	1.51
1	C	235	ARG	CZ-NH2	5.46	1.40	1.33
1	E	19	GLY	N-CA	-5.46	1.37	1.46
2	h	152	GLU	CD-OE1	5.46	1.31	1.25
3	J	185	GLY	N-CA	-5.46	1.37	1.46
1	a	100	ARG	CZ-NH1	5.46	1.40	1.33
3	I	140	TYR	CG-CD1	5.46	1.46	1.39
1	F	103	TYR	CD1-CE1	5.46	1.47	1.39
2	1	80	ARG	NE-CZ	5.45	1.40	1.33
3	H	397	PHE	CE1-CZ	5.45	1.47	1.37
1	C	232	TYR	CB-CG	-5.45	1.43	1.51
1	g	235	ARG	CZ-NH2	5.45	1.40	1.33
2	4	148	TYR	CZ-OH	5.45	1.47	1.37
2	h	173	TYR	CZ-OH	5.45	1.47	1.37
2	2	81	ARG	NE-CZ	5.45	1.40	1.33
3	K	129	GLY	N-CA	-5.44	1.37	1.46
1	F	185	PHE	CG-CD2	5.44	1.47	1.38
3	M	53	SER	CA-CB	5.44	1.61	1.52
2	m	203	GLU	CD-OE1	5.44	1.31	1.25
3	I	20	TYR	CZ-OH	5.44	1.47	1.37
3	L	66	GLY	CA-C	-5.44	1.43	1.51
1	F	238	GLU	CB-CG	5.44	1.62	1.52
3	K	187	GLY	CA-C	-5.44	1.43	1.51
2	j	152	GLU	CD-OE1	5.43	1.31	1.25
3	I	50	ARG	CZ-NH2	5.43	1.40	1.33
1	c	86	ARG	CD-NE	5.43	1.55	1.46
2	i	83	ARG	CZ-NH2	5.43	1.40	1.33
2	j	88	ARG	CD-NE	5.42	1.55	1.46
2	2	203	GLU	CD-OE1	5.42	1.31	1.25
3	I	224	ARG	CZ-NH2	5.42	1.40	1.33
1	b	180	ARG	CZ-NH1	5.41	1.40	1.33
2	1	154	ARG	NE-CZ	5.41	1.40	1.33
2	5	159	ILE	CA-C	-5.41	1.38	1.52
2	l	170	ARG	NE-CZ	5.41	1.40	1.33
1	B	28	ARG	CZ-NH1	5.40	1.40	1.33
2	m	174	SER	CA-CB	5.40	1.61	1.52
1	B	68	TYR	CZ-OH	5.40	1.47	1.37
1	f	93	ARG	CZ-NH2	5.40	1.40	1.33
1	d	93	ARG	NE-CZ	5.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	239	ARG	CZ-NH1	5.40	1.40	1.33
2	i	197	TYR	CB-CG	5.40	1.59	1.51
3	I	259	ARG	CZ-NH1	5.40	1.40	1.33
2	2	173	TYR	CE1-CZ	5.39	1.45	1.38
2	n	178	ARG	CD-NE	5.39	1.55	1.46
2	2	178	ARG	CD-NE	5.39	1.55	1.46
3	I	285	GLY	CA-C	-5.39	1.43	1.51
3	H	361	PHE	CG-CD1	5.39	1.46	1.38
3	K	181	TYR	CZ-OH	5.39	1.47	1.37
3	J	259	ARG	CZ-NH1	5.39	1.40	1.33
1	E	105	GLU	N-CA	-5.38	1.35	1.46
1	e	65	GLU	N-CA	-5.38	1.35	1.46
1	a	173	GLU	CD-OE1	5.38	1.31	1.25
2	3	118	GLU	CG-CD	5.38	1.60	1.51
2	l	213	LYS	CD-CE	5.38	1.64	1.51
3	L	59	ARG	CZ-NH1	5.38	1.40	1.33
1	A	28	ARG	NE-CZ	5.37	1.40	1.33
1	E	212	GLY	N-CA	-5.37	1.38	1.46
1	c	126	TYR	CG-CD1	5.37	1.46	1.39
3	I	259	ARG	CD-NE	5.37	1.55	1.46
3	K	224	ARG	CZ-NH2	5.37	1.40	1.33
2	1	172	ILE	N-CA	5.37	1.57	1.46
1	F	239	ARG	NE-CZ	5.37	1.40	1.33
2	1	68	ARG	CZ-NH1	5.37	1.40	1.33
2	j	50	ASP	C-N	5.37	1.46	1.34
2	1	170	ARG	CZ-NH1	5.36	1.40	1.33
1	A	239	ARG	CZ-NH1	5.36	1.40	1.33
3	J	308	GLU	CD-OE1	5.36	1.31	1.25
1	B	126	TYR	CE2-CZ	5.36	1.45	1.38
2	h	102	ARG	NE-CZ	5.36	1.40	1.33
3	I	154	ARG	CZ-NH1	5.36	1.40	1.33
3	H	27	TYR	CZ-OH	5.36	1.47	1.37
3	L	49	ARG	CD-NE	5.36	1.55	1.46
2	6	101	TYR	CB-CG	-5.35	1.43	1.51
3	M	207	VAL	CA-CB	-5.35	1.43	1.54
2	n	134	GLU	CD-OE2	5.35	1.31	1.25
3	J	305	ARG	CZ-NH1	5.35	1.40	1.33
1	e	228	GLU	CG-CD	5.35	1.59	1.51
1	c	96	ALA	CA-CB	5.35	1.63	1.52
3	I	203	PHE	CG-CD1	5.34	1.46	1.38
1	f	197	GLY	N-CA	-5.34	1.38	1.46
3	J	94	TYR	CE1-CZ	5.34	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	3	154	ARG	CZ-NH1	5.34	1.40	1.33
3	K	341	ARG	CZ-NH1	5.34	1.40	1.33
1	c	100	ARG	CZ-NH2	5.34	1.40	1.33
1	a	53	ARG	CZ-NH2	5.34	1.40	1.33
2	h	178	ARG	CZ-NH2	5.34	1.40	1.33
2	3	178	ARG	CD-NE	5.34	1.55	1.46
2	l	178	ARG	CZ-NH2	5.33	1.40	1.33
3	J	116	VAL	CB-CG1	5.33	1.64	1.52
1	C	158	GLU	CD-OE2	5.33	1.31	1.25
3	H	181	TYR	CD1-CE1	5.33	1.47	1.39
2	m	83	ARG	N-CA	-5.33	1.35	1.46
3	K	50	ARG	CZ-NH2	5.33	1.40	1.33
2	2	100	SER	CA-CB	5.32	1.60	1.52
3	J	336	PHE	CB-CG	-5.32	1.42	1.51
3	J	374	ASP	CB-CG	5.32	1.62	1.51
2	j	185	GLY	N-CA	-5.32	1.38	1.46
1	g	180	ARG	CZ-NH2	5.31	1.40	1.33
2	j	199	TYR	CG-CD2	-5.31	1.32	1.39
1	F	123	TYR	CD1-CE1	5.31	1.47	1.39
2	h	104	PHE	C-N	5.31	1.44	1.34
1	D	123	TYR	CG-CD1	5.31	1.46	1.39
1	G	22	PHE	CG-CD2	5.30	1.46	1.38
2	5	83	ARG	NE-CZ	5.30	1.40	1.33
1	b	180	ARG	N-CA	-5.30	1.35	1.46
2	i	101	TYR	CD1-CE1	5.30	1.47	1.39
2	4	197	TYR	CG-CD2	5.30	1.46	1.39
3	I	221	ARG	CZ-NH1	5.30	1.40	1.33
3	J	271	GLU	CG-CD	5.30	1.59	1.51
3	K	341	ARG	CZ-NH2	5.29	1.40	1.33
1	b	235	ARG	NE-CZ	5.29	1.40	1.33
1	C	60	GLU	CB-CG	5.28	1.62	1.52
1	d	132	PHE	CE2-CZ	5.28	1.47	1.37
1	f	219	ARG	CZ-NH2	5.28	1.40	1.33
2	5	154	ARG	NE-CZ	5.28	1.40	1.33
1	D	123	TYR	CZ-OH	5.28	1.46	1.37
3	J	367	ARG	CZ-NH2	5.28	1.40	1.33
3	M	377	LYS	CD-CE	5.27	1.64	1.51
2	l	141	GLY	N-CA	-5.27	1.38	1.46
3	K	50	ARG	CD-NE	5.27	1.55	1.46
1	b	45	GLY	CA-C	-5.27	1.43	1.51
1	a	158	GLU	CG-CD	5.26	1.59	1.51
3	I	317	ARG	CZ-NH1	5.26	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	241	ARG	CZ-NH1	5.26	1.39	1.33
1	D	221	PHE	CE2-CZ	5.26	1.47	1.37
1	F	144	VAL	CB-CG1	5.26	1.63	1.52
2	h	197	TYR	CG-CD2	5.26	1.46	1.39
2	k	121	SER	CA-CB	5.26	1.60	1.52
1	F	123	TYR	CG-CD2	5.25	1.46	1.39
1	F	44	GLU	C-N	5.25	1.42	1.33
1	D	20	ARG	CD-NE	5.25	1.55	1.46
2	2	51	ARG	CZ-NH1	5.25	1.39	1.33
3	L	250	ARG	CD-NE	5.24	1.55	1.46
2	2	101	TYR	CE1-CZ	5.24	1.45	1.38
1	b	79	SER	C-N	5.24	1.42	1.33
2	k	51	ARG	CZ-NH1	5.23	1.39	1.33
3	I	271	GLU	CD-OE2	5.23	1.31	1.25
3	M	249	ARG	CA-CB	5.23	1.65	1.53
3	M	305	ARG	CZ-NH2	5.23	1.39	1.33
1	b	213	TYR	CB-CG	5.23	1.59	1.51
3	H	364	ARG	CZ-NH2	5.23	1.39	1.33
1	A	185	PHE	CB-CG	-5.22	1.42	1.51
2	j	195	GLU	CD-OE1	5.22	1.31	1.25
1	c	93	ARG	CD-NE	5.22	1.55	1.46
1	D	232	TYR	CG-CD1	5.22	1.46	1.39
3	M	154	ARG	NE-CZ	5.22	1.39	1.33
3	M	173	GLU	CG-CD	5.22	1.59	1.51
1	a	180	ARG	CZ-NH2	5.22	1.39	1.33
1	a	203	GLU	CD-OE2	5.22	1.31	1.25
1	E	19	GLY	CA-C	-5.22	1.43	1.51
2	2	102	ARG	NE-CZ	5.22	1.39	1.33
2	7	154	ARG	CZ-NH1	5.22	1.39	1.33
3	I	341	ARG	NE-CZ	5.21	1.39	1.33
2	m	180	SER	CB-OG	-5.20	1.35	1.42
3	K	45	GLU	CD-OE1	5.20	1.31	1.25
1	a	53	ARG	CZ-NH1	5.20	1.39	1.33
1	C	246	LYS	CA-CB	5.20	1.65	1.53
2	j	195	GLU	CG-CD	5.20	1.59	1.51
2	4	178	ARG	NE-CZ	5.20	1.39	1.33
3	J	215	TYR	CZ-OH	5.20	1.46	1.37
1	a	225	SER	CA-CB	5.20	1.60	1.52
1	d	235	ARG	CZ-NH1	5.20	1.39	1.33
3	M	249	ARG	CZ-NH1	5.20	1.39	1.33
2	1	102	ARG	CZ-NH1	5.19	1.39	1.33
2	6	178	ARG	CZ-NH1	5.19	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	D	72	GLU	CD-OE2	-5.19	1.20	1.25
3	H	49	ARG	CD-NE	5.19	1.55	1.46
3	I	105	ARG	CZ-NH1	5.19	1.39	1.33
2	h	131	ALA	CA-CB	5.18	1.63	1.52
3	L	17	GLU	CD-OE1	5.18	1.31	1.25
3	L	152	GLU	CA-CB	5.18	1.65	1.53
2	k	117	SER	CA-CB	5.18	1.60	1.52
2	h	101	TYR	CG-CD2	5.17	1.45	1.39
2	3	68	ARG	CD-NE	5.17	1.55	1.46
2	h	196	PHE	CB-CG	-5.17	1.42	1.51
1	b	219	ARG	CZ-NH2	5.17	1.39	1.33
2	5	30	ARG	CZ-NH2	5.17	1.39	1.33
2	4	51	ARG	CZ-NH1	5.17	1.39	1.33
1	B	103	TYR	CG-CD1	5.17	1.45	1.39
2	6	95	SER	CA-CB	5.17	1.60	1.52
1	F	140	GLY	CA-C	-5.17	1.43	1.51
3	H	164	PRO	N-CA	-5.16	1.38	1.47
2	k	81	ARG	CZ-NH1	5.16	1.39	1.33
1	e	53	ARG	CA-CB	5.16	1.65	1.53
1	F	8	TYR	CE1-CZ	5.16	1.45	1.38
2	3	212	ARG	CD-NE	5.16	1.55	1.46
2	7	81	ARG	NE-CZ	5.16	1.39	1.33
1	C	93	ARG	CD-NE	5.15	1.55	1.46
1	f	219	ARG	NE-CZ	5.15	1.39	1.33
3	K	310	PRO	N-CA	-5.15	1.38	1.47
1	e	33	ARG	CZ-NH2	5.15	1.39	1.33
1	b	53	ARG	NE-CZ	5.15	1.39	1.33
1	F	130	ARG	CZ-NH2	5.14	1.39	1.33
1	C	93	ARG	CZ-NH2	5.14	1.39	1.33
1	F	33	ARG	CZ-NH1	5.13	1.39	1.33
2	7	197	TYR	CE1-CZ	5.13	1.45	1.38
1	e	152	PRO	N-CD	-5.13	1.40	1.47
3	K	56	GLU	CD-OE1	5.13	1.31	1.25
2	h	195	GLU	CG-CD	5.13	1.59	1.51
1	f	17	PRO	CA-CB	5.12	1.63	1.53
2	3	83	ARG	CZ-NH2	5.12	1.39	1.33
3	I	20	TYR	CG-CD2	5.12	1.45	1.39
3	K	177	GLY	CA-C	-5.12	1.43	1.51
2	7	81	ARG	CD-NE	5.12	1.55	1.46
3	K	29	ARG	CZ-NH1	5.12	1.39	1.33
1	g	53	ARG	CZ-NH2	5.12	1.39	1.33
2	5	100	SER	CA-C	-5.12	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	H	141	GLU	CD-OE2	5.12	1.31	1.25
3	I	341	ARG	CD-NE	5.12	1.55	1.46
3	I	50	ARG	CD-NE	5.12	1.55	1.46
3	K	48	VAL	CB-CG2	5.11	1.63	1.52
2	4	68	ARG	NE-CZ	5.11	1.39	1.33
3	I	11	GLU	CD-OE1	5.11	1.31	1.25
3	K	224	ARG	CD-NE	5.11	1.55	1.46
2	j	154	ARG	CZ-NH1	5.11	1.39	1.33
1	C	133	GLY	CA-C	5.11	1.60	1.51
2	l	123	TYR	CB-CG	5.11	1.59	1.51
3	K	112	THR	N-CA	-5.10	1.36	1.46
1	C	28	ARG	CZ-NH2	5.10	1.39	1.33
2	3	46	TYR	CD1-CE1	5.10	1.47	1.39
2	m	101	TYR	CE2-CZ	5.10	1.45	1.38
3	J	250	ARG	CD-NE	5.10	1.55	1.46
2	6	106	TYR	CZ-OH	5.10	1.46	1.37
1	A	130	ARG	CZ-NH1	5.09	1.39	1.33
1	g	28	ARG	NE-CZ	5.09	1.39	1.33
1	B	26	TYR	CG-CD2	5.09	1.45	1.39
2	6	117	SER	CA-CB	5.08	1.60	1.52
1	B	166	MET	C-N	5.08	1.42	1.33
1	b	130	ARG	NE-CZ	5.08	1.39	1.33
1	e	86	ARG	NE-CZ	5.08	1.39	1.33
1	c	180	ARG	CD-NE	5.08	1.55	1.46
2	m	30	ARG	CZ-NH2	5.08	1.39	1.33
3	H	44	TYR	CE1-CZ	5.08	1.45	1.38
3	L	259	ARG	NE-CZ	5.07	1.39	1.33
2	l	77	TYR	CD2-CE2	5.07	1.47	1.39
3	M	364	ARG	NE-CZ	5.07	1.39	1.33
3	K	171	GLY	CA-C	-5.06	1.43	1.51
1	B	221	PHE	CG-CD1	5.06	1.46	1.38
1	C	168	ARG	CD-NE	5.06	1.55	1.46
1	g	232	TYR	CE2-CZ	5.06	1.45	1.38
2	h	51	ARG	CD-NE	5.06	1.55	1.46
3	L	289	ARG	NE-CZ	5.06	1.39	1.33
1	c	35	ALA	CA-CB	5.06	1.63	1.52
1	d	80	GLY	N-CA	5.06	1.53	1.46
3	L	289	ARG	CZ-NH2	5.05	1.39	1.33
3	M	215	TYR	CD1-CE1	5.05	1.47	1.39
3	L	165	GLU	CB-CG	5.05	1.61	1.52
1	F	170	ALA	CA-CB	5.05	1.63	1.52
2	2	148	TYR	CZ-OH	5.05	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	5	205	GLU	CB-CG	5.05	1.61	1.52
1	b	180	ARG	NE-CZ	5.05	1.39	1.33
3	I	21	TYR	CG-CD2	5.05	1.45	1.39
3	I	76	ARG	NE-CZ	5.05	1.39	1.33
1	D	75	CYS	CB-SG	5.04	1.90	1.82
2	h	33	MET	C-N	5.04	1.42	1.33
1	c	79	SER	CB-OG	5.04	1.48	1.42
1	G	139	ALA	CA-CB	5.04	1.63	1.52
2	2	30	ARG	CZ-NH1	5.04	1.39	1.33
2	7	44	LYS	N-CA	-5.04	1.36	1.46
3	H	236	SER	CA-CB	5.04	1.60	1.52
3	J	181	TYR	C-N	5.04	1.42	1.33
2	4	136	ASP	CB-CG	5.04	1.62	1.51
1	G	16	SER	CA-CB	5.03	1.60	1.52
2	i	51	ARG	CZ-NH2	5.03	1.39	1.33
3	K	333	ASP	CB-CG	5.03	1.62	1.51
3	I	295	PRO	N-CD	-5.03	1.40	1.47
1	C	180	ARG	CZ-NH1	5.03	1.39	1.33
3	L	94	TYR	CE1-CZ	5.03	1.45	1.38
1	C	103	TYR	CG-CD1	5.03	1.45	1.39
2	h	211	PHE	CD2-CE2	5.03	1.49	1.39
2	k	102	ARG	CZ-NH2	5.02	1.39	1.33
1	g	85	ALA	CA-CB	5.02	1.62	1.52
3	K	249	ARG	NE-CZ	5.02	1.39	1.33
2	5	201	PRO	N-CD	-5.02	1.40	1.47
3	M	76	ARG	CZ-NH2	5.02	1.39	1.33
2	h	121	SER	CA-CB	5.01	1.60	1.52
1	c	78	THR	CA-C	-5.01	1.40	1.52
3	K	259	ARG	CZ-NH2	5.01	1.39	1.33
2	6	82	GLU	CG-CD	5.00	1.59	1.51
2	i	78	GLU	CD-OE2	5.00	1.31	1.25
2	n	144	SER	CB-OG	5.00	1.48	1.42

All (1787) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	170	ARG	NE-CZ-NH2	-46.06	97.27	120.30
2	5	170	ARG	NE-CZ-NH2	-36.96	101.82	120.30
2	l	170	ARG	NE-CZ-NH1	22.30	131.45	120.30
3	H	20	TYR	CB-CG-CD2	-22.19	107.68	121.00
1	e	26	TYR	CB-CG-CD1	20.64	133.38	121.00
3	H	20	TYR	CB-CG-CD1	19.51	132.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	20	ARG	NE-CZ-NH1	18.30	129.45	120.30
2	6	88	ARG	NE-CZ-NH2	17.90	129.25	120.30
2	m	102	ARG	NE-CZ-NH1	-17.75	111.43	120.30
1	e	26	TYR	CB-CG-CD2	-17.00	110.80	121.00
2	5	101	TYR	CB-CG-CD2	16.82	131.09	121.00
2	5	170	ARG	NE-CZ-NH1	16.78	128.69	120.30
1	D	33	ARG	NE-CZ-NH2	-16.67	111.97	120.30
3	K	41	ARG	NE-CZ-NH1	16.55	128.58	120.30
3	M	27	TYR	CB-CG-CD1	-16.28	111.23	121.00
3	M	27	TYR	CB-CG-CD2	15.81	130.49	121.00
2	4	68	ARG	NE-CZ-NH2	-15.78	112.41	120.30
1	B	100	ARG	NE-CZ-NH2	15.15	127.88	120.30
1	B	168	ARG	NE-CZ-NH1	14.42	127.51	120.30
1	E	10	ARG	NE-CZ-NH2	-14.37	113.11	120.30
3	K	263	ARG	NE-CZ-NH2	-14.37	113.11	120.30
1	f	20	ARG	NE-CZ-NH2	-14.33	113.13	120.30
1	F	213	TYR	CB-CG-CD1	-14.09	112.55	121.00
3	I	27	TYR	CB-CG-CD2	14.03	129.42	121.00
3	I	27	TYR	CB-CG-CD1	-13.89	112.67	121.00
3	J	275	PHE	CB-CG-CD2	13.76	130.43	120.80
1	B	179	TYR	CB-CG-CD1	-13.63	112.82	121.00
1	E	132	PHE	CB-CG-CD2	-13.61	111.28	120.80
3	I	140	TYR	CB-CG-CD2	13.58	129.15	121.00
1	D	86	ARG	NE-CZ-NH1	13.55	127.08	120.30
1	b	239	ARG	NE-CZ-NH2	13.45	127.03	120.30
1	g	168	ARG	NE-CZ-NH2	-13.37	113.62	120.30
3	K	29	ARG	NE-CZ-NH2	-13.34	113.63	120.30
3	K	215	TYR	CB-CG-CD2	-13.27	113.04	121.00
1	b	239	ARG	NE-CZ-NH1	-13.26	113.67	120.30
1	E	241	ARG	NE-CZ-NH2	13.24	126.92	120.30
2	i	106	TYR	CB-CG-CD2	-13.19	113.08	121.00
3	H	28	ARG	NE-CZ-NH2	-13.13	113.74	120.30
2	1	211	PHE	CB-CG-CD2	13.12	129.99	120.80
3	J	361	PHE	CB-CG-CD1	13.12	129.99	120.80
2	5	101	TYR	CB-CG-CD1	-13.07	113.16	121.00
3	K	41	ARG	NE-CZ-NH2	-13.07	113.76	120.30
1	G	159	TYR	CB-CG-CD1	-13.06	113.17	121.00
3	K	154	ARG	NE-CZ-NH2	-12.95	113.83	120.30
3	M	181	TYR	CB-CG-CD2	-12.85	113.29	121.00
3	I	317	ARG	NE-CZ-NH2	12.82	126.71	120.30
3	M	128	TYR	CB-CG-CD1	12.81	128.69	121.00
2	3	154	ARG	NE-CZ-NH2	12.80	126.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	L	263	ARG	NE-CZ-NH1	12.76	126.68	120.30
3	M	29	ARG	NE-CZ-NH2	-12.75	113.92	120.30
2	5	212	ARG	NE-CZ-NH1	12.65	126.63	120.30
1	d	180	ARG	NE-CZ-NH1	-12.63	113.98	120.30
3	M	317	ARG	NE-CZ-NH2	-12.61	114.00	120.30
3	J	215	TYR	CB-CG-CD1	-12.56	113.46	121.00
3	L	259	ARG	NE-CZ-NH2	12.56	126.58	120.30
2	4	148	TYR	CB-CG-CD2	-12.56	113.47	121.00
3	K	305	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	A	126	TYR	CB-CG-CD2	12.53	128.52	121.00
3	M	367	ARG	NE-CZ-NH2	-12.52	114.04	120.30
2	n	199	TYR	CB-CG-CD1	12.35	128.41	121.00
3	I	215	TYR	CB-CG-CD2	-12.33	113.60	121.00
3	K	130	PHE	CB-CG-CD2	-12.29	112.20	120.80
1	A	104	ASP	CB-CG-OD1	12.22	129.30	118.30
1	D	221	PHE	CB-CG-CD1	12.21	129.35	120.80
1	f	126	TYR	CB-CG-CD1	12.20	128.32	121.00
3	L	211	PHE	CB-CG-CD2	12.17	129.32	120.80
3	I	215	TYR	CB-CG-CD1	12.10	128.26	121.00
1	D	241	ARG	NE-CZ-NH2	12.09	126.34	120.30
2	4	102	ARG	NE-CZ-NH2	12.09	126.34	120.30
3	J	227	PHE	CB-CG-CD1	12.06	129.24	120.80
2	5	77	TYR	CB-CG-CD1	-12.06	113.77	121.00
2	n	103	TYR	CB-CG-CD2	-11.99	113.80	121.00
2	6	88	ARG	NE-CZ-NH1	-11.98	114.31	120.30
1	E	174	PHE	CB-CG-CD1	11.96	129.17	120.80
2	l	68	ARG	NE-CZ-NH2	-11.90	114.35	120.30
3	I	263	ARG	NE-CZ-NH2	-11.89	114.36	120.30
3	I	20	TYR	CB-CG-CD1	11.87	128.12	121.00
2	1	178	ARG	NE-CZ-NH2	-11.82	114.39	120.30
2	7	123	TYR	CB-CG-CD2	-11.82	113.91	121.00
1	D	182	ASP	CB-CG-OD1	-11.75	107.73	118.30
2	7	197	TYR	CB-CG-CD1	-11.74	113.95	121.00
1	d	20	ARG	NE-CZ-NH2	-11.74	114.43	120.30
2	m	83	ARG	NE-CZ-NH2	11.68	126.14	120.30
3	M	289	ARG	NE-CZ-NH1	11.65	126.13	120.30
3	H	59	ARG	NE-CZ-NH1	11.64	126.12	120.30
2	3	81	ARG	NE-CZ-NH2	11.64	126.12	120.30
2	m	81	ARG	NE-CZ-NH2	-11.63	114.48	120.30
1	D	221	PHE	CB-CG-CD2	-11.62	112.67	120.80
1	c	22	PHE	CB-CG-CD1	11.61	128.93	120.80
3	M	278	ARG	NE-CZ-NH1	11.51	126.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	168	ARG	NE-CZ-NH2	-11.51	114.55	120.30
1	B	100	ARG	NE-CZ-NH1	-11.50	114.55	120.30
2	5	77	TYR	CB-CG-CD2	11.49	127.89	121.00
1	F	28	ARG	NE-CZ-NH2	-11.49	114.56	120.30
2	6	211	PHE	CB-CG-CD2	11.45	128.81	120.80
2	l	83	ARG	NE-CZ-NH1	-11.39	114.60	120.30
3	L	211	PHE	CB-CG-CD1	-11.30	112.89	120.80
1	E	241	ARG	NE-CZ-NH1	-11.29	114.66	120.30
1	B	148	TYR	CB-CG-CD2	11.27	127.76	121.00
1	E	180	ARG	NE-CZ-NH2	11.27	125.93	120.30
3	I	76	ARG	NE-CZ-NH1	11.22	125.91	120.30
2	k	102	ARG	NE-CZ-NH2	11.19	125.89	120.30
1	a	68	TYR	CB-CG-CD2	-11.18	114.30	121.00
1	e	33	ARG	NE-CZ-NH2	11.14	125.87	120.30
1	f	126	TYR	CB-CG-CD2	-11.11	114.33	121.00
1	f	20	ARG	NE-CZ-NH1	11.09	125.84	120.30
3	L	249	ARG	NE-CZ-NH1	11.09	125.84	120.30
1	A	126	TYR	CB-CG-CD1	-10.99	114.40	121.00
2	6	197	TYR	CB-CG-CD1	-10.99	114.40	121.00
3	J	52	ARG	NE-CZ-NH2	-10.96	114.82	120.30
3	M	203	PHE	CB-CG-CD1	10.91	128.44	120.80
2	7	81	ARG	NE-CZ-NH2	-10.90	114.85	120.30
3	J	227	PHE	CB-CG-CD2	-10.88	113.18	120.80
2	4	80	ARG	NE-CZ-NH2	10.88	125.74	120.30
3	M	94	TYR	CB-CG-CD2	-10.88	114.47	121.00
1	E	91	ARG	NE-CZ-NH2	10.83	125.71	120.30
2	l	80	ARG	NE-CZ-NH1	-10.83	114.89	120.30
2	l	170	ARG	NH1-CZ-NH2	10.78	131.26	119.40
3	K	29	ARG	NE-CZ-NH1	10.78	125.69	120.30
3	M	367	ARG	NE-CZ-NH1	10.79	125.69	120.30
1	d	174	PHE	CB-CG-CD2	-10.78	113.25	120.80
2	2	103	TYR	CB-CG-CD1	-10.77	114.54	121.00
1	f	241	ARG	NE-CZ-NH1	-10.73	114.94	120.30
3	K	27	TYR	CB-CG-CD1	-10.69	114.58	121.00
3	M	326	ARG	NE-CZ-NH1	10.68	125.64	120.30
2	6	212	ARG	NE-CZ-NH1	10.68	125.64	120.30
1	d	123	TYR	CB-CG-CD2	10.62	127.37	121.00
3	I	142	ASP	CB-CG-OD2	-10.61	108.75	118.30
1	f	123	TYR	CB-CG-CD1	-10.57	114.66	121.00
2	k	81	ARG	NE-CZ-NH2	-10.56	115.02	120.30
2	2	103	TYR	CB-CG-CD2	10.55	127.33	121.00
1	F	235	ARG	NE-CZ-NH2	10.53	125.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	314	PHE	CB-CG-CD2	-10.48	113.46	120.80
2	m	46	TYR	CG-CD1-CE1	-10.44	112.94	121.30
1	B	33	ARG	NE-CZ-NH1	10.44	125.52	120.30
1	B	68	TYR	CB-CG-CD2	10.43	127.26	121.00
2	l	123	TYR	CB-CG-CD2	-10.42	114.75	121.00
3	J	76	ARG	NE-CZ-NH2	-10.42	115.09	120.30
2	h	30	ARG	NE-CZ-NH2	10.41	125.50	120.30
1	e	126	TYR	CB-CG-CD1	-10.40	114.76	121.00
2	3	30	ARG	NE-CZ-NH2	10.40	125.50	120.30
3	J	27	TYR	CB-CG-CD1	-10.38	114.77	121.00
3	I	249	ARG	NE-CZ-NH2	-10.33	115.13	120.30
1	E	174	PHE	CB-CG-CD2	-10.32	113.57	120.80
2	7	80	ARG	NE-CZ-NH1	-10.29	115.16	120.30
1	g	168	ARG	NE-CZ-NH1	10.27	125.44	120.30
2	j	123	TYR	CB-CG-CD1	-10.24	114.86	121.00
1	B	53	ARG	NE-CZ-NH1	10.21	125.41	120.30
1	f	28	ARG	NE-CZ-NH1	-10.20	115.20	120.30
3	I	302	ARG	NE-CZ-NH1	10.21	125.40	120.30
3	H	278	ARG	NE-CZ-NH2	-10.19	115.21	120.30
2	l	101	TYR	CB-CG-CD2	-10.18	114.89	121.00
1	e	10	ARG	NE-CZ-NH1	-10.16	115.22	120.30
1	b	91	ARG	NE-CZ-NH2	-10.13	115.23	120.30
1	a	100	ARG	NE-CZ-NH1	-10.13	115.23	120.30
3	L	46	ARG	NE-CZ-NH2	-10.11	115.24	120.30
1	e	62	ASP	CB-CG-OD2	10.07	127.37	118.30
3	H	50	ARG	NE-CZ-NH2	-10.07	115.27	120.30
1	b	126	TYR	CB-CG-CD2	10.06	127.03	121.00
1	G	213	TYR	CB-CG-CD1	10.04	127.02	121.00
1	G	119	PHE	CB-CG-CD2	10.03	127.82	120.80
1	g	232	TYR	CB-CG-CD1	10.01	127.01	121.00
1	c	132	PHE	CB-CG-CD1	10.01	127.81	120.80
1	d	239	ARG	NE-CZ-NH2	10.01	125.30	120.30
2	6	106	TYR	CB-CG-CD2	10.00	127.00	121.00
1	e	62	ASP	CB-CG-OD1	-9.97	109.32	118.30
3	K	20	TYR	CB-CG-CD2	-9.96	115.02	121.00
1	d	123	TYR	CB-CG-CD1	-9.96	115.02	121.00
1	d	22	PHE	CB-CG-CD1	-9.94	113.84	120.80
1	a	22	PHE	CB-CG-CD2	-9.92	113.86	120.80
3	L	224	ARG	NE-CZ-NH1	9.89	125.24	120.30
2	j	173	TYR	CB-CG-CD2	-9.84	115.10	121.00
1	C	218	ASP	CB-CG-OD2	-9.81	109.47	118.30
2	5	80	ARG	NE-CZ-NH1	-9.80	115.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	M	41	ARG	NE-CZ-NH2	-9.77	115.41	120.30
1	d	33	ARG	NE-CZ-NH1	9.76	125.18	120.30
2	4	30	ARG	NE-CZ-NH2	-9.76	115.42	120.30
3	I	20	TYR	CB-CG-CD2	-9.74	115.15	121.00
2	2	83	ARG	NE-CZ-NH1	-9.70	115.45	120.30
1	D	51	ASP	CB-CG-OD2	-9.68	109.59	118.30
1	C	180	ARG	NE-CZ-NH2	9.66	125.13	120.30
1	a	28	ARG	NE-CZ-NH2	-9.65	115.48	120.30
1	D	168	ARG	NE-CZ-NH1	9.64	125.12	120.30
3	K	239	PHE	CB-CG-CD2	-9.64	114.05	120.80
1	c	123	TYR	CB-CG-CD1	9.64	126.78	121.00
3	K	341	ARG	NE-CZ-NH1	9.64	125.12	120.30
3	I	43	ARG	NE-CZ-NH2	-9.62	115.49	120.30
2	5	126	ASP	CB-CG-OD2	-9.62	109.65	118.30
1	e	187	ASP	CB-CG-OD2	-9.59	109.67	118.30
2	1	211	PHE	CB-CG-CD1	-9.59	114.08	120.80
1	c	132	PHE	CB-CG-CD2	-9.59	114.09	120.80
1	B	235	ARG	NE-CZ-NH1	9.57	125.09	120.30
3	H	275	PHE	CB-CG-CD1	9.57	127.50	120.80
3	H	167	PHE	CB-CG-CD1	9.57	127.50	120.80
1	B	20	ARG	NE-CZ-NH1	-9.56	115.52	120.30
2	h	77	TYR	CB-CG-CD1	9.56	126.74	121.00
1	F	93	ARG	NE-CZ-NH2	-9.54	115.53	120.30
3	I	130	PHE	CB-CG-CD1	-9.53	114.13	120.80
2	k	140	THR	N-CA-CB	9.52	128.39	110.30
3	K	57	ARG	NE-CZ-NH2	-9.51	115.55	120.30
3	L	263	ARG	NE-CZ-NH2	-9.49	115.56	120.30
2	m	81	ARG	NE-CZ-NH1	9.45	125.03	120.30
1	D	26	TYR	CB-CG-CD2	9.44	126.66	121.00
1	A	26	TYR	CB-CG-CD2	9.43	126.66	121.00
1	c	53	ARG	NE-CZ-NH2	9.42	125.01	120.30
1	F	86	ARG	NE-CZ-NH2	-9.42	115.59	120.30
3	I	397	PHE	CB-CG-CD1	9.42	127.39	120.80
1	D	20	ARG	NE-CZ-NH2	-9.41	115.59	120.30
3	K	221	ARG	NE-CZ-NH1	9.39	124.99	120.30
1	a	179	TYR	CB-CG-CD1	-9.38	115.37	121.00
1	c	10	ARG	NE-CZ-NH1	-9.38	115.61	120.30
1	D	130	ARG	NE-CZ-NH2	-9.37	115.62	120.30
1	E	8	TYR	CG-CD1-CE1	-9.35	113.82	121.30
2	m	170	ARG	NE-CZ-NH1	-9.35	115.63	120.30
3	J	289	ARG	NE-CZ-NH1	9.34	124.97	120.30
2	1	83	ARG	NE-CZ-NH1	9.32	124.96	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	80	ARG	NE-CZ-NH2	9.30	124.95	120.30
1	a	168	ARG	NE-CZ-NH2	-9.27	115.67	120.30
3	K	259	ARG	NE-CZ-NH2	-9.26	115.67	120.30
1	F	100	ARG	NE-CZ-NH2	9.26	124.93	120.30
1	C	68	TYR	CB-CG-CD2	-9.22	115.47	121.00
2	4	212	ARG	NE-CZ-NH1	9.22	124.91	120.30
2	i	173	TYR	CB-CG-CD2	-9.22	115.47	121.00
3	M	302	ARG	NE-CZ-NH1	9.22	124.91	120.30
2	i	106	TYR	CB-CG-CD1	9.20	126.52	121.00
3	H	41	ARG	NE-CZ-NH2	9.19	124.89	120.30
1	E	26	TYR	CB-CG-CD1	-9.16	115.50	121.00
2	3	65	PHE	CB-CG-CD1	9.16	127.21	120.80
1	B	241	ARG	NE-CZ-NH2	9.15	124.87	120.30
3	H	50	ARG	NE-CZ-NH1	9.14	124.87	120.30
1	d	175	PHE	CB-CG-CD1	9.13	127.19	120.80
1	g	241	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	g	241	ARG	NE-CZ-NH2	9.09	124.85	120.30
2	h	68	ARG	NE-CZ-NH2	9.08	124.84	120.30
1	d	180	ARG	NE-CZ-NH2	9.07	124.84	120.30
3	I	221	ARG	NE-CZ-NH2	9.07	124.83	120.30
3	K	215	TYR	CB-CG-CD1	9.07	126.44	121.00
2	5	170	ARG	NH1-CZ-NH2	9.04	129.34	119.40
2	j	106	TYR	CB-CG-CD2	-9.02	115.59	121.00
1	c	179	TYR	CB-CG-CD1	9.02	126.41	121.00
1	G	26	TYR	CZ-CE2-CD2	9.01	127.91	119.80
2	3	187	ASP	CB-CG-OD1	-9.01	110.19	118.30
3	M	154	ARG	NE-CZ-NH1	-9.01	115.80	120.30
1	a	90	ASP	CB-CG-OD1	-9.01	110.19	118.30
1	F	103	TYR	CB-CG-CD2	-8.99	115.61	121.00
1	A	185	PHE	CB-CG-CD1	8.97	127.08	120.80
3	I	21	TYR	CB-CG-CD1	8.97	126.38	121.00
3	M	126	MET	CG-SD-CE	-8.97	85.85	100.20
1	E	53	ARG	NE-CZ-NH2	8.96	124.78	120.30
1	f	18	ASP	CB-CG-OD1	8.95	126.36	118.30
3	M	278	ARG	NE-CZ-NH2	-8.95	115.83	120.30
1	e	148	TYR	CB-CG-CD2	-8.95	115.63	121.00
3	K	181	TYR	CB-CG-CD1	-8.94	115.64	121.00
2	1	88	ARG	NE-CZ-NH1	8.93	124.76	120.30
3	L	224	ARG	NE-CZ-NH2	-8.93	115.84	120.30
3	H	221	ARG	NE-CZ-NH2	-8.92	115.84	120.30
3	I	21	TYR	CB-CG-CD2	-8.90	115.66	121.00
3	I	273	ASP	CB-CG-OD1	8.90	126.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	391	ASP	CB-CG-OD1	-8.89	110.30	118.30
1	D	119	PHE	CB-CG-CD1	-8.89	114.58	120.80
3	H	167	PHE	CB-CG-CD2	-8.88	114.58	120.80
1	d	93	ARG	NE-CZ-NH2	-8.88	115.86	120.30
3	M	305	ARG	NE-CZ-NH1	8.88	124.74	120.30
2	2	199	TYR	CB-CG-CD1	-8.87	115.68	121.00
1	c	33	ARG	NE-CZ-NH1	-8.84	115.88	120.30
2	j	154	ARG	NE-CZ-NH2	8.84	124.72	120.30
1	d	126	TYR	CB-CG-CD2	-8.84	115.70	121.00
3	J	361	PHE	CB-CG-CD2	-8.83	114.62	120.80
3	K	130	PHE	CB-CG-CD1	8.83	126.98	120.80
1	b	159	TYR	CB-CG-CD2	-8.82	115.70	121.00
1	C	26	TYR	CB-CG-CD1	-8.82	115.71	121.00
2	7	123	TYR	CB-CG-CD1	8.82	126.29	121.00
2	k	51	ARG	NE-CZ-NH1	-8.80	115.90	120.30
1	f	103	TYR	CB-CG-CD1	-8.79	115.72	121.00
3	H	181	TYR	CB-CG-CD1	-8.79	115.73	121.00
1	A	218	ASP	CB-CG-OD2	8.78	126.21	118.30
2	j	173	TYR	CB-CG-CD1	8.78	126.27	121.00
2	3	51	ARG	NE-CZ-NH1	-8.77	115.92	120.30
1	c	53	ARG	NE-CZ-NH1	-8.75	115.93	120.30
3	K	249	ARG	NE-CZ-NH2	-8.74	115.93	120.30
1	D	33	ARG	NE-CZ-NH1	8.71	124.66	120.30
1	d	174	PHE	CB-CG-CD1	8.70	126.89	120.80
1	e	28	ARG	NE-CZ-NH1	-8.70	115.95	120.30
2	i	211	PHE	CB-CG-CD1	8.70	126.89	120.80
3	M	304	ASP	CB-CG-OD2	8.69	126.12	118.30
1	c	148	TYR	CB-CG-CD1	-8.69	115.79	121.00
1	G	159	TYR	CB-CG-CD2	8.67	126.20	121.00
3	H	239	PHE	CB-CG-CD1	-8.67	114.73	120.80
1	E	93	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	g	10	ARG	NE-CZ-NH1	8.65	124.63	120.30
1	G	168	ARG	NE-CZ-NH1	-8.65	115.97	120.30
3	I	140	TYR	CB-CG-CD1	-8.65	115.81	121.00
3	I	205	ARG	NE-CZ-NH1	8.64	124.62	120.30
3	I	128	TYR	CG-CD2-CE2	-8.64	114.39	121.30
2	n	200	SER	N-CA-CB	8.63	123.44	110.50
1	F	159	TYR	CB-CG-CD1	-8.62	115.83	121.00
2	m	196	PHE	CB-CG-CD2	8.61	126.83	120.80
1	a	104	ASP	CB-CG-OD2	8.61	126.05	118.30
3	J	49	ARG	NE-CZ-NH1	8.61	124.60	120.30
1	D	100	ARG	NE-CZ-NH1	8.60	124.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	165	VAL	CA-CB-CG1	-8.60	98.01	110.90
1	c	103	TYR	CB-CG-CD1	8.59	126.16	121.00
1	a	26	TYR	CB-CG-CD2	-8.58	115.85	121.00
2	7	33	MET	CG-SD-CE	-8.58	86.47	100.20
2	5	178	ARG	NE-CZ-NH2	-8.57	116.02	120.30
2	3	53	ALA	N-CA-CB	8.56	122.08	110.10
1	f	217	ASP	CB-CG-OD1	-8.55	110.60	118.30
2	h	197	TYR	CB-CG-CD2	8.55	126.13	121.00
2	2	46	TYR	CB-CG-CD2	-8.55	115.87	121.00
2	n	46	TYR	CB-CG-CD1	-8.55	115.87	121.00
3	J	215	TYR	CB-CG-CD2	8.55	126.13	121.00
1	E	8	TYR	CD1-CE1-CZ	8.54	127.49	119.80
1	f	68	TYR	CB-CG-CD1	-8.53	115.88	121.00
2	h	123	TYR	CB-CG-CD2	-8.52	115.89	121.00
1	G	20	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	f	103	TYR	CB-CG-CD2	8.51	126.10	121.00
1	E	239	ARG	NE-CZ-NH1	8.50	124.55	120.30
2	n	178	ARG	NE-CZ-NH2	-8.50	116.05	120.30
3	H	341	ARG	NE-CZ-NH2	-8.50	116.05	120.30
2	2	80	ARG	NE-CZ-NH2	8.49	124.55	120.30
2	h	155	PHE	CB-CG-CD2	-8.49	114.86	120.80
2	6	154	ARG	NE-CZ-NH1	-8.48	116.06	120.30
3	J	275	PHE	CB-CG-CD1	-8.48	114.86	120.80
2	k	173	TYR	CB-CG-CD2	-8.47	115.92	121.00
2	i	155	PHE	CB-CG-CD2	-8.47	114.87	120.80
2	2	123	TYR	CG-CD2-CE2	8.47	128.07	121.30
2	i	155	PHE	CB-CG-CD1	8.46	126.72	120.80
1	b	93	ARG	NE-CZ-NH1	8.44	124.52	120.30
2	2	104	PHE	CG-CD2-CE2	8.44	130.08	120.80
1	E	100	ARG	NE-CZ-NH1	-8.43	116.08	120.30
3	L	305	ARG	NE-CZ-NH2	8.43	124.51	120.30
3	H	367	ARG	NE-CZ-NH2	8.42	124.51	120.30
2	6	178	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	C	26	TYR	CB-CG-CD2	8.39	126.03	121.00
3	I	87	PHE	CB-CG-CD2	-8.39	114.93	120.80
2	5	36	PHE	CB-CG-CD2	-8.38	114.93	120.80
1	b	10	ARG	NE-CZ-NH1	-8.36	116.12	120.30
2	6	106	TYR	CB-CG-CD1	-8.36	115.98	121.00
3	H	275	PHE	CB-CG-CD2	-8.35	114.96	120.80
1	G	241	ARG	NE-CZ-NH2	8.35	124.47	120.30
2	1	30	ARG	NE-CZ-NH1	-8.32	116.14	120.30
3	L	49	ARG	NE-CZ-NH1	8.32	124.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	221	PHE	CB-CG-CD1	-8.28	115.00	120.80
2	l	103	TYR	CB-CG-CD2	-8.28	116.03	121.00
1	d	185	PHE	CB-CG-CD2	8.28	126.59	120.80
1	G	119	PHE	CB-CG-CD1	-8.28	115.00	120.80
3	K	49	ARG	NE-CZ-NH1	-8.27	116.17	120.30
2	l	103	TYR	CB-CG-CD1	8.25	125.95	121.00
2	7	212	ARG	NE-CZ-NH2	-8.25	116.17	120.30
2	7	81	ARG	NH1-CZ-NH2	8.25	128.47	119.40
2	j	65	PHE	CB-CG-CD1	8.24	126.57	120.80
3	J	259	ARG	NE-CZ-NH2	-8.22	116.19	120.30
3	K	273	ASP	CB-CG-OD1	-8.22	110.90	118.30
2	i	211	PHE	CB-CG-CD2	-8.21	115.05	120.80
3	L	43	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	b	100	ARG	NE-CZ-NH1	-8.21	116.19	120.30
1	e	221	PHE	CB-CG-CD2	8.21	126.54	120.80
2	m	212	ARG	NE-CZ-NH2	-8.20	116.20	120.30
1	F	93	ARG	NE-CZ-NH1	8.19	124.40	120.30
1	c	103	TYR	CB-CG-CD2	-8.19	116.09	121.00
1	F	189	MET	CG-SD-CE	-8.19	87.10	100.20
1	B	91	ARG	NE-CZ-NH1	-8.18	116.21	120.30
1	e	239	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	F	91	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	g	26	TYR	CB-CG-CD2	-8.17	116.10	121.00
2	3	46	TYR	CB-CG-CD1	-8.16	116.10	121.00
1	F	213	TYR	CB-CG-CD2	8.15	125.89	121.00
1	f	15	PHE	CB-CG-CD2	8.15	126.50	120.80
2	i	173	TYR	CB-CG-CD1	8.14	125.89	121.00
2	1	51	ARG	NE-CZ-NH2	8.14	124.37	120.30
1	C	130	ARG	NE-CZ-NH1	8.12	124.36	120.30
1	A	123	TYR	CG-CD1-CE1	-8.11	114.81	121.30
1	f	15	PHE	CB-CG-CD1	-8.11	115.12	120.80
2	1	199	TYR	CG-CD2-CE2	-8.11	114.81	121.30
2	l	196	PHE	CB-CG-CD2	-8.11	115.12	120.80
1	G	130	ARG	NE-CZ-NH2	8.11	124.35	120.30
2	7	36	PHE	CB-CG-CD2	-8.10	115.13	120.80
1	F	235	ARG	NE-CZ-NH1	-8.10	116.25	120.30
2	6	123	TYR	CG-CD2-CE2	-8.10	114.82	121.30
2	h	173	TYR	CB-CG-CD2	-8.10	116.14	121.00
1	d	185	PHE	CB-CG-CD1	-8.09	115.14	120.80
2	4	49	ALA	N-CA-CB	8.08	121.42	110.10
1	E	28	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	C	213	TYR	CB-CG-CD1	-8.06	116.16	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	l	88	ARG	NE-CZ-NH2	8.06	124.33	120.30
3	I	123	LYS	C-N-CA	8.06	141.84	121.70
1	d	53	ARG	NE-CZ-NH1	-8.05	116.27	120.30
3	H	76	ARG	NE-CZ-NH1	8.05	124.33	120.30
3	I	346	ALA	N-CA-CB	8.05	121.37	110.10
1	a	33	ARG	NE-CZ-NH2	-8.02	116.29	120.30
2	l	123	TYR	CB-CG-CD1	8.02	125.81	121.00
1	E	33	ARG	NE-CZ-NH2	-8.01	116.29	120.30
3	J	43	ARG	NE-CZ-NH2	-8.01	116.29	120.30
1	C	179	TYR	CB-CG-CD1	-8.00	116.20	121.00
3	L	361	PHE	CB-CG-CD1	8.00	126.40	120.80
1	C	91	ARG	NE-CZ-NH1	-7.99	116.31	120.30
3	M	397	PHE	CB-CG-CD2	-7.98	115.21	120.80
1	b	175	PHE	CB-CG-CD1	7.98	126.39	120.80
2	k	83	ARG	NE-CZ-NH2	7.98	124.29	120.30
1	c	168	ARG	NE-CZ-NH1	-7.97	116.31	120.30
2	7	88	ARG	NE-CZ-NH2	-7.97	116.32	120.30
1	D	190	VAL	CA-CB-CG2	-7.95	98.97	110.90
1	E	103	TYR	CB-CG-CD2	-7.95	116.23	121.00
1	G	179	TYR	CB-CG-CD1	-7.95	116.23	121.00
2	5	155	PHE	CB-CG-CD2	7.91	126.34	120.80
1	b	180	ARG	NE-CZ-NH2	-7.91	116.35	120.30
3	M	20	TYR	CB-CG-CD1	7.90	125.74	121.00
2	h	106	TYR	CB-CG-CD1	-7.89	116.27	121.00
2	k	102	ARG	NE-CZ-NH1	-7.89	116.36	120.30
3	J	52	ARG	NE-CZ-NH1	7.87	124.24	120.30
3	L	364	ARG	NE-CZ-NH2	-7.87	116.36	120.30
2	3	123	TYR	CB-CG-CD2	-7.86	116.28	121.00
1	a	232	TYR	CB-CG-CD2	-7.85	116.29	121.00
2	l	14	THR	CA-CB-CG2	-7.85	101.41	112.40
2	h	51	ARG	NE-CZ-NH2	-7.85	116.38	120.30
1	f	93	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	e	91	ARG	NE-CZ-NH2	7.84	124.22	120.30
3	M	303	PHE	CB-CG-CD2	-7.84	115.31	120.80
1	A	213	TYR	CB-CG-CD1	-7.82	116.31	121.00
2	7	36	PHE	CB-CG-CD1	7.82	126.27	120.80
2	j	88	ARG	NE-CZ-NH1	-7.81	116.40	120.30
2	k	173	TYR	CG-CD2-CE2	-7.81	115.06	121.30
2	n	56	THR	CA-CB-CG2	-7.80	101.48	112.40
2	7	189	VAL	CA-CB-CG2	-7.80	99.20	110.90
1	G	68	TYR	CB-CG-CD2	-7.80	116.32	121.00
3	M	259	ARG	NE-CZ-NH1	-7.79	116.40	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	F	232	TYR	CB-CG-CD2	-7.79	116.33	121.00
1	a	68	TYR	CB-CG-CD1	7.78	125.67	121.00
1	C	196	MET	CG-SD-CE	-7.78	87.75	100.20
3	J	335	ASP	CB-CG-OD1	-7.77	111.30	118.30
3	I	49	ARG	NE-CZ-NH1	7.77	124.19	120.30
3	L	29	ARG	NE-CZ-NH1	-7.77	116.42	120.30
1	F	213	TYR	CG-CD1-CE1	-7.77	115.09	121.30
2	h	197	TYR	CG-CD1-CE1	7.77	127.51	121.30
1	F	150	THR	CA-CB-CG2	-7.76	101.54	112.40
2	k	51	ARG	NE-CZ-NH2	7.75	124.18	120.30
2	n	50	ASP	CB-CG-OD1	-7.75	111.33	118.30
2	4	80	ARG	NE-CZ-NH1	-7.75	116.43	120.30
3	H	302	ARG	NE-CZ-NH1	7.74	124.17	120.30
2	m	51	ARG	NE-CZ-NH2	7.74	124.17	120.30
1	E	93	ARG	NE-CZ-NH2	-7.74	116.43	120.30
2	h	106	TYR	CG-CD2-CE2	-7.74	115.11	121.30
2	i	123	TYR	CB-CG-CD2	7.73	125.64	121.00
1	E	142	ASP	CB-CG-OD2	7.72	125.25	118.30
1	c	28	ARG	NE-CZ-NH2	-7.71	116.44	120.30
3	H	154	ARG	NE-CZ-NH2	-7.71	116.45	120.30
3	L	336	PHE	CB-CG-CD2	-7.71	115.41	120.80
2	l	123	TYR	CB-CG-CD2	-7.69	116.39	121.00
3	H	259	ARG	NE-CZ-NH1	7.68	124.14	120.30
2	i	148	TYR	CB-CG-CD1	7.68	125.61	121.00
3	I	167	PHE	CB-CG-CD2	-7.67	115.43	120.80
3	M	397	PHE	CB-CG-CD1	7.67	126.17	120.80
2	j	197	TYR	CB-CG-CD1	-7.67	116.40	121.00
3	J	371	THR	CA-CB-CG2	-7.66	101.68	112.40
1	a	175	PHE	CB-CG-CD1	7.66	126.16	120.80
3	H	397	PHE	CB-CG-CD2	-7.66	115.44	120.80
3	M	128	TYR	CB-CG-CD2	-7.66	116.41	121.00
1	G	123	TYR	CB-CG-CD1	-7.65	116.41	121.00
2	j	101	TYR	CB-CG-CD2	-7.65	116.41	121.00
3	K	52	ARG	NE-CZ-NH2	-7.65	116.48	120.30
3	L	120	PRO	N-CA-CB	7.63	112.45	103.30
2	7	173	TYR	CG-CD2-CE2	-7.62	115.20	121.30
3	I	57	ARG	NE-CZ-NH1	7.62	124.11	120.30
3	K	346	ALA	N-CA-CB	7.62	120.76	110.10
2	2	104	PHE	CB-CG-CD1	7.61	126.13	120.80
2	l	170	ARG	CD-NE-CZ	7.61	134.25	123.60
2	h	170	ARG	NE-CZ-NH1	-7.60	116.50	120.30
2	k	62	ASP	CB-CG-OD2	-7.60	111.46	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	5	68	ARG	NE-CZ-NH2	-7.60	116.50	120.30
1	E	180	ARG	NE-CZ-NH1	-7.60	116.50	120.30
3	H	147	ASP	CB-CG-OD1	7.60	125.14	118.30
3	I	124	ASP	CB-CG-OD1	-7.59	111.47	118.30
2	l	184	ASP	CB-CG-OD1	7.58	125.12	118.30
1	F	239	ARG	NE-CZ-NH1	7.58	124.09	120.30
3	I	314	PHE	CB-CG-CD1	-7.58	115.50	120.80
3	L	282	LYS	N-CA-CB	7.56	124.21	110.60
2	k	77	TYR	CB-CG-CD1	7.55	125.53	121.00
3	M	94	TYR	CG-CD1-CE1	-7.55	115.26	121.30
2	l	33	MET	CG-SD-CE	-7.55	88.12	100.20
3	I	275	PHE	CB-CG-CD1	7.54	126.08	120.80
2	6	103	TYR	CB-CG-CD1	-7.54	116.48	121.00
1	A	235	ARG	NE-CZ-NH1	-7.53	116.53	120.30
2	j	81	ARG	NE-CZ-NH2	-7.52	116.54	120.30
2	7	81	ARG	NE-CZ-NH1	-7.52	116.54	120.30
3	I	178	VAL	CA-CB-CG1	-7.52	99.62	110.90
1	c	20	ARG	NE-CZ-NH1	7.52	124.06	120.30
1	B	175	PHE	CB-CG-CD2	-7.51	115.54	120.80
1	G	91	ARG	NE-CZ-NH1	-7.50	116.55	120.30
3	I	397	PHE	CB-CG-CD2	-7.50	115.55	120.80
3	I	128	TYR	CB-CG-CD1	-7.50	116.50	121.00
2	6	123	TYR	CZ-CE2-CD2	7.48	126.53	119.80
1	G	175	PHE	CB-CG-CD1	7.48	126.03	120.80
2	5	176	MET	CG-SD-CE	-7.48	88.23	100.20
1	B	179	TYR	CB-CG-CD2	7.48	125.49	121.00
1	a	100	ARG	NE-CZ-NH2	7.47	124.04	120.30
1	G	33	ARG	NE-CZ-NH1	7.47	124.04	120.30
1	A	232	TYR	CB-CG-CD2	-7.47	116.52	121.00
1	b	91	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	F	28	ARG	NE-CZ-NH1	7.47	124.03	120.30
1	G	232	TYR	CG-CD1-CE1	7.46	127.27	121.30
1	G	10	ARG	NE-CZ-NH1	7.46	124.03	120.30
1	A	51	ASP	CB-CG-OD2	-7.46	111.59	118.30
3	I	280	ASP	CB-CG-OD2	-7.44	111.60	118.30
2	5	83	ARG	NE-CZ-NH2	7.44	124.02	120.30
2	j	103	TYR	CB-CG-CD2	-7.44	116.54	121.00
1	c	187	ASP	CB-CG-OD2	-7.44	111.61	118.30
3	L	273	ASP	CB-CG-OD2	-7.43	111.61	118.30
3	L	94	TYR	CB-CG-CD2	-7.43	116.54	121.00
2	6	170	ARG	NE-CZ-NH2	7.42	124.01	120.30
2	6	104	PHE	CB-CG-CD2	-7.41	115.61	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	E	91	ARG	NE-CZ-NH1	-7.41	116.60	120.30
3	L	239	PHE	CB-CG-CD2	7.40	125.98	120.80
2	1	106	TYR	CB-CG-CD2	-7.40	116.56	121.00
3	L	239	PHE	CB-CG-CD1	-7.38	115.64	120.80
2	5	126	ASP	CB-CG-OD1	7.38	124.94	118.30
3	H	222	LEU	CB-CG-CD2	7.38	123.54	111.00
2	n	173	TYR	CZ-CE2-CD2	-7.37	113.16	119.80
1	G	123	TYR	CB-CG-CD2	7.37	125.42	121.00
2	k	30	ARG	N-CA-CB	7.37	123.86	110.60
1	a	90	ASP	CB-CG-OD2	7.36	124.93	118.30
1	a	232	TYR	CB-CG-CD1	7.35	125.41	121.00
2	h	80	ARG	NE-CZ-NH1	-7.35	116.62	120.30
2	5	154	ARG	NE-CZ-NH1	-7.35	116.63	120.30
2	1	173	TYR	CG-CD2-CE2	-7.34	115.42	121.30
1	G	22	PHE	CB-CG-CD2	7.33	125.94	120.80
1	A	53	ARG	NE-CZ-NH2	-7.33	116.63	120.30
2	j	77	TYR	CB-CG-CD1	7.32	125.39	121.00
1	B	241	ARG	NE-CZ-NH1	-7.31	116.64	120.30
2	n	25	MET	CG-SD-CE	-7.31	88.50	100.20
1	g	123	TYR	CB-CG-CD1	-7.30	116.62	121.00
2	4	148	TYR	CB-CG-CD1	7.30	125.38	121.00
2	h	155	PHE	CB-CG-CD1	7.30	125.91	120.80
1	B	148	TYR	CG-CD2-CE2	7.27	127.12	121.30
3	I	104	ALA	CB-CA-C	-7.27	99.20	110.10
1	E	142	ASP	CB-CG-OD1	-7.26	111.76	118.30
3	L	275	PHE	CB-CG-CD1	-7.25	115.72	120.80
1	A	15	PHE	CB-CG-CD1	7.24	125.87	120.80
3	I	36	PHE	CB-CG-CD2	7.24	125.87	120.80
1	a	168	ARG	NE-CZ-NH1	7.24	123.92	120.30
1	D	168	ARG	NH1-CZ-NH2	-7.23	111.45	119.40
1	D	235	ARG	NE-CZ-NH1	-7.23	116.69	120.30
2	l	106	TYR	CB-CG-CD2	-7.23	116.66	121.00
3	I	249	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	E	175	PHE	CB-CG-CD2	-7.22	115.75	120.80
1	E	132	PHE	CB-CG-CD1	7.21	125.85	120.80
3	L	278	ARG	NE-CZ-NH2	-7.21	116.69	120.30
2	1	33	MET	CG-SD-CE	-7.21	88.67	100.20
1	B	130	ARG	NE-CZ-NH2	-7.20	116.70	120.30
1	B	205	VAL	N-CA-C	-7.20	91.56	111.00
1	D	239	ARG	NE-CZ-NH1	7.20	123.90	120.30
1	d	219	ARG	NE-CZ-NH1	-7.20	116.70	120.30
1	c	159	TYR	CB-CG-CD2	-7.19	116.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	60	GLU	OE1-CD-OE2	-7.19	114.67	123.30
3	I	52	ARG	NE-CZ-NH2	-7.18	116.71	120.30
3	I	227	PHE	CB-CG-CD2	-7.18	115.77	120.80
3	H	239	PHE	CB-CG-CD2	7.18	125.82	120.80
3	I	335	ASP	CB-CG-OD2	-7.17	111.84	118.30
1	b	10	ARG	NE-CZ-NH2	7.17	123.89	120.30
2	2	212	ARG	NE-CZ-NH2	7.17	123.89	120.30
1	E	33	ARG	NE-CZ-NH1	7.17	123.88	120.30
1	A	123	TYR	CB-CG-CD2	-7.16	116.70	121.00
2	k	197	TYR	CB-CG-CD2	-7.16	116.70	121.00
1	d	20	ARG	NE-CZ-NH1	7.16	123.88	120.30
3	L	317	ARG	NE-CZ-NH2	7.16	123.88	120.30
2	i	46	TYR	CB-CG-CD2	-7.16	116.70	121.00
1	G	232	TYR	CB-CG-CD1	7.16	125.29	121.00
2	h	212	ARG	NE-CZ-NH2	7.16	123.88	120.30
3	K	94	TYR	CB-CG-CD2	-7.15	116.71	121.00
3	H	77	VAL	N-CA-C	-7.14	91.72	111.00
3	J	235	PRO	O-C-N	-7.14	111.28	122.70
3	M	104	ALA	N-CA-CB	7.14	120.09	110.10
3	I	303	PHE	CB-CG-CD2	-7.13	115.81	120.80
1	G	241	ARG	NE-CZ-NH1	-7.13	116.74	120.30
3	I	215	TYR	CZ-CE2-CD2	-7.13	113.39	119.80
1	c	182	ASP	CB-CG-OD1	-7.12	111.89	118.30
2	i	126	ASP	CB-CG-OD2	7.12	124.71	118.30
3	H	397	PHE	CB-CG-CD1	7.11	125.78	120.80
2	2	123	TYR	CZ-CE2-CD2	-7.11	113.40	119.80
1	F	232	TYR	CB-CG-CD1	7.10	125.26	121.00
2	6	211	PHE	CB-CG-CD1	-7.09	115.84	120.80
3	M	32	ASP	CB-CG-OD1	7.08	124.68	118.30
1	A	132	PHE	CB-CG-CD2	7.08	125.76	120.80
1	g	18	ASP	CB-CG-OD2	7.08	124.67	118.30
1	G	28	ARG	NE-CZ-NH1	7.07	123.84	120.30
2	4	178	ARG	NE-CZ-NH1	-7.07	116.77	120.30
2	4	187	ASP	CB-CG-OD2	7.07	124.66	118.30
1	B	224	VAL	CA-CB-CG2	7.07	121.50	110.90
1	e	148	TYR	CB-CG-CD1	7.06	125.24	121.00
1	a	189	MET	CG-SD-CE	-7.06	88.91	100.20
2	m	107	LEU	CB-CG-CD2	7.06	123.00	111.00
1	F	37	ALA	N-CA-CB	7.06	119.98	110.10
2	1	94	THR	CA-CB-CG2	-7.04	102.54	112.40
1	a	104	ASP	N-CA-CB	7.04	123.28	110.60
1	b	93	ARG	NE-CZ-NH2	-7.04	116.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	26	TYR	CB-CG-CD1	-7.03	116.78	121.00
1	a	175	PHE	CB-CG-CD2	-7.03	115.88	120.80
1	G	26	TYR	CG-CD2-CE2	-7.02	115.69	121.30
2	5	88	ARG	NE-CZ-NH1	-7.02	116.79	120.30
2	1	68	ARG	NE-CZ-NH2	7.02	123.81	120.30
2	3	123	TYR	CB-CG-CD1	7.02	125.21	121.00
3	H	375	PHE	CB-CG-CD1	-7.02	115.89	120.80
3	K	336	PHE	CB-CG-CD1	-7.02	115.89	120.80
2	k	139	ALA	N-CA-CB	7.01	119.91	110.10
2	l	68	ARG	NE-CZ-NH1	7.00	123.80	120.30
1	e	132	PHE	CB-CG-CD2	7.00	125.70	120.80
1	D	65	GLU	N-CA-CB	6.99	123.19	110.60
1	b	90	ASP	CB-CG-OD2	6.99	124.59	118.30
2	1	21	ASP	CB-CG-OD1	-6.99	112.01	118.30
1	b	201	GLU	N-CA-CB	6.99	123.18	110.60
2	n	134	GLU	N-CA-CB	6.98	123.17	110.60
1	D	22	PHE	CB-CG-CD2	-6.97	115.92	120.80
1	c	187	ASP	CB-CG-OD1	6.97	124.57	118.30
3	J	358	ALA	N-CA-CB	6.97	119.86	110.10
3	L	386	THR	CA-CB-CG2	-6.96	102.66	112.40
3	M	281	VAL	C-N-CA	6.96	139.10	121.70
3	J	335	ASP	CB-CG-OD2	6.96	124.56	118.30
2	7	30	ARG	NE-CZ-NH1	6.94	123.77	120.30
2	3	165	VAL	CA-CB-CG2	6.94	121.31	110.90
2	1	153	ASP	CB-CG-OD2	-6.94	112.06	118.30
2	h	30	ARG	NE-CZ-NH1	-6.93	116.83	120.30
2	l	80	ARG	NE-CZ-NH2	6.93	123.77	120.30
2	6	116	ASP	CB-CG-OD2	-6.93	112.06	118.30
3	I	205	ARG	NE-CZ-NH2	-6.93	116.83	120.30
2	6	36	PHE	CB-CG-CD1	6.93	125.65	120.80
3	K	361	PHE	CB-CG-CD2	-6.93	115.95	120.80
1	d	147	LEU	CB-CG-CD1	6.93	122.78	111.00
3	H	181	TYR	CB-CG-CD2	6.93	125.16	121.00
3	K	154	ARG	NE-CZ-NH1	6.92	123.76	120.30
1	A	104	ASP	CB-CG-OD2	-6.92	112.07	118.30
2	k	154	ARG	NE-CZ-NH1	-6.92	116.84	120.30
3	M	203	PHE	CB-CG-CD2	-6.91	115.96	120.80
2	1	33	MET	N-CA-CB	6.91	123.04	110.60
2	i	154	ARG	NE-CZ-NH1	-6.90	116.85	120.30
2	n	106	TYR	CB-CG-CD1	6.90	125.14	121.00
2	k	77	TYR	CB-CG-CD2	-6.90	116.86	121.00
2	l	185	GLY	N-CA-C	-6.90	95.86	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	179	ASP	CB-CG-OD1	-6.90	112.09	118.30
2	n	208	LEU	CB-CG-CD1	6.90	122.72	111.00
1	d	129	VAL	CG1-CB-CG2	6.89	121.92	110.90
2	l	176	MET	CG-SD-CE	6.89	111.22	100.20
2	7	179	ASP	CB-CG-OD2	6.89	124.50	118.30
1	A	123	TYR	CD1-CE1-CZ	6.88	126.00	119.80
1	F	241	ARG	NE-CZ-NH2	-6.88	116.86	120.30
3	J	339	LEU	CB-CG-CD2	6.87	122.68	111.00
3	M	46	ARG	NE-CZ-NH1	6.87	123.73	120.30
1	F	106	PRO	O-C-N	6.87	133.69	122.70
2	h	42	ALA	N-CA-CB	6.86	119.71	110.10
2	2	53	ALA	N-CA-CB	6.86	119.71	110.10
1	A	65	GLU	O-C-N	-6.86	111.73	122.70
2	2	199	TYR	CB-CG-CD2	6.86	125.11	121.00
1	A	168	ARG	CD-NE-CZ	-6.86	114.00	123.60
2	j	80	ARG	NE-CZ-NH1	-6.86	116.87	120.30
2	7	199	TYR	CB-CG-CD2	-6.86	116.89	121.00
1	a	148	TYR	CG-CD1-CE1	-6.85	115.82	121.30
1	f	150	THR	CA-CB-CG2	-6.85	102.81	112.40
2	j	50	ASP	CB-CG-OD1	-6.84	112.14	118.30
2	6	140	THR	N-CA-CB	6.84	123.29	110.30
2	l	106	TYR	CD1-CE1-CZ	-6.83	113.65	119.80
1	b	205	VAL	CA-CB-CG2	6.83	121.14	110.90
1	e	175	PHE	CB-CG-CD2	-6.82	116.03	120.80
1	b	22	PHE	CB-CG-CD1	-6.82	116.03	120.80
1	B	175	PHE	CB-CG-CD1	6.82	125.57	120.80
1	G	175	PHE	CB-CG-CD2	-6.82	116.03	120.80
3	J	46	ARG	NE-CZ-NH2	6.81	123.71	120.30
1	B	236	ALA	N-CA-CB	6.81	119.64	110.10
1	b	62	ASP	CB-CG-OD2	-6.80	112.17	118.30
2	5	62	ASP	CB-CG-OD2	6.80	124.42	118.30
1	a	86	ARG	NE-CZ-NH2	6.80	123.70	120.30
2	1	65	PHE	CB-CG-CD2	6.80	125.56	120.80
1	a	93	ARG	NE-CZ-NH2	-6.80	116.90	120.30
3	M	29	ARG	NE-CZ-NH1	6.80	123.70	120.30
2	h	17	LEU	N-CA-CB	6.80	124.00	110.40
2	2	154	ARG	NE-CZ-NH2	6.80	123.70	120.30
3	I	281	VAL	O-C-N	-6.79	111.83	122.70
1	C	175	PHE	CB-CG-CD2	-6.79	116.05	120.80
2	1	179	ASP	CB-CG-OD1	6.77	124.39	118.30
2	4	212	ARG	NE-CZ-NH2	-6.77	116.91	120.30
2	7	131	ALA	N-CA-C	-6.77	92.72	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	107	ALA	N-CA-CB	6.77	119.58	110.10
1	E	8	TYR	CB-CG-CD2	-6.77	116.94	121.00
2	m	178	ARG	NE-CZ-NH2	-6.77	116.92	120.30
2	h	194	ASP	CB-CG-OD1	-6.76	112.22	118.30
3	L	386	THR	N-CA-CB	6.76	123.14	110.30
2	k	83	ARG	N-CA-CB	6.75	122.76	110.60
1	b	68	TYR	CB-CG-CD2	-6.75	116.95	121.00
2	6	175	ALA	CB-CA-C	-6.75	99.98	110.10
2	n	51	ARG	NE-CZ-NH2	6.74	123.67	120.30
1	g	91	ARG	NE-CZ-NH2	-6.74	116.93	120.30
2	3	77	TYR	CB-CG-CD2	-6.74	116.96	121.00
1	b	219	ARG	NE-CZ-NH1	6.73	123.67	120.30
2	i	179	ASP	CB-CG-OD1	-6.73	112.25	118.30
1	D	103	TYR	CB-CG-CD1	6.72	125.03	121.00
2	3	51	ARG	NE-CZ-NH2	6.72	123.66	120.30
2	7	181	ALA	CB-CA-C	-6.72	100.02	110.10
1	f	123	TYR	CB-CG-CD2	6.72	125.03	121.00
1	G	132	PHE	CB-CG-CD2	-6.71	116.10	120.80
2	j	77	TYR	CB-CG-CD2	-6.71	116.97	121.00
1	g	126	TYR	CB-CG-CD1	-6.71	116.97	121.00
2	j	55	THR	N-CA-CB	6.71	123.04	110.30
1	c	148	TYR	CG-CD1-CE1	-6.70	115.94	121.30
1	F	103	TYR	CB-CG-CD1	6.70	125.02	121.00
3	L	44	TYR	CD1-CE1-CZ	6.70	125.83	119.80
3	J	203	PHE	CB-CG-CD1	6.70	125.49	120.80
2	4	148	TYR	CG-CD2-CE2	-6.70	115.94	121.30
1	e	53	ARG	NE-CZ-NH2	-6.70	116.95	120.30
2	1	169	VAL	CA-CB-CG2	-6.69	100.87	110.90
3	M	44	TYR	CB-CG-CD2	-6.68	116.99	121.00
2	7	173	TYR	CD1-CG-CD2	6.68	125.25	117.90
2	6	31	ALA	N-CA-CB	6.68	119.45	110.10
2	1	62	ASP	CB-CG-OD2	-6.67	112.29	118.30
3	L	76	ARG	NE-CZ-NH2	-6.67	116.97	120.30
1	f	132	PHE	CB-CG-CD2	-6.65	116.14	120.80
3	I	200	ARG	NE-CZ-NH1	6.65	123.62	120.30
2	m	83	ARG	NE-CZ-NH1	-6.64	116.98	120.30
1	D	232	TYR	CG-CD2-CE2	-6.64	115.99	121.30
3	H	273	ASP	N-CA-C	-6.64	93.07	111.00
2	7	101	TYR	CB-CG-CD2	-6.63	117.02	121.00
3	L	104	ALA	CB-CA-C	-6.63	100.15	110.10
1	D	6	MET	CG-SD-CE	-6.63	89.59	100.20
3	J	289	ARG	NE-CZ-NH2	-6.63	116.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	146	LEU	C-N-CA	6.63	138.27	121.70
2	2	80	ARG	NE-CZ-NH1	-6.62	116.99	120.30
2	n	103	TYR	CG-CD2-CE2	-6.61	116.01	121.30
3	J	314	PHE	CB-CG-CD1	6.61	125.43	120.80
1	e	213	TYR	CB-CG-CD1	6.61	124.97	121.00
1	G	213	TYR	CB-CG-CD2	-6.61	117.03	121.00
2	6	193	GLU	N-CA-CB	6.61	122.50	110.60
1	D	219	ARG	CD-NE-CZ	6.61	132.85	123.60
1	c	180	ARG	NE-CZ-NH1	-6.61	117.00	120.30
1	E	22	PHE	CB-CG-CD1	-6.60	116.18	120.80
3	I	226	VAL	CA-CB-CG2	-6.60	101.00	110.90
1	E	26	TYR	CB-CG-CD2	6.60	124.96	121.00
3	M	131	GLU	N-CA-CB	6.60	122.48	110.60
1	a	104	ASP	CB-CG-OD1	-6.59	112.37	118.30
1	g	91	ARG	NE-CZ-NH1	6.59	123.59	120.30
3	K	32	ASP	CB-CG-OD2	-6.59	112.37	118.30
2	4	123	TYR	CB-CG-CD1	-6.58	117.05	121.00
1	c	221	PHE	CB-CG-CD1	6.58	125.41	120.80
2	2	179	ASP	CB-CG-OD2	6.58	124.22	118.30
3	H	241	ASP	CB-CG-OD2	-6.58	112.38	118.30
2	i	77	TYR	CB-CG-CD1	6.58	124.95	121.00
2	5	88	ARG	NE-CZ-NH2	6.58	123.59	120.30
2	m	68	ARG	NE-CZ-NH1	6.57	123.58	120.30
3	M	309	VAL	CA-CB-CG2	-6.56	101.06	110.90
1	e	147	LEU	CB-CG-CD1	6.56	122.15	111.00
1	F	241	ARG	NE-CZ-NH1	-6.55	117.02	120.30
2	2	182	SER	N-CA-CB	6.55	120.33	110.50
2	7	88	ARG	NE-CZ-NH1	-6.54	117.03	120.30
1	a	186	ASP	CB-CG-OD1	6.54	124.18	118.30
1	E	126	TYR	CB-CG-CD2	6.54	124.92	121.00
3	L	215	TYR	CB-CG-CD1	-6.54	117.08	121.00
1	C	100	ARG	NE-CZ-NH1	6.53	123.57	120.30
3	H	69	SER	CB-CA-C	-6.53	97.69	110.10
2	k	103	TYR	CG-CD1-CE1	-6.53	116.08	121.30
2	7	104	PHE	CB-CG-CD2	6.53	125.37	120.80
2	7	147	ALA	N-CA-CB	6.53	119.24	110.10
3	I	212	VAL	N-CA-CB	6.53	125.86	111.50
3	K	27	TYR	CB-CG-CD2	6.52	124.91	121.00
1	f	18	ASP	CB-CG-OD2	-6.52	112.43	118.30
2	j	139	ALA	N-CA-CB	6.52	119.23	110.10
3	J	76	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	f	218	ASP	CB-CG-OD2	-6.52	112.44	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	7	88	ARG	NH1-CZ-NH2	6.52	126.57	119.40
3	H	63	LEU	CB-CG-CD1	6.51	122.07	111.00
2	h	68	ARG	NE-CZ-NH1	-6.51	117.04	120.30
1	b	123	TYR	CB-CG-CD1	-6.51	117.10	121.00
1	e	213	TYR	CG-CD1-CE1	6.50	126.50	121.30
1	C	100	ARG	NE-CZ-NH2	6.50	123.55	120.30
2	1	156	THR	CA-CB-CG2	-6.50	103.30	112.40
3	H	199	THR	CA-CB-CG2	-6.50	103.30	112.40
1	c	91	ARG	NE-CZ-NH2	6.50	123.55	120.30
2	n	154	ARG	NE-CZ-NH1	-6.49	117.05	120.30
3	J	65	VAL	CA-CB-CG2	-6.49	101.16	110.90
2	k	52	MET	CG-SD-CE	-6.49	89.82	100.20
1	a	180	ARG	NE-CZ-NH1	-6.49	117.06	120.30
1	F	26	TYR	CB-CG-CD1	-6.48	117.11	121.00
1	C	205	VAL	N-CA-C	-6.48	93.50	111.00
3	K	32	ASP	N-CA-CB	6.48	122.27	110.60
3	J	211	PHE	CB-CG-CD1	-6.47	116.27	120.80
1	D	175	PHE	CB-CG-CD2	-6.47	116.27	120.80
1	f	71	ASP	CB-CG-OD2	-6.47	112.48	118.30
1	f	219	ARG	NE-CZ-NH2	-6.47	117.07	120.30
2	6	187	ASP	CB-CG-OD2	-6.46	112.48	118.30
1	g	175	PHE	CB-CG-CD2	-6.46	116.28	120.80
1	a	190	VAL	CA-CB-CG2	-6.46	101.21	110.90
2	j	175	ALA	N-CA-CB	6.45	119.13	110.10
1	b	28	ARG	NE-CZ-NH1	-6.45	117.08	120.30
1	C	9	ASP	CB-CG-OD1	-6.45	112.50	118.30
1	g	232	TYR	CD1-CE1-CZ	6.45	125.60	119.80
2	h	56	THR	CA-CB-CG2	-6.44	103.38	112.40
2	k	63	ALA	N-CA-CB	6.44	119.12	110.10
1	d	175	PHE	CB-CG-CD2	-6.44	116.29	120.80
2	h	140	THR	N-CA-CB	6.44	122.53	110.30
1	A	130	ARG	NE-CZ-NH1	6.43	123.52	120.30
2	6	25	MET	CG-SD-CE	6.43	110.48	100.20
2	2	51	ARG	NE-CZ-NH2	6.42	123.51	120.30
1	D	213	TYR	CB-CG-CD1	6.42	124.85	121.00
3	K	364	ARG	NE-CZ-NH1	6.42	123.51	120.30
1	B	93	ARG	NE-CZ-NH2	-6.41	117.09	120.30
3	M	257	GLY	C-N-CA	6.41	137.72	121.70
1	A	168	ARG	NE-CZ-NH1	6.41	123.50	120.30
1	f	186	ASP	CB-CG-OD2	-6.40	112.54	118.30
2	4	74	ALA	CB-CA-C	-6.40	100.50	110.10
2	7	56	THR	CA-CB-CG2	-6.40	103.44	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	103	TYR	CB-CA-C	-6.40	97.61	110.40
3	L	259	ARG	NE-CZ-NH1	-6.40	117.10	120.30
3	J	224	ARG	NE-CZ-NH1	-6.40	117.10	120.30
1	B	174	PHE	CB-CG-CD1	6.39	125.28	120.80
3	K	40	GLU	N-CA-CB	6.39	122.11	110.60
3	I	211	PHE	CB-CG-CD2	-6.39	116.33	120.80
2	4	116	ASP	CB-CG-OD2	-6.39	112.55	118.30
3	M	265	MET	CG-SD-CE	-6.38	89.99	100.20
3	K	326	ARG	NE-CZ-NH2	6.38	123.49	120.30
1	A	135	SER	N-CA-CB	6.37	120.05	110.50
2	k	194	ASP	CB-CA-C	-6.36	97.69	110.40
1	E	218	ASP	CB-CG-OD2	-6.36	112.58	118.30
2	5	211	PHE	CB-CG-CD1	-6.36	116.35	120.80
1	a	228	GLU	OE1-CD-OE2	6.35	130.92	123.30
1	G	21	LEU	CB-CG-CD2	6.35	121.79	111.00
1	F	37	ALA	O-C-N	6.35	132.85	122.70
1	A	11	ALA	N-CA-CB	6.34	118.98	110.10
1	b	100	ARG	NE-CZ-NH2	6.34	123.47	120.30
3	M	140	TYR	CZ-CE2-CD2	6.34	125.51	119.80
1	a	62	ASP	CB-CG-OD2	-6.34	112.59	118.30
1	D	64	ILE	C-N-CA	6.34	137.55	121.70
2	j	211	PHE	CB-CG-CD2	-6.34	116.36	120.80
3	M	243	LEU	CB-CG-CD1	6.34	121.77	111.00
1	f	93	ARG	NE-CZ-NH2	-6.33	117.13	120.30
3	H	302	ARG	N-CA-C	-6.33	93.90	111.00
2	6	116	ASP	CB-CG-OD1	6.33	123.99	118.30
1	g	175	PHE	CB-CG-CD1	6.32	125.22	120.80
3	I	224	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	C	53	ARG	NE-CZ-NH1	6.32	123.46	120.30
1	E	221	PHE	CB-CG-CD2	-6.32	116.38	120.80
2	5	199	TYR	CB-CG-CD1	6.30	124.78	121.00
3	L	106	VAL	CG1-CB-CG2	6.30	120.99	110.90
2	n	106	TYR	CB-CG-CD2	-6.30	117.22	121.00
1	g	82	VAL	CG1-CB-CG2	6.30	120.98	110.90
2	7	173	TYR	CB-CG-CD1	-6.30	117.22	121.00
1	A	77	ALA	N-CA-CB	6.30	118.92	110.10
1	B	51	ASP	CB-CG-OD2	-6.30	112.63	118.30
2	6	103	TYR	CG-CD2-CE2	-6.29	116.27	121.30
2	7	134	GLU	N-CA-CB	6.29	121.91	110.60
1	a	130	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	m	178	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	m	46	TYR	CB-CG-CD1	-6.27	117.24	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	g	239	ARG	NE-CZ-NH2	6.27	123.44	120.30
2	6	134	GLU	N-CA-CB	6.27	121.88	110.60
2	1	178	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	C	231	PRO	N-CA-CB	6.26	110.81	103.30
2	5	101	TYR	CG-CD1-CE1	6.26	126.31	121.30
1	c	185	PHE	CB-CG-CD1	6.26	125.18	120.80
1	d	159	TYR	CB-CG-CD2	-6.26	117.25	121.00
2	j	144	SER	N-CA-CB	-6.26	101.11	110.50
2	n	173	TYR	CG-CD2-CE2	6.26	126.31	121.30
3	K	367	ARG	NE-CZ-NH1	6.26	123.43	120.30
1	B	5	GLN	CB-CA-C	6.25	122.91	110.40
1	D	168	ARG	NE-CZ-NH2	6.25	123.43	120.30
1	c	159	TYR	CB-CG-CD1	6.25	124.75	121.00
2	l	46	TYR	CB-CG-CD2	6.25	124.75	121.00
3	K	186	THR	CA-CB-CG2	-6.25	103.65	112.40
2	1	199	TYR	CD1-CE1-CZ	-6.25	114.18	119.80
1	C	53	ARG	NE-CZ-NH2	-6.24	117.18	120.30
3	L	270	ALA	N-CA-CB	6.24	118.84	110.10
1	c	179	TYR	CB-CG-CD2	-6.24	117.25	121.00
2	7	136	ASP	CB-CG-OD2	-6.24	112.68	118.30
1	b	168	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	G	33	ARG	NE-CZ-NH2	-6.24	117.18	120.30
1	F	123	TYR	CG-CD2-CE2	-6.24	116.31	121.30
1	a	210	GLU	CB-CA-C	6.24	122.87	110.40
2	h	197	TYR	CD1-CE1-CZ	-6.24	114.19	119.80
3	H	205	ARG	NE-CZ-NH1	6.24	123.42	120.30
2	i	111	LEU	N-CA-C	-6.23	94.17	111.00
2	2	65	PHE	CB-CG-CD2	6.23	125.16	120.80
2	k	187	ASP	CB-CG-OD2	-6.23	112.69	118.30
3	J	249	ARG	NE-CZ-NH2	-6.23	117.19	120.30
1	F	148	TYR	CB-CG-CD2	6.23	124.74	121.00
1	B	86	ARG	NE-CZ-NH1	6.22	123.41	120.30
1	c	65	GLU	OE1-CD-OE2	6.22	130.77	123.30
2	h	123	TYR	CB-CG-CD1	6.22	124.73	121.00
2	h	67	ALA	CB-CA-C	-6.21	100.78	110.10
1	e	103	TYR	CD1-CE1-CZ	-6.21	114.21	119.80
1	c	235	ARG	NE-CZ-NH2	-6.21	117.19	120.30
1	E	213	TYR	CB-CG-CD2	-6.21	117.27	121.00
2	3	62	ASP	CB-CG-OD2	-6.21	112.71	118.30
1	e	126	TYR	CB-CG-CD2	6.21	124.73	121.00
2	4	77	TYR	CB-CG-CD1	-6.21	117.28	121.00
3	H	70	ASP	CB-CG-OD1	-6.21	112.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	184	SER	N-CA-CB	6.20	119.80	110.50
1	G	40	ILE	CA-CB-CG1	6.20	122.78	111.00
1	d	136	LEU	N-CA-CB	6.20	122.80	110.40
2	2	190	LYS	N-CA-CB	6.20	121.76	110.60
3	J	391	ASP	CB-CG-OD1	-6.20	112.72	118.30
2	2	131	ALA	N-CA-CB	6.20	118.77	110.10
2	j	189	VAL	N-CA-C	-6.19	94.30	111.00
3	M	248	ALA	N-CA-CB	6.19	118.76	110.10
2	4	178	ARG	NE-CZ-NH2	-6.19	117.21	120.30
3	L	52	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	f	158	GLU	OE1-CD-OE2	-6.18	115.88	123.30
3	I	299	ARG	NE-CZ-NH2	-6.18	117.21	120.30
1	B	68	TYR	CG-CD2-CE2	6.18	126.24	121.30
3	K	124	ASP	CB-CG-OD2	-6.18	112.74	118.30
3	J	196	ALA	N-CA-CB	6.18	118.75	110.10
2	m	200	SER	N-CA-CB	6.17	119.76	110.50
1	B	119	PHE	CB-CG-CD2	6.17	125.12	120.80
3	M	325	THR	CA-CB-CG2	-6.17	103.76	112.40
2	m	51	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	D	161	ALA	CB-CA-C	-6.16	100.86	110.10
2	n	67	ALA	CB-CA-C	-6.16	100.86	110.10
3	L	361	PHE	CB-CG-CD2	-6.16	116.49	120.80
2	k	104	PHE	CB-CG-CD1	6.15	125.11	120.80
2	5	187	ASP	CB-CG-OD1	-6.15	112.76	118.30
2	1	65	PHE	CD1-CE1-CZ	6.15	127.48	120.10
1	B	142	ASP	CB-CG-OD2	-6.15	112.77	118.30
3	L	76	ARG	NE-CZ-NH1	6.15	123.38	120.30
1	a	22	PHE	CB-CG-CD1	6.15	125.10	120.80
3	I	317	ARG	NH1-CZ-NH2	-6.14	112.64	119.40
3	H	321	PHE	N-CA-CB	6.14	121.65	110.60
2	h	136	ASP	CB-CG-OD2	6.14	123.83	118.30
2	3	65	PHE	CB-CG-CD2	-6.13	116.51	120.80
2	4	88	ARG	NE-CZ-NH2	6.13	123.36	120.30
2	1	148	TYR	CZ-CE2-CD2	6.13	125.31	119.80
2	i	185	GLY	N-CA-C	-6.12	97.80	113.10
2	7	173	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	F	33	ARG	N-CA-CB	6.12	121.61	110.60
1	B	44	GLU	OE1-CD-OE2	6.12	130.64	123.30
3	H	368	ALA	CB-CA-C	-6.12	100.93	110.10
1	a	163	ALA	C-N-CA	6.11	136.98	121.70
2	5	191	ILE	N-CA-C	-6.11	94.49	111.00
1	f	179	TYR	CB-CG-CD1	-6.11	117.33	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	258	ASP	CB-CG-OD2	-6.11	112.80	118.30
3	I	41	ARG	NE-CZ-NH1	6.11	123.35	120.30
2	2	191	ILE	N-CA-C	-6.10	94.52	111.00
1	c	119	PHE	CB-CG-CD2	-6.10	116.53	120.80
1	D	163	ALA	CB-CA-C	-6.10	100.95	110.10
1	b	84	ASP	CB-CG-OD2	-6.09	112.82	118.30
1	d	103	TYR	CB-CG-CD1	6.08	124.65	121.00
2	h	197	TYR	CB-CG-CD1	-6.08	117.35	121.00
1	a	142	ASP	O-C-N	6.08	132.43	122.70
1	D	161	ALA	N-CA-CB	6.08	118.61	110.10
2	2	68	ARG	NE-CZ-NH2	-6.08	117.26	120.30
3	H	278	ARG	N-CA-C	-6.08	94.59	111.00
1	G	68	TYR	CB-CG-CD1	6.08	124.65	121.00
1	e	233	VAL	CA-CB-CG2	-6.08	101.79	110.90
1	A	68	TYR	CG-CD2-CE2	-6.07	116.44	121.30
1	A	159	TYR	CZ-CE2-CD2	6.07	125.27	119.80
1	F	224	VAL	CA-CB-CG2	-6.07	101.80	110.90
3	J	254	ASP	CB-CG-OD2	6.07	123.76	118.30
3	J	221	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	g	100	ARG	NE-CZ-NH1	-6.06	117.27	120.30
3	J	367	ARG	NE-CZ-NH1	-6.06	117.27	120.30
3	H	364	ARG	NE-CZ-NH1	6.06	123.33	120.30
1	b	235	ARG	N-CA-CB	6.05	121.49	110.60
2	1	62	ASP	CB-CG-OD1	6.05	123.74	118.30
2	h	106	TYR	CD1-CG-CD2	6.04	124.55	117.90
2	i	170	ARG	CG-CD-NE	-6.04	99.11	111.80
1	C	100	ARG	NH1-CZ-NH2	-6.04	112.75	119.40
2	1	31	ALA	N-CA-CB	6.04	118.55	110.10
3	K	313	THR	CA-CB-CG2	-6.04	103.95	112.40
2	6	196	PHE	CB-CG-CD1	-6.04	116.58	120.80
1	D	91	ARG	NE-CZ-NH1	-6.03	117.28	120.30
3	J	128	TYR	CA-CB-CG	-6.03	101.94	113.40
1	A	148	TYR	CG-CD2-CE2	-6.03	116.48	121.30
2	l	55	THR	CA-CB-CG2	-6.03	103.96	112.40
1	a	132	PHE	CB-CG-CD1	-6.03	116.58	120.80
1	D	93	ARG	NE-CZ-NH2	-6.03	117.29	120.30
2	2	101	TYR	CZ-CE2-CD2	6.03	125.22	119.80
1	A	9	ASP	CB-CG-OD1	6.02	123.72	118.30
1	E	219	ARG	NE-CZ-NH1	6.02	123.31	120.30
1	f	200	ILE	CA-CB-CG2	-6.02	98.86	110.90
3	L	207	VAL	CA-CB-CG1	6.02	119.93	110.90
1	C	20	ARG	NE-CZ-NH1	6.02	123.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	235	ARG	NE-CZ-NH1	6.01	123.31	120.30
3	M	94	TYR	CD1-CG-CD2	6.01	124.52	117.90
2	3	139	ALA	C-N-CA	6.01	136.73	121.70
3	K	223	VAL	CA-CB-CG1	-6.01	101.89	110.90
1	e	235	ARG	NE-CZ-NH1	-6.00	117.30	120.30
3	I	104	ALA	N-CA-CB	6.00	118.50	110.10
1	b	216	VAL	CA-CB-CG2	-6.00	101.90	110.90
1	e	205	VAL	CA-CB-CG2	-6.00	101.90	110.90
2	n	199	TYR	CD1-CG-CD2	-6.00	111.30	117.90
3	H	218	GLU	N-CA-CB	6.00	121.40	110.60
1	f	138	ILE	CA-CB-CG1	-6.00	99.61	111.00
3	J	206	VAL	CG1-CB-CG2	6.00	120.49	110.90
1	C	217	ASP	CB-CG-OD1	-5.99	112.91	118.30
2	1	123	TYR	CB-CG-CD1	5.99	124.59	121.00
3	L	181	TYR	CB-CG-CD2	-5.99	117.41	121.00
1	E	221	PHE	CG-CD2-CE2	-5.99	114.21	120.80
1	A	185	PHE	CB-CG-CD2	-5.98	116.61	120.80
2	5	14	THR	N-CA-CB	5.98	121.67	110.30
1	b	123	TYR	CB-CG-CD2	5.98	124.59	121.00
1	D	28	ARG	NE-CZ-NH2	-5.98	117.31	120.30
1	E	210	GLU	N-CA-C	-5.98	94.85	111.00
3	I	374	ASP	CB-CG-OD2	-5.98	112.92	118.30
1	e	53	ARG	NE-CZ-NH1	5.98	123.29	120.30
2	j	139	ALA	N-CA-C	-5.97	94.87	111.00
1	g	213	TYR	CB-CG-CD2	-5.97	117.42	121.00
1	d	213	TYR	CG-CD1-CE1	-5.97	116.52	121.30
3	J	284	ILE	N-CA-C	-5.97	94.88	111.00
1	C	136	LEU	CB-CG-CD2	5.97	121.14	111.00
3	L	140	TYR	CG-CD1-CE1	-5.96	116.53	121.30
1	c	33	ARG	NE-CZ-NH2	5.96	123.28	120.30
2	n	57	ALA	N-CA-CB	5.96	118.44	110.10
3	K	181	TYR	CD1-CG-CD2	5.95	124.45	117.90
2	1	106	TYR	CB-CG-CD1	5.95	124.57	121.00
3	M	95	ILE	N-CA-C	-5.95	94.93	111.00
2	3	204	VAL	CG1-CB-CG2	-5.95	101.38	110.90
1	D	26	TYR	CB-CG-CD1	-5.95	117.43	121.00
2	4	33	MET	N-CA-CB	5.94	121.30	110.60
3	H	251	THR	N-CA-CB	5.94	121.59	110.30
2	4	178	ARG	NH1-CZ-NH2	5.94	125.93	119.40
2	7	197	TYR	CB-CG-CD2	5.94	124.56	121.00
2	j	54	MET	CA-CB-CG	5.94	123.39	113.30
2	l	29	LYS	N-CA-C	-5.94	94.97	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	3	63	ALA	CB-CA-C	-5.93	101.20	110.10
3	M	395	VAL	CA-CB-CG2	5.93	119.80	110.90
2	3	211	PHE	CG-CD2-CE2	-5.92	114.28	120.80
2	5	75	ASN	CB-CA-C	-5.92	98.56	110.40
3	L	397	PHE	CB-CG-CD1	-5.92	116.66	120.80
1	g	204	LEU	CB-CG-CD1	5.92	121.06	111.00
1	F	195	ALA	CB-CA-C	-5.92	101.22	110.10
2	3	39	SER	CB-CA-C	-5.92	98.86	110.10
1	E	231	PRO	N-CA-CB	5.92	110.40	103.30
1	G	221	PHE	CB-CG-CD1	-5.91	116.66	120.80
2	4	83	ARG	NE-CZ-NH2	5.91	123.26	120.30
2	k	50	ASP	CB-CG-OD2	5.91	123.62	118.30
3	L	275	PHE	CB-CG-CD2	5.91	124.94	120.80
2	1	170	ARG	NE-CZ-NH2	-5.90	117.35	120.30
1	f	103	TYR	CD1-CE1-CZ	-5.90	114.49	119.80
2	6	77	TYR	CG-CD1-CE1	-5.90	116.58	121.30
2	l	121	SER	N-CA-CB	5.90	119.35	110.50
3	H	120	PRO	N-CA-CB	-5.90	96.11	102.60
2	4	104	PHE	CB-CG-CD1	-5.89	116.67	120.80
2	i	80	ARG	NE-CZ-NH1	-5.89	117.35	120.30
2	i	116	ASP	CB-CA-C	5.89	122.18	110.40
3	J	147	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	G	69	LYS	N-CA-CB	5.88	121.19	110.60
2	4	16	GLY	N-CA-C	-5.88	98.40	113.10
1	c	65	GLU	N-CA-CB	5.88	121.18	110.60
2	n	17	LEU	N-CA-CB	5.88	122.16	110.40
2	m	14	THR	CA-CB-CG2	-5.88	104.17	112.40
1	a	86	ARG	NH1-CZ-NH2	-5.87	112.94	119.40
1	d	241	ARG	NE-CZ-NH1	5.87	123.24	120.30
2	3	27	THR	CA-CB-CG2	-5.87	104.18	112.40
2	l	106	TYR	CG-CD1-CE1	5.87	126.00	121.30
1	E	88	LEU	CB-CG-CD1	5.87	120.98	111.00
1	G	23	GLN	CA-CB-CG	5.87	126.32	113.40
2	3	196	PHE	CB-CG-CD1	5.87	124.91	120.80
2	k	62	ASP	CB-CG-OD1	5.87	123.58	118.30
3	L	397	PHE	CB-CG-CD2	5.87	124.91	120.80
1	c	186	ASP	CB-CG-OD2	5.87	123.58	118.30
1	B	186	ASP	CB-CG-OD2	-5.87	113.02	118.30
1	b	129	VAL	CG1-CB-CG2	5.86	120.28	110.90
1	D	118	ASP	N-CA-CB	5.86	121.15	110.60
1	F	241	ARG	NH1-CZ-NH2	5.86	125.85	119.40
2	5	23	VAL	N-CA-C	-5.86	95.19	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	304	ASP	CB-CG-OD1	5.86	123.57	118.30
3	L	15	LYS	O-C-N	5.85	132.07	122.70
1	d	239	ARG	NE-CZ-NH1	-5.85	117.37	120.30
1	c	20	ARG	C-N-CA	5.85	136.33	121.70
1	a	91	ARG	NE-CZ-NH2	-5.85	117.38	120.30
1	d	26	TYR	CB-CG-CD2	5.85	124.51	121.00
2	5	134	GLU	N-CA-CB	5.84	121.12	110.60
2	k	155	PHE	CB-CG-CD1	5.84	124.89	120.80
2	j	36	PHE	CB-CG-CD2	-5.84	116.71	120.80
3	K	95	ILE	N-CA-C	-5.84	95.23	111.00
1	A	219	ARG	NE-CZ-NH2	5.84	123.22	120.30
2	m	212	ARG	CB-CA-C	-5.84	98.73	110.40
2	n	194	ASP	CB-CA-C	-5.84	98.73	110.40
1	e	10	ARG	NE-CZ-NH2	5.83	123.22	120.30
2	n	170	ARG	CD-NE-CZ	-5.83	115.44	123.60
3	L	328	MET	CA-CB-CG	5.83	123.21	113.30
2	k	103	TYR	CB-CG-CD1	-5.83	117.50	121.00
2	k	177	LYS	N-CA-CB	5.83	121.09	110.60
3	K	239	PHE	CG-CD1-CE1	-5.83	114.39	120.80
1	e	46	VAL	N-CA-C	-5.82	95.29	111.00
1	G	53	ARG	NE-CZ-NH2	5.82	123.21	120.30
2	5	212	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	C	88	LEU	CB-CG-CD1	5.82	120.89	111.00
1	G	22	PHE	CB-CG-CD1	-5.82	116.73	120.80
1	G	26	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	g	130	ARG	NE-CZ-NH2	-5.82	117.39	120.30
1	E	129	VAL	N-CA-C	-5.81	95.31	111.00
2	l	37	ILE	O-C-N	-5.80	113.41	122.70
1	c	20	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	2	205	GLU	OE1-CD-OE2	5.80	130.26	123.30
1	d	84	ASP	CB-CG-OD1	-5.80	113.08	118.30
1	g	20	ARG	NE-CZ-NH1	5.80	123.20	120.30
3	K	241	ASP	CB-CG-OD1	5.80	123.52	118.30
1	G	26	TYR	CB-CG-CD2	5.80	124.48	121.00
2	k	30	ARG	NE-CZ-NH2	-5.80	117.40	120.30
2	5	152	GLU	O-C-N	-5.80	113.42	122.70
3	I	119	LEU	CB-CA-C	-5.79	99.19	110.20
2	l	102	ARG	NE-CZ-NH1	5.79	123.19	120.30
2	h	191	ILE	N-CA-C	-5.79	95.37	111.00
1	a	20	ARG	NE-CZ-NH1	-5.78	117.41	120.30
3	L	101	LYS	N-CA-CB	5.78	121.00	110.60
2	n	123	TYR	O-C-N	5.78	131.94	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	I	142	ASP	CB-CG-OD1	5.78	123.50	118.30
1	A	132	PHE	CB-CG-CD1	-5.77	116.76	120.80
3	L	44	TYR	CB-CG-CD1	-5.77	117.53	121.00
2	l	184	ASP	CB-CG-OD2	-5.77	113.11	118.30
2	6	148	TYR	CD1-CE1-CZ	5.77	124.99	119.80
1	B	144	VAL	CG1-CB-CG2	-5.77	101.67	110.90
1	c	18	ASP	N-CA-CB	5.77	120.98	110.60
2	2	154	ARG	NE-CZ-NH1	-5.77	117.42	120.30
2	j	178	ARG	NE-CZ-NH2	-5.77	117.42	120.30
2	4	77	TYR	CD1-CE1-CZ	-5.77	114.61	119.80
1	b	84	ASP	CB-CG-OD1	5.77	123.49	118.30
3	J	299	ARG	NE-CZ-NH1	-5.77	117.42	120.30
2	5	152	GLU	CA-C-N	5.76	129.88	117.20
2	l	100	SER	N-CA-CB	5.76	119.15	110.50
2	k	136	ASP	CB-CG-OD1	-5.76	113.12	118.30
1	b	175	PHE	CB-CG-CD2	-5.76	116.77	120.80
1	e	61	ALA	N-CA-CB	-5.76	102.04	110.10
2	n	101	TYR	CG-CD2-CE2	5.76	125.91	121.30
3	H	49	ARG	NE-CZ-NH2	-5.75	117.42	120.30
1	E	221	PHE	CZ-CE2-CD2	5.75	127.00	120.10
1	e	199	SER	N-CA-CB	5.75	119.13	110.50
1	c	15	PHE	CB-CG-CD1	-5.75	116.78	120.80
3	I	126	MET	CG-SD-CE	5.75	109.40	100.20
1	C	213	TYR	CG-CD2-CE2	-5.75	116.70	121.30
2	l	128	ILE	CA-CB-CG1	5.74	121.91	111.00
2	m	135	LYS	N-CA-CB	5.74	120.94	110.60
3	K	280	ASP	N-CA-C	-5.74	95.49	111.00
3	M	200	ARG	NE-CZ-NH1	-5.74	117.43	120.30
3	L	212	VAL	N-CA-CB	5.74	124.13	111.50
1	b	119	PHE	CB-CG-CD2	-5.74	116.78	120.80
2	7	21	ASP	CB-CG-OD1	5.74	123.47	118.30
3	I	67	VAL	N-CA-C	-5.74	95.51	111.00
3	I	154	ARG	NE-CZ-NH1	-5.74	117.43	120.30
3	K	261	VAL	CG1-CB-CG2	-5.74	101.72	110.90
2	k	181	ALA	CB-CA-C	-5.74	101.50	110.10
1	g	123	TYR	CG-CD1-CE1	-5.74	116.71	121.30
1	g	232	TYR	CB-CG-CD2	-5.74	117.56	121.00
2	i	199	TYR	CB-CG-CD1	-5.73	117.56	121.00
2	5	148	TYR	CG-CD2-CE2	5.73	125.88	121.30
1	B	239	ARG	NE-CZ-NH2	-5.73	117.44	120.30
2	5	161	VAL	CA-CB-CG1	-5.72	102.31	110.90
2	j	196	PHE	N-CA-C	-5.72	95.55	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	J	238	ILE	O-C-N	-5.72	113.55	122.70
1	F	11	ALA	N-CA-CB	5.72	118.11	110.10
3	J	305	ARG	NE-CZ-NH1	-5.72	117.44	120.30
2	3	80	ARG	NE-CZ-NH1	5.72	123.16	120.30
3	H	119	LEU	CB-CG-CD2	5.72	120.72	111.00
2	4	198	GLN	N-CA-C	-5.72	95.57	111.00
2	n	80	ARG	NE-CZ-NH1	-5.71	117.44	120.30
3	L	252	ASN	N-CA-CB	5.71	120.88	110.60
1	c	128	GLY	O-C-N	-5.71	113.56	122.70
3	M	304	ASP	N-CA-CB	5.71	120.88	110.60
3	I	121	THR	C-N-CA	5.71	135.97	121.70
3	I	304	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	g	56	SER	N-CA-CB	5.70	119.05	110.50
3	K	192	ALA	N-CA-CB	5.70	118.08	110.10
3	M	20	TYR	CG-CD1-CE1	5.70	125.86	121.30
1	f	14	VAL	CA-CB-CG2	5.69	119.44	110.90
3	M	59	ARG	NE-CZ-NH2	-5.69	117.45	120.30
2	2	196	PHE	CB-CG-CD1	5.69	124.78	120.80
3	L	77	VAL	CA-CB-CG2	5.69	119.44	110.90
1	e	54	VAL	C-N-CA	5.69	134.25	122.30
2	2	14	THR	CA-CB-CG2	-5.69	104.43	112.40
2	3	52	MET	N-CA-C	-5.69	95.64	111.00
2	6	49	ALA	N-CA-CB	5.69	118.06	110.10
1	g	219	ARG	NE-CZ-NH2	-5.69	117.46	120.30
2	i	153	ASP	CB-CG-OD2	5.69	123.42	118.30
1	a	189	MET	CA-CB-CG	5.69	122.97	113.30
1	C	219	ARG	NE-CZ-NH1	5.68	123.14	120.30
2	n	47	GLN	N-CA-CB	5.68	120.83	110.60
2	m	36	PHE	CB-CG-CD1	-5.68	116.82	120.80
3	L	302	ARG	NE-CZ-NH1	-5.68	117.46	120.30
1	b	194	VAL	CA-CB-CG1	5.68	119.42	110.90
1	B	187	ASP	CB-CA-C	-5.68	99.04	110.40
2	l	148	TYR	CB-CG-CD2	-5.68	117.59	121.00
3	I	130	PHE	CB-CG-CD2	5.68	124.78	120.80
1	D	233	VAL	CA-CB-CG2	-5.68	102.38	110.90
1	G	185	PHE	CB-CG-CD2	-5.68	116.83	120.80
2	j	21	ASP	CB-CG-OD1	-5.68	113.19	118.30
2	4	68	ARG	NE-CZ-NH1	5.68	123.14	120.30
1	C	175	PHE	CB-CG-CD1	5.67	124.77	120.80
3	K	105	ARG	NE-CZ-NH2	-5.67	117.47	120.30
3	K	205	ARG	CG-CD-NE	-5.66	99.91	111.80
3	M	65	VAL	CA-CB-CG1	5.66	119.39	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	d	161	ALA	CB-CA-C	-5.66	101.61	110.10
1	B	159	TYR	CB-CG-CD2	-5.66	117.61	121.00
1	g	76	ALA	CB-CA-C	-5.66	101.62	110.10
2	4	52	MET	CG-SD-CE	-5.66	91.15	100.20
2	5	102	ARG	NE-CZ-NH2	-5.66	117.47	120.30
1	B	134	VAL	CA-CB-CG2	-5.65	102.42	110.90
2	m	80	ARG	NE-CZ-NH1	-5.65	117.47	120.30
2	j	103	TYR	CG-CD2-CE2	-5.65	116.78	121.30
3	L	309	VAL	CA-CB-CG2	-5.65	102.42	110.90
1	D	244	LEU	CB-CG-CD2	5.65	120.60	111.00
1	f	151	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	B	103	TYR	CB-CG-CD1	5.65	124.39	121.00
2	1	173	TYR	CZ-CE2-CD2	5.65	124.88	119.80
2	j	108	VAL	CA-CB-CG1	5.65	119.37	110.90
1	f	100	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	2	178	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	b	86	ARG	NE-CZ-NH1	-5.64	117.48	120.30
1	f	103	TYR	CG-CD1-CE1	5.64	125.81	121.30
3	K	302	ARG	NE-CZ-NH2	-5.64	117.48	120.30
2	1	154	ARG	NE-CZ-NH2	5.64	123.12	120.30
2	i	118	GLU	CB-CA-C	-5.64	99.12	110.40
3	H	215	TYR	CD1-CE1-CZ	-5.63	114.73	119.80
3	I	248	ALA	N-CA-CB	5.63	117.98	110.10
1	G	14	VAL	CA-CB-CG2	-5.63	102.46	110.90
2	5	112	ILE	N-CA-CB	5.63	123.74	110.80
2	6	77	TYR	CG-CD2-CE2	5.63	125.80	121.30
1	f	216	VAL	CA-CB-CG1	5.62	119.34	110.90
1	C	239	ARG	NE-CZ-NH2	5.62	123.11	120.30
1	f	219	ARG	CD-NE-CZ	-5.62	115.73	123.60
2	5	189	VAL	N-CA-CB	5.62	123.86	111.50
3	L	95	ILE	CA-CB-CG1	5.62	121.67	111.00
3	I	255	THR	CA-CB-CG2	-5.61	104.54	112.40
1	D	10	ARG	NE-CZ-NH1	5.61	123.11	120.30
2	n	178	ARG	NE-CZ-NH1	5.61	123.11	120.30
1	E	40	ILE	N-CA-C	-5.61	95.86	111.00
3	M	242	GLU	CA-CB-CG	5.61	125.73	113.40
2	5	56	THR	CA-CB-CG2	-5.60	104.55	112.40
2	1	101	TYR	CB-CG-CD1	5.60	124.36	121.00
3	M	235	PRO	N-CA-CB	5.60	110.02	103.30
3	J	59	ARG	N-CA-CB	5.60	120.68	110.60
3	J	302	ARG	NE-CZ-NH2	-5.60	117.50	120.30
3	H	29	ARG	NE-CZ-NH1	-5.60	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	2	212	ARG	NE-CZ-NH1	-5.59	117.50	120.30
1	B	104	ASP	CB-CG-OD2	-5.59	113.27	118.30
1	E	120	LYS	CB-CG-CD	5.59	126.14	111.60
1	E	124	THR	CA-CB-CG2	-5.59	104.57	112.40
1	G	137	LEU	N-CA-C	-5.59	95.91	111.00
3	H	335	ASP	CB-CG-OD1	-5.59	113.27	118.30
1	D	51	ASP	CB-CG-OD1	5.59	123.33	118.30
3	M	21	TYR	CG-CD1-CE1	-5.59	116.83	121.30
1	d	62	ASP	CB-CG-OD2	-5.59	113.27	118.30
2	h	136	ASP	CB-CG-OD1	-5.59	113.27	118.30
3	H	314	PHE	CB-CG-CD1	-5.59	116.89	120.80
2	m	148	TYR	CB-CG-CD2	-5.58	117.65	121.00
2	i	162	ASP	O-C-N	-5.58	113.77	122.70
1	C	68	TYR	CG-CD1-CE1	-5.58	116.84	121.30
3	K	255	THR	N-CA-CB	5.58	120.90	110.30
2	2	36	PHE	CB-CG-CD2	-5.58	116.89	120.80
2	n	134	GLU	N-CA-C	-5.58	95.94	111.00
2	3	51	ARG	O-C-N	-5.58	113.78	122.70
3	I	134	GLU	OE1-CD-OE2	5.58	129.99	123.30
2	3	187	ASP	CB-CG-OD2	5.57	123.31	118.30
2	6	42	ALA	N-CA-CB	5.57	117.90	110.10
1	G	150	THR	CA-CB-OG1	-5.57	97.31	109.00
1	f	241	ARG	NH1-CZ-NH2	5.57	125.52	119.40
1	g	11	ALA	CB-CA-C	5.57	118.45	110.10
2	6	53	ALA	N-CA-CB	5.57	117.89	110.10
2	n	196	PHE	N-CA-C	-5.57	95.97	111.00
1	E	218	ASP	CB-CG-OD1	5.56	123.31	118.30
3	K	295	PRO	N-CA-CB	5.56	109.97	103.30
1	c	22	PHE	CB-CG-CD2	-5.56	116.91	120.80
1	A	15	PHE	CB-CG-CD2	-5.56	116.91	120.80
3	L	254	ASP	O-C-N	-5.56	113.81	122.70
1	B	199	SER	N-CA-CB	5.56	118.83	110.50
3	H	76	ARG	NE-CZ-NH2	-5.55	117.52	120.30
2	i	39	SER	N-CA-CB	5.55	118.83	110.50
2	4	196	PHE	N-CA-C	-5.55	96.01	111.00
3	L	373	LEU	CB-CG-CD1	-5.55	101.57	111.00
1	D	137	LEU	CB-CA-C	-5.55	99.66	110.20
2	1	199	TYR	CG-CD1-CE1	5.55	125.74	121.30
3	I	19	ASP	O-C-N	5.55	131.57	122.70
3	L	41	ARG	NE-CZ-NH2	5.55	123.07	120.30
3	I	358	ALA	N-CA-CB	5.54	117.86	110.10
2	7	197	TYR	CG-CD2-CE2	-5.54	116.87	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	K	28	ARG	CG-CD-NE	-5.54	100.16	111.80
2	7	37	ILE	N-CA-C	-5.54	96.04	111.00
3	M	70	ASP	CB-CG-OD2	-5.54	113.32	118.30
2	3	110	LEU	CB-CA-C	-5.54	99.68	110.20
2	j	154	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
3	H	278	ARG	N-CA-CB	5.54	120.56	110.60
2	m	196	PHE	CB-CG-CD1	-5.53	116.93	120.80
3	M	124	ASP	CB-CG-OD1	5.53	123.28	118.30
2	4	46	TYR	CB-CG-CD1	-5.53	117.68	121.00
3	M	258	ASP	N-CA-CB	5.53	120.55	110.60
1	D	174	PHE	CB-CG-CD2	-5.53	116.93	120.80
2	5	47	GLN	O-C-N	-5.53	113.86	122.70
2	i	123	TYR	CG-CD1-CE1	5.52	125.72	121.30
2	l	66	LEU	CB-CG-CD1	5.52	120.39	111.00
2	h	55	THR	CA-CB-CG2	-5.52	104.67	112.40
3	M	43	ARG	O-C-N	5.52	131.53	122.70
1	D	239	ARG	NE-CZ-NH2	-5.52	117.54	120.30
2	i	23	VAL	N-CA-C	-5.52	96.10	111.00
1	g	132	PHE	CB-CG-CD2	-5.51	116.94	120.80
2	h	77	TYR	CD1-CG-CD2	-5.51	111.83	117.90
2	7	136	ASP	CB-CG-OD1	5.51	123.26	118.30
2	k	18	VAL	CG1-CB-CG2	-5.51	102.09	110.90
2	l	27	THR	CA-CB-CG2	-5.51	104.69	112.40
2	1	33	MET	CB-CA-C	-5.50	99.39	110.40
2	1	101	TYR	CG-CD1-CE1	-5.50	116.90	121.30
2	7	62	ASP	CB-CG-OD1	-5.50	113.35	118.30
3	K	239	PHE	CD1-CG-CD2	5.50	125.45	118.30
1	g	10	ARG	NH1-CZ-NH2	-5.50	113.35	119.40
2	k	179	ASP	N-CA-CB	5.50	120.50	110.60
2	4	196	PHE	N-CA-CB	5.50	120.49	110.60
3	M	236	SER	N-CA-CB	5.50	118.74	110.50
1	E	132	PHE	CG-CD1-CE1	-5.50	114.75	120.80
3	K	87	PHE	CB-CG-CD2	-5.50	116.95	120.80
3	K	181	TYR	CG-CD1-CE1	-5.50	116.90	121.30
3	H	178	VAL	N-CA-C	-5.49	96.17	111.00
3	M	27	TYR	CB-CA-C	-5.49	99.42	110.40
1	A	36	THR	CA-CB-OG1	5.49	120.53	109.00
2	4	103	TYR	N-CA-CB	5.49	120.48	110.60
1	a	206	PRO	O-C-N	5.49	131.48	122.70
2	6	86	THR	CA-CB-CG2	-5.49	104.72	112.40
1	B	28	ARG	NE-CZ-NH1	5.48	123.04	120.30
1	b	21	LEU	CB-CG-CD2	-5.48	101.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	95	GLU	OE1-CD-OE2	-5.48	116.72	123.30
3	L	262	GLN	CG-CD-OE1	5.48	132.56	121.60
2	4	187	ASP	CB-CG-OD1	-5.48	113.37	118.30
3	K	20	TYR	CG-CD2-CE2	-5.48	116.92	121.30
2	i	196	PHE	N-CA-C	-5.48	96.21	111.00
1	A	31	VAL	CA-CB-CG2	-5.48	102.68	110.90
2	h	148	TYR	CB-CG-CD2	-5.48	117.71	121.00
1	e	132	PHE	CB-CG-CD1	-5.47	116.97	120.80
3	L	391	ASP	CB-CG-OD2	-5.47	113.38	118.30
3	M	317	ARG	NH1-CZ-NH2	5.47	125.42	119.40
2	5	21	ASP	CB-CG-OD2	-5.47	113.38	118.30
1	d	68	TYR	CB-CG-CD1	-5.46	117.72	121.00
1	F	123	TYR	CZ-CE2-CD2	5.46	124.72	119.80
2	5	51	ARG	NE-CZ-NH2	5.46	123.03	120.30
1	f	180	ARG	NE-CZ-NH2	5.46	123.03	120.30
2	6	54	MET	CG-SD-CE	5.46	108.94	100.20
2	7	51	ARG	NE-CZ-NH1	5.46	123.03	120.30
3	M	362	ALA	N-CA-CB	5.46	117.75	110.10
2	m	33	MET	N-CA-C	-5.46	96.26	111.00
1	E	115	LYS	O-C-N	-5.46	113.97	122.70
1	B	65	GLU	CB-CA-C	5.46	121.31	110.40
3	I	19	ASP	CB-CG-OD2	-5.46	113.39	118.30
2	1	36	PHE	CB-CG-CD2	-5.46	116.98	120.80
1	g	141	VAL	N-CA-C	-5.45	96.28	111.00
2	5	95	SER	N-CA-CB	5.45	118.68	110.50
2	n	102	ARG	CD-NE-CZ	-5.45	115.97	123.60
2	n	163	GLU	C-N-CA	5.45	135.32	121.70
1	a	20	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	F	26	TYR	CG-CD2-CE2	-5.45	116.94	121.30
2	7	178	ARG	NE-CZ-NH1	5.45	123.02	120.30
1	F	41	LYS	N-CA-CB	5.45	120.41	110.60
2	6	80	ARG	NE-CZ-NH1	-5.44	117.58	120.30
3	L	105	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	C	130	ARG	NH1-CZ-NH2	-5.44	113.41	119.40
2	i	184	ASP	CB-CG-OD1	5.44	123.20	118.30
2	6	87	VAL	CA-CB-CG2	-5.44	102.74	110.90
3	J	190	LEU	CB-CG-CD1	5.44	120.25	111.00
1	d	155	ALA	CB-CA-C	-5.44	101.94	110.10
1	f	168	ARG	NE-CZ-NH2	-5.44	117.58	120.30
2	n	179	ASP	CB-CG-OD1	-5.44	113.41	118.30
1	E	37	ALA	N-CA-CB	5.43	117.71	110.10
3	J	50	ARG	NE-CZ-NH2	-5.43	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	179	TYR	CG-CD1-CE1	-5.43	116.96	121.30
3	L	23	LEU	C-N-CA	5.43	135.27	121.70
3	M	312	PRO	N-CA-CB	5.43	109.81	103.30
1	a	105	GLU	OE1-CD-OE2	5.43	129.81	123.30
3	I	330	LEU	N-CA-CB	5.43	121.25	110.40
3	M	324	HIS	C-N-CA	5.43	135.26	121.70
1	A	76	ALA	C-N-CA	5.42	135.26	121.70
1	C	15	PHE	CB-CG-CD2	5.42	124.60	120.80
1	D	179	TYR	CG-CD2-CE2	-5.42	116.96	121.30
2	k	103	TYR	CD1-CG-CD2	5.42	123.87	117.90
1	A	53	ARG	NE-CZ-NH1	5.42	123.01	120.30
1	g	18	ASP	CB-CG-OD1	-5.42	113.42	118.30
3	K	49	ARG	CG-CD-NE	-5.42	100.42	111.80
2	4	45	ILE	N-CA-C	-5.42	96.37	111.00
2	k	134	GLU	OE1-CD-OE2	5.42	129.80	123.30
2	2	197	TYR	CG-CD2-CE2	-5.42	116.97	121.30
3	H	259	ARG	NE-CZ-NH2	-5.41	117.59	120.30
3	L	100	LEU	CB-CG-CD2	5.41	120.20	111.00
2	3	188	VAL	O-C-N	-5.41	114.04	122.70
2	i	33	MET	N-CA-C	-5.41	96.40	111.00
1	B	136	LEU	CB-CG-CD1	5.40	120.19	111.00
1	E	84	ASP	CB-CG-OD1	-5.40	113.44	118.30
2	2	162	ASP	CB-CG-OD1	-5.40	113.44	118.30
3	I	294	ASP	CB-CA-C	-5.40	99.60	110.40
3	I	137	GLU	N-CA-CB	5.40	120.32	110.60
3	M	24	ARG	NE-CZ-NH2	5.40	123.00	120.30
3	M	226	VAL	CA-CB-CG2	-5.40	102.80	110.90
3	H	202	THR	O-C-N	-5.40	114.06	122.70
1	d	21	LEU	CB-CG-CD1	5.40	120.18	111.00
1	C	244	LEU	CB-CG-CD2	5.40	120.17	111.00
2	2	77	TYR	CB-CG-CD2	-5.40	117.76	121.00
3	I	278	ARG	NE-CZ-NH2	-5.40	117.60	120.30
1	g	134	VAL	CA-CB-CG1	5.39	118.99	110.90
1	E	62	ASP	CB-CG-OD2	5.39	123.15	118.30
2	6	20	LYS	N-CA-CB	5.39	120.30	110.60
1	a	179	TYR	CB-CG-CD2	5.39	124.23	121.00
1	F	156	LEU	CB-CG-CD1	5.39	120.16	111.00
2	1	204	VAL	CA-CB-CG2	-5.39	102.82	110.90
2	l	193	GLU	N-CA-CB	5.39	120.30	110.60
1	f	124	THR	CA-CB-CG2	5.38	119.94	112.40
3	L	61	PRO	N-CD-CG	5.38	111.28	103.20
1	g	68	TYR	CD1-CE1-CZ	5.38	124.64	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	350	ASP	CB-CG-OD1	-5.38	113.45	118.30
1	d	104	ASP	CB-CG-OD2	5.38	123.14	118.30
1	E	28	ARG	NE-CZ-NH1	5.38	122.99	120.30
1	F	168	ARG	NE-CZ-NH2	-5.38	117.61	120.30
2	n	98	LEU	CB-CG-CD2	5.38	120.14	111.00
3	I	203	PHE	CB-CG-CD2	5.38	124.56	120.80
2	2	148	TYR	CB-CG-CD2	5.38	124.22	121.00
2	j	106	TYR	CB-CG-CD1	5.38	124.23	121.00
1	b	33	ARG	NE-CZ-NH2	5.38	122.99	120.30
2	1	144	SER	N-CA-CB	5.37	118.56	110.50
3	M	94	TYR	CG-CD2-CE2	-5.37	117.00	121.30
1	f	116	ILE	CA-CB-CG2	-5.37	100.17	110.90
2	n	213	LYS	CA-CB-CG	5.36	125.19	113.40
1	f	217	ASP	CB-CG-OD2	5.36	123.12	118.30
2	5	46	TYR	CG-CD2-CE2	-5.36	117.01	121.30
2	3	148	TYR	CZ-CE2-CD2	5.36	124.62	119.80
3	I	20	TYR	CG-CD2-CE2	-5.36	117.02	121.30
3	K	14	LYS	CA-CB-CG	5.36	125.18	113.40
1	b	36	THR	CA-CB-CG2	-5.35	104.91	112.40
3	H	107	ALA	CB-CA-C	-5.35	102.07	110.10
3	K	270	ALA	CB-CA-C	-5.35	102.07	110.10
1	d	187	ASP	CB-CG-OD1	5.35	123.11	118.30
3	K	199	THR	CA-CB-CG2	-5.35	104.92	112.40
3	K	201	ALA	CB-CA-C	-5.35	102.08	110.10
2	6	81	ARG	NE-CZ-NH2	-5.34	117.63	120.30
1	C	180	ARG	NE-CZ-NH1	-5.34	117.63	120.30
2	k	104	PHE	N-CA-C	-5.34	96.58	111.00
1	c	62	ASP	CB-CG-OD2	-5.34	113.50	118.30
1	e	46	VAL	CG1-CB-CG2	5.34	119.44	110.90
2	2	118	GLU	CG-CD-OE1	5.34	128.98	118.30
3	M	375	PHE	CB-CG-CD1	-5.34	117.06	120.80
3	L	88	VAL	CG1-CB-CG2	-5.34	102.36	110.90
1	D	159	TYR	O-C-N	5.34	131.24	122.70
3	H	146	LEU	CB-CG-CD1	5.34	120.07	111.00
1	B	232	TYR	CA-CB-CG	-5.33	103.26	113.40
2	j	176	MET	CG-SD-CE	-5.33	91.66	100.20
3	H	287	THR	N-CA-C	-5.33	96.59	111.00
1	B	118	ASP	CB-CG-OD2	-5.33	113.50	118.30
2	m	165	VAL	CA-CB-CG1	-5.33	102.90	110.90
3	I	112	THR	CA-CB-CG2	-5.33	104.94	112.40
1	a	65	GLU	N-CA-CB	5.33	120.19	110.60
1	B	22	PHE	N-CA-CB	5.33	120.19	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	232	TYR	CB-CG-CD2	-5.32	117.81	121.00
1	c	181	ASP	CA-CB-CG	-5.32	101.69	113.40
3	K	133	GLU	C-N-CA	5.32	135.00	121.70
1	b	144	VAL	N-CA-C	-5.32	96.64	111.00
1	e	155	ALA	N-CA-C	-5.32	96.64	111.00
1	b	159	TYR	CG-CD2-CE2	-5.32	117.05	121.30
1	E	168	ARG	NE-CZ-NH2	-5.32	117.64	120.30
1	g	72	GLU	OE1-CD-OE2	5.32	129.68	123.30
3	M	36	PHE	CB-CG-CD1	-5.32	117.08	120.80
1	g	151	ASP	CB-CG-OD1	-5.31	113.52	118.30
2	7	25	MET	CG-SD-CE	-5.31	91.70	100.20
2	1	85	PRO	N-CA-CB	5.31	109.67	103.30
3	I	85	PRO	O-C-N	5.31	131.20	122.70
1	B	201	GLU	N-CA-CB	5.31	120.16	110.60
2	2	87	VAL	CA-CB-CG1	-5.31	102.93	110.90
1	G	179	TYR	CB-CG-CD2	5.31	124.19	121.00
2	3	30	ARG	N-CA-CB	5.31	120.16	110.60
3	M	289	ARG	NH1-CZ-NH2	-5.31	113.56	119.40
3	J	276	ASP	CB-CG-OD1	5.31	123.08	118.30
1	f	218	ASP	CB-CG-OD1	5.31	123.08	118.30
3	H	302	ARG	N-CA-CB	5.31	120.15	110.60
1	b	77	ALA	N-CA-CB	5.31	117.53	110.10
2	5	191	ILE	N-CA-CB	5.31	123.00	110.80
2	2	123	TYR	CB-CG-CD1	5.30	124.18	121.00
2	4	112	ILE	O-C-N	-5.30	114.18	123.20
3	I	280	ASP	CB-CG-OD1	5.30	123.07	118.30
3	H	270	ALA	N-CA-CB	5.30	117.52	110.10
1	d	205	VAL	CA-CB-CG1	-5.30	102.95	110.90
2	5	196	PHE	N-CA-C	-5.30	96.69	111.00
3	M	398	VAL	CA-C-O	-5.30	108.97	120.10
1	c	117	CYS	N-CA-CB	5.30	120.14	110.60
2	5	173	TYR	CZ-CE2-CD2	-5.30	115.03	119.80
3	H	211	PHE	CB-CG-CD1	5.30	124.51	120.80
1	E	22	PHE	CB-CG-CD2	5.30	124.51	120.80
1	G	131	PRO	N-CA-CB	5.30	109.66	103.30
3	K	398	VAL	CA-C-O	-5.30	108.98	120.10
2	3	197	TYR	CA-CB-CG	5.29	123.46	113.40
1	A	88	LEU	CB-CG-CD2	-5.29	102.00	111.00
2	m	55	THR	N-CA-CB	5.29	120.36	110.30
3	L	398	VAL	CA-C-O	-5.29	108.98	120.10
1	A	159	TYR	CG-CD2-CE2	-5.29	117.07	121.30
2	m	88	ARG	NE-CZ-NH1	-5.29	117.65	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	e	30	ALA	CB-CA-C	-5.29	102.16	110.10
2	1	83	ARG	NE-CZ-NH2	-5.29	117.66	120.30
3	H	220	ALA	N-CA-CB	5.29	117.50	110.10
3	J	398	VAL	CA-C-O	-5.29	108.99	120.10
1	f	130	ARG	NE-CZ-NH2	-5.29	117.66	120.30
3	H	398	VAL	CA-C-O	-5.29	109.00	120.10
3	M	62	PRO	N-CA-CB	5.29	109.64	103.30
3	M	65	VAL	CA-CB-CG2	-5.29	102.97	110.90
1	A	93	ARG	NE-CZ-NH1	5.28	122.94	120.30
1	a	53	ARG	NE-CZ-NH2	5.28	122.94	120.30
1	B	217	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	E	193	LEU	CB-CG-CD1	5.28	119.98	111.00
1	D	241	ARG	NE-CZ-NH1	-5.28	117.66	120.30
1	e	15	PHE	CB-CG-CD2	5.28	124.50	120.80
2	h	111	LEU	N-CA-C	-5.28	96.75	111.00
1	e	233	VAL	CA-CB-CG1	5.28	118.81	110.90
3	I	398	VAL	CA-C-O	-5.28	109.02	120.10
3	M	212	VAL	CA-CB-CG2	5.27	118.81	110.90
1	F	178	GLU	OE1-CD-OE2	5.27	129.63	123.30
2	2	43	LYS	CB-CA-C	-5.27	99.86	110.40
3	I	123	LYS	N-CA-CB	5.27	120.09	110.60
3	I	196	ALA	N-CA-CB	5.27	117.48	110.10
1	C	86	ARG	NE-CZ-NH2	5.27	122.94	120.30
1	D	150	THR	CA-CB-CG2	-5.27	105.02	112.40
1	c	185	PHE	CB-CG-CD2	-5.27	117.11	120.80
3	L	162	LEU	CB-CG-CD2	5.27	119.96	111.00
2	k	14	THR	CA-CB-CG2	-5.26	105.03	112.40
3	I	250	ARG	NH1-CZ-NH2	-5.26	113.61	119.40
1	B	182	ASP	CB-CA-C	-5.26	99.87	110.40
1	B	44	GLU	CB-CA-C	-5.26	99.88	110.40
3	K	65	VAL	CA-CB-CG1	5.26	118.79	110.90
1	a	144	VAL	N-CA-C	-5.26	96.80	111.00
1	B	140	GLY	N-CA-C	-5.26	99.95	113.10
2	l	18	VAL	CA-CB-CG1	-5.26	103.01	110.90
1	g	214	VAL	N-CA-C	-5.26	96.80	111.00
3	H	367	ARG	NE-CZ-NH1	-5.26	117.67	120.30
1	a	37	ALA	N-CA-CB	5.25	117.46	110.10
1	C	67	ILE	N-CA-CB	5.25	122.89	110.80
1	F	185	PHE	CB-CG-CD1	5.25	124.48	120.80
2	4	189	VAL	CG1-CB-CG2	5.25	119.30	110.90
2	h	37	ILE	CG1-CB-CG2	5.25	122.95	111.40
3	L	155	GLU	OE1-CD-OE2	-5.25	117.00	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	H	203	PHE	N-CA-C	-5.25	96.82	111.00
3	I	146	LEU	C-N-CA	5.25	134.82	121.70
2	h	74	ALA	N-CA-CB	5.25	117.45	110.10
1	a	181	ASP	CB-CG-OD2	-5.25	113.58	118.30
3	K	336	PHE	N-CA-CB	5.25	120.05	110.60
1	B	18	ASP	CB-CG-OD2	-5.24	113.58	118.30
3	J	140	TYR	CB-CG-CD2	5.24	124.15	121.00
1	E	175	PHE	CG-CD2-CE2	-5.24	115.03	120.80
3	H	363	ILE	O-C-N	-5.24	114.31	122.70
2	i	100	SER	CB-CA-C	-5.24	100.14	110.10
3	H	374	ASP	N-CA-CB	5.24	120.03	110.60
3	K	349	ALA	N-CA-CB	5.24	117.44	110.10
3	K	205	ARG	N-CA-CB	5.24	120.03	110.60
1	B	159	TYR	CG-CD2-CE2	-5.24	117.11	121.30
1	G	240	ILE	N-CA-CB	5.24	122.84	110.80
1	G	161	ALA	N-CA-CB	5.23	117.43	110.10
1	D	100	ARG	NH1-CZ-NH2	-5.23	113.64	119.40
1	E	220	THR	N-CA-C	-5.23	96.87	111.00
1	g	217	ASP	O-C-N	5.23	131.07	122.70
3	K	397	PHE	N-CA-CB	5.23	120.01	110.60
3	M	282	LYS	N-CA-CB	5.23	120.02	110.60
2	7	51	ARG	NE-CZ-NH2	-5.23	117.69	120.30
3	M	314	PHE	CB-CG-CD2	5.23	124.46	120.80
1	c	239	ARG	NE-CZ-NH1	-5.23	117.69	120.30
1	d	28	ARG	NE-CZ-NH1	5.23	122.91	120.30
2	n	199	TYR	CG-CD1-CE1	5.23	125.48	121.30
2	3	162	ASP	CB-CA-C	-5.23	99.95	110.40
2	7	148	TYR	CB-CG-CD1	-5.22	117.87	121.00
1	D	28	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	5	68	ARG	NE-CZ-NH1	5.22	122.91	120.30
1	e	93	ARG	NE-CZ-NH1	-5.22	117.69	120.30
2	6	196	PHE	N-CA-C	-5.22	96.91	111.00
3	I	156	ALA	CB-CA-C	-5.22	102.27	110.10
2	2	173	TYR	CB-CG-CD2	5.22	124.13	121.00
2	i	83	ARG	NE-CZ-NH2	5.22	122.91	120.30
2	j	191	ILE	N-CA-C	-5.22	96.92	111.00
1	d	122	GLN	N-CA-CB	5.21	119.99	110.60
2	j	109	GLN	N-CA-CB	5.21	119.99	110.60
1	c	126	TYR	CZ-CE2-CD2	5.21	124.49	119.80
2	m	64	GLN	CB-CA-C	-5.21	99.97	110.40
3	L	29	ARG	NH1-CZ-NH2	5.21	125.14	119.40
2	j	179	ASP	N-CA-CB	5.21	119.98	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	G	48	LEU	CB-CG-CD2	-5.21	102.14	111.00
1	A	123	TYR	CB-CG-CD1	5.21	124.12	121.00
1	E	171	VAL	CA-CB-CG2	-5.21	103.09	110.90
1	f	73	HIS	CA-CB-CG	5.21	122.45	113.60
1	G	238	GLU	OE1-CD-OE2	5.21	129.54	123.30
1	d	194	VAL	CA-CB-CG2	-5.20	103.09	110.90
2	5	124	SER	N-CA-CB	5.20	118.30	110.50
3	I	155	GLU	O-C-N	5.20	131.02	122.70
2	h	67	ALA	N-CA-CB	5.20	117.38	110.10
2	3	63	ALA	N-CA-CB	5.20	117.38	110.10
2	m	23	VAL	CA-CB-CG2	5.20	118.70	110.90
2	m	201	PRO	O-C-N	5.19	131.01	122.70
3	M	239	PHE	CB-CG-CD1	5.19	124.43	120.80
1	g	139	ALA	O-C-N	5.19	132.02	123.20
1	d	12	ILE	C-N-CA	5.19	134.67	121.70
1	f	103	TYR	CB-CA-C	-5.19	100.03	110.40
2	6	197	TYR	CB-CG-CD2	5.19	124.11	121.00
3	H	21	TYR	CG-CD2-CE2	-5.19	117.15	121.30
2	4	38	ALA	N-CA-CB	5.18	117.36	110.10
3	H	19	ASP	O-C-N	-5.18	114.41	122.70
2	i	126	ASP	N-CA-CB	-5.18	101.27	110.60
3	J	280	ASP	CA-CB-CG	-5.18	102.00	113.40
3	J	298	LEU	CB-CG-CD2	5.18	119.81	111.00
1	e	123	TYR	CG-CD2-CE2	-5.18	117.16	121.30
2	2	15	VAL	CG1-CB-CG2	5.18	119.19	110.90
3	I	250	ARG	NE-CZ-NH1	5.18	122.89	120.30
1	d	40	ILE	CA-CB-CG1	5.18	120.84	111.00
2	h	95	SER	N-CA-CB	5.18	118.26	110.50
2	6	81	ARG	CB-CA-C	-5.18	100.05	110.40
2	n	170	ARG	CB-CA-C	5.18	120.75	110.40
2	k	148	TYR	CB-CG-CD2	-5.17	117.89	121.00
2	1	52	MET	CA-CB-CG	-5.17	104.51	113.30
3	H	107	ALA	N-CA-CB	5.17	117.34	110.10
3	K	294	ASP	CB-CG-OD2	-5.17	113.65	118.30
3	K	397	PHE	CB-CG-CD2	5.17	124.42	120.80
1	C	19	GLY	N-CA-C	-5.16	100.19	113.10
2	5	60	VAL	CA-CB-CG2	-5.16	103.16	110.90
2	5	118	GLU	CB-CA-C	-5.16	100.07	110.40
2	5	189	VAL	CA-CB-CG2	5.16	118.64	110.90
1	b	33	ARG	NE-CZ-NH1	5.16	122.88	120.30
1	d	196	MET	N-CA-CB	5.16	119.89	110.60
2	2	209	ALA	CB-CA-C	-5.16	102.36	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	92	ALA	CB-CA-C	-5.16	102.36	110.10
2	n	60	VAL	CA-CB-CG2	5.16	118.64	110.90
1	C	22	PHE	CB-CG-CD1	5.16	124.41	120.80
2	n	180	SER	N-CA-CB	5.16	118.23	110.50
2	4	102	ARG	NE-CZ-NH1	-5.15	117.72	120.30
2	k	136	ASP	CB-CA-C	5.15	120.71	110.40
1	c	230	LYS	CA-C-N	5.15	131.53	117.10
1	F	68	TYR	CG-CD1-CE1	-5.15	117.18	121.30
2	k	102	ARG	CD-NE-CZ	-5.15	116.39	123.60
2	7	152	GLU	N-CA-CB	5.15	119.87	110.60
2	n	103	TYR	CD1-CG-CD2	5.15	123.57	117.90
1	d	175	PHE	N-CA-CB	5.15	119.87	110.60
1	B	8	TYR	CD1-CE1-CZ	5.15	124.43	119.80
1	C	89	ILE	N-CA-CB	5.15	122.64	110.80
1	F	95	GLU	N-CA-CB	5.15	119.87	110.60
3	K	94	TYR	CG-CD1-CE1	-5.15	117.18	121.30
3	M	211	PHE	CB-CG-CD2	-5.15	117.20	120.80
2	1	197	TYR	CZ-CE2-CD2	5.14	124.43	119.80
3	K	20	TYR	CG-CD1-CE1	-5.14	117.18	121.30
1	A	8	TYR	CB-CG-CD1	5.14	124.08	121.00
1	e	14	VAL	N-CA-CB	5.14	122.81	111.50
2	2	112	ILE	N-CA-C	-5.14	97.11	111.00
3	H	265	MET	CG-SD-CE	-5.14	91.97	100.20
2	k	55	THR	CA-CB-CG2	-5.14	105.21	112.40
2	k	192	THR	O-C-N	5.14	130.92	122.70
2	m	173	TYR	CB-CG-CD2	5.14	124.08	121.00
3	K	142	ASP	CB-CG-OD2	5.14	122.92	118.30
3	M	135	LYS	CB-CA-C	5.14	120.68	110.40
3	I	100	LEU	N-CA-CB	5.13	120.67	110.40
1	A	51	ASP	CB-CG-OD1	5.13	122.92	118.30
2	3	27	THR	CA-CB-OG1	5.13	119.78	109.00
2	n	25	MET	CA-CB-CG	-5.13	104.57	113.30
1	b	64	ILE	O-C-N	5.13	130.91	122.70
1	c	194	VAL	CA-CB-CG1	5.13	118.60	110.90
2	l	112	ILE	N-CA-C	-5.13	97.15	111.00
2	6	55	THR	CA-CB-CG2	-5.13	105.22	112.40
3	J	28	ARG	CG-CD-NE	-5.13	101.03	111.80
1	g	123	TYR	CB-CG-CD2	5.13	124.08	121.00
1	d	216	VAL	CA-CB-CG1	5.13	118.59	110.90
3	K	16	LEU	CB-CG-CD2	5.13	119.72	111.00
2	h	81	ARG	NE-CZ-NH1	5.13	122.86	120.30
3	M	18	GLU	N-CA-CB	5.13	119.83	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	k	123	TYR	N-CA-CB	5.12	119.83	110.60
3	K	392	LEU	N-CA-CB	5.12	120.65	110.40
1	B	245	LYS	N-CA-CB	5.12	119.82	110.60
1	b	179	TYR	CD1-CE1-CZ	-5.12	115.19	119.80
1	G	67	ILE	N-CA-C	-5.12	97.17	111.00
3	M	250	ARG	NE-CZ-NH1	-5.12	117.74	120.30
1	A	16	SER	N-CA-CB	5.12	118.18	110.50
1	a	205	VAL	CA-CB-CG1	5.12	118.58	110.90
1	E	78	THR	CA-CB-CG2	5.12	119.57	112.40
1	e	213	TYR	CB-CG-CD2	-5.12	117.93	121.00
2	j	169	VAL	CG1-CB-CG2	-5.12	102.71	110.90
3	H	370	VAL	CG1-CB-CG2	-5.12	102.70	110.90
3	H	276	ASP	CB-CG-OD1	-5.12	113.69	118.30
3	I	305	ARG	NE-CZ-NH2	-5.12	117.74	120.30
1	f	180	ARG	NE-CZ-NH1	-5.11	117.74	120.30
2	5	36	PHE	CB-CG-CD1	5.11	124.38	120.80
1	G	147	LEU	N-CA-C	-5.11	97.20	111.00
2	k	187	ASP	CB-CG-OD1	5.11	122.90	118.30
1	C	20	ARG	O-C-N	-5.11	114.53	122.70
2	k	25	MET	N-CA-C	-5.11	97.20	111.00
2	h	173	TYR	CB-CG-CD1	5.11	124.06	121.00
2	l	199	TYR	N-CA-CB	5.11	119.79	110.60
2	k	199	TYR	CA-C-O	-5.11	109.38	120.10
2	m	109	GLN	N-CA-CB	5.11	119.79	110.60
3	I	384	LYS	O-C-N	5.10	130.87	122.70
2	h	196	PHE	CB-CG-CD1	-5.10	117.23	120.80
2	m	102	ARG	NH1-CZ-NH2	5.10	125.01	119.40
3	H	278	ARG	NH1-CZ-NH2	5.10	125.01	119.40
1	E	84	ASP	CB-CG-OD2	5.10	122.89	118.30
2	2	46	TYR	CA-CB-CG	-5.10	103.71	113.40
2	6	82	GLU	N-CA-CB	5.10	119.77	110.60
3	L	207	VAL	N-CA-C	-5.10	97.24	111.00
3	L	215	TYR	CG-CD1-CE1	-5.10	117.22	121.30
1	g	163	ALA	CB-CA-C	-5.09	102.46	110.10
2	h	173	TYR	O-C-N	-5.09	114.55	122.70
2	5	211	PHE	CB-CG-CD2	5.09	124.37	120.80
3	H	227	PHE	CB-CG-CD2	-5.09	117.23	120.80
3	K	299	ARG	N-CA-CB	5.09	119.77	110.60
3	M	76	ARG	NE-CZ-NH1	5.09	122.85	120.30
1	C	241	ARG	CB-CA-C	-5.09	100.21	110.40
1	e	168	ARG	NE-CZ-NH2	5.09	122.84	120.30
3	M	108	LEU	CB-CA-C	-5.09	100.53	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	j	24	VAL	CA-CB-CG2	-5.09	103.27	110.90
2	h	109	GLN	CB-CA-C	5.09	120.57	110.40
3	I	223	VAL	CA-CB-CG2	5.09	118.53	110.90
1	A	175	PHE	O-C-N	-5.08	114.57	122.70
1	E	20	ARG	NE-CZ-NH2	-5.08	117.76	120.30
2	h	53	ALA	N-CA-CB	5.08	117.22	110.10
1	C	28	ARG	NE-CZ-NH1	5.08	122.84	120.30
3	K	281	VAL	CG1-CB-CG2	5.08	119.03	110.90
3	H	324	HIS	CB-CA-C	-5.08	100.24	110.40
2	l	12	THR	N-CA-CB	5.08	119.94	110.30
2	4	35	ASN	N-CA-CB	5.08	119.74	110.60
1	e	238	GLU	N-CA-CB	5.07	119.73	110.60
1	F	168	ARG	NE-CZ-NH1	5.07	122.84	120.30
2	h	81	ARG	NE-CZ-NH2	-5.07	117.76	120.30
2	j	98	LEU	N-CA-CB	5.07	120.54	110.40
2	k	31	ALA	N-CA-CB	5.07	117.20	110.10
1	g	22	PHE	CG-CD2-CE2	5.07	126.38	120.80
2	5	49	ALA	N-CA-CB	5.07	117.20	110.10
2	5	112	ILE	N-CA-C	-5.07	97.31	111.00
1	C	93	ARG	NE-CZ-NH2	-5.07	117.77	120.30
2	l	191	ILE	N-CA-CB	5.07	122.46	110.80
1	C	6	MET	N-CA-C	-5.07	97.33	111.00
1	C	222	LYS	CB-CA-C	-5.06	100.27	110.40
1	b	62	ASP	CB-CG-OD1	5.06	122.86	118.30
2	n	175	ALA	CB-CA-C	-5.06	102.51	110.10
2	5	197	TYR	CB-CG-CD2	-5.06	117.96	121.00
3	H	251	THR	CA-CB-CG2	-5.06	105.32	112.40
3	K	34	LYS	O-C-N	-5.06	114.60	122.70
3	K	142	ASP	CB-CG-OD1	-5.06	113.75	118.30
1	e	202	SER	N-CA-CB	5.06	118.09	110.50
2	l	81	ARG	NE-CZ-NH2	5.06	122.83	120.30
3	K	258	ASP	CB-CG-OD1	5.06	122.85	118.30
1	b	220	THR	CA-CB-OG1	5.06	119.62	109.00
1	e	235	ARG	NE-CZ-NH2	5.05	122.83	120.30
2	n	47	GLN	O-C-N	-5.05	114.62	122.70
3	J	303	PHE	CB-CG-CD1	-5.05	117.26	120.80
1	f	129	VAL	CG1-CB-CG2	5.05	118.98	110.90
3	I	281	VAL	CA-C-N	5.05	128.31	117.20
3	L	57	ARG	NE-CZ-NH2	-5.05	117.78	120.30
1	G	118	ASP	CB-CG-OD1	5.04	122.84	118.30
2	k	201	PRO	N-CA-CB	5.04	109.35	103.30
2	7	123	TYR	CG-CD1-CE1	-5.04	117.27	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	f	237	ASN	N-CA-CB	5.04	119.68	110.60
2	4	118	GLU	CB-CA-C	-5.04	100.32	110.40
1	e	213	TYR	CD1-CE1-CZ	-5.04	115.27	119.80
1	D	220	THR	N-CA-C	-5.04	97.40	111.00
2	n	146	THR	CA-CB-CG2	-5.04	105.35	112.40
2	k	165	VAL	CA-CB-CG2	5.04	118.45	110.90
2	6	210	LYS	O-C-N	-5.04	114.64	122.70
2	7	28	GLU	N-CA-CB	5.04	119.67	110.60
2	n	110	LEU	CB-CG-CD1	5.04	119.56	111.00
3	H	203	PHE	CB-CA-C	5.04	120.47	110.40
1	D	53	ARG	NE-CZ-NH1	5.03	122.82	120.30
1	F	238	GLU	OE1-CD-OE2	-5.03	117.26	123.30
1	f	204	LEU	CB-CG-CD1	-5.03	102.44	111.00
1	G	65	GLU	N-CA-C	-5.03	97.41	111.00
2	i	56	THR	CA-CB-CG2	-5.03	105.35	112.40
2	5	111	LEU	N-CA-C	-5.03	97.41	111.00
1	F	71	ASP	CB-CG-OD2	-5.03	113.77	118.30
1	b	148	TYR	CB-CA-C	-5.03	100.34	110.40
1	d	55	GLY	C-N-CA	5.03	134.28	121.70
2	1	173	TYR	CB-CG-CD2	-5.03	117.98	121.00
2	4	56	THR	CA-CB-CG2	-5.03	105.36	112.40
3	M	289	ARG	CB-CA-C	-5.03	100.34	110.40
1	c	218	ASP	CB-CG-OD1	5.03	122.83	118.30
1	d	10	ARG	NE-CZ-NH1	5.03	122.81	120.30
2	3	208	LEU	N-CA-CB	-5.03	100.34	110.40
3	L	101	LYS	CA-CB-CG	5.03	124.46	113.40
1	B	155	ALA	CB-CA-C	-5.03	102.56	110.10
1	D	33	ARG	CB-CA-C	-5.03	100.35	110.40
3	H	286	ALA	N-CA-CB	5.03	117.14	110.10
3	I	130	PHE	CB-CA-C	-5.02	100.35	110.40
1	B	136	LEU	N-CA-CB	5.02	120.44	110.40
2	7	199	TYR	CG-CD1-CE1	-5.02	117.28	121.30
1	B	119	PHE	CB-CG-CD1	-5.02	117.29	120.80
1	e	180	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	B	168	ARG	CG-CD-NE	-5.02	101.26	111.80
1	b	195	ALA	N-CA-CB	5.02	117.12	110.10
2	j	21	ASP	CA-C-N	5.02	126.23	116.20
3	J	167	PHE	CB-CG-CD2	5.02	124.31	120.80
3	I	308	GLU	N-CA-CB	5.01	119.63	110.60
3	K	178	VAL	CB-CA-C	-5.01	101.87	111.40
3	L	207	VAL	CG1-CB-CG2	-5.01	102.88	110.90
2	j	124	SER	N-CA-CB	5.01	118.02	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	D	120	LYS	CB-CG-CD	5.01	124.63	111.60
1	e	175	PHE	CB-CG-CD1	5.01	124.31	120.80
1	c	58	LEU	CB-CA-C	-5.01	100.69	110.20
1	G	51	ASP	CB-CG-OD1	5.01	122.81	118.30
2	k	41	ALA	CB-CA-C	5.01	117.61	110.10
2	k	103	TYR	CG-CD2-CE2	-5.01	117.29	121.30
2	k	139	ALA	C-N-CA	5.01	134.22	121.70
2	m	135	LYS	N-CA-C	-5.01	97.48	111.00
2	m	136	ASP	CB-CG-OD2	-5.01	113.79	118.30
2	l	121	SER	N-CA-C	-5.00	97.49	111.00
1	b	186	ASP	CB-CG-OD1	-5.00	113.80	118.30
1	G	65	GLU	OE1-CD-OE2	5.00	129.30	123.30
2	h	198	GLN	N-CA-C	-5.00	97.49	111.00
2	2	197	TYR	CZ-CE2-CD2	5.00	124.30	119.80
2	k	36	PHE	CB-CG-CD2	-5.00	117.30	120.80
3	H	346	ALA	CB-CA-C	-5.00	102.60	110.10
3	J	387	THR	N-CA-CB	5.00	119.81	110.30

There are no chirality outliers.

All (321) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	101	TYR	Sidechain
2	1	103	TYR	Sidechain
2	1	106	TYR	Sidechain
2	1	123	TYR	Sidechain
2	1	170	ARG	Sidechain
2	1	199	TYR	Sidechain
2	1	46	TYR	Sidechain
2	1	81	ARG	Sidechain
2	2	106	TYR	Sidechain
2	2	123	TYR	Sidechain
2	2	139	ALA	Peptide
2	2	148	TYR	Sidechain
2	2	178	ARG	Sidechain
2	2	197	TYR	Sidechain
2	2	212	ARG	Sidechain
2	3	102	ARG	Sidechain
2	3	106	TYR	Sidechain
2	3	197	TYR	Sidechain
2	3	51	ARG	Sidechain
2	3	83	ARG	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
2	4	101	TYR	Sidechain
2	4	103	TYR	Sidechain
2	4	106	TYR	Sidechain
2	4	139	ALA	Peptide
2	4	68	ARG	Sidechain
2	4	88	ARG	Sidechain
2	5	101	TYR	Sidechain
2	5	103	TYR	Sidechain
2	5	132	ILE	Peptide
2	5	170	ARG	Sidechain
2	5	173	TYR	Sidechain
2	5	51	ARG	Sidechain
2	5	77	TYR	Sidechain
2	6	102	ARG	Sidechain
2	6	154	ARG	Sidechain
2	6	199	TYR	Sidechain
2	6	77	TYR	Sidechain
2	7	106	TYR	Sidechain
2	7	123	TYR	Sidechain
2	7	132	ILE	Peptide
2	7	139	ALA	Peptide
2	7	68	ARG	Sidechain
2	7	77	TYR	Sidechain
2	7	88	ARG	Sidechain
1	A	105	GLU	Peptide
1	A	148	TYR	Sidechain
1	A	168	ARG	Sidechain
1	A	179	TYR	Sidechain
1	A	22	PHE	Sidechain
1	A	53	ARG	Sidechain
1	A	65	GLU	Peptide
1	A	68	TYR	Sidechain
1	A	8	TYR	Sidechain
1	A	86	ARG	Sidechain
1	B	103	TYR	Sidechain
1	B	123	TYR	Sidechain
1	B	14	VAL	Peptide
1	B	159	TYR	Sidechain
1	B	179	TYR	Sidechain
1	B	20	ARG	Sidechain
1	B	213	TYR	Sidechain
1	B	219	ARG	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	B	220	THR	Peptide
1	B	232	TYR	Sidechain
1	B	66	LYS	Peptide
1	C	10	ARG	Sidechain
1	C	123	TYR	Sidechain
1	C	159	TYR	Sidechain
1	C	168	ARG	Sidechain
1	C	179	TYR	Sidechain
1	C	20	ARG	Sidechain
1	C	220	THR	Peptide
1	C	65	GLU	Peptide
1	C	66	LYS	Peptide
1	C	8	TYR	Sidechain
1	D	126	TYR	Sidechain
1	D	180	ARG	Sidechain
1	D	185	PHE	Sidechain
1	D	220	THR	Peptide
1	D	232	TYR	Sidechain
1	D	26	TYR	Sidechain
1	D	8	TYR	Sidechain
1	E	100	ARG	Sidechain
1	E	179	TYR	Sidechain
1	E	213	TYR	Sidechain
1	E	220	THR	Peptide
1	E	26	TYR	Sidechain
1	E	86	ARG	Sidechain
1	E	93	ARG	Sidechain
1	F	10	ARG	Sidechain
1	F	130	ARG	Sidechain
1	F	179	TYR	Sidechain
1	F	219	ARG	Sidechain
1	F	220	THR	Peptide
1	F	232	TYR	Sidechain
1	F	8	TYR	Sidechain
1	F	83	ALA	Mainchain
1	F	93	ARG	Sidechain
1	G	100	ARG	Sidechain
1	G	103	TYR	Sidechain
1	G	148	TYR	Sidechain
1	G	179	TYR	Sidechain
1	G	180	ARG	Sidechain
1	G	219	ARG	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	G	220	THR	Peptide
1	G	232	TYR	Sidechain
1	G	241	ARG	Sidechain
1	G	28	ARG	Sidechain
1	G	5	GLN	Peptide
3	H	105	ARG	Sidechain
3	H	181	TYR	Sidechain
3	H	201	ALA	Mainchain,Peptide
3	H	205	ARG	Sidechain
3	H	21	TYR	Sidechain
3	H	221	ARG	Sidechain
3	H	250	ARG	Sidechain
3	H	269	LEU	Peptide
3	H	27	TYR	Sidechain
3	H	277	PRO	Peptide
3	H	317	ARG	Sidechain
3	H	367	ARG	Sidechain
3	H	386	THR	Peptide
3	H	387	THR	Peptide
3	H	41	ARG	Sidechain
3	H	44	TYR	Sidechain
3	H	94	TYR	Sidechain
3	I	121	THR	Peptide
3	I	140	TYR	Sidechain
3	I	167	PHE	Sidechain
3	I	221	ARG	Sidechain
3	I	224	ARG	Sidechain
3	I	24	ARG	Sidechain
3	I	27	TYR	Sidechain
3	I	278	ARG	Sidechain
3	I	289	ARG	Sidechain
3	I	386	THR	Peptide
3	I	387	THR	Peptide
3	I	57	ARG	Sidechain
3	J	140	TYR	Sidechain
3	J	154	ARG	Sidechain
3	J	20	TYR	Sidechain
3	J	200	ARG	Sidechain
3	J	205	ARG	Sidechain
3	J	215	TYR	Peptide
3	J	254	ASP	Peptide
3	J	29	ARG	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
3	J	305	ARG	Sidechain
3	J	314	PHE	Sidechain
3	J	336	PHE	Sidechain
3	J	371	THR	Peptide
3	J	385	LYS	Peptide
3	J	386	THR	Peptide
3	J	49	ARG	Sidechain
3	J	52	ARG	Sidechain
3	K	140	TYR	Sidechain
3	K	20	TYR	Sidechain
3	K	211	PHE	Sidechain
3	K	215	TYR	Sidechain,Peptide
3	K	217	GLY	Peptide
3	K	218	GLU	Peptide
3	K	236	SER	Peptide
3	K	240	ILE	Peptide
3	K	249	ARG	Sidechain
3	K	254	ASP	Peptide
3	K	276	ASP	Peptide
3	K	311	LEU	Peptide
3	K	326	ARG	Sidechain
3	K	364	ARG	Sidechain
3	K	386	THR	Peptide
3	K	44	TYR	Sidechain
3	K	76	ARG	Sidechain
3	L	121	THR	Peptide
3	L	154	ARG	Sidechain
3	L	181	TYR	Peptide
3	L	21	TYR	Sidechain
3	L	215	TYR	Sidechain
3	L	224	ARG	Sidechain
3	L	254	ASP	Peptide
3	L	269	LEU	Mainchain
3	L	278	ARG	Sidechain
3	L	29	ARG	Sidechain
3	L	303	PHE	Sidechain,Peptide
3	L	305	ARG	Sidechain
3	L	317	ARG	Sidechain
3	L	386	THR	Peptide
3	L	387	THR	Peptide
3	L	52	ARG	Sidechain
3	M	121	THR	Peptide

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
3	M	128	TYR	Sidechain
3	M	181	TYR	Sidechain
3	M	186	THR	Peptide
3	M	190	LEU	Peptide
3	M	20	TYR	Sidechain
3	M	207	VAL	Peptide
3	M	215	TYR	Sidechain
3	M	263	ARG	Sidechain
3	M	27	TYR	Sidechain
3	M	28	ARG	Sidechain
3	M	299	ARG	Sidechain
3	M	302	ARG	Sidechain
3	M	321	PHE	Sidechain
3	M	341	ARG	Sidechain
3	M	385	LYS	Peptide
3	M	386	THR	Peptide
3	M	44	TYR	Sidechain
3	M	46	ARG	Sidechain
3	M	49	ARG	Sidechain
1	a	148	TYR	Sidechain
1	a	159	TYR	Sidechain
1	a	179	TYR	Sidechain
1	a	213	TYR	Sidechain
1	a	220	THR	Peptide
1	a	221	PHE	Sidechain
1	a	232	TYR	Sidechain
1	a	235	ARG	Sidechain
1	b	10	ARG	Sidechain
1	b	123	TYR	Sidechain
1	b	179	TYR	Sidechain
1	b	185	PHE	Sidechain
1	b	220	THR	Peptide
1	b	221	PHE	Sidechain
1	b	235	ARG	Sidechain
1	b	239	ARG	Sidechain
1	b	68	TYR	Sidechain
1	b	91	ARG	Sidechain
1	c	10	ARG	Sidechain
1	c	15	PHE	Sidechain
1	c	179	TYR	Sidechain
1	c	213	TYR	Sidechain
1	c	232	TYR	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
1	c	241	ARG	Sidechain
1	c	53	ARG	Sidechain
1	c	68	TYR	Sidechain
1	c	86	ARG	Sidechain
1	d	126	TYR	Sidechain
1	d	213	TYR	Sidechain
1	d	22	PHE	Sidechain
1	d	220	THR	Peptide
1	d	239	ARG	Sidechain
1	d	26	TYR	Sidechain
1	d	86	ARG	Sidechain
1	d	91	ARG	Sidechain
1	e	10	ARG	Sidechain
1	e	175	PHE	Sidechain
1	e	179	TYR	Sidechain
1	e	213	TYR	Sidechain
1	e	220	THR	Peptide
1	e	53	ARG	Sidechain
1	e	86	ARG	Sidechain
1	e	93	ARG	Sidechain
1	f	119	PHE	Sidechain
1	f	132	PHE	Sidechain
1	f	148	TYR	Sidechain
1	f	159	TYR	Sidechain
1	f	20	ARG	Sidechain
1	f	219	ARG	Sidechain
1	f	220	THR	Peptide
1	f	239	ARG	Sidechain
1	f	86	ARG	Sidechain
1	f	93	ARG	Sidechain
1	g	126	TYR	Sidechain
1	g	148	TYR	Sidechain
1	g	213	TYR	Sidechain
1	g	219	ARG	Sidechain
1	g	220	THR	Peptide
1	g	241	ARG	Sidechain
2	h	103	TYR	Sidechain
2	h	139	ALA	Peptide
2	h	170	ARG	Sidechain
2	h	178	ARG	Sidechain
2	h	197	TYR	Sidechain
2	h	199	TYR	Sidechain

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>	<b>Group</b>
2	i	103	TYR	Sidechain
2	i	113	GLY	Peptide
2	i	139	ALA	Peptide
2	i	199	TYR	Sidechain
2	i	46	TYR	Sidechain
2	i	51	ARG	Sidechain
2	i	65	PHE	Sidechain
2	i	77	TYR	Sidechain
2	i	83	ARG	Sidechain
2	j	104	PHE	Sidechain
2	j	154	ARG	Sidechain
2	j	197	TYR	Sidechain
2	j	30	ARG	Sidechain
2	k	101	TYR	Sidechain
2	k	103	TYR	Sidechain
2	k	123	TYR	Sidechain
2	k	178	ARG	Sidechain
2	k	199	TYR	Sidechain
2	k	212	ARG	Sidechain
2	k	30	ARG	Sidechain
2	k	65	PHE	Sidechain
2	k	68	ARG	Sidechain
2	k	77	TYR	Sidechain
2	k	80	ARG	Sidechain
2	l	101	TYR	Sidechain
2	l	123	TYR	Sidechain
2	l	154	ARG	Sidechain
2	l	170	ARG	Sidechain
2	l	211	PHE	Sidechain
2	l	212	ARG	Sidechain
2	l	68	ARG	Sidechain
2	l	77	TYR	Sidechain
2	l	81	ARG	Sidechain
2	l	83	ARG	Sidechain
2	m	103	TYR	Sidechain
2	m	106	TYR	Sidechain
2	m	212	ARG	Sidechain
2	m	83	ARG	Sidechain
2	n	101	TYR	Sidechain
2	n	132	ILE	Peptide
2	n	139	ALA	Peptide
2	n	178	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	n	197	TYR	Sidechain
2	n	199	TYR	Sidechain
2	n	30	ARG	Sidechain
2	n	77	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	240/242 (99%)	221 (92%)	13 (5%)	6 (2%)	5	32
1	B	240/242 (99%)	229 (95%)	7 (3%)	4 (2%)	9	42
1	C	240/242 (99%)	226 (94%)	9 (4%)	5 (2%)	7	36
1	D	240/242 (99%)	223 (93%)	12 (5%)	5 (2%)	7	36
1	E	240/242 (99%)	226 (94%)	10 (4%)	4 (2%)	9	42
1	F	240/242 (99%)	229 (95%)	8 (3%)	3 (1%)	12	48
1	G	240/242 (99%)	226 (94%)	9 (4%)	5 (2%)	7	36
1	a	235/242 (97%)	223 (95%)	8 (3%)	4 (2%)	9	42
1	b	235/242 (97%)	219 (93%)	16 (7%)	0	100	100
1	c	235/242 (97%)	223 (95%)	9 (4%)	3 (1%)	12	48
1	d	235/242 (97%)	221 (94%)	10 (4%)	4 (2%)	9	42
1	e	235/242 (97%)	217 (92%)	15 (6%)	3 (1%)	12	48
1	f	235/242 (97%)	221 (94%)	11 (5%)	3 (1%)	12	48
1	g	235/242 (97%)	223 (95%)	9 (4%)	3 (1%)	12	48
2	1	200/202 (99%)	192 (96%)	7 (4%)	1 (0%)	29	69

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
2	2	200/202 (99%)	176 (88%)	19 (10%)	5 (2%)	5	32
2	3	200/202 (99%)	185 (92%)	10 (5%)	5 (2%)	5	32
2	4	200/202 (99%)	185 (92%)	11 (6%)	4 (2%)	7	38
2	5	200/202 (99%)	182 (91%)	12 (6%)	6 (3%)	4	28
2	6	200/202 (99%)	181 (90%)	14 (7%)	5 (2%)	5	32
2	7	200/202 (99%)	186 (93%)	9 (4%)	5 (2%)	5	32
2	h	200/202 (99%)	180 (90%)	9 (4%)	11 (6%)	2	19
2	i	200/202 (99%)	189 (94%)	8 (4%)	3 (2%)	10	46
2	j	200/202 (99%)	186 (93%)	10 (5%)	4 (2%)	7	38
2	k	200/202 (99%)	185 (92%)	11 (6%)	4 (2%)	7	38
2	l	200/202 (99%)	183 (92%)	13 (6%)	4 (2%)	7	38
2	m	200/202 (99%)	191 (96%)	6 (3%)	3 (2%)	10	46
2	n	200/202 (99%)	181 (90%)	10 (5%)	9 (4%)	2	22
3	H	388/390 (100%)	344 (89%)	31 (8%)	13 (3%)	3	26
3	I	388/390 (100%)	354 (91%)	21 (5%)	13 (3%)	3	26
3	J	388/390 (100%)	353 (91%)	29 (8%)	6 (2%)	10	46
3	K	388/390 (100%)	344 (89%)	25 (6%)	19 (5%)	2	20
3	L	388/390 (100%)	348 (90%)	24 (6%)	16 (4%)	3	22
3	M	388/390 (100%)	336 (87%)	36 (9%)	16 (4%)	3	22
All	All	8453/8556 (99%)	7788 (92%)	461 (6%)	204 (2%)	9	33

All (204) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	a	54	VAL
1	B	64	ILE
1	C	20	ARG
1	C	66	LYS
1	C	67	ILE
1	c	219	ARG
1	D	56	SER
1	D	65	GLU
1	F	64	ILE
1	G	56	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	g	143	GLU
2	h	128	ILE
2	h	140	THR
2	2	140	THR
2	2	182	SER
2	3	212	ARG
2	4	140	THR
2	m	200	SER
2	n	131	ALA
2	n	139	ALA
3	H	120	PRO
3	H	270	ALA
3	H	278	ARG
3	H	280	ASP
3	I	124	ASP
3	I	282	LYS
3	K	163	LYS
3	K	215	TYR
3	K	237	ILE
3	K	313	THR
3	K	387	THR
3	L	125	PRO
3	L	255	THR
3	L	270	ALA
3	L	292	ILE
3	M	131	GLU
3	M	190	LEU
3	M	191	LEU
3	J	212	VAL
3	J	386	THR
1	A	106	PRO
1	A	143	GLU
1	a	34	GLY
1	B	65	GLU
1	B	143	GLU
1	c	73	HIS
1	D	161	ALA
1	d	12	ILE
1	d	161	ALA
1	d	221	PHE
1	E	221	PHE
1	F	221	PHE

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	f	143	GLU
1	f	179	TYR
1	G	221	PHE
2	h	21	ASP
2	2	139	ALA
2	i	44	LYS
2	i	193	GLU
2	3	139	ALA
2	3	193	GLU
2	j	212	ARG
2	k	30	ARG
2	k	193	GLU
2	5	136	ASP
2	6	19	CYS
2	6	41	ALA
2	6	139	ALA
2	7	133	GLU
2	n	132	ILE
3	H	212	VAL
3	H	269	LEU
3	I	74	ASP
3	I	242	GLU
3	I	273	ASP
3	I	387	THR
3	K	255	THR
3	K	280	ASP
3	K	296	ALA
3	K	333	ASP
3	K	391	ASP
3	L	61	PRO
3	L	247	ALA
3	L	269	LEU
3	L	282	LYS
3	L	330	LEU
3	M	93	GLN
3	M	134	GLU
3	M	282	LYS
3	M	304	ASP
3	M	313	THR
3	M	333	ASP
3	M	386	THR
1	A	9	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	35	ALA
1	A	57	LYS
1	a	161	ALA
1	B	221	PHE
1	C	221	PHE
1	c	62	ASP
1	e	161	ALA
1	F	9	ASP
1	G	6	MET
1	g	221	PHE
2	1	136	ASP
2	h	51	ARG
2	h	183	GLY
2	h	191	ILE
2	h	193	GLU
2	3	181	ALA
2	j	136	ASP
2	4	33	MET
2	4	44	LYS
2	5	193	GLU
2	l	40	LYS
2	6	136	ASP
2	7	83	ARG
3	H	126	MET
3	H	302	ARG
3	H	387	THR
3	I	131	GLU
3	I	212	VAL
3	K	149	GLN
3	K	201	ALA
3	K	392	LEU
3	L	146	LEU
3	L	212	VAL
3	L	221	ARG
3	L	331	ALA
3	M	122	SER
3	M	183	PRO
3	J	92	SER
1	D	55	GLY
1	d	143	GLU
1	E	6	MET
1	E	9	ASP

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Mol	Chain	Res	Type
1	E	73	HIS
1	g	218	ASP
2	h	106	TYR
2	h	137	ILE
2	2	106	TYR
2	2	212	ARG
2	k	140	THR
2	k	194	ASP
2	5	181	ALA
2	l	194	ASP
2	6	140	THR
2	m	106	TYR
2	m	193	GLU
2	n	137	ILE
2	n	140	THR
2	n	181	ALA
2	n	200	SER
3	H	209	SER
3	K	242	GLU
3	K	247	ALA
3	M	214	LYS
3	M	258	ASP
3	J	74	ASP
3	J	254	ASP
1	a	221	PHE
1	C	9	ASP
1	e	14	VAL
1	f	62	ASP
1	G	9	ASP
1	G	143	GLU
2	h	127	PRO
2	h	200	SER
2	i	200	SER
2	3	41	ALA
2	j	185	GLY
2	4	130	GLY
2	5	105	PRO
2	n	107	LEU
3	H	134	GLU
3	H	254	ASP
3	I	122	SER
3	I	135	LYS

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Mol	Chain	Res	Type
3	I	310	PRO
3	K	91	THR
3	K	187	GLY
3	L	135	LYS
3	L	396	MET
3	J	126	MET
2	5	133	GLU
2	1	136	ASP
2	7	34	GLY
3	I	284	ILE
3	I	388	PRO
3	K	135	LYS
1	D	64	ILE
2	5	191	ILE
2	7	105	PRO
3	L	310	PRO
2	7	85	PRO
3	M	124	ASP
2	j	200	SER
3	H	132	VAL
2	n	129	GLY
3	K	277	PRO
3	M	212	VAL
1	e	17	PRO
2	l	137	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	203/203 (100%)	201 (99%)	2 (1%)	76	86
1	B	203/203 (100%)	200 (98%)	3 (2%)	65	80
1	C	203/203 (100%)	193 (95%)	10 (5%)	25	50
1	D	203/203 (100%)	199 (98%)	4 (2%)	55	74
1	E	203/203 (100%)	194 (96%)	9 (4%)	28	53

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	F	203/203 (100%)	196 (97%)	7 (3%)	37	60
1	G	203/203 (100%)	197 (97%)	6 (3%)	41	63
1	a	199/203 (98%)	189 (95%)	10 (5%)	24	49
1	b	199/203 (98%)	193 (97%)	6 (3%)	41	63
1	c	199/203 (98%)	192 (96%)	7 (4%)	36	59
1	d	199/203 (98%)	193 (97%)	6 (3%)	41	63
1	e	199/203 (98%)	187 (94%)	12 (6%)	19	44
1	f	199/203 (98%)	191 (96%)	8 (4%)	31	55
1	g	199/203 (98%)	197 (99%)	2 (1%)	76	86
2	1	164/164 (100%)	158 (96%)	6 (4%)	34	58
2	2	164/164 (100%)	158 (96%)	6 (4%)	34	58
2	3	164/164 (100%)	160 (98%)	4 (2%)	49	69
2	4	164/164 (100%)	154 (94%)	10 (6%)	18	44
2	5	164/164 (100%)	157 (96%)	7 (4%)	29	53
2	6	164/164 (100%)	157 (96%)	7 (4%)	29	53
2	7	164/164 (100%)	159 (97%)	5 (3%)	41	63
2	h	164/164 (100%)	159 (97%)	5 (3%)	41	63
2	i	164/164 (100%)	155 (94%)	9 (6%)	21	47
2	j	164/164 (100%)	155 (94%)	9 (6%)	21	47
2	k	164/164 (100%)	159 (97%)	5 (3%)	41	63
2	l	164/164 (100%)	159 (97%)	5 (3%)	41	63
2	m	164/164 (100%)	163 (99%)	1 (1%)	86	92
2	n	164/164 (100%)	159 (97%)	5 (3%)	41	63
3	H	338/338 (100%)	330 (98%)	8 (2%)	49	69
3	I	338/338 (100%)	331 (98%)	7 (2%)	53	72
3	J	338/338 (100%)	326 (96%)	12 (4%)	35	59
3	K	338/338 (100%)	328 (97%)	10 (3%)	41	63
3	L	338/338 (100%)	324 (96%)	14 (4%)	30	55
3	M	338/338 (100%)	327 (97%)	11 (3%)	38	61
All	All	7138/7166 (100%)	6900 (97%)	238 (3%)	41	61

All (238) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	162	THR
1	a	13	THR
1	a	21	LEU
1	a	33	ARG
1	a	58	LEU
1	a	121	GLN
1	a	129	VAL
1	a	142	ASP
1	a	166	MET
1	a	213	TYR
1	a	217	ASP
1	B	130	ARG
1	B	166	MET
1	B	205	VAL
1	b	15	PHE
1	b	28	ARG
1	b	42	CYS
1	b	182	ASP
1	b	209	ILE
1	b	224	VAL
1	C	5	GLN
1	C	57	LYS
1	C	63	THR
1	C	86	ARG
1	C	144	VAL
1	C	151	ASP
1	C	156	LEU
1	C	166	MET
1	C	208	ASN
1	C	227	GLU
1	c	121	GLN
1	c	144	VAL
1	c	166	MET
1	c	182	ASP
1	c	187	ASP
1	c	213	TYR
1	c	215	LYS
1	D	121	GLN
1	D	213	TYR
1	D	215	LYS
1	D	231	PRO
1	d	21	LEU

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	d	40	ILE
1	d	130	ARG
1	d	142	ASP
1	d	145	PRO
1	d	160	LYS
1	E	6	MET
1	E	33	ARG
1	E	75	CYS
1	E	104	ASP
1	E	121	GLN
1	E	130	ARG
1	E	145	PRO
1	E	178	GLU
1	E	191	LEU
1	e	22	PHE
1	e	40	ILE
1	e	57	LYS
1	e	59	LEU
1	e	63	THR
1	e	99	ASN
1	e	102	THR
1	e	118	ASP
1	e	121	GLN
1	e	151	ASP
1	e	189	MET
1	e	208	ASN
1	F	84	ASP
1	F	102	THR
1	F	182	ASP
1	F	208	ASN
1	F	217	ASP
1	F	229	LEU
1	F	230	LYS
1	f	21	LEU
1	f	40	ILE
1	f	102	THR
1	f	105	GLU
1	f	129	VAL
1	f	144	VAL
1	f	213	TYR
1	f	229	LEU
1	G	5	GLN

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	G	21	LEU
1	G	57	LYS
1	G	97	GLN
1	G	187	ASP
1	G	216	VAL
1	g	121	GLN
1	g	219	ARG
2	1	14	THR
2	1	27	THR
2	1	28	GLU
2	1	45	ILE
2	1	121	SER
2	1	202	GLU
2	h	17	LEU
2	h	52	MET
2	h	106	TYR
2	h	116	ASP
2	h	205	GLU
2	2	14	THR
2	2	45	ILE
2	2	106	TYR
2	2	121	SER
2	2	148	TYR
2	2	212	ARG
2	i	17	LEU
2	i	45	ILE
2	i	104	PHE
2	i	110	LEU
2	i	121	SER
2	i	122	ILE
2	i	137	ILE
2	i	140	THR
2	i	173	TYR
2	3	12	THR
2	3	17	LEU
2	3	72	ILE
2	3	197	TYR
2	j	14	THR
2	j	39	SER
2	j	77	TYR
2	j	116	ASP
2	j	121	SER

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	j	148	TYR
2	j	184	ASP
2	j	204	VAL
2	j	205	GLU
2	4	27	THR
2	4	28	GLU
2	4	56	THR
2	4	72	ILE
2	4	108	VAL
2	4	110	LEU
2	4	123	TYR
2	4	140	THR
2	4	188	VAL
2	4	208	LEU
2	k	13	THR
2	k	33	MET
2	k	120	LYS
2	k	148	TYR
2	k	212	ARG
2	5	15	VAL
2	5	17	LEU
2	5	27	THR
2	5	39	SER
2	5	45	ILE
2	5	198	GLN
2	5	208	LEU
2	1	27	THR
2	1	104	PHE
2	1	109	GLN
2	1	116	ASP
2	1	146	THR
2	6	28	GLU
2	6	45	ILE
2	6	62	ASP
2	6	126	ASP
2	6	136	ASP
2	6	201	PRO
2	6	202	GLU
2	m	212	ARG
2	7	28	GLU
2	7	64	GLN
2	7	153	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
2	7	163	GLU
2	7	205	GLU
2	n	60	VAL
2	n	87	VAL
2	n	117	SER
2	n	179	ASP
2	n	194	ASP
3	H	54	GLU
3	H	116	VAL
3	H	120	PRO
3	H	127	VAL
3	H	137	GLU
3	H	206	VAL
3	H	329	LYS
3	H	360	MET
3	I	88	VAL
3	I	174	PRO
3	I	214	LYS
3	I	276	ASP
3	I	277	PRO
3	I	283	VAL
3	I	352	LYS
3	K	74	ASP
3	K	121	THR
3	K	123	LYS
3	K	189	THR
3	K	241	ASP
3	K	250	ARG
3	K	260	GLU
3	K	304	ASP
3	K	311	LEU
3	K	319	GLN
3	L	11	GLU
3	L	67	VAL
3	L	85	PRO
3	L	101	LYS
3	L	122	SER
3	L	175	PRO
3	L	179	LEU
3	L	183	PRO
3	L	250	ARG
3	L	304	ASP

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<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
3	L	332	GLU
3	L	333	ASP
3	L	344	GLU
3	L	350	ASP
3	M	48	VAL
3	M	67	VAL
3	M	79	VAL
3	M	127	VAL
3	M	165	GLU
3	M	190	LEU
3	M	249	ARG
3	M	272	LEU
3	M	347	SER
3	M	380	GLU
3	M	386	THR
3	J	85	PRO
3	J	101	LYS
3	J	122	SER
3	J	148	VAL
3	J	227	PHE
3	J	244	ASP
3	J	256	SER
3	J	300	PRO
3	J	311	LEU
3	J	315	GLU
3	J	332	GLU
3	J	375	PHE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (40) such sidechains are listed below:

<b>Mol</b>	<b>Chain</b>	<b>Res</b>	<b>Type</b>
1	A	121	GLN
1	A	125	GLN
1	B	122	GLN
1	B	125	GLN
1	b	97	GLN
1	b	121	GLN
1	b	237	ASN
1	C	23	GLN
1	C	237	ASN
1	c	97	GLN
1	c	99	ASN

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Mol	Chain	Res	Type
1	c	121	GLN
1	d	99	ASN
1	d	125	GLN
1	d	237	ASN
1	E	23	GLN
1	E	73	HIS
1	E	237	ASN
1	e	73	HIS
1	F	237	ASN
1	f	121	GLN
1	f	237	ASN
1	G	97	GLN
1	G	237	ASN
2	i	47	GLN
2	3	75	ASN
2	3	109	GLN
2	j	47	GLN
2	j	75	ASN
2	4	96	ASN
2	4	99	ASN
2	7	64	GLN
2	n	64	GLN
3	H	109	ASN
3	H	213	GLN
3	I	90	ASN
3	K	117	ASN
3	K	252	ASN
3	L	324	HIS
3	M	262	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.



## 5.6 Ligand geometry

Of 10 ligands modelled in this entry, 5 are monoatomic - leaving 5 for Mogul analysis.

In the following table, the Counts columns list the number of bonds (or angles) for which Mogul statistics could be retrieved, the number of bonds (or angles) that are observed in the model and the number of bonds (or angles) that are defined in the Chemical Component Dictionary. The Link column lists molecule types, if any, to which the group is linked. 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  $|Z| > 2$  is considered an outlier worth inspection. RMSZ is the root-mean-square of all Z scores of the bond lengths (or angles).

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
4	ATP	H	401	5	26,33,33	1.58	6 (23%)	31,52,52	1.86	6 (19%)
4	ATP	L	401	5	26,33,33	1.08	2 (7%)	31,52,52	2.39	6 (19%)
4	ATP	M	401	5	26,33,33	1.47	4 (15%)	31,52,52	2.34	7 (22%)
4	ATP	K	401	5	26,33,33	1.18	4 (15%)	31,52,52	2.35	7 (22%)
6	ADP	I	401	5	24,29,29	1.48	3 (12%)	29,45,45	1.93	5 (17%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
4	ATP	H	401	5	-	4/18/38/38	0/3/3/3
4	ATP	L	401	5	-	6/18/38/38	0/3/3/3
4	ATP	M	401	5	-	4/18/38/38	0/3/3/3
4	ATP	K	401	5	-	7/18/38/38	0/3/3/3
6	ADP	I	401	5	-	1/12/32/32	0/3/3/3

All (19) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	I	401	ADP	C2'-C1'	-3.99	1.47	1.53
4	M	401	ATP	C2'-C1'	3.76	1.59	1.53
4	H	401	ATP	C2-N3	3.35	1.37	1.32
4	M	401	ATP	C4-N3	-3.29	1.31	1.35
4	H	401	ATP	O4'-C1'	2.73	1.44	1.41
4	H	401	ATP	C8-N7	-2.68	1.29	1.34
4	H	401	ATP	O4'-C4'	-2.62	1.39	1.45
6	I	401	ADP	C8-N7	-2.58	1.30	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	M	401	ATP	C8-N7	-2.56	1.30	1.34
4	K	401	ATP	C8-N7	-2.56	1.30	1.34
4	M	401	ATP	O4'-C1'	2.55	1.44	1.41
4	L	401	ATP	O4'-C1'	2.46	1.44	1.41
4	H	401	ATP	C5'-C4'	2.34	1.58	1.51
6	I	401	ADP	PB-O1B	2.31	1.58	1.50
4	K	401	ATP	C4-N3	-2.27	1.32	1.35
4	L	401	ATP	C5'-C4'	2.25	1.58	1.51
4	K	401	ATP	C2-N1	2.09	1.37	1.33
4	H	401	ATP	O3'-C3'	2.08	1.47	1.43
4	K	401	ATP	PA-O2A	-2.04	1.45	1.55

All (31) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	401	ATP	PB-O3B-PG	8.33	161.41	132.83
4	L	401	ATP	PB-O3B-PG	7.65	159.08	132.83
4	K	401	ATP	PB-O3B-PG	7.62	158.98	132.83
4	K	401	ATP	PA-O3A-PB	7.26	157.74	132.83
4	M	401	ATP	PA-O3A-PB	7.21	157.58	132.83
6	I	401	ADP	PA-O3A-PB	7.13	157.29	132.83
4	L	401	ATP	PA-O3A-PB	6.93	156.60	132.83
4	H	401	ATP	PB-O3B-PG	6.34	154.60	132.83
4	H	401	ATP	PA-O3A-PB	4.89	149.62	132.83
4	L	401	ATP	C5-C6-N1	-4.25	110.72	120.35
6	I	401	ADP	N6-C6-N1	3.75	126.37	118.57
4	K	401	ATP	C5'-C4'-C3'	-3.57	101.79	115.18
4	K	401	ATP	C5-C6-N6	3.51	125.69	120.35
6	I	401	ADP	C5-C6-N1	-3.43	112.58	120.35
4	M	401	ATP	N6-C6-N1	3.07	124.95	118.57
4	L	401	ATP	N6-C6-N1	3.00	124.80	118.57
4	M	401	ATP	C5-C6-N1	-2.87	113.84	120.35
4	L	401	ATP	C5-C6-N6	2.71	124.47	120.35
4	H	401	ATP	O5'-C5'-C4'	2.69	118.27	108.99
4	K	401	ATP	O3G-PG-O2G	2.64	117.72	107.64
4	K	401	ATP	C1'-N9-C4	2.62	131.25	126.64
4	H	401	ATP	C5-C6-N1	-2.49	114.71	120.35
4	H	401	ATP	N6-C6-N1	2.46	123.68	118.57
4	H	401	ATP	C5'-C4'-C3'	2.32	123.87	115.18
4	M	401	ATP	O4'-C1'-C2'	-2.28	103.59	106.93
6	I	401	ADP	O2B-PB-O1B	2.25	119.50	110.68
4	M	401	ATP	C4-C5-N7	-2.24	107.07	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	M	401	ATP	O4'-C4'-C3'	2.19	109.45	105.11
4	K	401	ATP	C5-C6-N1	-2.19	115.40	120.35
4	L	401	ATP	C2-N1-C6	2.13	122.39	118.75
6	I	401	ADP	N3-C2-N1	2.02	131.83	128.68

There are no chirality outliers.

All (22) torsion outliers are listed below:

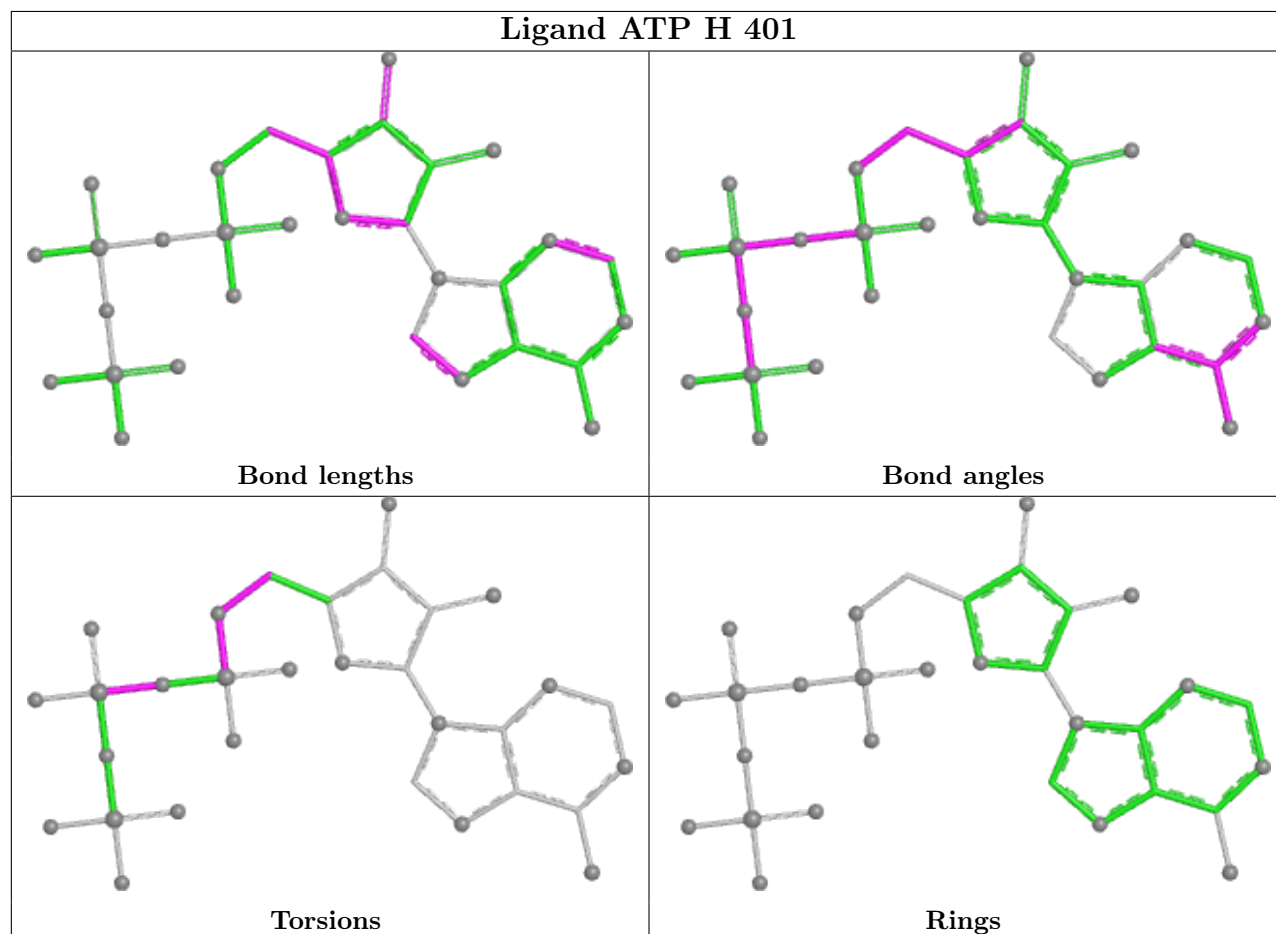
Mol	Chain	Res	Type	Atoms
4	H	401	ATP	C5'-O5'-PA-O3A
4	K	401	ATP	PB-O3B-PG-O2G
4	K	401	ATP	PB-O3B-PG-O3G
4	K	401	ATP	C5'-O5'-PA-O1A
4	L	401	ATP	PB-O3B-PG-O2G
4	L	401	ATP	C5'-O5'-PA-O1A
4	L	401	ATP	C5'-O5'-PA-O2A
4	M	401	ATP	C5'-O5'-PA-O2A
4	M	401	ATP	C5'-O5'-PA-O3A
4	K	401	ATP	C4'-C5'-O5'-PA
4	K	401	ATP	PB-O3A-PA-O5'
4	H	401	ATP	C4'-C5'-O5'-PA
4	K	401	ATP	PG-O3B-PB-O2B
4	H	401	ATP	C5'-O5'-PA-O1A
4	M	401	ATP	PB-O3B-PG-O1G
4	M	401	ATP	PA-O3A-PB-O1B
4	K	401	ATP	PB-O3B-PG-O1G
4	L	401	ATP	PB-O3B-PG-O1G
6	I	401	ADP	PA-O3A-PB-O1B
4	L	401	ATP	C5'-O5'-PA-O3A
4	H	401	ATP	PA-O3A-PB-O1B
4	L	401	ATP	PG-O3B-PB-O2B

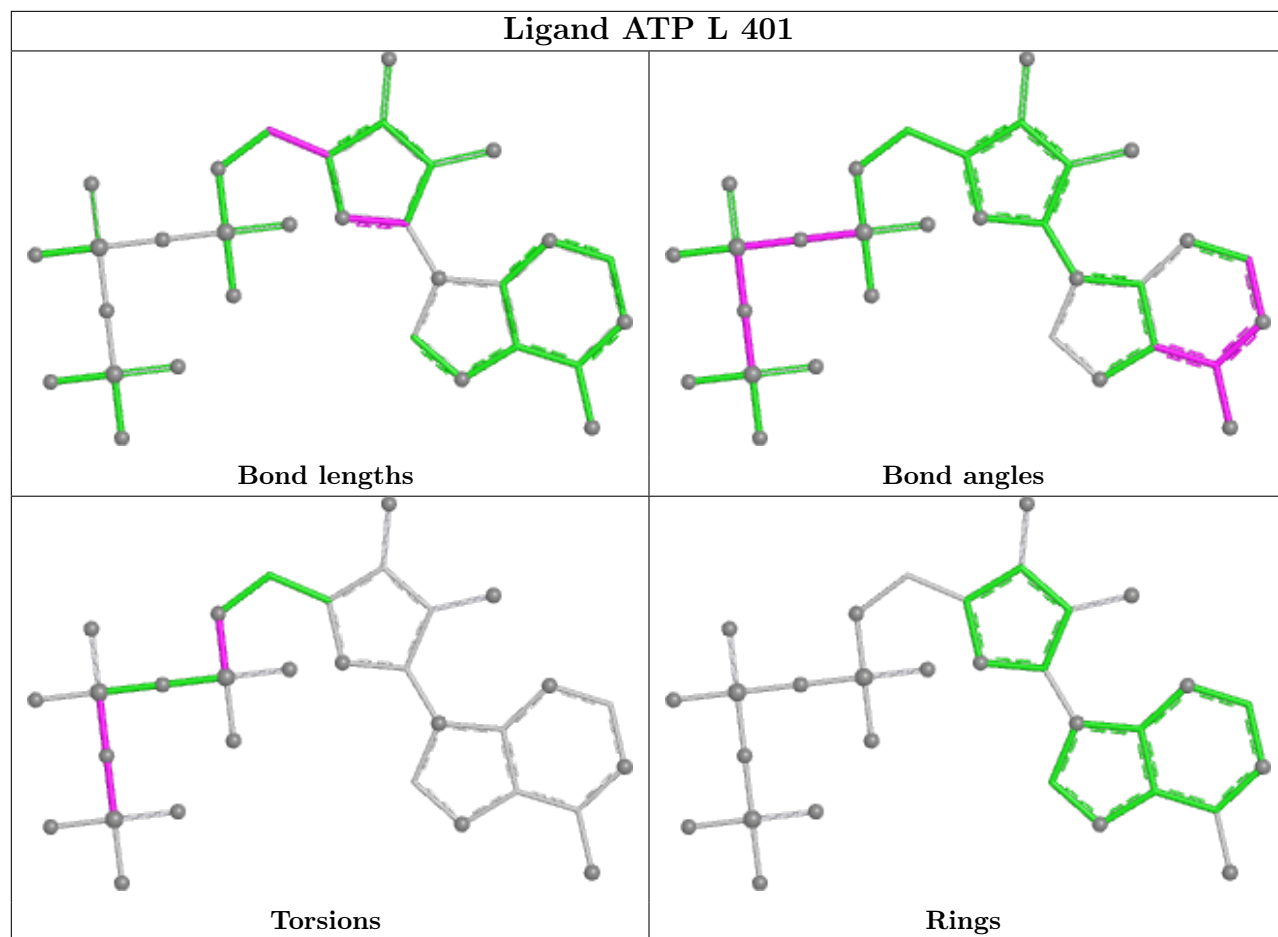
There are no ring outliers.

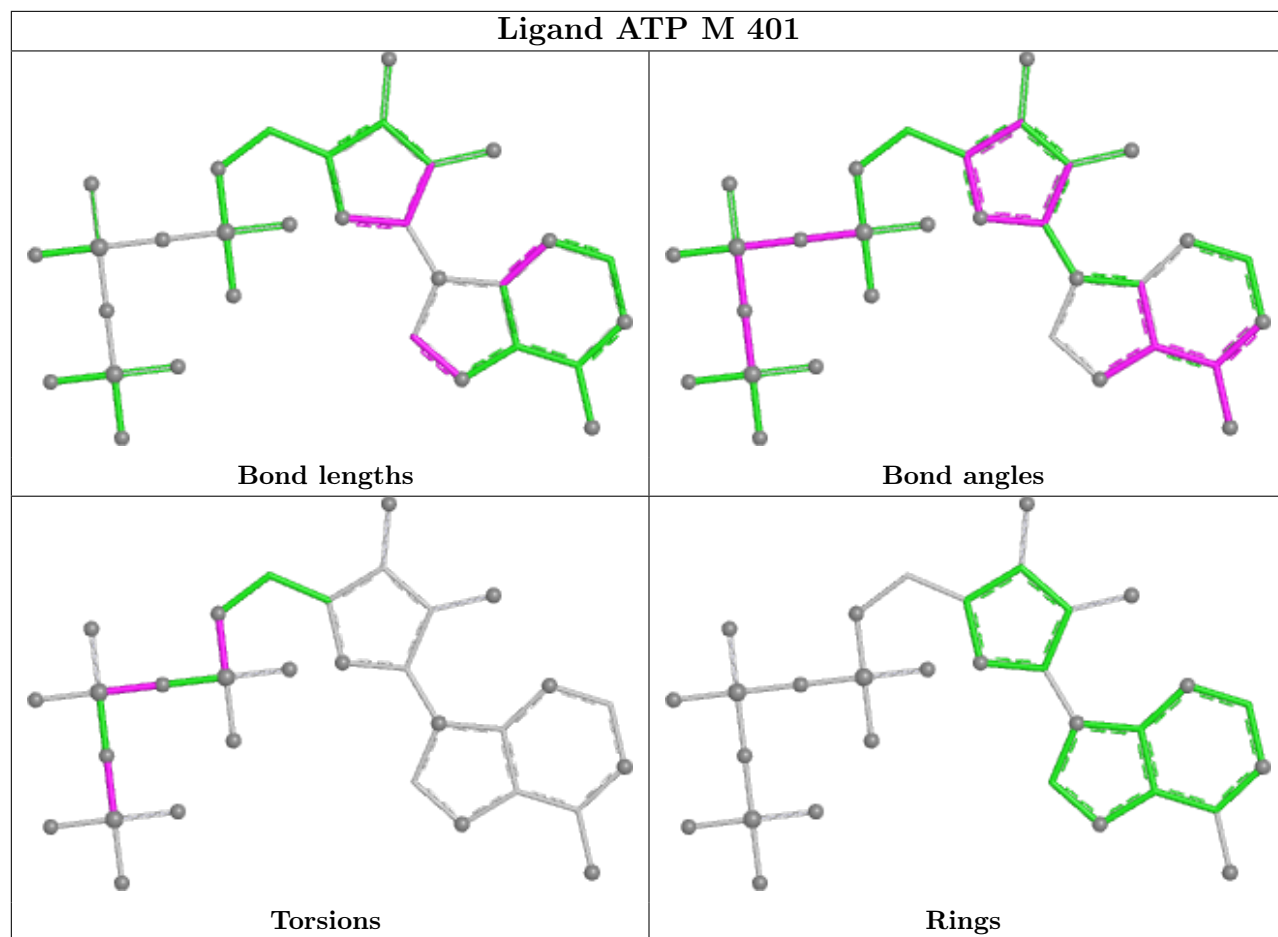
No monomer is involved in short contacts.

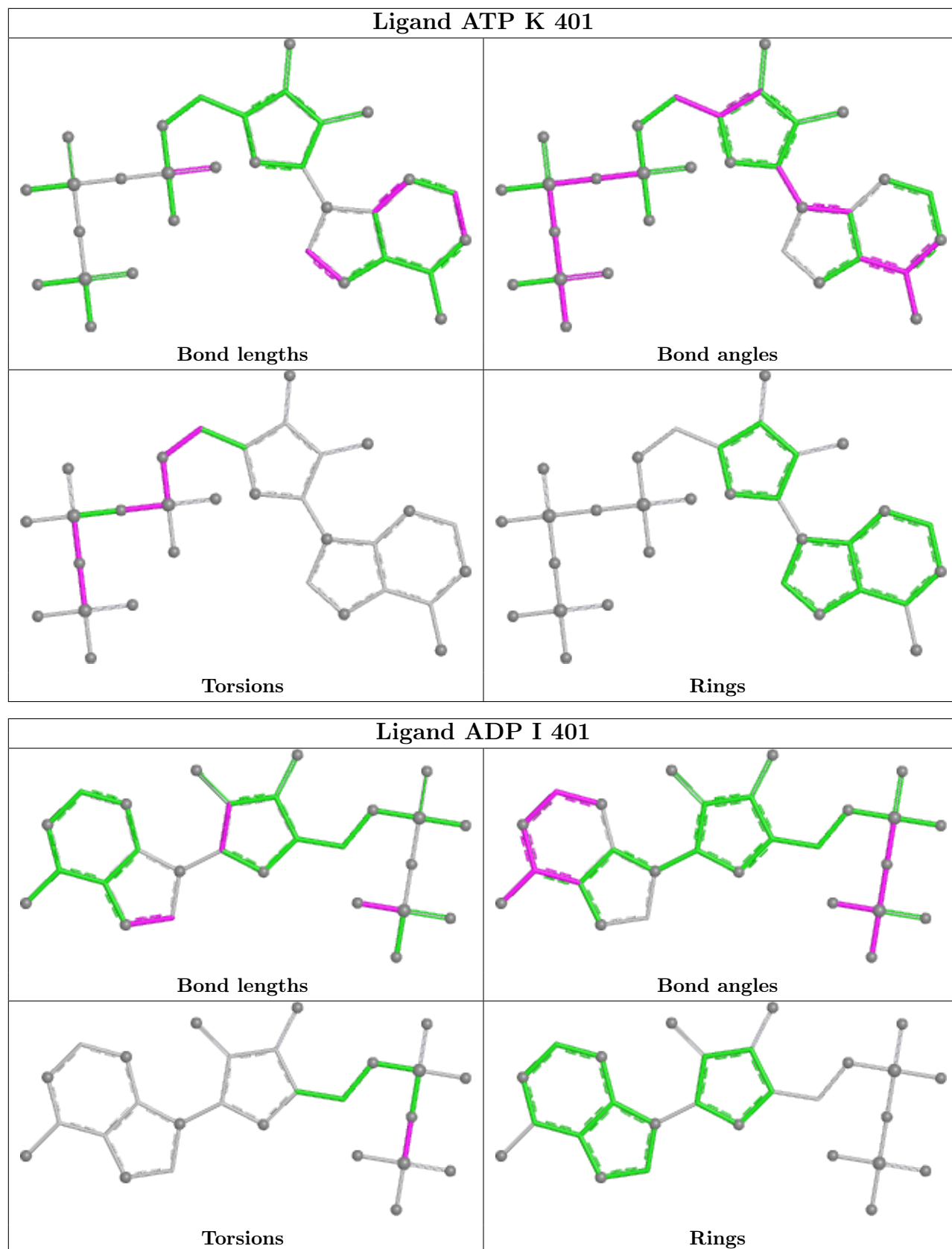
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring

in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.









## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.



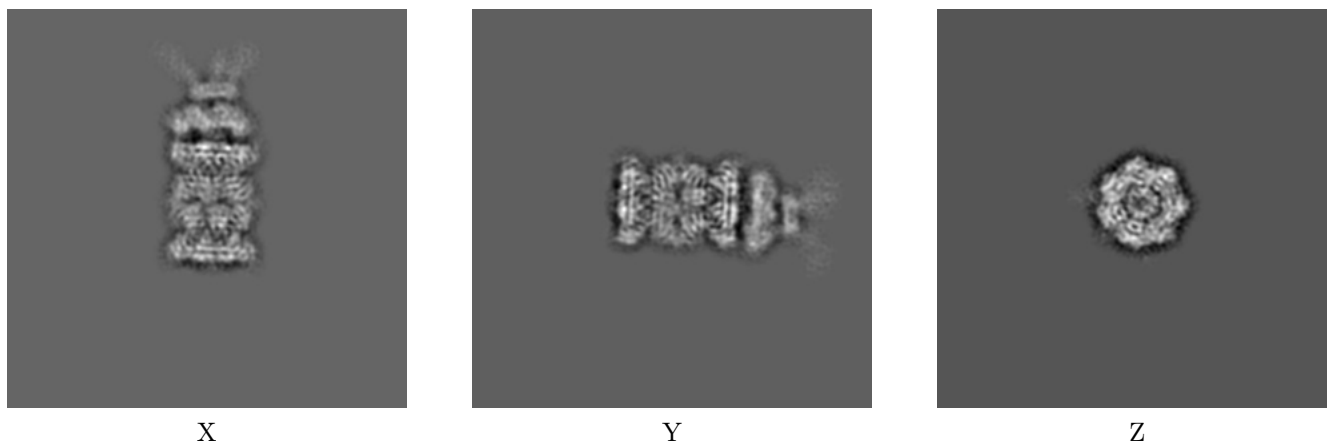
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-0216. These allow visual inspection of the internal detail of the map and identification of artifacts.

No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

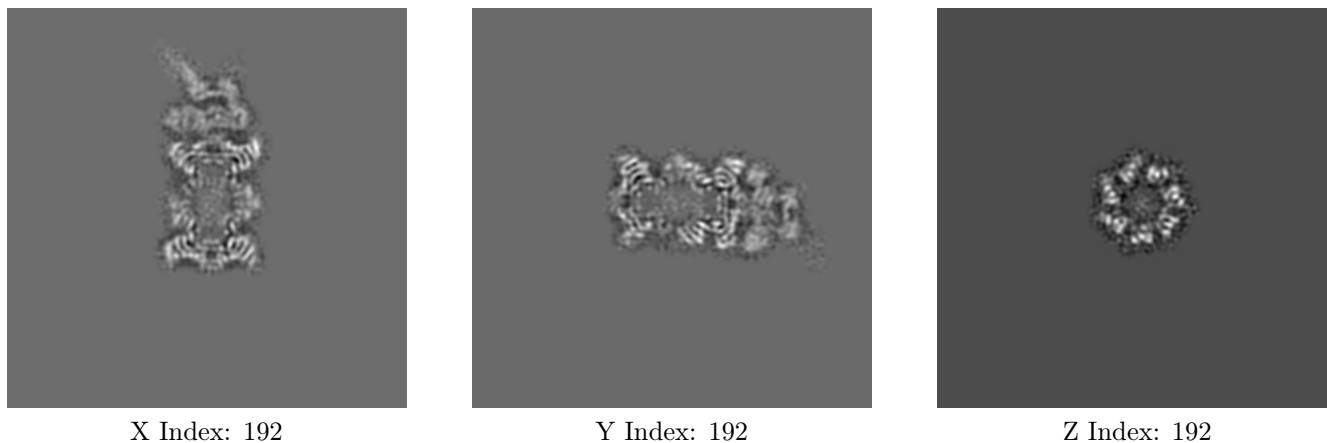
#### 6.1.1 Primary map



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

### 6.2 Central slices [i](#)

#### 6.2.1 Primary map



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: 179



Y Index: 211



Z Index: 251

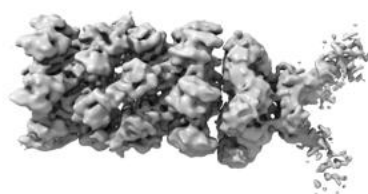
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

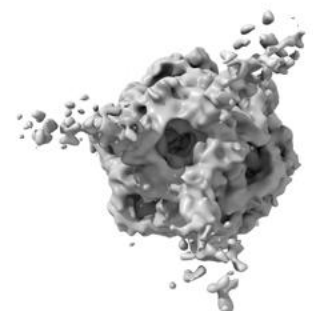
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0068. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

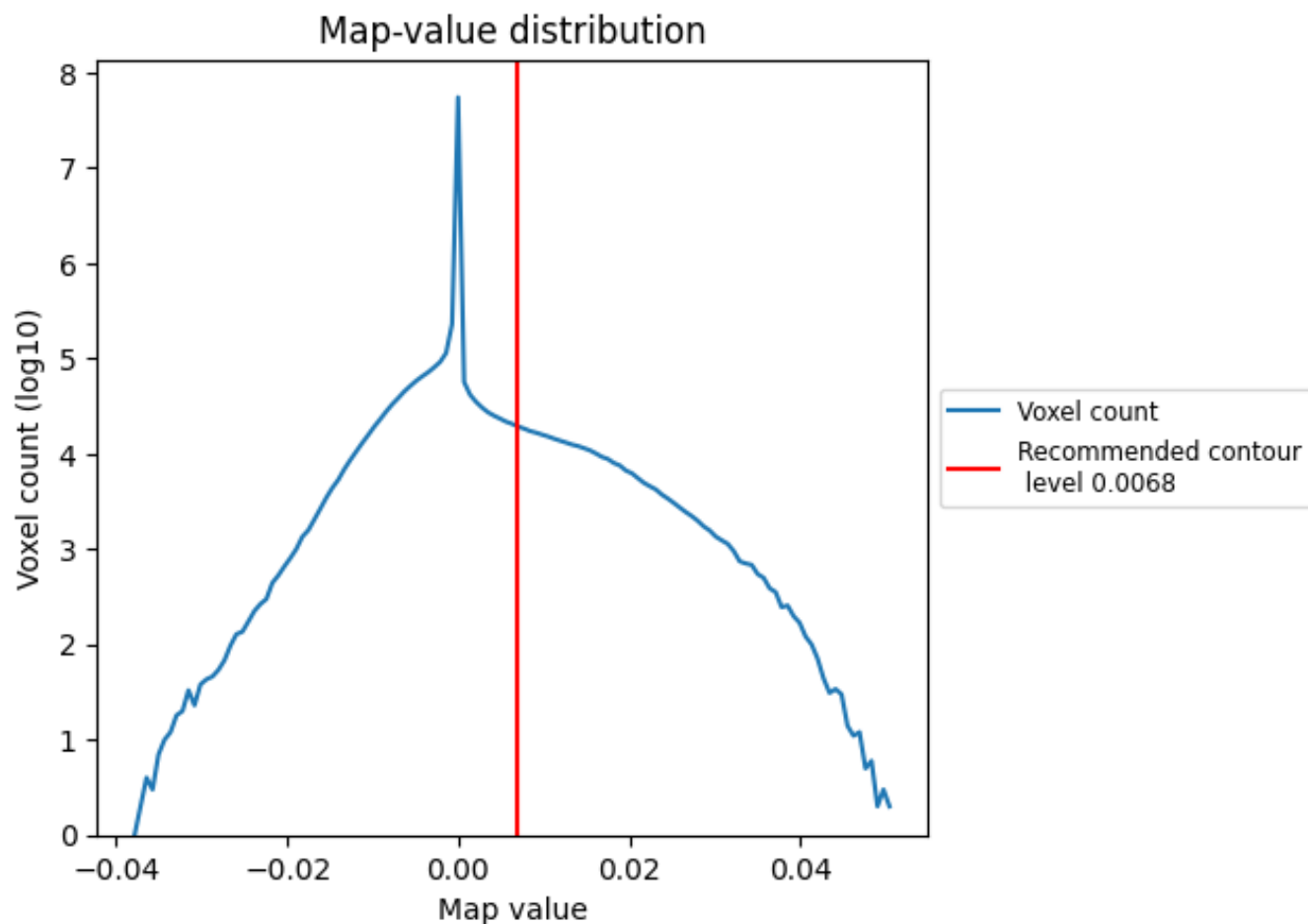
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

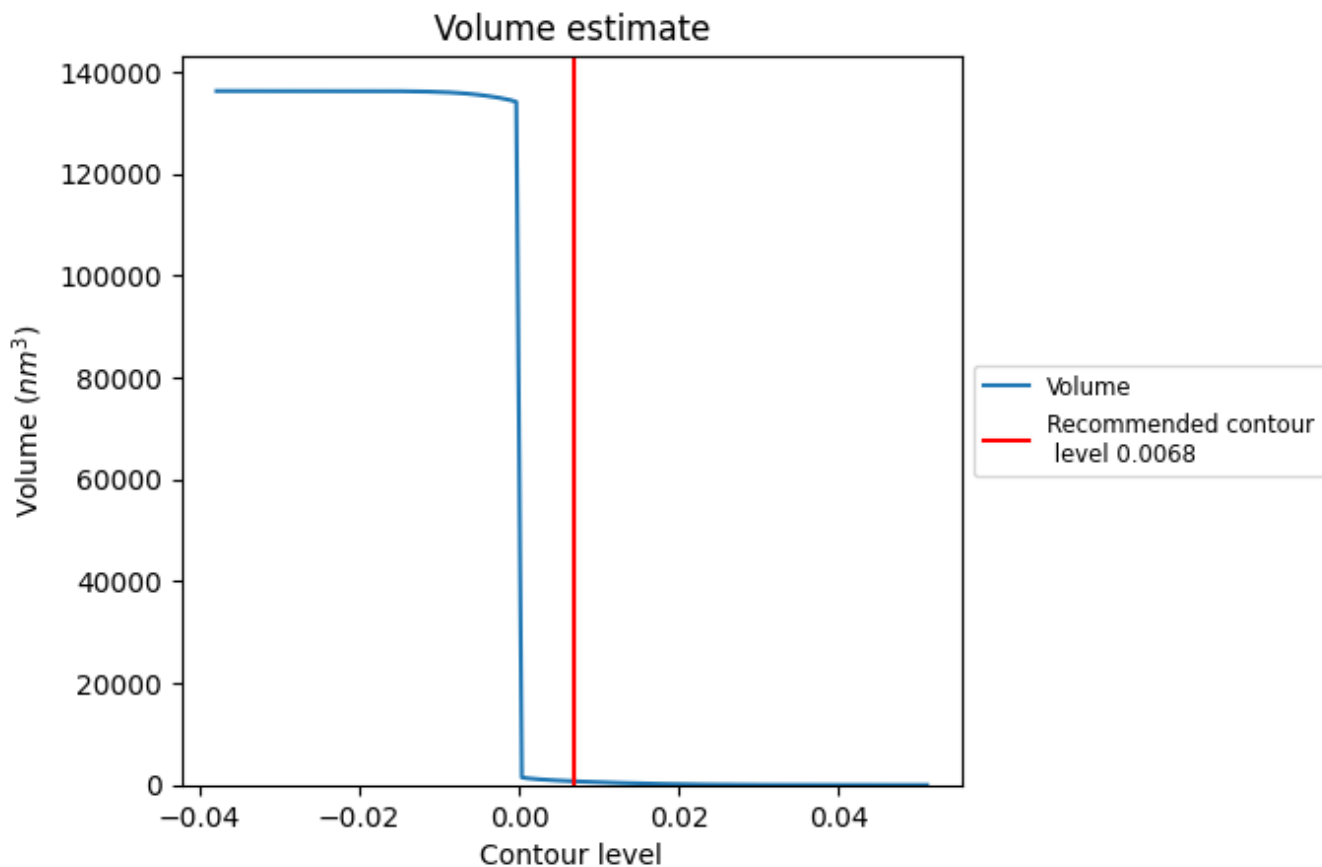
This section contains the results of statistical analysis of the map.

### 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.

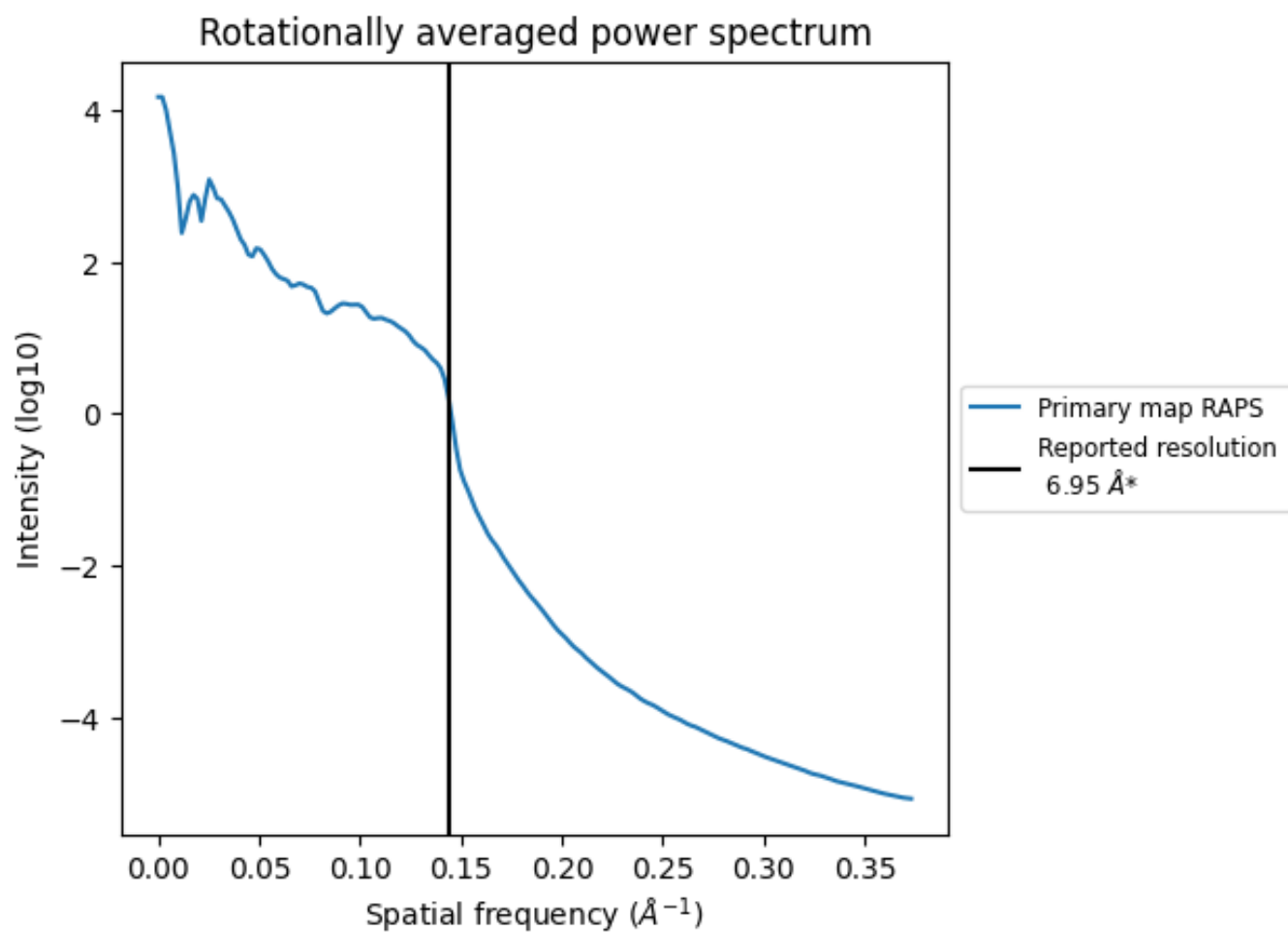
## 7.2 Volume estimate [\(i\)](#)



The volume at the recommended contour level is 735 nm<sup>3</sup>; this corresponds to an approximate mass of 664 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 [i](#)



\*Reported resolution corresponds to spatial frequency of  $0.144 \text{\AA}^{-1}$

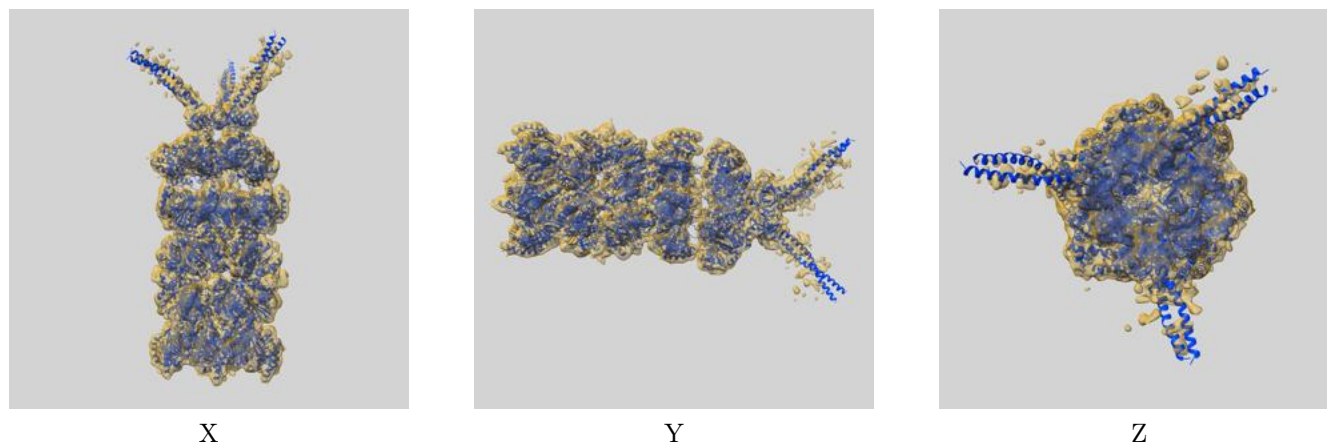
## 8 Fourier-Shell correlation

This section was not generated. No FSC curve or half-maps provided.

## 9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-0216 and PDB model 6HED. Per-residue inclusion information can be found in section 3 on page 8.

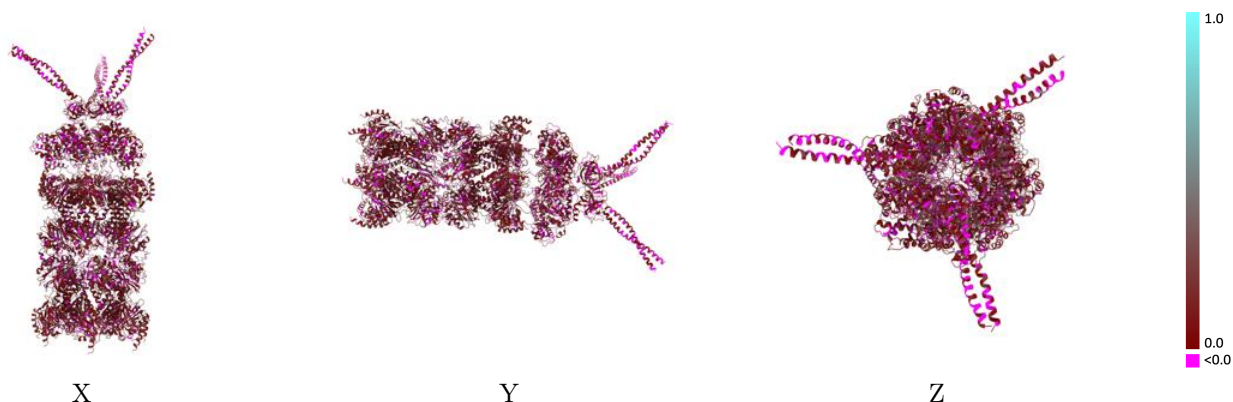
### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.0068 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.

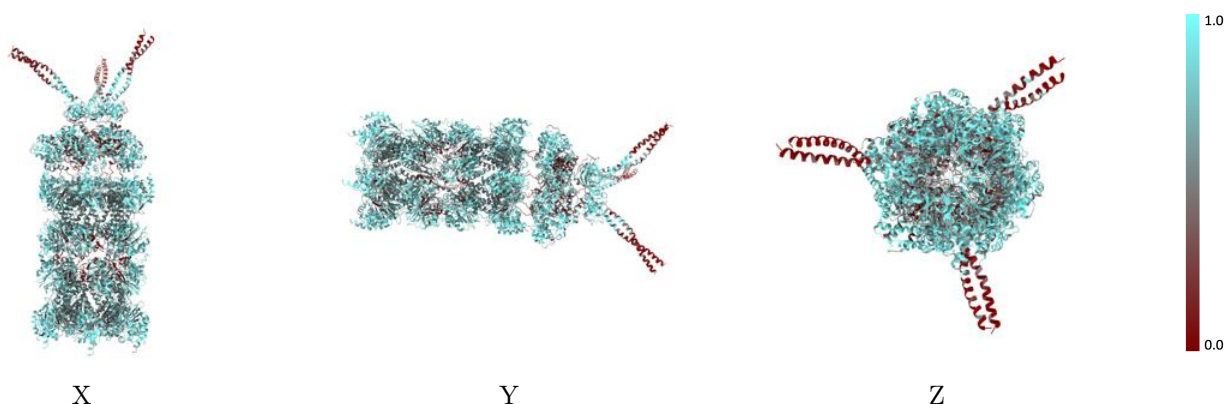


## 9.2 Q-score mapped to coordinate model [\(i\)](#)



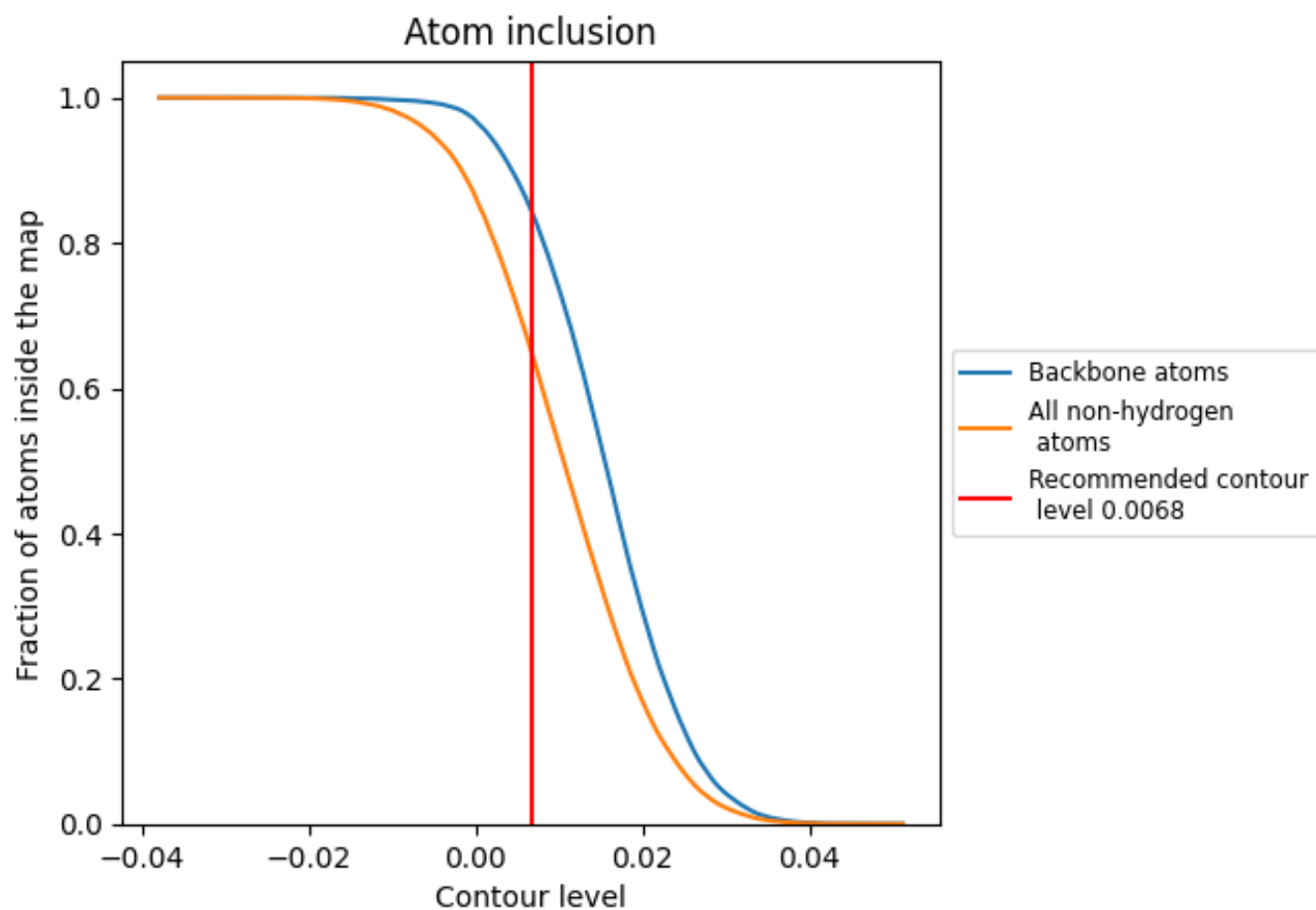
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (0.0068).







































































## 9.4 Atom inclusion [i](#)



At the recommended contour level, 84% of all backbone atoms, 65% 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 (0.0068) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.6451	 0.1140
1	 0.6195	 0.1150
2	 0.6373	 0.1220
3	 0.6504	 0.1250
4	 0.6300	 0.1240
5	 0.6392	 0.1210
6	 0.6313	 0.1130
7	 0.6254	 0.1180
A	 0.7017	 0.1320
B	 0.7076	 0.1380
C	 0.6964	 0.1320
D	 0.6824	 0.1340
E	 0.6990	 0.1300
F	 0.7049	 0.1370
G	 0.7012	 0.1310
H	 0.6149	 0.0960
I	 0.6147	 0.0860
J	 0.5682	 0.0880
K	 0.6054	 0.0950
L	 0.5940	 0.0860
M	 0.6120	 0.1000
a	 0.6924	 0.1210
b	 0.6880	 0.1220
c	 0.6826	 0.1180
d	 0.6732	 0.1160
e	 0.6941	 0.1220
f	 0.6683	 0.1160
g	 0.6886	 0.1270
h	 0.6399	 0.1210
i	 0.6195	 0.1210
j	 0.6096	 0.1160
k	 0.6129	 0.1210
l	 0.6228	 0.1210
m	 0.6024	 0.1080
n	 0.6274	 0.1080

