Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 07:24 am GMT

PDB ID	:	6HEA
EMDB ID	:	EMD-0214
Title	:	PAN-proteasome in state 3
Authors	:	Majumder, P.; Rudack, T.; Beck, F.; Baumeister, W.
Deposited on	:	2018-08-20
Resolution	:	7.04 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at
http://www.wwpdb.org/validation/2017/FAQs#types.

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

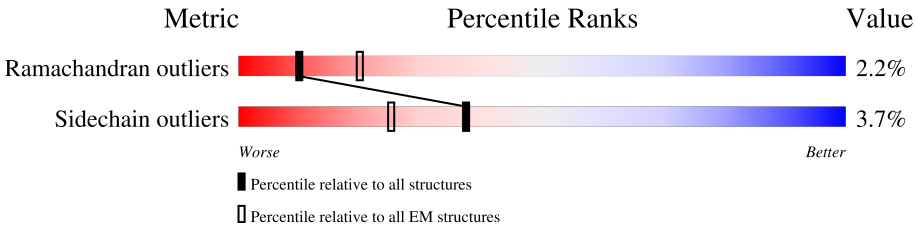
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 7.04 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 >=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 <=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	10% 75% 21% ·
1	B	242	12% 74% 23% ·
1	C	242	11% 73% 24% ·
1	D	242	10% 74% 20% 6%
1	E	242	8% 77% 19% ·
1	F	242	8% 76% 21% ·
1	G	242	9% 74% 23% ·
1	a	242	7% 75% 18% · ·
1	b	242	11% 74% 22% · ·

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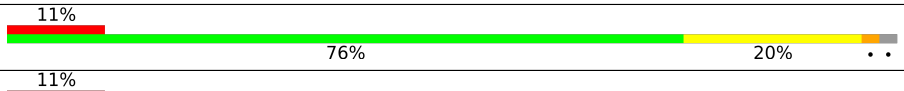
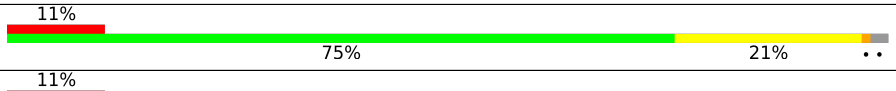
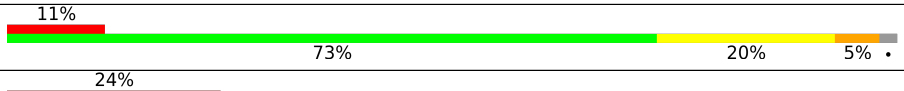
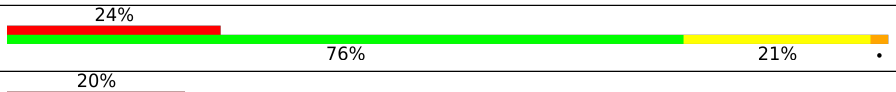
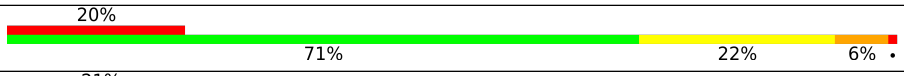
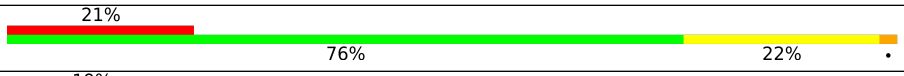
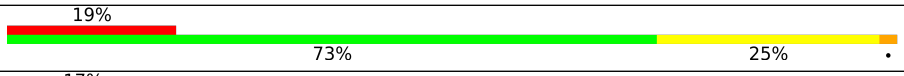
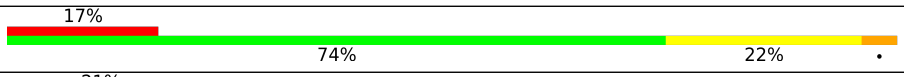
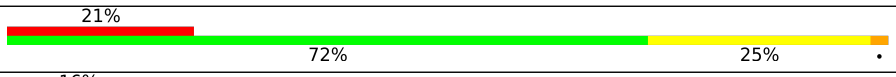
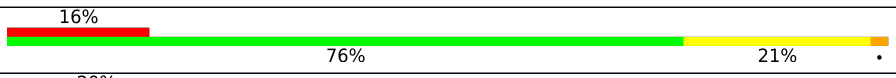
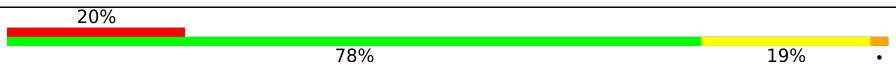
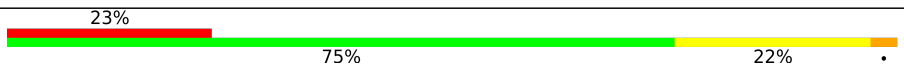
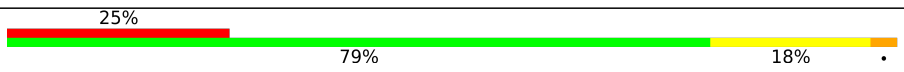
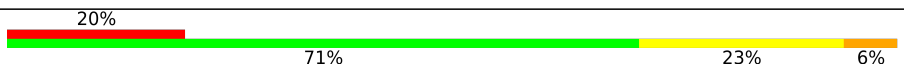
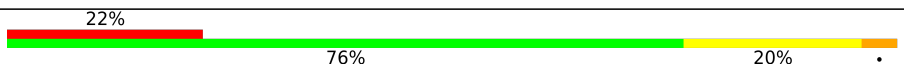
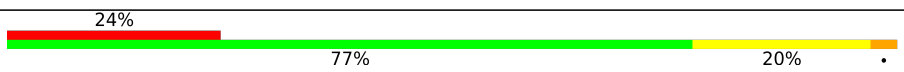
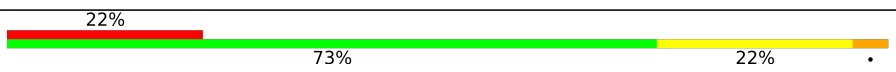
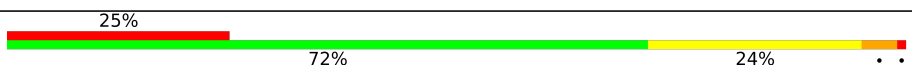
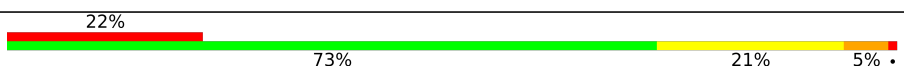
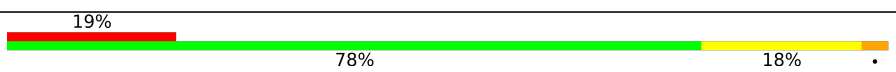
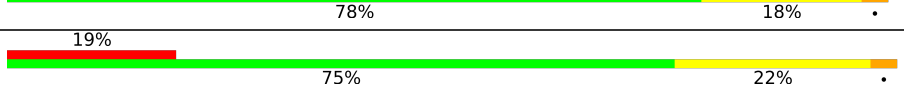
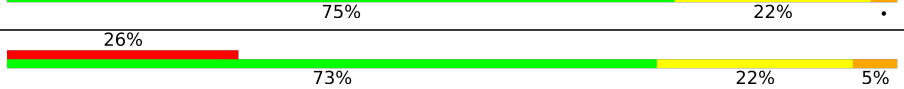
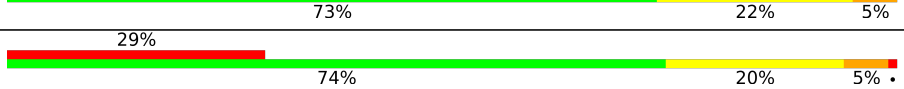
Mol	Chain	Length	Quality of chain
1	c	242	
1	d	242	
1	e	242	
1	f	242	
1	g	242	
2	1	202	
2	2	202	
2	3	202	
2	4	202	
2	5	202	
2	6	202	
2	7	202	
2	h	202	
2	i	202	
2	j	202	
2	k	202	
2	l	202	
2	m	202	
2	n	202	
3	H	390	
3	I	390	
3	J	390	
3	K	390	
3	L	390	
3	M	390	

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

- Molecule 2 is a protein called Proteasome subunit beta.

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

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

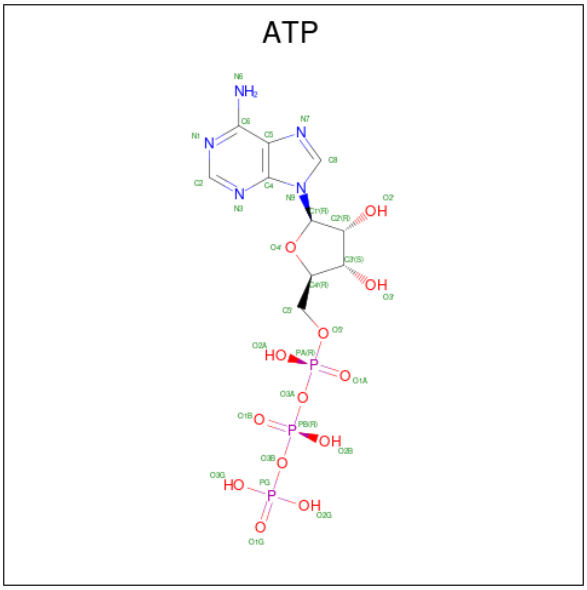
- Molecule 3 is a protein called Proteasome-activating nucleotidase.

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

- Molecule 4 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

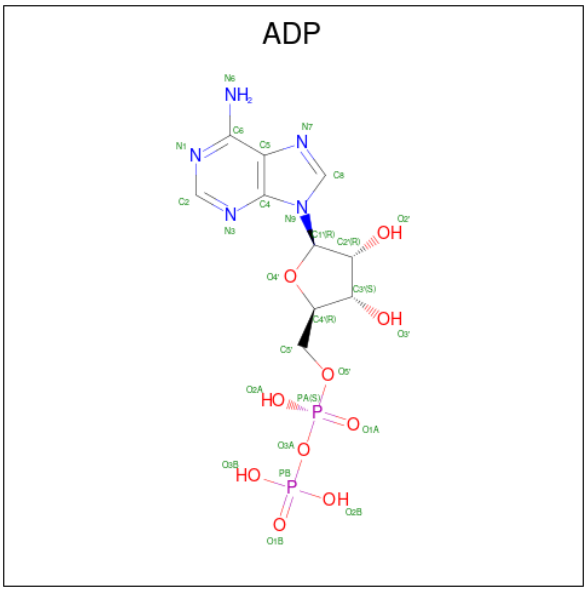
Mol	Chain	Residues	Atoms	AltConf
4	H	1	Total Mg 1 1	0
4	I	1	Total Mg 1 1	0
4	K	1	Total Mg 1 1	0
4	M	1	Total Mg 1 1	0
4	J	1	Total Mg 1 1	0

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



Mol	Chain	Residues	Atoms	AltConf
5	I	1	Total C N O P 62 20 10 26 6	0
5	I	1	Total C N O P 62 20 10 26 6	0
5	M	1	Total C N O P 31 10 5 13 3	0
5	J	1	Total C N O P 31 10 5 13 3	0

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

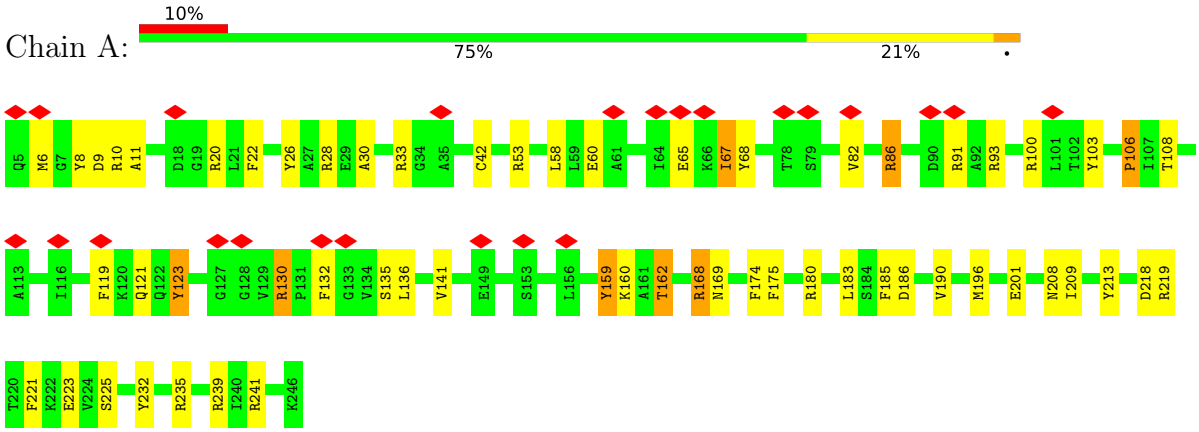


Mol	Chain	Residues	Atoms					AltConf
6	K	1	Total	C	N	O	P	0
			27	10	5	10	2	

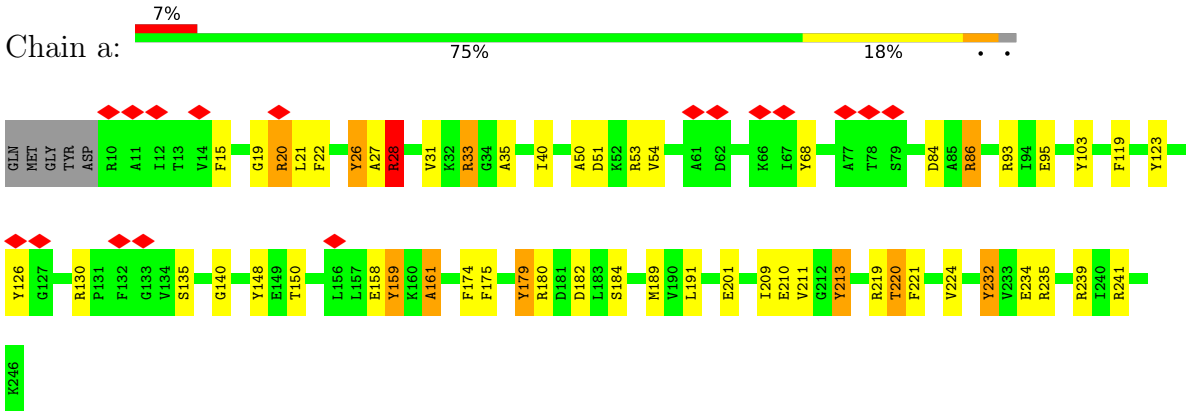
3 Residue-property plots (i)

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.

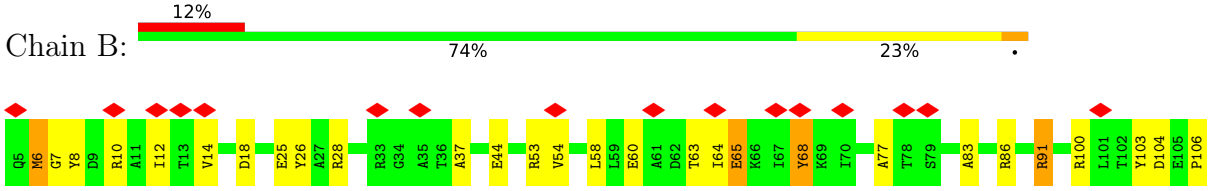
• Molecule 1: Proteasome subunit alpha

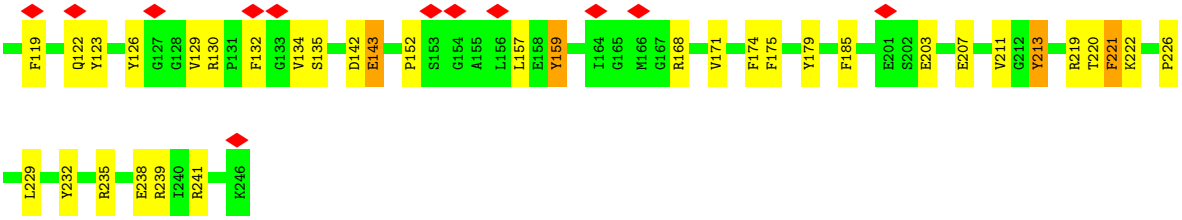


• Molecule 1: Proteasome subunit alpha



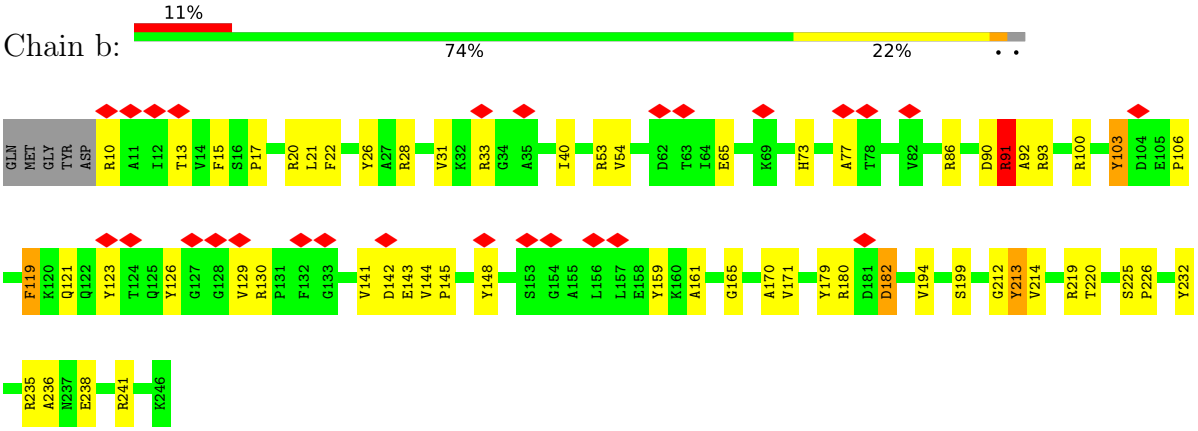
• Molecule 1: Proteasome subunit alpha





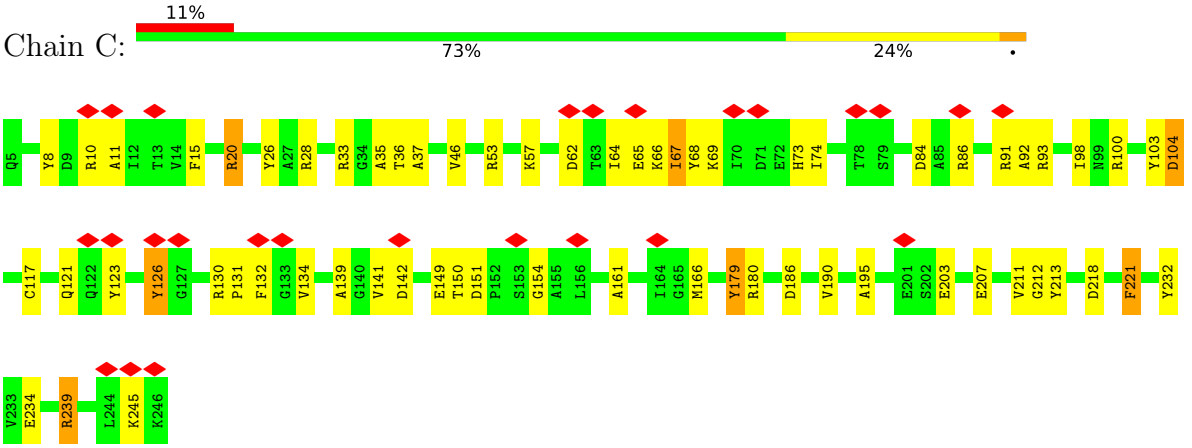
• Molecule 1: Proteasome subunit alpha

Chain b:



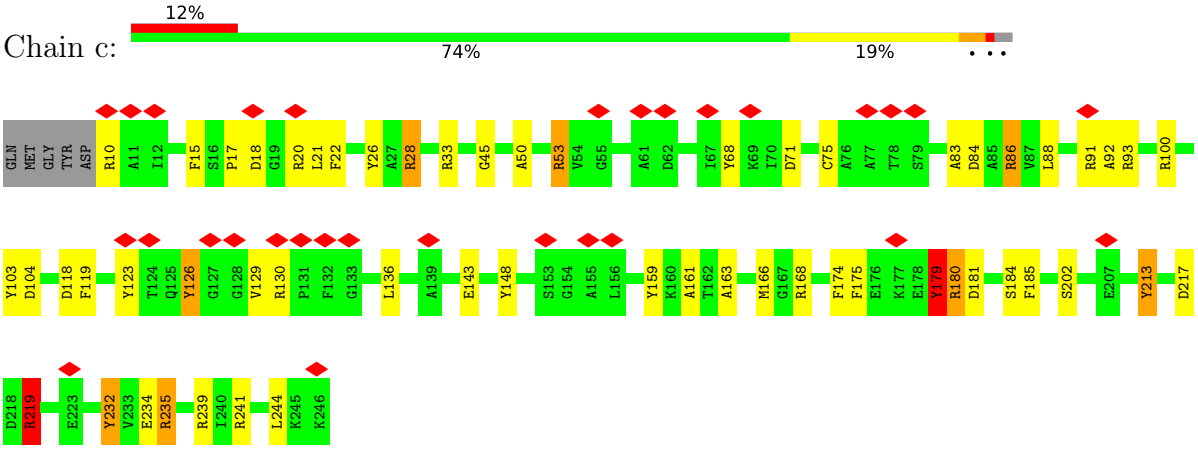
• Molecule 1: Proteasome subunit alpha

Chain C:



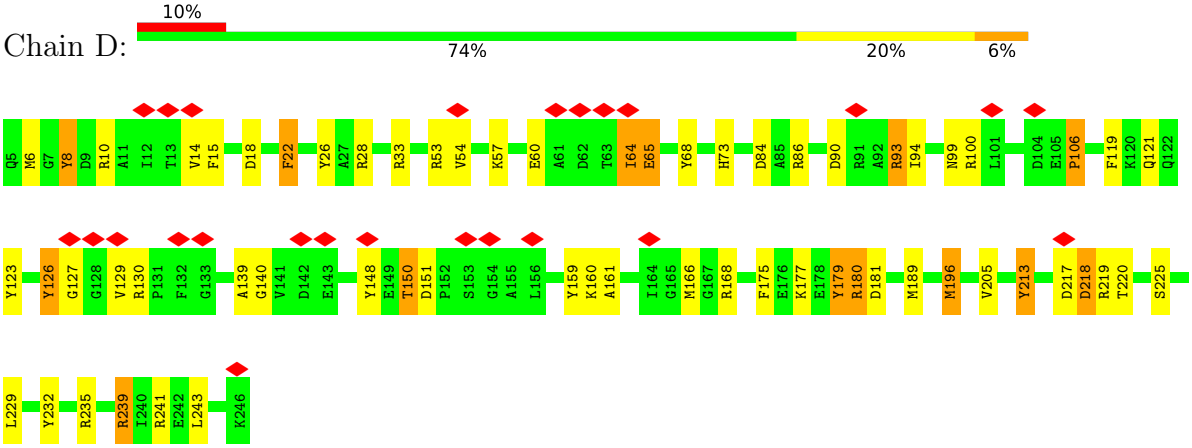
• Molecule 1: Proteasome subunit alpha

Chain c:



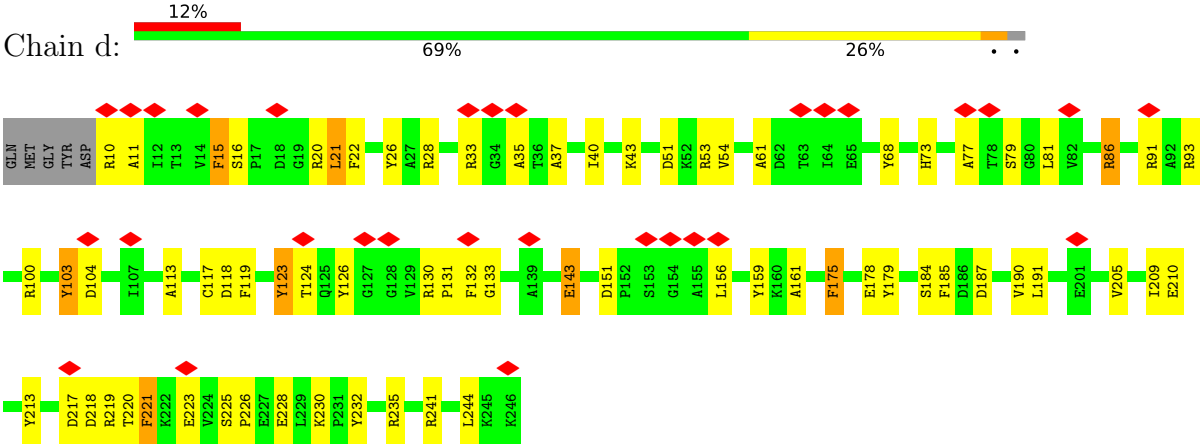
• Molecule 1: Proteasome subunit alpha

Chain D:



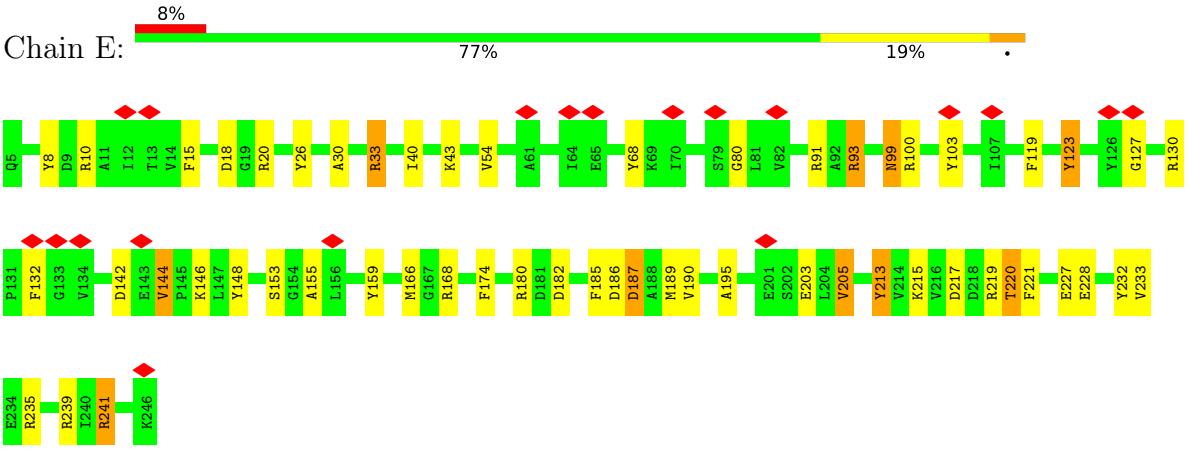
• Molecule 1: Proteasome subunit alpha

Chain d:



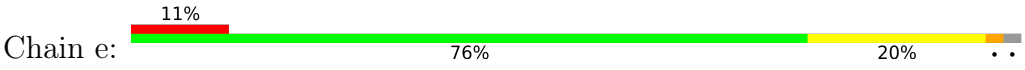
• Molecule 1: Proteasome subunit alpha

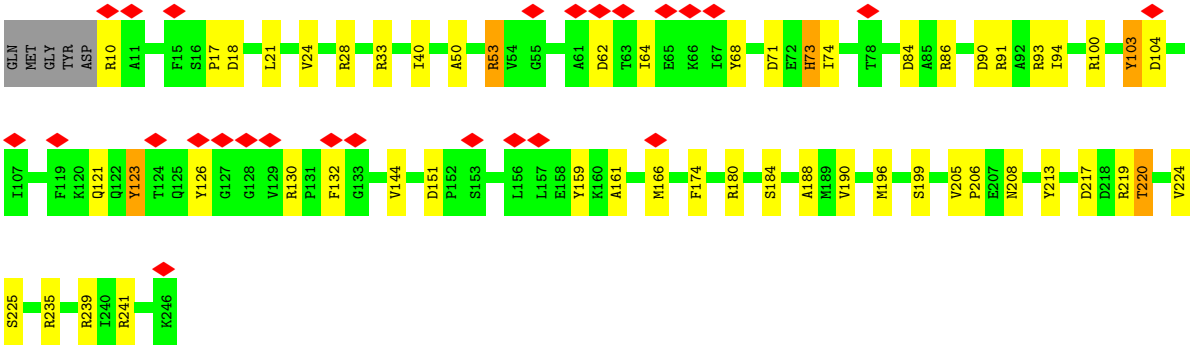
Chain E:



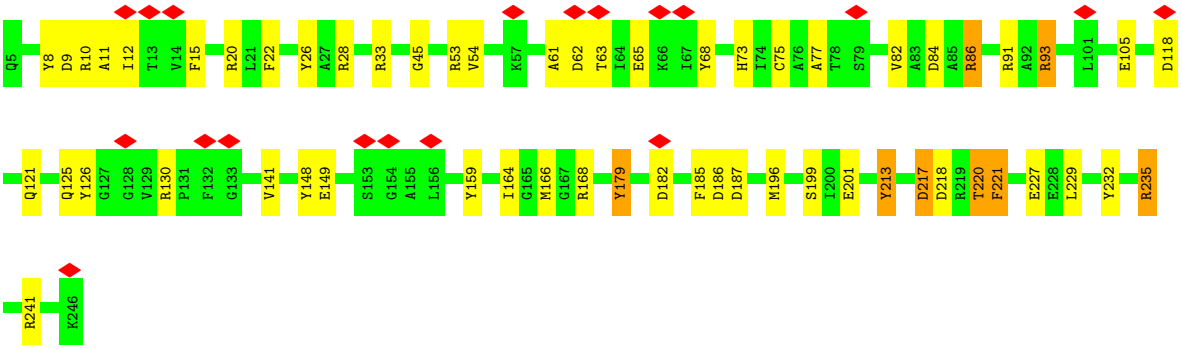
• Molecule 1: Proteasome subunit alpha

Chain e:

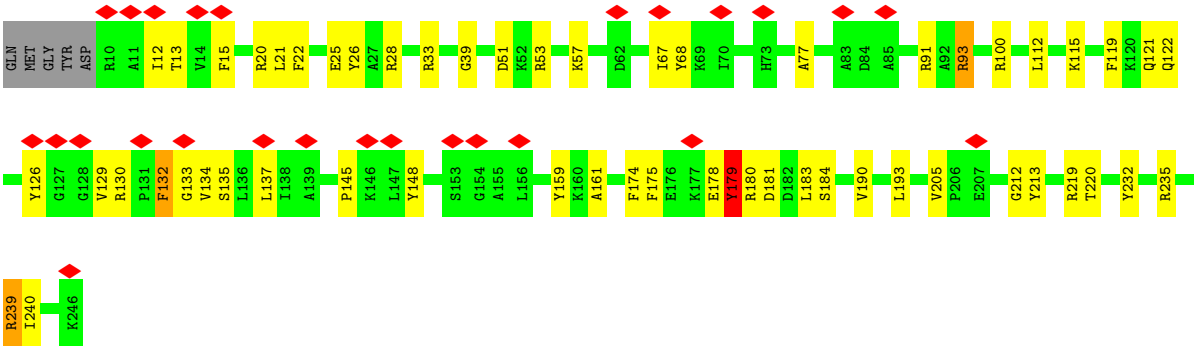




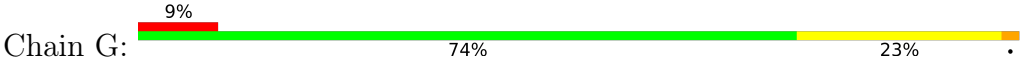
• Molecule 1: Proteasome subunit alpha

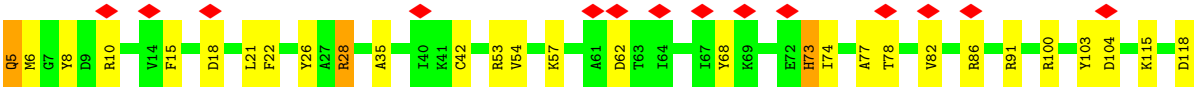


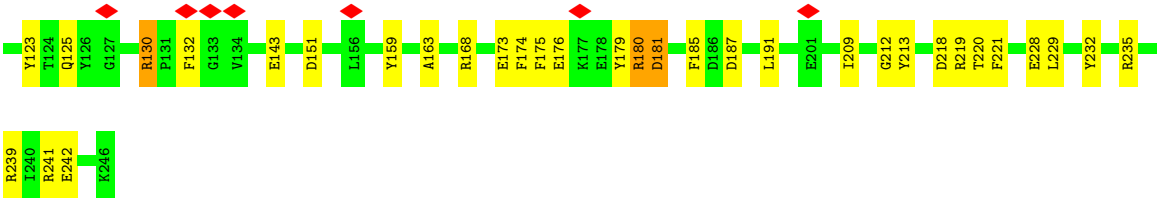
• Molecule 1: Proteasome subunit alpha



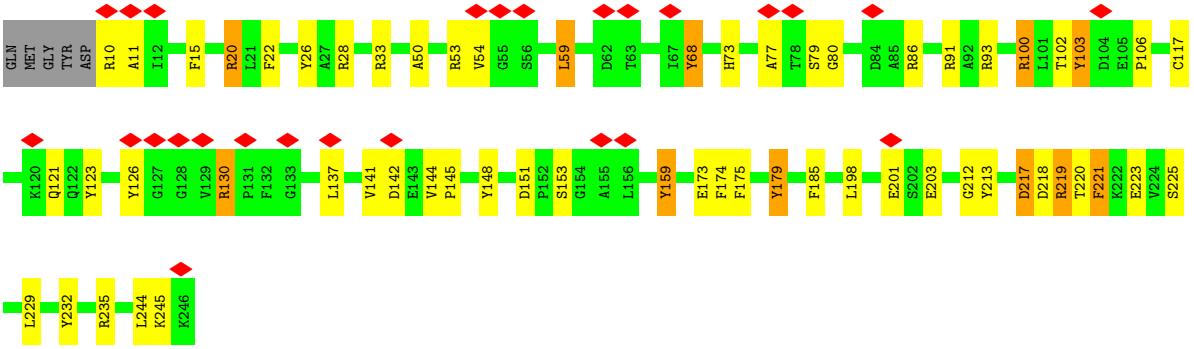
• Molecule 1: Proteasome subunit alpha



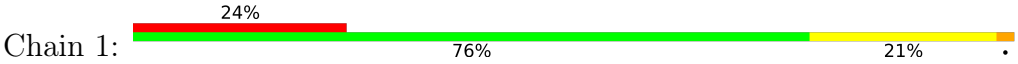


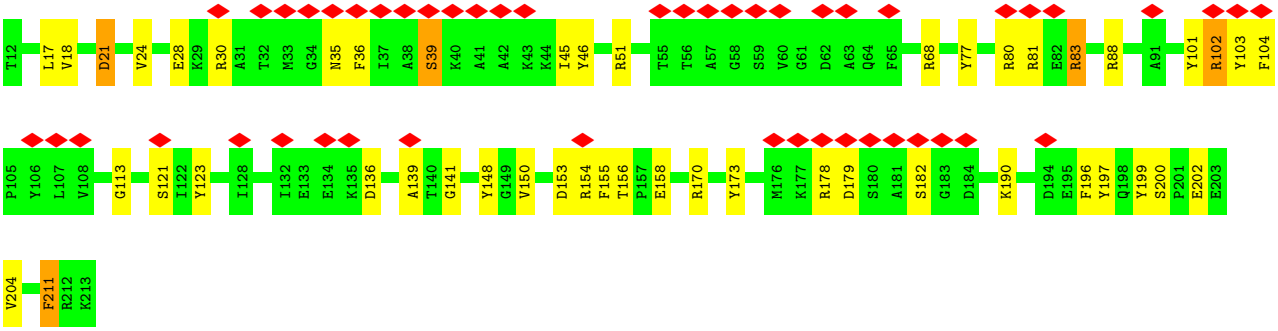


• Molecule 1: Proteasome subunit alpha

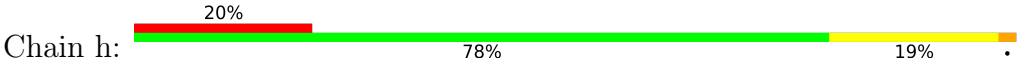


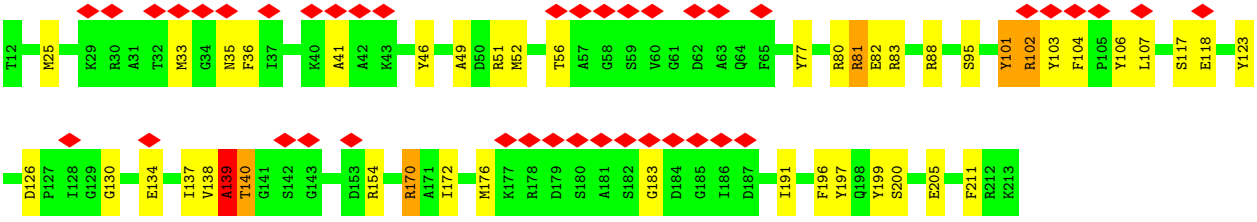
• Molecule 2: Proteasome subunit beta



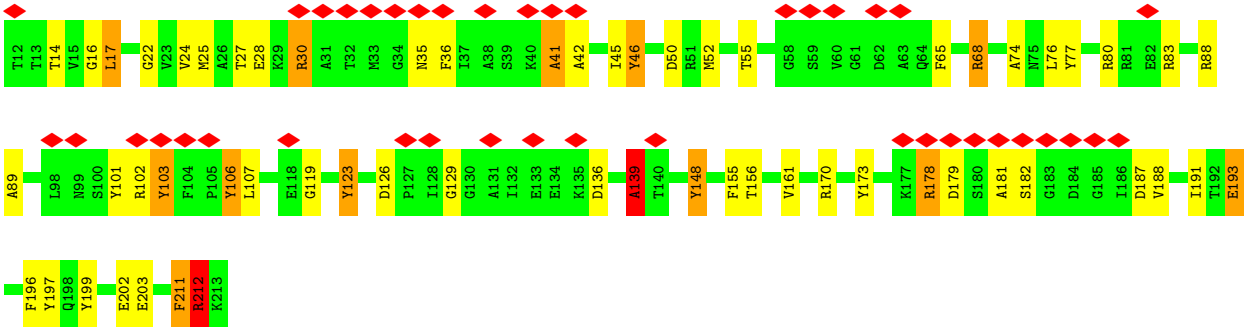


• Molecule 2: Proteasome subunit beta



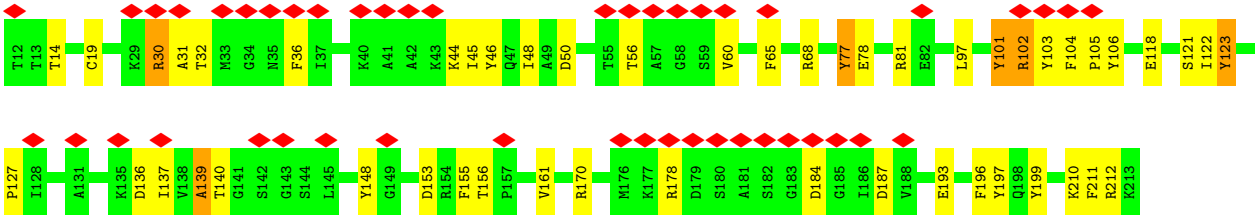


• Molecule 2: Proteasome subunit beta



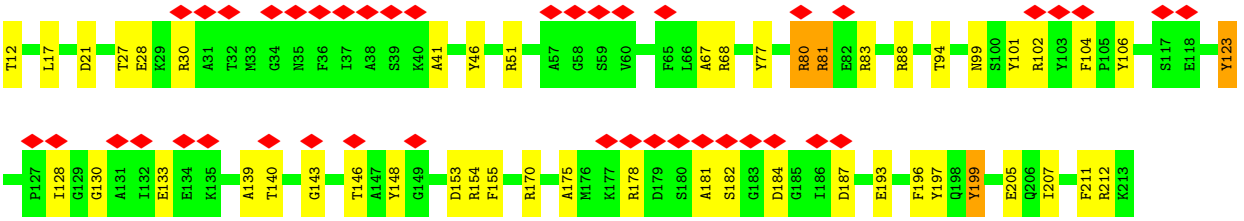
• Molecule 2: Proteasome subunit beta

Chain i:



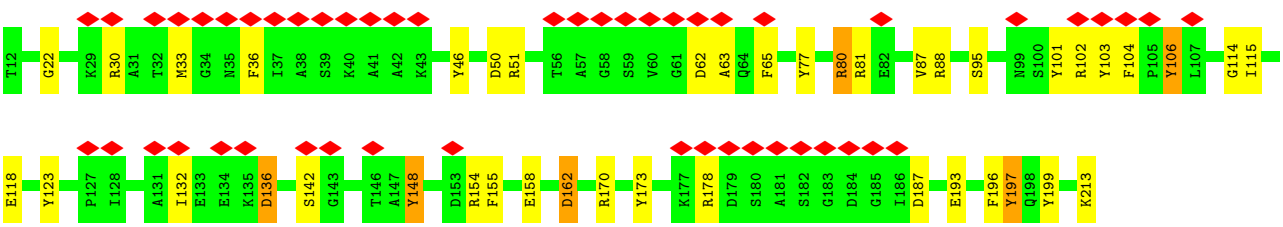
• Molecule 2: Proteasome subunit beta

Chain 3:



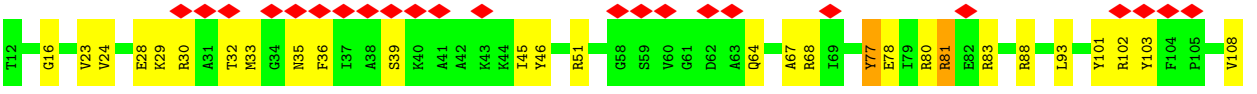
• Molecule 2: Proteasome subunit beta

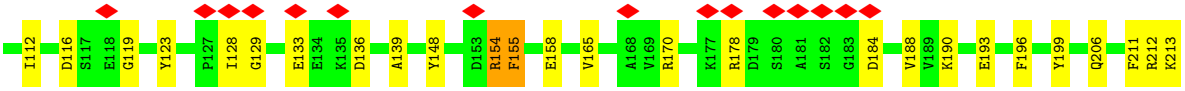
Chain j:



• Molecule 2: Proteasome subunit beta

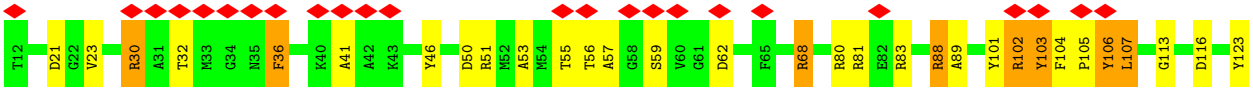
Chain 4:

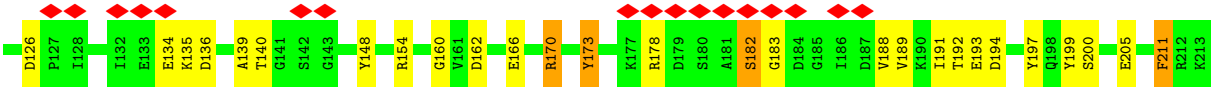




• Molecule 2: Proteasome subunit beta

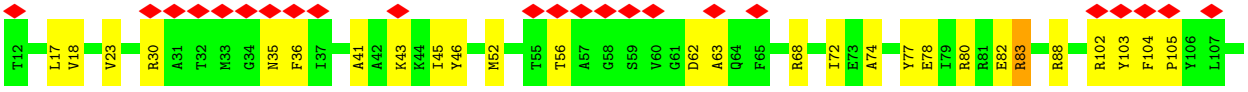
Chain k:





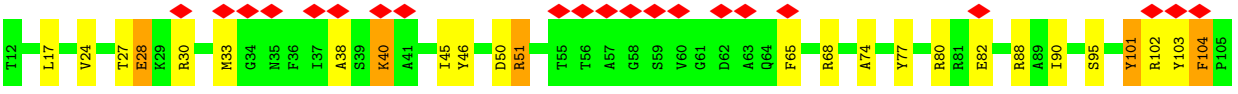
• Molecule 2: Proteasome subunit beta

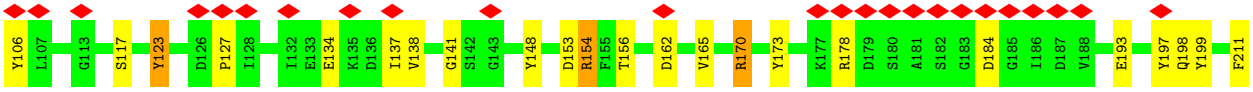
Chain 5:



• Molecule 2: Proteasome subunit beta

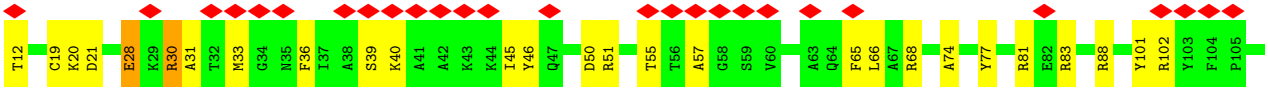
Chain l:





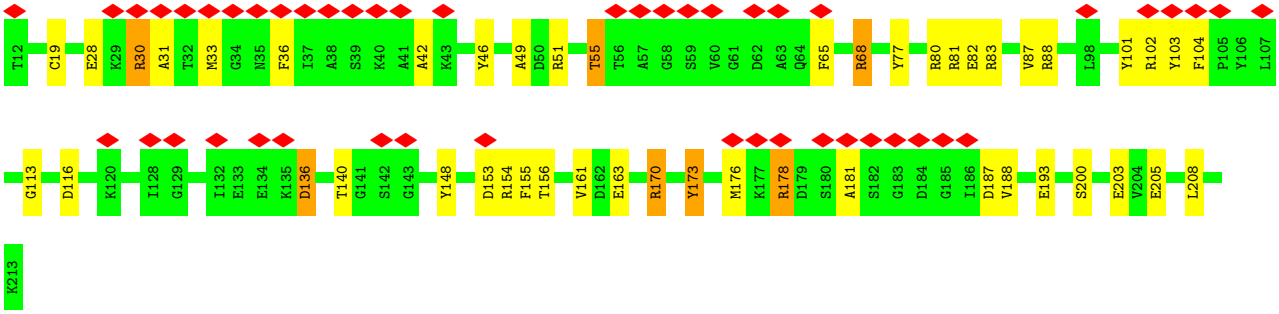
• Molecule 2: Proteasome subunit beta

Chain 6:



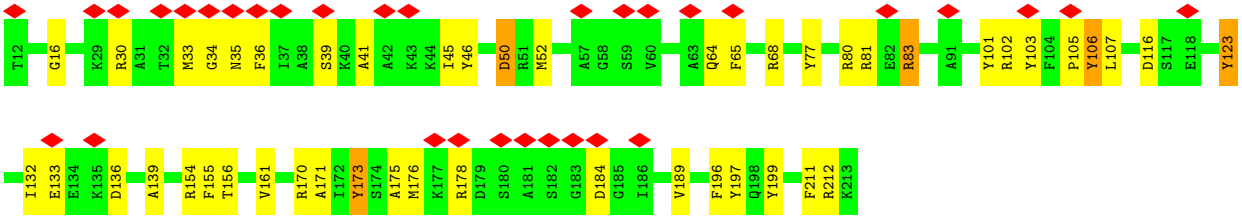
• Molecule 2: Proteasome subunit beta

Chain m:



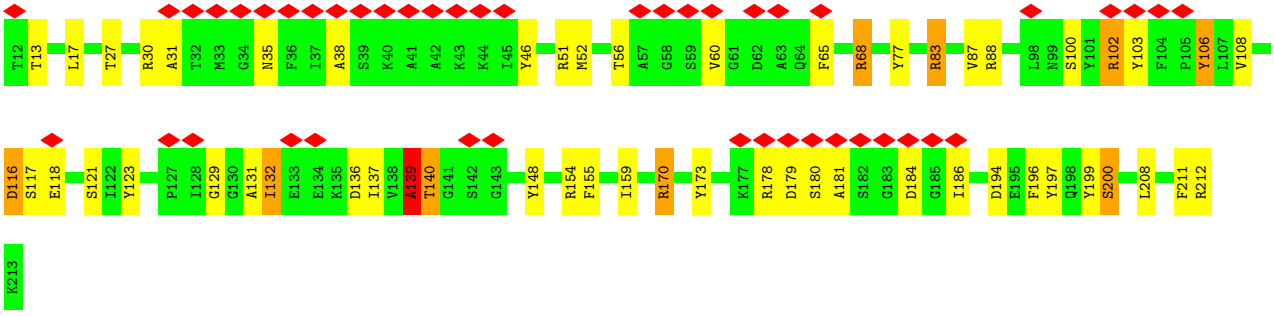
• Molecule 2: Proteasome subunit beta

Chain 7:



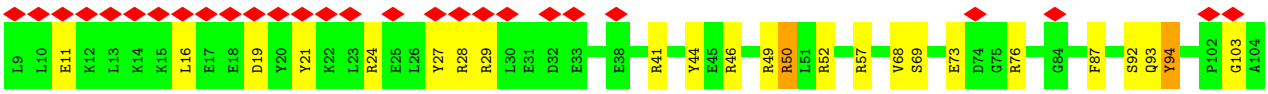
• Molecule 2: Proteasome subunit beta

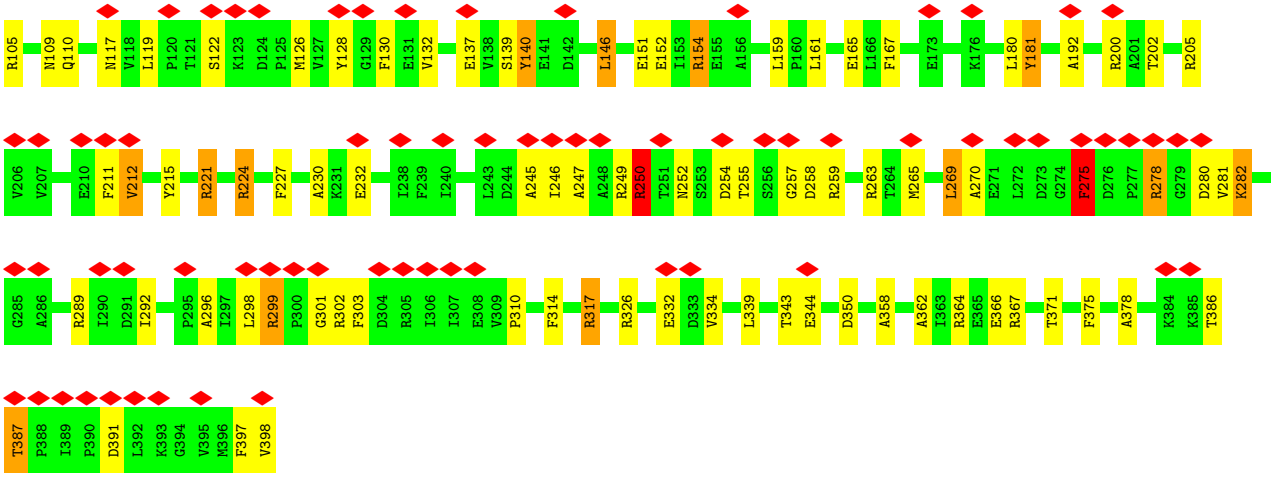
Chain n:



• Molecule 3: Proteasome-activating nucleotidase

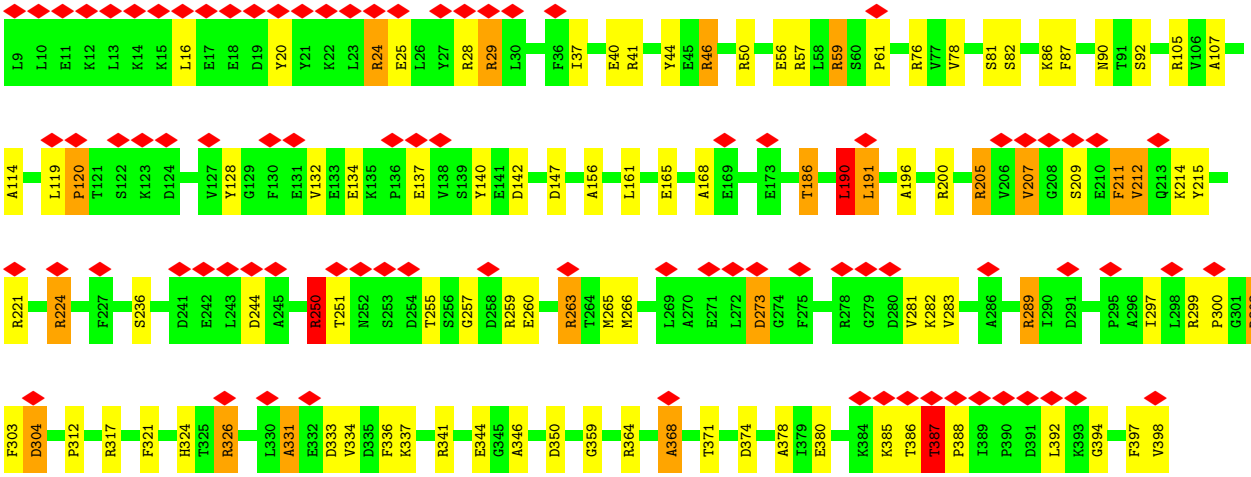
Chain H:





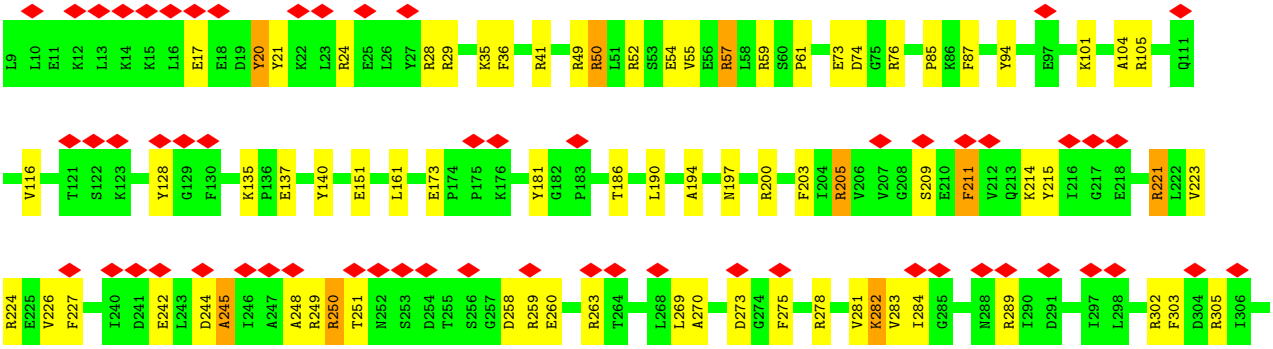
• Molecule 3: Proteasome-activating nucleotidase

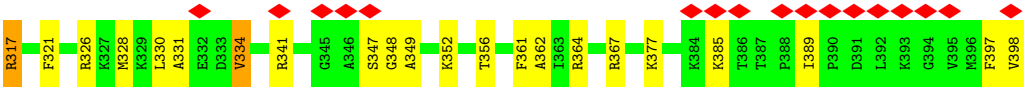
Chain I:



• Molecule 3: Proteasome-activating nucleotidase

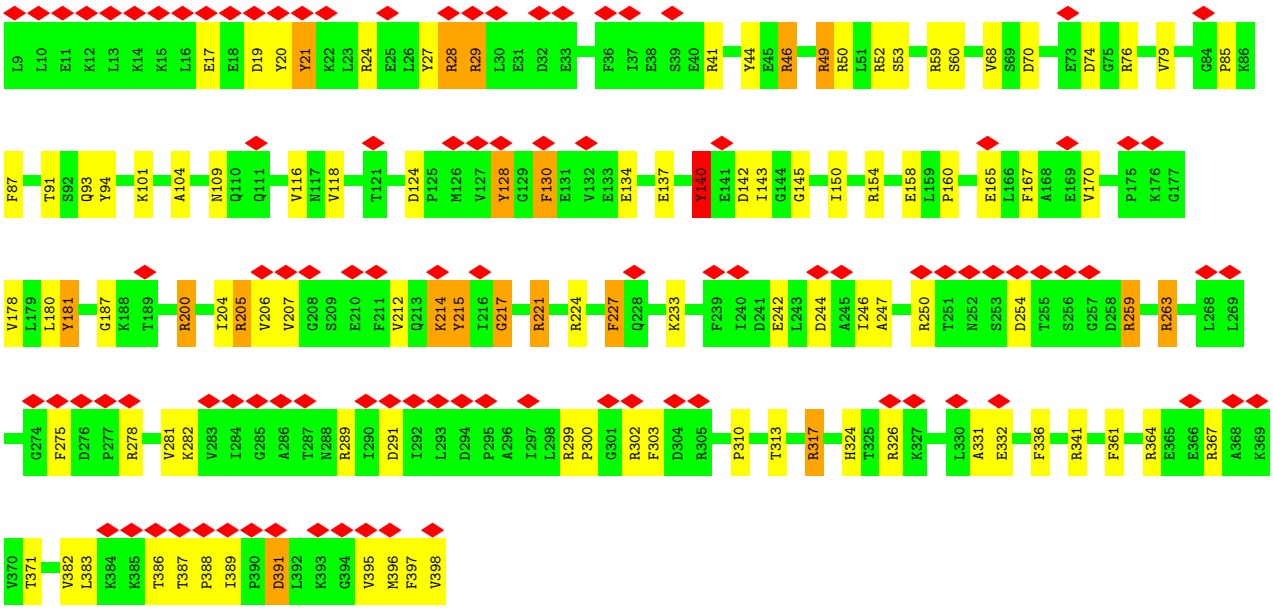
Chain K:





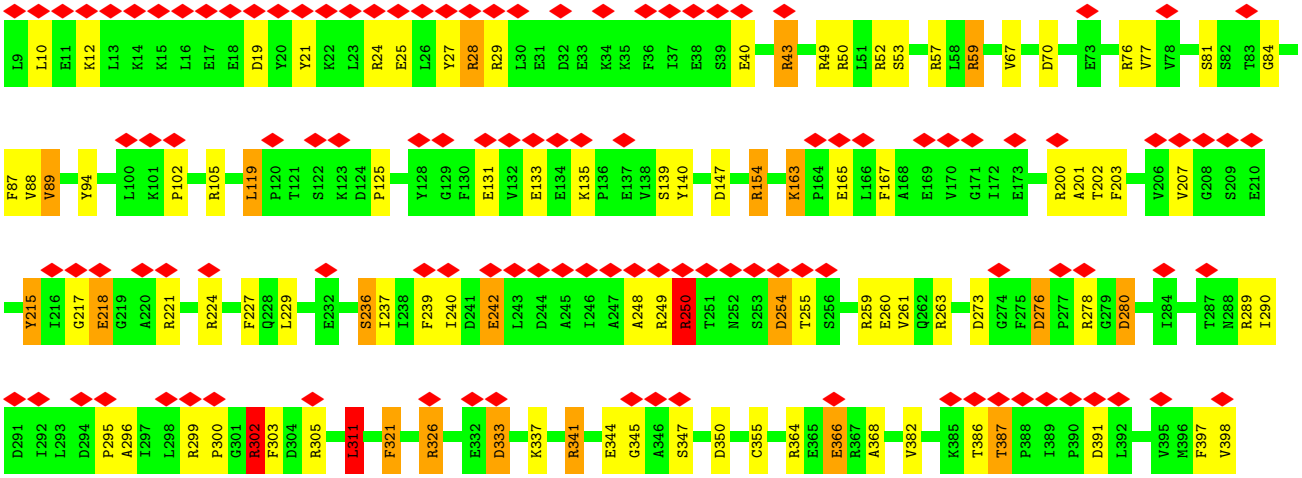
• Molecule 3: Proteasome-activating nucleotidase

Chain L:



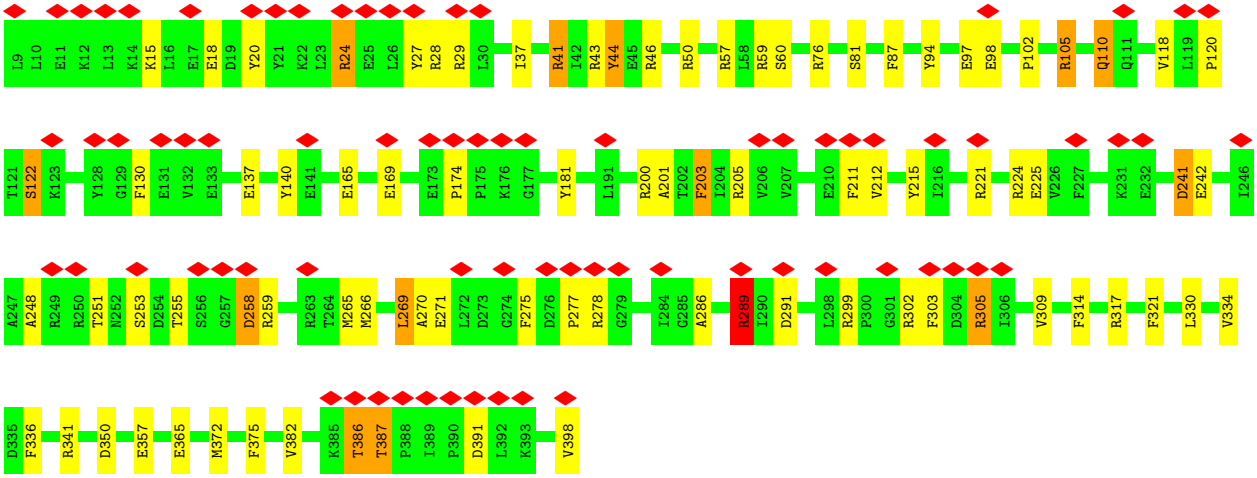
• Molecule 3: Proteasome-activating nucleotidase

Chain M:



• Molecule 3: Proteasome-activating nucleotidase

Chain J:


L9 L10 E11 K12 L13 K14 K15 L16 E17 E18 D19 Y20 Y21 K22 L23 R24 E25 L26 Y27 R28 R29 L30 I37 R41 I42 R43 Y44 E45 R46 R50 R57 L58 R59 S60 R76 S81 F87 Y94 E97 E98 P102 R105 Q110 Q111 V118 L119 P120
T121 S122 K123 Y128 G129 F130 E131 V132 E133 E137 Y140 E141 E165 E169 E173 P174 P175 K176 G177 Y181 L191 R200 A201 T202 F203 T204 R205 V206 V207 E210 F211 V212 Y215 I216 R221 R224 E225 V226 F227 K231 E232 D241 E242 I246
A247 A248 R249 R250 T251 N252 S253 D254 T255 S256 G257 D258 R259 R263 T264 M265 M266 L269 A270 E271 L272 D273 G274 F275 D276 P277 R278 G279 I284 G285 A286 R289 T290 D291 L298 R299 P300 G301 R302 F303 D304 R306 I306 V309 F314 R317 F321 L330 V334
D335 F336 R341 D350 E357 E365 M372 F375 V382 K385 T386 T387 P388 I389 P390 D391 L392 K393 V398

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	31471	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 ($e^-/Å^2$)	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	0.054	Depositor
Minimum map value	-0.040	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.002	Depositor
Recommended contour level	0.0072	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

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: ADP, ATP, 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	1.77	19/1934 (1.0%)	2.04	60/2605 (2.3%)
1	B	1.82	27/1934 (1.4%)	1.96	53/2605 (2.0%)
1	C	1.76	16/1934 (0.8%)	2.00	53/2605 (2.0%)
1	D	1.73	22/1934 (1.1%)	2.13	69/2605 (2.6%)
1	E	1.75	19/1934 (1.0%)	2.04	54/2605 (2.1%)
1	F	1.78	15/1934 (0.8%)	2.03	55/2605 (2.1%)
1	G	1.79	19/1934 (1.0%)	1.92	49/2605 (1.9%)
1	a	1.78	22/1892 (1.2%)	2.00	52/2549 (2.0%)
1	b	1.79	27/1892 (1.4%)	1.96	49/2549 (1.9%)
1	c	1.78	24/1892 (1.3%)	2.04	58/2549 (2.3%)
1	d	1.70	20/1892 (1.1%)	2.04	54/2549 (2.1%)
1	e	1.75	17/1892 (0.9%)	1.94	44/2549 (1.7%)
1	f	1.73	16/1892 (0.8%)	2.01	53/2549 (2.1%)
1	g	1.75	23/1892 (1.2%)	2.03	51/2549 (2.0%)
2	1	1.76	16/1573 (1.0%)	2.02	44/2121 (2.1%)
2	2	1.78	18/1573 (1.1%)	2.09	58/2121 (2.7%)
2	3	1.70	18/1573 (1.1%)	1.98	47/2121 (2.2%)
2	4	1.74	27/1573 (1.7%)	2.01	38/2121 (1.8%)
2	5	3.30	25/1573 (1.6%)	2.22	41/2121 (1.9%)
2	6	1.75	11/1573 (0.7%)	2.06	56/2121 (2.6%)
2	7	1.75	14/1573 (0.9%)	2.04	44/2121 (2.1%)
2	h	1.76	16/1573 (1.0%)	1.88	29/2121 (1.4%)
2	i	1.71	13/1573 (0.8%)	1.98	36/2121 (1.7%)
2	j	1.78	14/1573 (0.9%)	1.97	40/2121 (1.9%)
2	k	1.75	18/1573 (1.1%)	2.14	64/2121 (3.0%)
2	l	3.30	23/1573 (1.5%)	2.21	41/2121 (1.9%)
2	m	1.73	17/1573 (1.1%)	1.90	39/2121 (1.8%)
2	n	1.75	17/1573 (1.1%)	2.07	58/2121 (2.7%)
3	H	1.80	35/3146 (1.1%)	1.95	83/4240 (2.0%)
3	I	1.73	33/3146 (1.0%)	1.97	90/4240 (2.1%)
3	J	1.77	33/3146 (1.0%)	1.83	56/4240 (1.3%)
3	K	1.72	31/3146 (1.0%)	1.95	79/4240 (1.9%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\|>5$	RMSZ	$\#\|Z\|>5$
3	L	1.76	38/3146 (1.2%)	1.96	88/4240 (2.1%)
3	M	1.76	34/3146 (1.1%)	1.95	82/4240 (1.9%)
All	All	1.86	737/67680 (1.1%)	2.00	1867/91212 (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	7
1	B	0	9
1	C	0	4
1	D	0	11
1	E	0	5
1	F	0	8
1	G	0	9
1	a	0	9
1	b	0	6
1	c	0	8
1	d	0	10
1	e	0	7
1	f	0	7
1	g	0	8
2	1	0	4
2	2	0	8
2	3	0	6
2	4	0	7
2	5	0	9
2	6	0	3
2	7	0	8
2	h	0	7
2	i	0	6
2	j	0	4
2	k	0	10
2	l	0	8
2	m	0	6
2	n	0	6
3	H	0	22
3	I	0	19
3	J	0	14
3	K	0	11

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Mol	Chain	#Chirality outliers	#Planarity outliers
3	L	0	21
3	M	0	19
All	All	0	306

All (737) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	170	ARG	CZ-NH1	60.89	2.12	1.33
2	5	170	ARG	CZ-NH1	60.38	2.11	1.33
2	5	211	PHE	CG-CD2	49.71	2.13	1.38
2	l	211	PHE	CG-CD2	47.70	2.10	1.38
2	l	211	PHE	CG-CD1	45.23	2.06	1.38
2	5	211	PHE	CG-CD1	43.27	2.03	1.38
2	5	211	PHE	CE2-CZ	36.76	2.07	1.37
2	l	211	PHE	CE2-CZ	35.49	2.04	1.37
2	l	211	PHE	CE1-CZ	34.65	2.03	1.37
2	5	211	PHE	CE1-CZ	32.77	1.99	1.37
2	l	211	PHE	CD1-CE1	32.77	2.04	1.39
2	5	211	PHE	CD1-CE1	31.06	2.01	1.39
2	5	211	PHE	CD2-CE2	30.82	2.00	1.39
2	l	211	PHE	CD2-CE2	30.46	2.00	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	c	148	TYR	CG-CD1	9.75	1.51	1.39
2	1	113	GLY	CA-C	-9.18	1.37	1.51
1	c	68	TYR	CE2-CZ	8.88	1.50	1.38
3	M	59	ARG	CZ-NH2	8.81	1.44	1.33
1	b	238	GLU	CG-CD	8.72	1.65	1.51
2	h	117	SER	CA-CB	8.51	1.65	1.52
1	A	241	ARG	CD-NE	8.41	1.60	1.46
3	L	41	ARG	CZ-NH1	8.28	1.43	1.33
2	6	212	ARG	CZ-NH2	8.26	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	45	GLY	CA-C	-8.25	1.38	1.51
3	I	128	TYR	CG-CD2	8.17	1.49	1.39
1	F	130	ARG	NE-CZ	8.15	1.43	1.33
2	m	173	TYR	CD1-CE1	8.11	1.51	1.39
1	e	100	ARG	CD-NE	8.09	1.60	1.46
2	j	199	TYR	CE1-CZ	7.97	1.49	1.38
3	H	165	GLU	CG-CD	7.97	1.64	1.51
1	a	180	ARG	NE-CZ	7.95	1.43	1.33
1	B	238	GLU	CD-OE1	7.92	1.34	1.25
3	J	76	ARG	CZ-NH2	7.91	1.43	1.33
1	b	20	ARG	CZ-NH2	7.90	1.43	1.33
1	e	225	SER	CA-CB	7.89	1.64	1.52
3	I	56	GLU	CD-OE2	7.85	1.34	1.25
3	M	347	SER	CB-OG	7.84	1.52	1.42
3	J	278	ARG	CZ-NH1	7.83	1.43	1.33
1	a	68	TYR	CB-CG	-7.81	1.40	1.51
2	k	68	ARG	NE-CZ	7.80	1.43	1.33
2	2	16	GLY	N-CA	-7.78	1.34	1.46
2	6	124	SER	CA-CB	7.68	1.64	1.52
3	K	260	GLU	CD-OE1	7.62	1.34	1.25
3	J	305	ARG	CZ-NH2	7.54	1.42	1.33
3	H	152	GLU	CG-CD	7.52	1.63	1.51
1	G	26	TYR	CG-CD2	7.51	1.49	1.39
1	f	180	ARG	CZ-NH2	7.42	1.42	1.33
3	H	232	GLU	CG-CD	7.41	1.63	1.51
1	b	26	TYR	CE1-CZ	7.40	1.48	1.38
3	L	205	ARG	NE-CZ	7.39	1.42	1.33
1	e	53	ARG	CZ-NH1	7.35	1.42	1.33
3	H	278	ARG	CD-NE	7.35	1.58	1.46
1	b	130	ARG	CZ-NH2	7.35	1.42	1.33
2	6	77	TYR	CG-CD2	7.35	1.48	1.39
1	a	53	ARG	CD-NE	7.34	1.58	1.46
1	c	235	ARG	CD-NE	7.33	1.58	1.46
1	A	174	PHE	CG-CD1	7.26	1.49	1.38
1	B	241	ARG	NE-CZ	7.25	1.42	1.33
3	M	81	SER	CB-OG	7.25	1.51	1.42
2	5	103	TYR	CG-CD1	7.23	1.48	1.39
1	e	100	ARG	NE-CZ	7.22	1.42	1.33
1	E	213	TYR	CZ-OH	7.22	1.50	1.37
1	C	68	TYR	CE2-CZ	7.21	1.48	1.38
1	e	213	TYR	CG-CD1	7.21	1.48	1.39
1	E	100	ARG	CD-NE	7.18	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	83	ARG	CD-NE	7.18	1.58	1.46
3	I	364	ARG	CD-NE	7.16	1.58	1.46
2	1	80	ARG	NE-CZ	7.14	1.42	1.33
2	n	83	ARG	NE-CZ	7.13	1.42	1.33
1	E	235	ARG	NE-CZ	7.12	1.42	1.33
1	A	235	ARG	NE-CZ	7.11	1.42	1.33
1	f	175	PHE	CE1-CZ	7.08	1.50	1.37
2	4	102	ARG	CD-NE	7.06	1.58	1.46
1	A	219	ARG	NE-CZ	7.03	1.42	1.33
2	n	197	TYR	CG-CD2	7.03	1.48	1.39
1	g	219	ARG	NE-CZ	7.02	1.42	1.33
2	4	81	ARG	NE-CZ	7.01	1.42	1.33
1	F	213	TYR	CG-CD1	6.99	1.48	1.39
3	M	278	ARG	CD-NE	6.98	1.58	1.46
2	5	154	ARG	NE-CZ	6.98	1.42	1.33
2	i	81	ARG	NE-CZ	6.95	1.42	1.33
1	a	126	TYR	CG-CD1	6.95	1.48	1.39
1	e	224	VAL	CB-CG2	6.94	1.67	1.52
3	K	76	ARG	NE-CZ	6.93	1.42	1.33
2	4	28	GLU	CD-OE1	6.92	1.33	1.25
2	l	123	TYR	CB-CG	-6.91	1.41	1.51
3	H	140	TYR	CG-CD2	6.90	1.48	1.39
3	L	299	ARG	CZ-NH2	6.89	1.42	1.33
1	C	232	TYR	CE1-CZ	6.89	1.47	1.38
1	A	82	VAL	CB-CG1	6.89	1.67	1.52
1	E	180	ARG	CD-NE	6.89	1.58	1.46
3	M	224	ARG	NE-CZ	6.88	1.42	1.33
1	b	219	ARG	CZ-NH1	6.87	1.42	1.33
2	k	160	GLY	CA-C	-6.87	1.40	1.51
3	J	259	ARG	NE-CZ	6.87	1.42	1.33
2	k	113	GLY	N-CA	-6.86	1.35	1.46
2	n	196	PHE	CG-CD2	6.83	1.49	1.38
2	n	83	ARG	CD-NE	6.81	1.58	1.46
2	5	88	ARG	CZ-NH1	6.79	1.41	1.33
2	4	129	GLY	N-CA	-6.78	1.35	1.46
1	A	123	TYR	CB-CG	6.77	1.61	1.51
2	4	51	ARG	NE-CZ	6.77	1.41	1.33
1	E	148	TYR	CG-CD2	6.77	1.48	1.39
3	H	137	GLU	CD-OE2	6.75	1.33	1.25
3	I	224	ARG	CZ-NH2	6.74	1.41	1.33
1	b	226	PRO	N-CD	-6.74	1.38	1.47
1	c	91	ARG	CZ-NH1	6.73	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	f	130	ARG	NE-CZ	6.73	1.41	1.33
1	a	201	GLU	CG-CD	6.69	1.61	1.51
1	A	232	TYR	CG-CD1	6.65	1.47	1.39
1	E	235	ARG	CZ-NH1	6.65	1.41	1.33
1	f	180	ARG	NE-CZ	6.63	1.41	1.33
2	n	103	TYR	CG-CD1	6.63	1.47	1.39
1	a	86	ARG	CZ-NH2	6.62	1.41	1.33
2	l	106	TYR	CE1-CZ	6.62	1.47	1.38
1	c	168	ARG	NE-CZ	6.59	1.41	1.33
3	L	165	GLU	CB-CG	6.59	1.64	1.52
1	F	91	ARG	CZ-NH2	6.58	1.41	1.33
1	b	100	ARG	CD-NE	6.58	1.57	1.46
1	G	219	ARG	CD-NE	6.57	1.57	1.46
1	D	219	ARG	CD-NE	6.55	1.57	1.46
2	l	102	ARG	CZ-NH1	6.55	1.41	1.33
2	1	200	SER	CA-CB	6.55	1.62	1.52
2	7	80	ARG	CZ-NH2	6.54	1.41	1.33
1	e	53	ARG	CZ-NH2	6.54	1.41	1.33
1	f	28	ARG	CD-NE	6.53	1.57	1.46
2	2	102	ARG	CD-NE	6.52	1.57	1.46
3	H	41	ARG	CZ-NH2	6.50	1.41	1.33
3	I	28	ARG	NE-CZ	6.50	1.41	1.33
1	e	100	ARG	CZ-NH2	6.47	1.41	1.33
2	h	103	TYR	CB-CG	6.47	1.61	1.51
2	i	68	ARG	CZ-NH1	6.46	1.41	1.33
2	3	68	ARG	CZ-NH1	6.46	1.41	1.33
2	m	83	ARG	CZ-NH1	6.46	1.41	1.33
3	I	46	ARG	CZ-NH1	6.46	1.41	1.33
1	a	19	GLY	CA-C	-6.46	1.41	1.51
3	J	98	GLU	CD-OE2	6.44	1.32	1.25
1	a	50	ALA	CA-CB	6.44	1.66	1.52
1	D	28	ARG	NE-CZ	6.43	1.41	1.33
3	L	87	PHE	CG-CD2	6.42	1.48	1.38
3	L	94	TYR	CB-CG	6.41	1.61	1.51
2	m	28	GLU	CG-CD	6.40	1.61	1.51
1	A	22	PHE	CG-CD1	6.40	1.48	1.38
3	J	43	ARG	CZ-NH2	6.39	1.41	1.33
1	c	130	ARG	CD-NE	6.38	1.57	1.46
1	a	179	TYR	CE1-CZ	6.38	1.46	1.38
2	5	78	GLU	CD-OE1	6.38	1.32	1.25
2	7	39	SER	CA-CB	6.37	1.62	1.52
1	D	10	ARG	CD-NE	6.37	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	26	TYR	CE2-CZ	6.36	1.46	1.38
1	B	8	TYR	CE1-CZ	6.35	1.46	1.38
2	2	182	SER	CA-CB	6.35	1.62	1.52
3	L	278	ARG	NE-CZ	6.34	1.41	1.33
3	H	49	ARG	NE-CZ	6.32	1.41	1.33
2	i	118	GLU	CD-OE1	6.31	1.32	1.25
1	B	100	ARG	CD-NE	6.31	1.57	1.46
1	A	180	ARG	CZ-NH1	6.29	1.41	1.33
3	M	200	ARG	NE-CZ	6.29	1.41	1.33
3	L	130	PHE	CG-CD2	6.28	1.48	1.38
3	K	302	ARG	CZ-NH1	6.27	1.41	1.33
2	2	199	TYR	CG-CD2	6.26	1.47	1.39
3	J	59	ARG	CZ-NH2	6.25	1.41	1.33
2	h	46	TYR	CG-CD1	6.24	1.47	1.39
1	E	233	VAL	CB-CG1	6.24	1.66	1.52
2	k	81	ARG	NE-CZ	6.23	1.41	1.33
1	b	103	TYR	CE1-CZ	6.23	1.46	1.38
2	h	51	ARG	CZ-NH1	6.23	1.41	1.33
2	m	205	GLU	CD-OE1	6.23	1.32	1.25
2	1	51	ARG	CD-NE	6.22	1.57	1.46
1	F	65	GLU	CG-CD	6.21	1.61	1.51
3	L	341	ARG	CZ-NH1	6.21	1.41	1.33
3	I	259	ARG	NE-CZ	6.19	1.41	1.33
2	n	68	ARG	CZ-NH2	6.19	1.41	1.33
2	k	104	PHE	CG-CD1	6.18	1.48	1.38
2	2	148	TYR	CE1-CZ	6.18	1.46	1.38
1	d	10	ARG	CD-NE	6.17	1.56	1.46
3	M	302	ARG	NE-CZ	6.17	1.41	1.33
1	B	65	GLU	CD-OE2	6.16	1.32	1.25
3	K	209	SER	CA-CB	6.16	1.62	1.52
3	I	300	PRO	N-CD	6.14	1.56	1.47
1	G	73	HIS	N-CA	-6.13	1.34	1.46
1	c	10	ARG	CD-NE	6.13	1.56	1.46
1	E	168	ARG	NE-CZ	6.13	1.41	1.33
2	2	101	TYR	CE2-CZ	6.13	1.46	1.38
1	f	184	SER	CA-CB	6.12	1.62	1.52
2	3	193	GLU	CD-OE1	6.12	1.32	1.25
1	e	86	ARG	CZ-NH1	6.12	1.41	1.33
3	H	302	ARG	CZ-NH2	6.11	1.41	1.33
2	n	60	VAL	CA-CB	6.11	1.67	1.54
3	I	40	GLU	CB-CG	6.11	1.63	1.52
1	D	180	ARG	NE-CZ	6.11	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	G	100	ARG	NE-CZ	6.11	1.41	1.33
2	k	200	SER	CA-CB	6.11	1.62	1.52
2	m	173	TYR	CZ-OH	6.10	1.48	1.37
2	l	117	SER	CA-CB	6.09	1.62	1.52
2	2	22	GLY	N-CA	-6.09	1.36	1.46
1	b	103	TYR	CE2-CZ	6.09	1.46	1.38
1	C	179	TYR	CB-CG	6.08	1.60	1.51
1	g	173	GLU	CD-OE2	6.08	1.32	1.25
3	K	305	ARG	NE-CZ	6.08	1.41	1.33
1	E	227	GLU	CD-OE2	6.07	1.32	1.25
1	a	158	GLU	CG-CD	6.07	1.61	1.51
2	4	154	ARG	NE-CZ	6.07	1.41	1.33
2	1	196	PHE	CA-CB	6.06	1.67	1.53
3	M	305	ARG	CD-NE	6.06	1.56	1.46
2	1	170	ARG	NE-CZ	6.06	1.41	1.33
1	d	223	GLU	CG-CD	6.05	1.61	1.51
2	h	200	SER	CA-CB	6.04	1.62	1.52
2	i	30	ARG	CD-NE	6.04	1.56	1.46
1	e	199	SER	CB-OG	-6.04	1.34	1.42
1	c	119	PHE	CG-CD1	6.03	1.47	1.38
3	K	200	ARG	NE-CZ	6.03	1.40	1.33
1	b	126	TYR	CG-CD2	6.02	1.47	1.39
1	c	148	TYR	CD1-CE1	6.02	1.48	1.39
1	B	53	ARG	NE-CZ	6.02	1.40	1.33
1	D	225	SER	CA-CB	6.02	1.61	1.52
2	5	80	ARG	CZ-NH2	6.01	1.40	1.33
1	g	126	TYR	CB-CG	-5.98	1.42	1.51
1	g	73	HIS	CB-CG	5.98	1.60	1.50
3	I	312	PRO	CA-C	-5.98	1.40	1.52
3	H	46	ARG	CZ-NH1	5.96	1.40	1.33
3	M	299	ARG	CZ-NH1	5.96	1.40	1.33
3	K	54	GLU	CD-OE1	5.96	1.32	1.25
2	6	81	ARG	CD-NE	5.95	1.56	1.46
2	l	173	TYR	CD2-CE2	5.94	1.48	1.39
1	d	133	GLY	CA-C	-5.94	1.42	1.51
2	j	199	TYR	CB-CG	5.93	1.60	1.51
1	f	53	ARG	CD-NE	5.93	1.56	1.46
1	g	153	SER	CA-CB	5.93	1.61	1.52
1	g	79	SER	CB-OG	-5.93	1.34	1.42
1	g	235	ARG	CZ-NH2	5.93	1.40	1.33
3	H	299	ARG	CZ-NH2	5.92	1.40	1.33
1	G	26	TYR	CE2-CZ	5.92	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	1	199	TYR	CE1-CZ	5.91	1.46	1.38
1	B	86	ARG	CZ-NH2	5.90	1.40	1.33
1	b	106	PRO	N-CD	-5.89	1.39	1.47
1	c	45	GLY	CA-C	-5.89	1.42	1.51
2	2	211	PHE	CG-CD2	5.89	1.47	1.38
2	m	163	GLU	CD-OE1	5.89	1.32	1.25
2	m	82	GLU	CD-OE1	5.88	1.32	1.25
3	J	94	TYR	CG-CD2	5.88	1.46	1.39
2	4	103	TYR	CG-CD1	5.88	1.46	1.39
3	H	29	ARG	CZ-NH2	5.88	1.40	1.33
1	B	126	TYR	CZ-OH	5.87	1.47	1.37
1	d	241	ARG	NE-CZ	5.87	1.40	1.33
2	7	46	TYR	CB-CG	5.87	1.60	1.51
3	K	24	ARG	CZ-NH1	5.86	1.40	1.33
2	2	196	PHE	CA-CB	5.86	1.66	1.53
2	j	101	TYR	CG-CD1	5.86	1.46	1.39
2	6	117	SER	CA-CB	5.86	1.61	1.52
3	L	76	ARG	CZ-NH2	5.85	1.40	1.33
3	M	300	PRO	N-CD	5.85	1.56	1.47
3	M	53	SER	CA-CB	5.85	1.61	1.52
1	f	68	TYR	CZ-OH	5.85	1.47	1.37
3	K	259	ARG	CD-NE	5.84	1.56	1.46
3	J	221	ARG	CD-NE	5.84	1.56	1.46
1	F	93	ARG	NE-CZ	5.84	1.40	1.33
1	a	68	TYR	CE1-CZ	5.83	1.46	1.38
3	L	299	ARG	CZ-NH1	5.83	1.40	1.33
1	c	100	ARG	CZ-NH1	5.83	1.40	1.33
2	3	106	TYR	CG-CD2	5.83	1.46	1.39
2	i	121	SER	CA-CB	5.83	1.61	1.52
3	J	169	GLU	CD-OE2	5.83	1.32	1.25
1	b	180	ARG	CZ-NH1	5.82	1.40	1.33
1	D	33	ARG	N-CA	-5.82	1.34	1.46
2	h	102	ARG	NE-CZ	5.82	1.40	1.33
3	M	259	ARG	CD-NE	5.81	1.56	1.46
3	L	87	PHE	N-CA	-5.80	1.34	1.46
1	d	86	ARG	NE-CZ	5.80	1.40	1.33
2	2	77	TYR	CE1-CZ	5.80	1.46	1.38
1	d	228	GLU	CD-OE2	5.79	1.32	1.25
2	j	22	GLY	N-CA	-5.79	1.37	1.46
3	K	205	ARG	NE-CZ	5.79	1.40	1.33
1	B	211	VAL	C-N	5.79	1.43	1.33
1	D	127	GLY	N-CA	-5.79	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	c	20	ARG	CZ-NH2	5.78	1.40	1.33
2	3	196	PHE	CB-CG	-5.78	1.41	1.51
3	L	341	ARG	CD-NE	5.78	1.56	1.46
2	3	99	ASN	CA-CB	5.78	1.68	1.53
2	m	170	ARG	NE-CZ	5.78	1.40	1.33
2	5	118	GLU	CD-OE2	5.77	1.32	1.25
1	c	33	ARG	CZ-NH2	5.77	1.40	1.33
1	A	33	ARG	NE-CZ	5.77	1.40	1.33
3	J	27	TYR	CZ-OH	5.77	1.47	1.37
1	G	159	TYR	N-CA	-5.77	1.34	1.46
2	3	81	ARG	CZ-NH2	5.77	1.40	1.33
3	M	43	ARG	NE-CZ	5.76	1.40	1.33
1	G	130	ARG	NE-CZ	5.76	1.40	1.33
1	D	189	MET	CA-CB	5.76	1.66	1.53
1	A	86	ARG	CZ-NH1	5.75	1.40	1.33
3	M	344	GLU	CG-CD	5.75	1.60	1.51
1	B	219	ARG	CZ-NH2	5.75	1.40	1.33
3	J	102	PRO	N-CD	-5.75	1.39	1.47
1	B	226	PRO	N-CD	-5.74	1.39	1.47
3	J	29	ARG	NE-CZ	5.74	1.40	1.33
3	L	275	PHE	CA-CB	5.74	1.66	1.53
1	b	213	TYR	CG-CD1	5.73	1.46	1.39
1	C	91	ARG	NE-CZ	5.72	1.40	1.33
3	K	41	ARG	NE-CZ	5.72	1.40	1.33
1	A	180	ARG	CZ-NH2	5.72	1.40	1.33
1	G	18	ASP	CA-CB	5.72	1.66	1.53
1	f	126	TYR	CG-CD1	5.72	1.46	1.39
2	3	83	ARG	NE-CZ	5.72	1.40	1.33
3	J	37	ILE	CA-CB	-5.72	1.41	1.54
1	d	91	ARG	CZ-NH2	5.71	1.40	1.33
3	K	348	GLY	CA-C	5.71	1.60	1.51
3	J	278	ARG	CZ-NH2	5.70	1.40	1.33
2	6	180	SER	CA-CB	5.70	1.61	1.52
1	C	207	GLU	CG-CD	5.70	1.60	1.51
3	K	50	ARG	NE-CZ	5.70	1.40	1.33
3	M	24	ARG	CZ-NH2	5.69	1.40	1.33
1	D	241	ARG	NE-CZ	5.69	1.40	1.33
1	D	235	ARG	CZ-NH1	5.69	1.40	1.33
1	c	180	ARG	CD-NE	5.68	1.56	1.46
1	d	86	ARG	CZ-NH1	5.68	1.40	1.33
1	g	28	ARG	CZ-NH2	5.68	1.40	1.33
2	4	103	TYR	CE1-CZ	5.68	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	170	ARG	NE-CZ	5.67	1.40	1.33
2	4	148	TYR	CG-CD1	5.67	1.46	1.39
2	4	123	TYR	CE1-CZ	5.66	1.46	1.38
2	6	178	ARG	CZ-NH2	5.66	1.40	1.33
1	g	179	TYR	CG-CD2	5.65	1.46	1.39
3	K	302	ARG	NE-CZ	5.65	1.40	1.33
3	K	367	ARG	CZ-NH1	5.65	1.40	1.33
3	H	11	GLU	CD-OE2	5.65	1.31	1.25
1	E	20	ARG	NE-CZ	5.65	1.40	1.33
1	f	28	ARG	CZ-NH1	5.64	1.40	1.33
1	f	91	ARG	NE-CZ	5.64	1.40	1.33
1	D	140	GLY	CA-C	-5.64	1.42	1.51
1	C	130	ARG	CD-NE	5.64	1.56	1.46
2	h	80	ARG	CZ-NH2	5.64	1.40	1.33
1	b	130	ARG	CZ-NH1	5.63	1.40	1.33
3	K	341	ARG	CZ-NH1	5.63	1.40	1.33
1	A	53	ARG	CZ-NH1	5.63	1.40	1.33
3	K	203	PHE	CG-CD1	5.63	1.47	1.38
3	I	341	ARG	CZ-NH2	5.63	1.40	1.33
1	G	6	MET	C-N	5.63	1.43	1.33
3	K	52	ARG	NE-CZ	5.62	1.40	1.33
3	K	55	VAL	C-N	5.62	1.47	1.34
2	l	74	ALA	C-N	5.62	1.47	1.34
3	I	263	ARG	NE-CZ	5.61	1.40	1.33
3	L	60	SER	CA-CB	5.61	1.61	1.52
1	d	93	ARG	NE-CZ	5.61	1.40	1.33
2	i	193	GLU	CD-OE1	5.61	1.31	1.25
2	7	199	TYR	CE1-CZ	5.61	1.45	1.38
3	L	275	PHE	CG-CD1	5.61	1.47	1.38
1	a	135	SER	CA-CB	5.60	1.61	1.52
3	L	263	ARG	CZ-NH1	5.60	1.40	1.33
2	n	102	ARG	CZ-NH2	5.59	1.40	1.33
2	n	170	ARG	NE-CZ	5.59	1.40	1.33
2	5	80	ARG	CD-NE	5.58	1.55	1.46
2	j	170	ARG	CZ-NH2	5.58	1.40	1.33
1	B	143	GLU	CD-OE2	5.58	1.31	1.25
2	h	170	ARG	CD-NE	5.58	1.55	1.46
1	g	130	ARG	CZ-NH2	5.57	1.40	1.33
2	h	83	ARG	NE-CZ	5.57	1.40	1.33
2	7	170	ARG	NE-CZ	5.57	1.40	1.33
3	H	94	TYR	CE2-CZ	5.57	1.45	1.38
2	4	119	GLY	CA-C	-5.56	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	7	68	ARG	NE-CZ	5.56	1.40	1.33
1	a	95	GLU	CB-CG	-5.56	1.41	1.52
3	J	200	ARG	CZ-NH2	5.56	1.40	1.33
1	B	132	PHE	CG-CD2	5.55	1.47	1.38
2	5	80	ARG	CZ-NH1	5.55	1.40	1.33
3	L	154	ARG	NE-CZ	5.55	1.40	1.33
2	k	88	ARG	CD-NE	5.54	1.55	1.46
1	F	168	ARG	CZ-NH1	5.54	1.40	1.33
1	c	91	ARG	NE-CZ	5.54	1.40	1.33
2	4	46	TYR	CG-CD2	5.54	1.46	1.39
3	M	300	PRO	N-CA	-5.53	1.37	1.47
1	d	178	GLU	CD-OE2	5.53	1.31	1.25
2	1	68	ARG	CD-NE	5.53	1.55	1.46
2	7	46	TYR	CG-CD1	5.53	1.46	1.39
1	G	91	ARG	CD-NE	5.52	1.55	1.46
3	I	302	ARG	NE-CZ	5.52	1.40	1.33
2	3	212	ARG	CZ-NH2	5.52	1.40	1.33
3	H	105	ARG	NE-CZ	5.51	1.40	1.33
1	g	10	ARG	NE-CZ	5.51	1.40	1.33
1	g	91	ARG	CZ-NH1	5.50	1.40	1.33
3	L	167	PHE	CG-CD2	5.50	1.47	1.38
2	4	190	LYS	CA-CB	5.50	1.66	1.53
2	l	88	ARG	NE-CZ	5.50	1.40	1.33
3	L	227	PHE	CE2-CZ	5.50	1.47	1.37
2	j	178	ARG	NE-CZ	5.50	1.40	1.33
3	I	57	ARG	CZ-NH1	5.50	1.40	1.33
2	3	88	ARG	CD-NE	5.50	1.55	1.46
1	b	225	SER	CA-CB	5.49	1.61	1.52
1	e	239	ARG	CD-NE	5.49	1.55	1.46
3	I	24	ARG	CD-NE	5.49	1.55	1.46
3	L	263	ARG	CD-NE	5.49	1.55	1.46
3	M	140	TYR	CE1-CZ	5.49	1.45	1.38
2	2	107	LEU	CA-CB	5.49	1.66	1.53
2	3	130	GLY	N-CA	-5.49	1.37	1.46
3	J	309	VAL	CB-CG2	5.49	1.64	1.52
2	i	197	TYR	CE1-CZ	5.49	1.45	1.38
3	I	105	ARG	CZ-NH1	5.48	1.40	1.33
1	B	44	GLU	CB-CG	5.48	1.62	1.52
2	2	155	PHE	CE1-CZ	5.48	1.47	1.37
2	3	182	SER	C-N	5.48	1.43	1.33
2	n	88	ARG	NE-CZ	5.48	1.40	1.33
3	K	341	ARG	CD-NE	5.48	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	I	236	SER	CA-CB	5.48	1.61	1.52
1	A	93	ARG	CZ-NH2	5.48	1.40	1.33
2	m	88	ARG	CZ-NH2	5.47	1.40	1.33
2	l	51	ARG	CZ-NH2	5.47	1.40	1.33
2	3	102	ARG	NE-CZ	5.47	1.40	1.33
1	E	10	ARG	CD-NE	5.46	1.55	1.46
3	K	347	SER	CB-OG	5.46	1.49	1.42
2	4	68	ARG	NE-CZ	5.46	1.40	1.33
1	F	53	ARG	N-CA	-5.45	1.35	1.46
3	H	397	PHE	CE1-CZ	5.45	1.47	1.37
1	G	8	TYR	CG-CD1	-5.45	1.32	1.39
2	k	30	ARG	NE-CZ	5.45	1.40	1.33
3	H	302	ARG	CD-NE	5.45	1.55	1.46
3	M	366	GLU	CB-CG	5.45	1.62	1.52
3	I	137	GLU	CD-OE2	5.44	1.31	1.25
3	M	21	TYR	CG-CD2	5.44	1.46	1.39
3	H	76	ARG	NE-CZ	5.44	1.40	1.33
1	B	235	ARG	CZ-NH1	5.44	1.40	1.33
2	4	112	ILE	N-CA	-5.44	1.35	1.46
3	L	158	GLU	CD-OE2	5.44	1.31	1.25
2	l	138	VAL	CA-CB	-5.43	1.43	1.54
2	i	199	TYR	CE1-CZ	5.43	1.45	1.38
1	c	83	ALA	CA-CB	5.43	1.63	1.52
2	k	103	TYR	CE2-CZ	5.43	1.45	1.38
1	B	68	TYR	CZ-OH	5.42	1.47	1.37
1	c	219	ARG	NE-CZ	5.42	1.40	1.33
1	d	10	ARG	N-CA	5.42	1.57	1.46
1	D	205	VAL	CB-CG1	5.42	1.64	1.52
2	j	123	TYR	CE2-CZ	5.42	1.45	1.38
2	k	134	GLU	CD-OE2	5.42	1.31	1.25
2	k	101	TYR	CG-CD1	5.42	1.46	1.39
1	b	126	TYR	CD2-CE2	5.42	1.47	1.39
1	C	117	CYS	CB-SG	-5.42	1.73	1.81
1	a	239	ARG	CZ-NH1	5.41	1.40	1.33
2	i	212	ARG	CD-NE	5.41	1.55	1.46
3	I	221	ARG	CA-C	-5.41	1.38	1.52
2	n	123	TYR	CG-CD1	5.41	1.46	1.39
2	m	102	ARG	CZ-NH2	5.41	1.40	1.33
1	g	53	ARG	CA-C	-5.41	1.38	1.52
2	4	212	ARG	CZ-NH2	5.40	1.40	1.33
1	E	155	ALA	CA-CB	5.40	1.63	1.52
1	f	28	ARG	CZ-NH2	5.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	l	95	SER	CB-OG	-5.40	1.35	1.42
3	I	259	ARG	CZ-NH2	5.40	1.40	1.33
1	B	122	GLN	CB-CG	5.40	1.67	1.52
2	h	118	GLU	CD-OE1	5.40	1.31	1.25
1	a	140	GLY	CA-C	-5.40	1.43	1.51
1	b	26	TYR	CG-CD2	5.40	1.46	1.39
1	C	195	ALA	CA-CB	5.40	1.63	1.52
2	i	127	PRO	CA-CB	5.40	1.64	1.53
1	D	93	ARG	CZ-NH1	5.39	1.40	1.33
2	1	178	ARG	CZ-NH1	5.39	1.40	1.33
2	6	118	GLU	CG-CD	5.39	1.60	1.51
3	H	259	ARG	CZ-NH1	5.39	1.40	1.33
1	B	10	ARG	NE-CZ	5.39	1.40	1.33
3	H	296	ALA	CA-CB	5.39	1.63	1.52
2	m	51	ARG	NE-CZ	5.38	1.40	1.33
1	b	22	PHE	CE2-CZ	5.38	1.47	1.37
3	H	282	LYS	CA-C	-5.38	1.39	1.52
3	I	61	PRO	N-CD	5.38	1.55	1.47
1	C	26	TYR	CG-CD1	5.38	1.46	1.39
2	3	154	ARG	CZ-NH2	5.38	1.40	1.33
2	k	59	SER	CA-CB	5.38	1.61	1.52
3	M	40	GLU	CD-OE1	5.37	1.31	1.25
1	A	241	ARG	CZ-NH2	5.37	1.40	1.33
2	7	197	TYR	CE2-CZ	5.37	1.45	1.38
3	I	59	ARG	CZ-NH1	5.37	1.40	1.33
3	M	52	ARG	CD-NE	5.37	1.55	1.46
1	c	143	GLU	CD-OE2	5.37	1.31	1.25
2	j	132	ILE	CA-CB	-5.37	1.42	1.54
1	A	168	ARG	CZ-NH1	5.36	1.40	1.33
1	b	194	VAL	CB-CG1	5.36	1.64	1.52
3	I	190	LEU	CA-CB	5.36	1.66	1.53
3	M	201	ALA	CA-CB	5.35	1.63	1.52
2	m	104	PHE	CG-CD1	5.35	1.46	1.38
2	4	133	GLU	CB-CG	5.34	1.62	1.52
2	k	182	SER	CA-CB	5.34	1.60	1.52
3	K	190	LEU	CA-C	-5.34	1.39	1.52
2	j	80	ARG	NE-CZ	5.34	1.40	1.33
1	F	33	ARG	CZ-NH2	5.34	1.40	1.33
3	L	118	VAL	CB-CG1	5.34	1.64	1.52
1	D	130	ARG	NE-CZ	5.34	1.40	1.33
1	G	173	GLU	CD-OE1	5.33	1.31	1.25
1	F	159	TYR	CG-CD1	5.33	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	209	ILE	N-CA	-5.33	1.35	1.46
2	7	212	ARG	NE-CZ	5.33	1.40	1.33
3	L	364	ARG	CD-NE	5.33	1.55	1.46
1	G	191	LEU	C-N	5.33	1.42	1.33
2	i	170	ARG	NE-CZ	5.33	1.40	1.33
3	I	82	SER	CA-CB	5.33	1.60	1.52
1	c	184	SER	CA-CB	5.32	1.60	1.52
1	D	239	ARG	CD-NE	5.32	1.55	1.46
1	d	104	ASP	CA-CB	5.32	1.65	1.53
3	K	137	GLU	CD-OE1	5.32	1.31	1.25
1	b	199	SER	CA-CB	5.31	1.60	1.52
2	7	101	TYR	CD2-CE2	5.31	1.47	1.39
3	H	358	ALA	CA-CB	5.31	1.63	1.52
1	b	148	TYR	CZ-OH	5.31	1.46	1.37
2	l	82	GLU	CD-OE2	5.31	1.31	1.25
3	J	303	PHE	CB-CG	5.31	1.60	1.51
1	e	206	PRO	N-CD	-5.31	1.40	1.47
3	L	154	ARG	CZ-NH1	5.31	1.40	1.33
1	D	180	ARG	CZ-NH1	5.30	1.40	1.33
2	1	148	TYR	CB-CG	-5.30	1.43	1.51
1	c	68	TYR	CE1-CZ	5.30	1.45	1.38
1	b	91	ARG	CZ-NH2	5.29	1.40	1.33
1	a	174	PHE	CG-CD1	5.29	1.46	1.38
2	5	173	TYR	CE2-CZ	5.29	1.45	1.38
3	J	46	ARG	CD-NE	5.29	1.55	1.46
1	a	179	TYR	CB-CG	-5.29	1.43	1.51
1	e	17	PRO	N-CD	5.29	1.55	1.47
1	e	219	ARG	CZ-NH2	5.29	1.40	1.33
1	g	86	ARG	CZ-NH1	5.29	1.40	1.33
2	5	77	TYR	CB-CG	5.29	1.59	1.51
3	H	44	TYR	CZ-OH	5.28	1.46	1.37
1	B	91	ARG	CZ-NH2	5.28	1.40	1.33
2	1	102	ARG	NE-CZ	5.28	1.40	1.33
3	K	105	ARG	CD-NE	5.28	1.55	1.46
1	c	241	ARG	CZ-NH1	5.28	1.40	1.33
1	G	86	ARG	CZ-NH1	5.28	1.40	1.33
2	j	197	TYR	CB-CG	-5.28	1.43	1.51
3	K	224	ARG	NE-CZ	5.28	1.40	1.33
2	3	205	GLU	CB-CG	5.27	1.62	1.52
3	J	357	GLU	CA-C	-5.27	1.39	1.52
1	d	132	PHE	C-N	5.27	1.42	1.33
1	e	219	ARG	NE-CZ	5.27	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	i	178	ARG	CD-NE	5.27	1.55	1.46
3	H	69	SER	CA-CB	5.27	1.60	1.52
2	n	100	SER	CA-CB	5.26	1.60	1.52
2	1	36	PHE	CG-CD2	5.26	1.46	1.38
3	L	46	ARG	NE-CZ	5.26	1.39	1.33
2	4	102	ARG	CZ-NH1	5.26	1.39	1.33
1	B	86	ARG	CZ-NH1	5.26	1.39	1.33
2	6	101	TYR	CG-CD2	-5.26	1.32	1.39
1	g	28	ARG	CD-NE	5.25	1.55	1.46
2	h	183	GLY	CA-C	-5.25	1.43	1.51
2	n	148	TYR	CZ-OH	5.25	1.46	1.37
2	j	95	SER	CA-CB	5.25	1.60	1.52
1	B	135	SER	C-N	5.25	1.46	1.34
1	D	119	PHE	C-N	5.25	1.46	1.34
3	H	200	ARG	CD-NE	5.25	1.55	1.46
3	L	49	ARG	CZ-NH2	5.25	1.39	1.33
1	B	100	ARG	CZ-NH1	5.24	1.39	1.33
1	d	210	GLU	CD-OE1	-5.24	1.19	1.25
3	H	301	GLY	CA-C	-5.24	1.43	1.51
2	h	211	PHE	CG-CD2	5.23	1.46	1.38
1	A	106	PRO	N-CD	5.23	1.55	1.47
2	2	80	ARG	CZ-NH2	5.23	1.39	1.33
2	3	178	ARG	CZ-NH1	5.23	1.39	1.33
2	3	199	TYR	CG-CD1	5.23	1.46	1.39
1	B	25	GLU	CB-CG	5.23	1.62	1.52
1	G	28	ARG	CD-NE	5.23	1.55	1.46
2	n	123	TYR	CG-CD2	5.23	1.46	1.39
1	c	185	PHE	CE2-CZ	5.22	1.47	1.37
2	1	46	TYR	CG-CD2	5.22	1.46	1.39
2	7	136	ASP	CA-CB	5.22	1.65	1.53
1	C	130	ARG	NE-CZ	5.22	1.39	1.33
3	H	151	GLU	CA-CB	5.22	1.65	1.53
3	M	215	TYR	CG-CD1	5.22	1.46	1.39
1	C	33	ARG	NE-CZ	5.22	1.39	1.33
3	K	367	ARG	CA-CB	5.22	1.65	1.53
3	L	52	ARG	NE-CZ	5.21	1.39	1.33
3	M	24	ARG	NE-CZ	5.21	1.39	1.33
2	1	154	ARG	CZ-NH2	5.20	1.39	1.33
3	M	221	ARG	CZ-NH1	5.20	1.39	1.33
1	D	219	ARG	CZ-NH1	5.20	1.39	1.33
3	I	326	ARG	CZ-NH1	5.20	1.39	1.33
1	d	68	TYR	CE2-CZ	5.20	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	E	127	GLY	CA-C	-5.20	1.43	1.51
2	h	130	GLY	N-CA	-5.20	1.38	1.46
2	3	143	GLY	N-CA	5.20	1.53	1.46
1	E	68	TYR	CB-CG	-5.20	1.43	1.51
1	g	80	GLY	N-CA	-5.20	1.38	1.46
2	2	203	GLU	CD-OE1	5.19	1.31	1.25
3	K	57	ARG	CZ-NH1	5.19	1.39	1.33
3	L	224	ARG	CD-NE	5.19	1.55	1.46
3	M	263	ARG	CZ-NH2	5.19	1.39	1.33
1	B	68	TYR	CD1-CE1	5.18	1.47	1.39
1	g	68	TYR	CZ-OH	5.18	1.46	1.37
3	J	365	GLU	CB-CG	5.18	1.61	1.52
1	G	91	ARG	NE-CZ	5.18	1.39	1.33
2	k	154	ARG	CD-NE	5.18	1.55	1.46
1	a	239	ARG	NE-CZ	5.17	1.39	1.33
2	4	16	GLY	N-CA	-5.17	1.38	1.46
1	f	133	GLY	N-CA	-5.17	1.38	1.46
2	j	81	ARG	NE-CZ	5.17	1.39	1.33
3	I	299	ARG	CZ-NH2	5.17	1.39	1.33
2	m	178	ARG	CD-NE	5.17	1.55	1.46
3	J	375	PHE	CG-CD1	5.17	1.46	1.38
1	c	123	TYR	CB-CG	-5.17	1.44	1.51
1	d	68	TYR	CZ-OH	5.17	1.46	1.37
1	a	213	TYR	CZ-OH	5.16	1.46	1.37
2	l	154	ARG	CZ-NH2	5.16	1.39	1.33
1	E	153	SER	CB-OG	5.16	1.49	1.42
2	m	203	GLU	CG-CD	5.16	1.59	1.51
2	7	170	ARG	CZ-NH1	5.16	1.39	1.33
3	J	28	ARG	CD-NE	5.16	1.55	1.46
2	n	199	TYR	CG-CD1	5.16	1.45	1.39
1	e	213	TYR	CG-CD2	5.15	1.45	1.39
3	L	17	GLU	CD-OE1	5.15	1.31	1.25
2	i	123	TYR	CD2-CE2	5.15	1.47	1.39
1	B	53	ARG	CD-NE	5.15	1.55	1.46
1	C	239	ARG	CZ-NH2	5.15	1.39	1.33
1	b	119	PHE	CE2-CZ	5.15	1.47	1.37
3	J	253	SER	CA-CB	5.15	1.60	1.52
1	D	22	PHE	CA-CB	5.14	1.65	1.53
1	b	179	TYR	CZ-OH	5.14	1.46	1.37
1	A	28	ARG	NE-CZ	5.14	1.39	1.33
2	h	170	ARG	NE-CZ	5.14	1.39	1.33
2	k	154	ARG	CZ-NH1	5.14	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	F	10	ARG	CZ-NH2	5.14	1.39	1.33
2	5	105	PRO	C-N	5.13	1.45	1.34
1	A	239	ARG	CZ-NH2	5.13	1.39	1.33
2	5	83	ARG	CZ-NH1	5.13	1.39	1.33
3	L	59	ARG	NE-CZ	5.13	1.39	1.33
1	G	228	GLU	CD-OE1	5.13	1.31	1.25
2	5	160	GLY	CA-C	-5.13	1.43	1.51
3	I	209	SER	CA-CB	5.13	1.60	1.52
3	I	302	ARG	CZ-NH2	5.13	1.39	1.33
3	K	49	ARG	CZ-NH2	5.13	1.39	1.33
2	4	206	GLN	CD-NE2	5.13	1.45	1.32
2	k	170	ARG	NE-CZ	5.13	1.39	1.33
3	H	128	TYR	CG-CD2	5.13	1.45	1.39
2	j	142	SER	CA-CB	5.13	1.60	1.52
2	5	114	GLY	N-CA	5.12	1.53	1.46
3	M	49	ARG	CZ-NH1	5.12	1.39	1.33
2	1	30	ARG	CA-CB	5.11	1.65	1.53
2	4	213	LYS	C-OXT	5.11	1.33	1.23
1	F	86	ARG	CZ-NH2	5.11	1.39	1.33
1	C	212	GLY	N-CA	-5.11	1.38	1.46
3	H	103	GLY	CA-C	-5.11	1.43	1.51
1	E	219	ARG	NE-CZ	5.11	1.39	1.33
1	F	126	TYR	CG-CD1	5.11	1.45	1.39
1	D	53	ARG	NE-CZ	5.11	1.39	1.33
2	3	178	ARG	NE-CZ	5.11	1.39	1.33
3	I	359	GLY	CA-C	-5.11	1.43	1.51
2	2	106	TYR	CG-CD2	5.11	1.45	1.39
2	4	80	ARG	NE-CZ	5.11	1.39	1.33
3	J	317	ARG	NE-CZ	5.10	1.39	1.33
1	g	217	ASP	C-N	5.10	1.45	1.34
3	I	260	GLU	CG-CD	5.10	1.59	1.51
1	e	126	TYR	CB-CG	-5.09	1.44	1.51
2	h	82	GLU	CB-CG	5.09	1.61	1.52
2	k	68	ARG	CZ-NH2	5.09	1.39	1.33
3	K	21	TYR	CG-CD1	5.09	1.45	1.39
3	J	299	ARG	CZ-NH2	5.09	1.39	1.33
1	D	54	VAL	C-N	5.09	1.42	1.33
2	h	134	GLU	CA-C	-5.09	1.39	1.52
3	L	44	TYR	CZ-OH	5.09	1.46	1.37
3	M	59	ARG	CD-NE	5.09	1.55	1.46
3	J	60	SER	C-N	5.09	1.44	1.34
3	J	41	ARG	CD-NE	5.09	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	d	184	SER	CA-CB	5.09	1.60	1.52
3	M	345	GLY	N-CA	-5.09	1.38	1.46
1	b	236	ALA	N-CA	-5.08	1.36	1.46
1	C	103	TYR	CE1-CZ	5.08	1.45	1.38
2	6	83	ARG	NE-CZ	5.08	1.39	1.33
1	a	184	SER	CA-CB	5.08	1.60	1.52
1	B	103	TYR	CG-CD2	5.08	1.45	1.39
1	C	20	ARG	NE-CZ	5.07	1.39	1.33
1	G	132	PHE	N-CA	-5.07	1.36	1.46
2	1	51	ARG	NE-CZ	5.07	1.39	1.33
2	l	193	GLU	CB-CG	5.07	1.61	1.52
3	J	317	ARG	CD-NE	5.07	1.55	1.46
1	g	53	ARG	CZ-NH1	5.07	1.39	1.33
2	2	129	GLY	CA-C	5.07	1.59	1.51
2	4	154	ARG	CD-NE	5.07	1.55	1.46
2	4	29	LYS	CA-C	-5.06	1.39	1.52
2	k	154	ARG	NE-CZ	5.06	1.39	1.33
2	5	123	TYR	CG-CD2	5.06	1.45	1.39
3	M	321	PHE	CG-CD1	5.06	1.46	1.38
1	c	22	PHE	CG-CD2	5.06	1.46	1.38
1	E	130	ARG	NE-CZ	5.06	1.39	1.33
1	g	50	ALA	CA-CB	5.06	1.63	1.52
2	4	158	GLU	CB-CG	5.06	1.61	1.52
1	f	25	GLU	CD-OE2	5.06	1.31	1.25
3	M	89	VAL	CA-C	-5.06	1.39	1.52
3	L	361	PHE	CA-C	-5.05	1.39	1.52
2	4	80	ARG	CZ-NH2	5.05	1.39	1.33
2	7	16	GLY	N-CA	-5.05	1.38	1.46
1	d	159	TYR	CE2-CZ	5.05	1.45	1.38
3	H	257	GLY	N-CA	-5.05	1.38	1.46
2	5	119	GLY	N-CA	-5.04	1.38	1.46
2	n	178	ARG	CZ-NH1	5.04	1.39	1.33
1	B	60	GLU	CG-CD	5.04	1.59	1.51
1	D	123	TYR	CG-CD1	5.04	1.45	1.39
1	d	159	TYR	CG-CD2	5.04	1.45	1.39
2	5	82	GLU	CB-CG	5.04	1.61	1.52
3	L	145	GLY	CA-C	5.04	1.59	1.51
3	I	344	GLU	CD-OE2	5.04	1.31	1.25
2	6	195	GLU	CD-OE2	5.04	1.31	1.25
2	m	81	ARG	CZ-NH1	5.04	1.39	1.33
3	M	218	GLU	CG-CD	5.04	1.59	1.51
1	f	190	VAL	CA-CB	-5.03	1.44	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	2	102	ARG	NE-CZ	5.03	1.39	1.33
1	F	199	SER	CA-CB	5.03	1.60	1.52
1	b	93	ARG	CZ-NH1	5.03	1.39	1.33
1	g	103	TYR	CD1-CE1	5.03	1.46	1.39
2	m	113	GLY	CA-C	5.03	1.59	1.51
1	G	125	GLN	CA-CB	5.03	1.65	1.53
1	g	175	PHE	CG-CD1	5.03	1.46	1.38
2	5	30	ARG	NE-CZ	5.03	1.39	1.33
3	L	217	GLY	CA-C	-5.03	1.43	1.51
1	f	39	GLY	CA-C	-5.03	1.43	1.51
3	H	154	ARG	CD-NE	5.03	1.54	1.46
2	m	154	ARG	C-N	5.02	1.45	1.34
2	l	80	ARG	CD-NE	5.02	1.54	1.46
2	4	30	ARG	NE-CZ	5.02	1.39	1.33
1	d	53	ARG	CZ-NH2	5.02	1.39	1.33
2	n	46	TYR	CB-CG	5.02	1.59	1.51
2	j	193	GLU	CA-CB	5.01	1.65	1.53
3	J	44	TYR	CG-CD2	5.01	1.45	1.39
1	b	171	VAL	CA-CB	-5.01	1.44	1.54
1	C	35	ALA	CA-CB	5.01	1.62	1.52
1	E	232	TYR	CG-CD1	-5.01	1.32	1.39
1	E	228	GLU	CD-OE1	-5.01	1.20	1.25
3	L	134	GLU	CD-OE2	5.01	1.31	1.25
3	J	205	ARG	CZ-NH1	5.01	1.39	1.33
1	g	28	ARG	CZ-NH1	5.01	1.39	1.33
1	a	159	TYR	CE1-CZ	5.00	1.45	1.38
2	l	127	PRO	N-CD	-5.00	1.40	1.47
3	H	221	ARG	NE-CZ	5.00	1.39	1.33
2	l	170	ARG	NE-CZ	5.00	1.39	1.33
3	H	332	GLU	CG-CD	5.00	1.59	1.51

All (1867) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	170	ARG	NE-CZ-NH2	-42.88	98.86	120.30
2	l	170	ARG	NE-CZ-NH2	-41.57	99.51	120.30
2	5	170	ARG	NE-CZ-NH1	18.88	129.74	120.30
2	l	170	ARG	NE-CZ-NH1	18.38	129.49	120.30
1	F	28	ARG	NE-CZ-NH2	-18.01	111.29	120.30
1	a	126	TYR	CB-CG-CD1	17.83	131.70	121.00
3	K	259	ARG	NE-CZ-NH2	-16.65	111.97	120.30
2	k	68	ARG	NE-CZ-NH2	-16.27	112.16	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	l	148	TYR	CB-CG-CD2	-15.98	111.41	121.00
1	g	20	ARG	NE-CZ-NH1	15.97	128.29	120.30
1	D	33	ARG	NE-CZ-NH1	15.27	127.94	120.30
3	L	128	TYR	CB-CG-CD2	-15.24	111.85	121.00
1	g	20	ARG	NE-CZ-NH2	-14.97	112.81	120.30
3	H	94	TYR	CB-CG-CD2	14.90	129.94	121.00
3	I	259	ARG	NE-CZ-NH2	-14.89	112.86	120.30
2	6	77	TYR	CB-CG-CD1	14.77	129.86	121.00
2	6	68	ARG	NE-CZ-NH2	-14.61	113.00	120.30
3	H	46	ARG	NE-CZ-NH2	14.49	127.55	120.30
2	1	101	TYR	CB-CG-CD2	-14.48	112.31	121.00
1	f	148	TYR	CB-CG-CD2	-14.34	112.40	121.00
1	E	20	ARG	NE-CZ-NH2	-14.33	113.14	120.30
1	F	33	ARG	NE-CZ-NH1	14.23	127.42	120.30
2	6	68	ARG	NE-CZ-NH1	14.16	127.38	120.30
2	l	80	ARG	NE-CZ-NH2	14.14	127.37	120.30
2	2	83	ARG	NE-CZ-NH1	-14.14	113.23	120.30
3	I	57	ARG	NE-CZ-NH2	13.90	127.25	120.30
2	k	81	ARG	NE-CZ-NH2	-13.82	113.39	120.30
1	a	28	ARG	NE-CZ-NH1	13.68	127.14	120.30
1	b	53	ARG	NE-CZ-NH2	13.60	127.10	120.30
1	a	28	ARG	NE-CZ-NH2	-13.48	113.56	120.30
2	1	101	TYR	CB-CG-CD1	13.47	129.08	121.00
2	2	123	TYR	CB-CG-CD1	13.45	129.07	121.00
2	4	211	PHE	CB-CG-CD2	13.31	130.11	120.80
2	h	88	ARG	NE-CZ-NH2	13.28	126.94	120.30
1	F	241	ARG	NE-CZ-NH1	-13.19	113.70	120.30
1	C	26	TYR	CB-CG-CD2	13.15	128.89	121.00
1	d	175	PHE	CB-CG-CD1	-12.96	111.73	120.80
3	K	20	TYR	CB-CG-CD2	-12.95	113.23	121.00
2	j	30	ARG	NE-CZ-NH2	12.94	126.77	120.30
1	a	126	TYR	CB-CG-CD2	-12.90	113.26	121.00
1	d	33	ARG	NE-CZ-NH2	12.87	126.74	120.30
2	n	68	ARG	NE-CZ-NH2	-12.85	113.88	120.30
1	c	175	PHE	CB-CG-CD2	-12.83	111.82	120.80
1	F	130	ARG	NE-CZ-NH2	-12.82	113.89	120.30
2	n	68	ARG	NE-CZ-NH1	12.80	126.70	120.30
2	5	62	ASP	CB-CG-OD1	12.76	129.78	118.30
1	c	93	ARG	NE-CZ-NH2	-12.73	113.93	120.30
1	a	20	ARG	NE-CZ-NH1	12.68	126.64	120.30
3	I	24	ARG	NE-CZ-NH2	-12.61	114.00	120.30
3	I	259	ARG	NE-CZ-NH1	12.54	126.57	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7	170	ARG	NE-CZ-NH1	-12.52	114.04	120.30
1	B	213	TYR	CB-CG-CD2	-12.50	113.50	121.00
2	n	51	ARG	NE-CZ-NH1	12.45	126.52	120.30
1	E	174	PHE	CB-CG-CD2	-12.42	112.10	120.80
2	k	102	ARG	NE-CZ-NH1	-12.40	114.10	120.30
3	I	59	ARG	NE-CZ-NH2	-12.38	114.11	120.30
1	a	239	ARG	NE-CZ-NH2	12.35	126.47	120.30
3	L	215	TYR	CB-CG-CD2	12.31	128.38	121.00
3	M	49	ARG	NE-CZ-NH2	12.24	126.42	120.30
1	b	93	ARG	NE-CZ-NH1	12.21	126.41	120.30
1	e	159	TYR	CB-CG-CD1	-12.17	113.70	121.00
2	4	36	PHE	CB-CG-CD2	12.17	129.32	120.80
2	7	212	ARG	NE-CZ-NH2	-12.16	114.22	120.30
2	i	212	ARG	NE-CZ-NH1	12.07	126.33	120.30
2	7	68	ARG	NE-CZ-NH2	-12.06	114.27	120.30
3	L	224	ARG	NE-CZ-NH2	12.05	126.33	120.30
1	D	123	TYR	CB-CG-CD2	-12.05	113.77	121.00
2	7	211	PHE	CB-CG-CD1	-12.04	112.38	120.80
2	i	103	TYR	CB-CG-CD2	-12.03	113.78	121.00
3	M	250	ARG	NE-CZ-NH2	-12.01	114.29	120.30
1	f	235	ARG	NE-CZ-NH1	-11.98	114.31	120.30
1	C	123	TYR	CB-CG-CD2	-11.97	113.82	121.00
1	c	174	PHE	CB-CG-CD2	-11.97	112.42	120.80
1	f	239	ARG	NE-CZ-NH2	11.93	126.26	120.30
1	A	26	TYR	CB-CG-CD2	11.84	128.11	121.00
2	4	212	ARG	NE-CZ-NH1	11.83	126.22	120.30
2	i	212	ARG	NE-CZ-NH2	-11.78	114.41	120.30
2	2	199	TYR	CB-CG-CD1	11.77	128.06	121.00
3	M	278	ARG	NE-CZ-NH1	11.73	126.16	120.30
1	e	53	ARG	NE-CZ-NH2	11.69	126.15	120.30
3	H	227	PHE	CB-CG-CD2	-11.65	112.64	120.80
1	g	26	TYR	CB-CG-CD2	-11.61	114.04	121.00
1	d	100	ARG	NE-CZ-NH2	11.60	126.10	120.30
1	d	10	ARG	NE-CZ-NH2	11.53	126.07	120.30
1	C	26	TYR	CB-CG-CD1	-11.53	114.08	121.00
3	H	57	ARG	NE-CZ-NH2	-11.53	114.54	120.30
1	f	235	ARG	NE-CZ-NH2	11.52	126.06	120.30
3	K	250	ARG	NE-CZ-NH1	11.49	126.05	120.30
3	I	41	ARG	NE-CZ-NH2	-11.49	114.56	120.30
1	c	100	ARG	NE-CZ-NH2	11.47	126.03	120.30
2	j	104	PHE	CB-CG-CD1	-11.44	112.79	120.80
2	2	123	TYR	CB-CG-CD2	-11.44	114.14	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	d	103	TYR	CB-CG-CD2	-11.42	114.15	121.00
1	F	33	ARG	NE-CZ-NH2	-11.35	114.62	120.30
1	c	123	TYR	CB-CG-CD1	11.35	127.81	121.00
2	4	211	PHE	CB-CG-CD1	-11.35	112.86	120.80
1	g	22	PHE	CB-CG-CD1	-11.34	112.86	120.80
2	4	199	TYR	CB-CG-CD1	11.33	127.80	121.00
1	D	126	TYR	CB-CG-CD2	11.29	127.78	121.00
3	H	263	ARG	NE-CZ-NH1	11.29	125.94	120.30
2	n	196	PHE	CB-CG-CD1	11.29	128.70	120.80
3	K	250	ARG	NE-CZ-NH2	-11.22	114.69	120.30
1	G	22	PHE	CB-CG-CD1	11.21	128.65	120.80
2	5	199	TYR	CB-CG-CD2	-11.20	114.28	121.00
1	c	91	ARG	NE-CZ-NH1	-11.16	114.72	120.30
2	i	46	TYR	CB-CG-CD1	-11.16	114.31	121.00
3	I	128	TYR	CB-CG-CD1	-11.14	114.31	121.00
3	L	278	ARG	NE-CZ-NH1	11.10	125.85	120.30
1	B	168	ARG	NE-CZ-NH2	-11.08	114.76	120.30
1	b	180	ARG	NE-CZ-NH2	11.06	125.83	120.30
3	L	59	ARG	NE-CZ-NH2	-11.05	114.77	120.30
3	H	250	ARG	NE-CZ-NH2	-11.03	114.78	120.30
1	c	71	ASP	CB-CG-OD2	10.99	128.19	118.30
1	B	241	ARG	NE-CZ-NH1	-10.95	114.82	120.30
1	b	148	TYR	CB-CG-CD1	-10.92	114.45	121.00
2	5	170	ARG	NH1-CZ-NH2	10.90	131.39	119.40
3	K	52	ARG	NE-CZ-NH2	-10.87	114.87	120.30
1	c	86	ARG	NE-CZ-NH2	-10.85	114.88	120.30
2	n	77	TYR	CB-CG-CD2	10.84	127.50	121.00
3	H	94	TYR	CB-CG-CD1	-10.84	114.50	121.00
3	H	263	ARG	NE-CZ-NH2	-10.83	114.89	120.30
1	A	175	PHE	CB-CG-CD1	10.81	128.37	120.80
1	E	213	TYR	CB-CG-CD2	-10.80	114.52	121.00
1	D	33	ARG	NE-CZ-NH2	-10.75	114.92	120.30
3	K	302	ARG	NE-CZ-NH1	10.73	125.66	120.30
3	L	140	TYR	CB-CG-CD2	10.72	127.43	121.00
1	G	239	ARG	NE-CZ-NH1	10.71	125.66	120.30
1	g	93	ARG	NE-CZ-NH1	10.71	125.66	120.30
2	k	211	PHE	CB-CG-CD1	-10.71	113.31	120.80
1	D	126	TYR	CB-CG-CD1	-10.69	114.59	121.00
3	H	41	ARG	NE-CZ-NH2	-10.69	114.96	120.30
1	A	235	ARG	NE-CZ-NH2	-10.68	114.96	120.30
2	7	77	TYR	CB-CG-CD1	10.68	127.41	121.00
3	L	20	TYR	CB-CG-CD2	-10.66	114.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	j	30	ARG	NE-CZ-NH1	-10.65	114.97	120.30
2	l	104	PHE	CB-CG-CD1	10.65	128.25	120.80
1	D	148	TYR	CB-CG-CD1	-10.64	114.62	121.00
2	7	46	TYR	CB-CG-CD1	-10.63	114.62	121.00
3	H	140	TYR	CB-CG-CD1	10.63	127.38	121.00
2	3	148	TYR	CB-CG-CD2	-10.63	114.62	121.00
3	I	76	ARG	NE-CZ-NH1	10.63	125.61	120.30
3	I	128	TYR	CB-CG-CD2	10.63	127.38	121.00
3	I	289	ARG	NE-CZ-NH2	-10.63	114.99	120.30
2	k	50	ASP	CB-CG-OD2	10.62	127.86	118.30
2	2	178	ARG	NE-CZ-NH2	-10.57	115.01	120.30
2	j	173	TYR	CB-CG-CD2	-10.57	114.66	121.00
3	I	50	ARG	NE-CZ-NH2	-10.57	115.02	120.30
3	M	341	ARG	NE-CZ-NH1	10.54	125.57	120.30
3	L	128	TYR	CB-CG-CD1	10.53	127.32	121.00
1	C	180	ARG	NE-CZ-NH2	10.52	125.56	120.30
1	b	86	ARG	NE-CZ-NH1	10.51	125.55	120.30
1	f	213	TYR	CB-CG-CD1	-10.50	114.70	121.00
2	3	46	TYR	CB-CG-CD1	-10.48	114.71	121.00
1	a	33	ARG	NE-CZ-NH1	-10.46	115.07	120.30
1	e	123	TYR	CB-CG-CD2	-10.45	114.73	121.00
1	B	239	ARG	NE-CZ-NH1	-10.45	115.08	120.30
1	f	91	ARG	NE-CZ-NH1	-10.42	115.09	120.30
2	l	170	ARG	NH1-CZ-NH2	10.41	130.85	119.40
1	A	86	ARG	NE-CZ-NH1	10.39	125.49	120.30
1	d	100	ARG	NE-CZ-NH1	-10.36	115.12	120.30
2	h	196	PHE	CB-CG-CD2	-10.36	113.55	120.80
3	H	21	TYR	CB-CG-CD2	-10.35	114.79	121.00
1	G	219	ARG	NE-CZ-NH1	10.34	125.47	120.30
2	2	106	TYR	CB-CG-CD1	-10.32	114.81	121.00
1	G	241	ARG	NE-CZ-NH1	-10.30	115.15	120.30
2	k	102	ARG	NE-CZ-NH2	10.28	125.44	120.30
1	A	11	ALA	N-CA-CB	10.27	124.48	110.10
1	G	22	PHE	CB-CG-CD2	-10.25	113.63	120.80
1	f	93	ARG	NE-CZ-NH1	-10.21	115.20	120.30
1	e	33	ARG	NE-CZ-NH2	10.19	125.40	120.30
1	g	175	PHE	CB-CG-CD2	-10.19	113.67	120.80
2	1	123	TYR	CB-CG-CD1	10.17	127.10	121.00
3	H	21	TYR	CB-CG-CD1	10.17	127.10	121.00
3	L	20	TYR	CB-CG-CD1	10.17	127.10	121.00
2	7	30	ARG	NE-CZ-NH2	-10.16	115.22	120.30
2	k	197	TYR	CB-CG-CD1	10.12	127.07	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	159	TYR	CB-CG-CD2	-10.10	114.94	121.00
2	k	88	ARG	NE-CZ-NH1	-10.10	115.25	120.30
1	B	26	TYR	CB-CG-CD1	-10.06	114.96	121.00
1	C	8	TYR	CB-CG-CD2	-10.05	114.97	121.00
3	K	221	ARG	NE-CZ-NH2	-10.05	115.27	120.30
2	7	178	ARG	NE-CZ-NH2	10.05	125.33	120.30
3	H	200	ARG	NE-CZ-NH2	-10.02	115.29	120.30
1	D	219	ARG	NE-CZ-NH2	-10.01	115.30	120.30
1	A	91	ARG	NE-CZ-NH1	-9.99	115.31	120.30
2	n	154	ARG	NE-CZ-NH2	9.95	125.28	120.30
3	H	94	TYR	CG-CD2-CE2	9.93	129.25	121.30
3	K	181	TYR	CB-CG-CD2	-9.93	115.04	121.00
3	L	215	TYR	CB-CG-CD1	-9.91	115.05	121.00
1	B	219	ARG	NE-CZ-NH2	-9.90	115.35	120.30
2	m	68	ARG	NE-CZ-NH2	-9.90	115.35	120.30
2	5	83	ARG	NE-CZ-NH2	9.89	125.24	120.30
1	D	26	TYR	CB-CG-CD1	-9.88	115.07	121.00
3	H	364	ARG	NE-CZ-NH2	-9.85	115.37	120.30
2	2	178	ARG	NE-CZ-NH1	9.84	125.22	120.30
1	c	28	ARG	NE-CZ-NH1	9.83	125.22	120.30
1	c	100	ARG	NE-CZ-NH1	-9.82	115.39	120.30
2	2	187	ASP	CB-CG-OD1	9.79	127.11	118.30
2	5	148	TYR	CB-CG-CD1	-9.79	115.13	121.00
1	A	53	ARG	NE-CZ-NH2	9.77	125.19	120.30
1	d	118	ASP	CB-CG-OD2	9.76	127.08	118.30
1	F	22	PHE	CB-CG-CD2	9.72	127.61	120.80
1	d	175	PHE	CB-CG-CD2	9.72	127.60	120.80
3	K	278	ARG	NE-CZ-NH1	9.72	125.16	120.30
1	F	53	ARG	NE-CZ-NH1	9.63	125.12	120.30
3	M	59	ARG	NE-CZ-NH2	-9.59	115.50	120.30
2	k	136	ASP	CB-CG-OD2	9.59	126.93	118.30
1	e	130	ARG	NE-CZ-NH2	-9.59	115.51	120.30
3	H	224	ARG	NE-CZ-NH1	-9.55	115.53	120.30
2	2	148	TYR	CB-CG-CD1	-9.54	115.27	121.00
3	J	24	ARG	NE-CZ-NH2	9.54	125.07	120.30
3	I	371	THR	CA-CB-CG2	-9.53	99.05	112.40
1	G	168	ARG	NE-CZ-NH2	-9.51	115.54	120.30
1	C	100	ARG	NE-CZ-NH1	-9.51	115.55	120.30
1	E	130	ARG	NE-CZ-NH2	9.50	125.05	120.30
1	c	239	ARG	NE-CZ-NH2	-9.50	115.55	120.30
2	k	197	TYR	CB-CG-CD2	-9.48	115.31	121.00
1	F	93	ARG	NE-CZ-NH1	9.48	125.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	n	170	ARG	NE-CZ-NH1	-9.46	115.57	120.30
2	2	68	ARG	NE-CZ-NH2	-9.42	115.59	120.30
3	I	397	PHE	CB-CG-CD1	9.42	127.39	120.80
2	7	175	ALA	N-CA-CB	9.41	123.27	110.10
1	a	235	ARG	NE-CZ-NH2	9.38	124.99	120.30
3	K	227	PHE	CB-CG-CD1	-9.37	114.24	120.80
1	f	51	ASP	CB-CG-OD1	-9.35	109.89	118.30
2	n	178	ARG	NE-CZ-NH1	9.35	124.97	120.30
3	M	19	ASP	CB-CG-OD1	9.34	126.70	118.30
1	E	182	ASP	CB-CG-OD1	-9.33	109.90	118.30
1	B	26	TYR	CB-CG-CD2	9.32	126.59	121.00
1	b	33	ARG	NE-CZ-NH1	-9.32	115.64	120.30
1	E	239	ARG	NE-CZ-NH2	-9.31	115.64	120.30
3	H	24	ARG	NE-CZ-NH1	9.30	124.95	120.30
1	f	180	ARG	NE-CZ-NH1	9.30	124.95	120.30
2	4	199	TYR	CB-CG-CD2	-9.30	115.42	121.00
1	c	26	TYR	CB-CG-CD2	9.29	126.58	121.00
3	K	270	ALA	N-CA-CB	9.27	123.08	110.10
3	K	20	TYR	CB-CG-CD1	9.25	126.55	121.00
2	3	197	TYR	CB-CG-CD1	9.25	126.55	121.00
1	C	126	TYR	CB-CG-CD2	-9.23	115.47	121.00
3	K	326	ARG	NE-CZ-NH2	-9.22	115.69	120.30
2	i	199	TYR	CB-CG-CD1	-9.21	115.48	121.00
1	D	28	ARG	NE-CZ-NH1	-9.20	115.70	120.30
3	M	299	ARG	NE-CZ-NH2	9.19	124.89	120.30
1	d	81	LEU	CB-CG-CD1	9.18	126.60	111.00
2	i	103	TYR	CB-CG-CD1	9.18	126.50	121.00
1	c	33	ARG	NE-CZ-NH1	-9.16	115.72	120.30
1	A	10	ARG	NE-CZ-NH1	9.16	124.88	120.30
2	k	104	PHE	CB-CG-CD2	9.13	127.19	120.80
1	E	213	TYR	CB-CG-CD1	9.12	126.47	121.00
2	6	154	ARG	NE-CZ-NH1	-9.12	115.74	120.30
1	D	123	TYR	CB-CG-CD1	9.10	126.46	121.00
2	1	21	ASP	CB-CG-OD2	9.09	126.48	118.30
1	C	123	TYR	CB-CG-CD1	9.09	126.45	121.00
1	E	185	PHE	CB-CG-CD1	-9.09	114.44	120.80
3	M	19	ASP	CB-CG-OD2	-9.08	110.13	118.30
1	E	123	TYR	CB-CG-CD2	-9.07	115.56	121.00
2	k	173	TYR	CB-CG-CD2	-9.06	115.56	121.00
1	b	148	TYR	CB-CG-CD2	9.05	126.43	121.00
2	m	116	ASP	CB-CG-OD1	9.05	126.45	118.30
1	e	159	TYR	CB-CG-CD2	9.05	126.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3	104	PHE	CB-CG-CD1	-9.04	114.47	120.80
2	2	36	PHE	CB-CG-CD1	9.04	127.13	120.80
1	F	20	ARG	NE-CZ-NH1	9.03	124.81	120.30
3	L	70	ASP	CB-CG-OD2	-9.03	110.17	118.30
3	L	278	ARG	NE-CZ-NH2	-9.01	115.80	120.30
2	7	106	TYR	CB-CG-CD1	8.99	126.39	121.00
1	D	65	GLU	N-CA-CB	8.98	126.77	110.60
2	1	21	ASP	CB-CG-OD1	-8.95	110.24	118.30
3	J	130	PHE	CB-CG-CD2	-8.95	114.53	120.80
1	b	241	ARG	NE-CZ-NH1	8.95	124.78	120.30
1	F	168	ARG	NE-CZ-NH2	8.95	124.78	120.30
2	j	123	TYR	CB-CG-CD1	8.95	126.37	121.00
2	l	148	TYR	CB-CG-CD1	8.95	126.37	121.00
2	i	68	ARG	NE-CZ-NH1	-8.94	115.83	120.30
1	a	86	ARG	NE-CZ-NH1	8.93	124.76	120.30
2	4	67	ALA	N-CA-CB	8.93	122.59	110.10
2	k	126	ASP	CB-CG-OD1	8.91	126.32	118.30
3	H	29	ARG	NE-CZ-NH2	-8.90	115.85	120.30
1	a	123	TYR	CB-CG-CD2	-8.89	115.66	121.00
1	b	232	TYR	CB-CG-CD1	-8.89	115.67	121.00
1	b	119	PHE	CB-CG-CD1	8.88	127.01	120.80
1	b	180	ARG	NE-CZ-NH1	-8.87	115.86	120.30
2	n	199	TYR	CB-CG-CD1	8.87	126.32	121.00
3	M	24	ARG	CD-NE-CZ	8.86	136.01	123.60
1	C	132	PHE	CB-CG-CD1	8.86	127.00	120.80
3	I	140	TYR	CB-CG-CD1	-8.86	115.69	121.00
1	D	68	TYR	CB-CG-CD2	8.85	126.31	121.00
2	7	106	TYR	CB-CG-CD2	-8.85	115.69	121.00
2	n	103	TYR	CB-CG-CD2	-8.85	115.69	121.00
3	M	154	ARG	NE-CZ-NH2	-8.83	115.89	120.30
1	F	126	TYR	CB-CG-CD2	-8.83	115.70	121.00
2	l	153	ASP	CB-CG-OD1	-8.83	110.36	118.30
1	D	151	ASP	CB-CG-OD2	-8.80	110.38	118.30
3	K	328	MET	CG-SD-CE	-8.79	86.13	100.20
1	g	179	TYR	CB-CG-CD2	-8.77	115.74	121.00
1	f	26	TYR	CB-CG-CD1	8.76	126.26	121.00
2	1	102	ARG	NE-CZ-NH1	-8.76	115.92	120.30
2	j	123	TYR	CB-CG-CD2	-8.75	115.75	121.00
3	L	116	VAL	CA-CB-CG2	-8.75	97.77	110.90
2	k	173	TYR	CB-CG-CD1	8.72	126.23	121.00
1	C	132	PHE	CB-CG-CD2	-8.71	114.70	120.80
3	K	244	ASP	CB-CG-OD1	8.71	126.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	317	ARG	NE-CZ-NH2	8.71	124.65	120.30
3	L	367	ARG	NE-CZ-NH1	8.70	124.65	120.30
3	J	258	ASP	CB-CG-OD1	-8.70	110.47	118.30
1	f	159	TYR	CB-CG-CD1	8.69	126.22	121.00
3	M	105	ARG	NE-CZ-NH1	8.68	124.64	120.30
1	D	181	ASP	CB-CG-OD1	8.66	126.10	118.30
1	G	68	TYR	CB-CG-CD1	-8.66	115.80	121.00
3	H	87	PHE	CB-CG-CD1	8.65	126.86	120.80
2	j	46	TYR	CG-CD2-CE2	-8.65	114.38	121.30
1	G	86	ARG	NE-CZ-NH1	8.64	124.62	120.30
1	A	218	ASP	CB-CG-OD1	-8.63	110.53	118.30
3	I	200	ARG	NE-CZ-NH2	-8.63	115.98	120.30
1	a	180	ARG	NE-CZ-NH1	-8.63	115.99	120.30
2	3	197	TYR	CB-CG-CD2	-8.63	115.82	121.00
1	c	53	ARG	NE-CZ-NH1	-8.62	115.99	120.30
2	4	78	GLU	OE1-CD-OE2	8.62	133.65	123.30
3	I	50	ARG	NE-CZ-NH1	8.62	124.61	120.30
1	e	91	ARG	NE-CZ-NH2	8.61	124.60	120.30
1	e	53	ARG	NE-CZ-NH1	-8.60	116.00	120.30
2	7	212	ARG	NE-CZ-NH1	8.60	124.60	120.30
1	g	219	ARG	NE-CZ-NH1	-8.59	116.01	120.30
2	1	121	SER	N-CA-CB	8.58	123.37	110.50
3	K	259	ARG	NE-CZ-NH1	8.58	124.59	120.30
3	I	29	ARG	NE-CZ-NH2	-8.56	116.02	120.30
3	H	87	PHE	CB-CG-CD2	-8.55	114.82	120.80
1	D	239	ARG	NE-CZ-NH2	-8.54	116.03	120.30
1	b	20	ARG	NE-CZ-NH1	8.53	124.56	120.30
3	H	299	ARG	NE-CZ-NH2	-8.52	116.04	120.30
2	5	77	TYR	CB-CG-CD2	8.52	126.11	121.00
1	C	213	TYR	CB-CG-CD1	8.51	126.11	121.00
2	6	178	ARG	NE-CZ-NH1	8.51	124.56	120.30
1	D	232	TYR	CB-CG-CD1	-8.51	115.89	121.00
3	K	278	ARG	NE-CZ-NH2	-8.51	116.05	120.30
3	I	128	TYR	CG-CD2-CE2	-8.50	114.50	121.30
3	J	50	ARG	NE-CZ-NH1	8.49	124.55	120.30
1	f	239	ARG	NE-CZ-NH1	-8.48	116.06	120.30
1	F	221	PHE	CB-CG-CD2	8.47	126.73	120.80
3	H	326	ARG	NE-CZ-NH2	-8.46	116.07	120.30
3	J	130	PHE	CB-CG-CD1	8.46	126.72	120.80
1	f	159	TYR	CB-CG-CD2	-8.45	115.93	121.00
3	H	258	ASP	CB-CG-OD1	-8.45	110.70	118.30
3	M	250	ARG	NE-CZ-NH1	8.45	124.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	j	173	TYR	CB-CG-CD1	8.43	126.06	121.00
1	A	130	ARG	NE-CZ-NH1	8.43	124.51	120.30
1	a	239	ARG	NE-CZ-NH1	-8.42	116.09	120.30
1	E	33	ARG	NE-CZ-NH1	8.41	124.50	120.30
1	g	26	TYR	CG-CD1-CE1	-8.40	114.58	121.30
3	L	24	ARG	NE-CZ-NH2	-8.39	116.10	120.30
1	B	8	TYR	CB-CG-CD2	8.39	126.03	121.00
1	D	239	ARG	NE-CZ-NH1	8.38	124.49	120.30
1	g	28	ARG	NE-CZ-NH2	-8.37	116.11	120.30
2	7	68	ARG	NE-CZ-NH1	8.34	124.47	120.30
3	L	130	PHE	CB-CG-CD1	8.34	126.64	120.80
1	c	235	ARG	NE-CZ-NH1	-8.34	116.13	120.30
3	L	205	ARG	NE-CZ-NH2	-8.34	116.13	120.30
2	n	121	SER	N-CA-CB	8.33	122.99	110.50
2	h	140	THR	CA-CB-CG2	-8.32	100.75	112.40
3	J	181	TYR	CB-CG-CD1	-8.32	116.01	121.00
2	5	178	ARG	NE-CZ-NH1	-8.31	116.14	120.30
1	g	179	TYR	CB-CG-CD1	8.31	125.98	121.00
2	4	83	ARG	NE-CZ-NH1	-8.30	116.15	120.30
3	M	273	ASP	CB-CG-OD2	-8.30	110.83	118.30
1	E	174	PHE	CB-CG-CD1	8.29	126.61	120.80
3	I	105	ARG	NE-CZ-NH2	8.29	124.44	120.30
3	H	259	ARG	NE-CZ-NH1	8.28	124.44	120.30
2	5	62	ASP	CB-CG-OD2	-8.27	110.86	118.30
1	B	171	VAL	CA-CB-CG2	-8.26	98.50	110.90
2	k	80	ARG	NE-CZ-NH2	8.25	124.43	120.30
3	K	28	ARG	NE-CZ-NH1	8.25	124.42	120.30
1	G	185	PHE	CB-CG-CD1	-8.24	115.03	120.80
1	C	28	ARG	NE-CZ-NH2	-8.22	116.19	120.30
2	l	104	PHE	CB-CG-CD2	-8.22	115.05	120.80
3	L	140	TYR	CB-CG-CD1	-8.22	116.07	121.00
3	I	76	ARG	NE-CZ-NH2	-8.21	116.19	120.30
1	C	15	PHE	CB-CG-CD1	-8.21	115.05	120.80
1	B	86	ARG	NE-CZ-NH2	-8.21	116.20	120.30
2	6	88	ARG	NE-CZ-NH1	-8.20	116.20	120.30
2	n	102	ARG	NE-CZ-NH1	-8.19	116.20	120.30
1	G	103	TYR	CB-CG-CD2	8.19	125.91	121.00
3	M	50	ARG	NE-CZ-NH2	-8.19	116.21	120.30
2	j	102	ARG	NE-CZ-NH1	-8.18	116.21	120.30
3	H	76	ARG	NE-CZ-NH2	-8.17	116.22	120.30
3	I	336	PHE	CB-CG-CD2	-8.16	115.09	120.80
1	D	100	ARG	NE-CZ-NH1	8.16	124.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	5	77	TYR	CB-CG-CD1	-8.16	116.11	121.00
1	A	20	ARG	NE-CZ-NH1	-8.15	116.22	120.30
1	E	20	ARG	NH1-CZ-NH2	8.15	128.37	119.40
2	k	50	ASP	CB-CG-OD1	-8.15	110.97	118.30
2	5	211	PHE	CB-CG-CD2	-8.14	115.10	120.80
1	d	235	ARG	NE-CZ-NH1	-8.13	116.24	120.30
2	3	77	TYR	CB-CG-CD2	8.13	125.88	121.00
2	4	30	ARG	NE-CZ-NH2	-8.13	116.24	120.30
3	J	27	TYR	CB-CG-CD2	8.12	125.87	121.00
3	I	105	ARG	NE-CZ-NH1	-8.11	116.24	120.30
1	f	126	TYR	CB-CG-CD1	-8.10	116.14	121.00
3	K	36	PHE	CB-CG-CD2	-8.09	115.14	120.80
3	J	59	ARG	NE-CZ-NH1	-8.09	116.26	120.30
1	D	218	ASP	CB-CG-OD2	8.08	125.57	118.30
1	d	16	SER	N-CA-CB	8.07	122.60	110.50
1	d	77	ALA	N-CA-CB	8.07	121.39	110.10
1	A	10	ARG	NE-CZ-NH2	-8.06	116.27	120.30
2	l	178	ARG	NE-CZ-NH2	-8.06	116.27	120.30
2	6	81	ARG	NE-CZ-NH2	-8.06	116.27	120.30
1	g	86	ARG	NE-CZ-NH2	-8.05	116.28	120.30
2	2	173	TYR	CB-CG-CD2	-8.04	116.18	121.00
2	2	52	MET	CG-SD-CE	-8.03	87.35	100.20
2	2	77	TYR	CG-CD2-CE2	-8.03	114.87	121.30
2	h	77	TYR	CB-CG-CD1	8.01	125.81	121.00
3	I	57	ARG	NE-CZ-NH1	-8.01	116.29	120.30
1	e	241	ARG	NE-CZ-NH1	-8.01	116.30	120.30
2	k	30	ARG	NE-CZ-NH1	8.00	124.30	120.30
3	H	275	PHE	CB-CG-CD1	7.99	126.39	120.80
3	M	397	PHE	CB-CG-CD2	-7.98	115.21	120.80
1	A	93	ARG	NE-CZ-NH2	-7.97	116.31	120.30
1	a	180	ARG	NE-CZ-NH2	7.96	124.28	120.30
1	A	100	ARG	NE-CZ-NH1	-7.96	116.32	120.30
1	a	93	ARG	NE-CZ-NH1	7.94	124.27	120.30
2	5	41	ALA	N-CA-CB	7.93	121.21	110.10
1	e	151	ASP	CB-CG-OD2	-7.93	111.17	118.30
1	e	219	ARG	NE-CZ-NH1	-7.92	116.34	120.30
2	3	21	ASP	CB-CG-OD1	-7.92	111.17	118.30
3	L	28	ARG	NE-CZ-NH2	-7.92	116.34	120.30
2	6	36	PHE	CB-CG-CD1	7.92	126.34	120.80
2	n	116	ASP	CB-CG-OD2	7.91	125.42	118.30
2	3	199	TYR	CB-CG-CD1	7.89	125.73	121.00
3	I	215	TYR	CB-CG-CD1	-7.89	116.27	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	123	TYR	CG-CD1-CE1	-7.89	114.99	121.30
1	c	219	ARG	NE-CZ-NH1	-7.87	116.36	120.30
1	c	123	TYR	CB-CG-CD2	-7.86	116.28	121.00
1	D	8	TYR	CD1-CE1-CZ	-7.86	112.72	119.80
3	M	391	ASP	CB-CG-OD2	-7.86	111.22	118.30
1	D	8	TYR	CG-CD1-CE1	7.85	127.58	121.30
3	H	41	ARG	NE-CZ-NH1	7.84	124.22	120.30
1	D	8	TYR	CB-CG-CD1	7.81	125.69	121.00
2	m	102	ARG	NE-CZ-NH2	7.81	124.20	120.30
2	3	46	TYR	CB-CG-CD2	7.81	125.68	121.00
2	3	170	ARG	NE-CZ-NH1	-7.80	116.40	120.30
1	b	119	PHE	CB-CG-CD2	-7.79	115.34	120.80
2	i	102	ARG	NE-CZ-NH2	7.79	124.20	120.30
3	L	289	ARG	NE-CZ-NH1	7.79	124.19	120.30
3	K	361	PHE	CB-CG-CD2	-7.78	115.35	120.80
2	1	153	ASP	CB-CG-OD1	-7.77	111.31	118.30
1	E	132	PHE	CB-CG-CD2	7.75	126.23	120.80
1	C	86	ARG	NE-CZ-NH1	7.75	124.17	120.30
1	C	218	ASP	CB-CG-OD2	7.73	125.26	118.30
1	A	103	TYR	CB-CG-CD2	-7.72	116.37	121.00
3	M	299	ARG	NE-CZ-NH1	-7.72	116.44	120.30
2	n	148	TYR	CB-CG-CD2	-7.72	116.37	121.00
2	n	31	ALA	N-CA-CB	7.71	120.89	110.10
3	I	331	ALA	N-CA-CB	7.70	120.88	110.10
1	F	61	ALA	CB-CA-C	-7.70	98.55	110.10
2	m	173	TYR	CB-CG-CD1	7.69	125.62	121.00
2	1	83	ARG	NE-CZ-NH1	7.69	124.14	120.30
2	m	103	TYR	CB-CG-CD2	-7.69	116.39	121.00
2	1	197	TYR	CB-CG-CD1	-7.68	116.39	121.00
1	C	221	PHE	CB-CG-CD1	-7.67	115.43	120.80
3	M	397	PHE	CB-CG-CD1	7.67	126.17	120.80
1	F	118	ASP	CB-CG-OD1	7.66	125.20	118.30
2	1	158	GLU	N-CA-CB	7.66	124.39	110.60
1	D	123	TYR	CD1-CE1-CZ	7.66	126.69	119.80
3	H	397	PHE	CB-CG-CD2	-7.66	115.44	120.80
1	F	11	ALA	N-CA-CB	7.65	120.81	110.10
1	E	132	PHE	CB-CG-CD1	-7.63	115.45	120.80
1	e	28	ARG	NE-CZ-NH2	7.63	124.12	120.30
2	n	65	PHE	CB-CG-CD2	-7.63	115.46	120.80
2	h	196	PHE	CB-CG-CD1	7.63	126.14	120.80
2	k	162	ASP	CB-CG-OD2	-7.62	111.44	118.30
2	6	46	TYR	CB-CG-CD2	7.62	125.57	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	241	ARG	NE-CZ-NH1	7.61	124.10	120.30
2	6	46	TYR	CB-CG-CD1	-7.61	116.44	121.00
3	L	140	TYR	CD1-CE1-CZ	-7.60	112.96	119.80
1	a	235	ARG	NE-CZ-NH1	-7.59	116.50	120.30
1	E	91	ARG	NE-CZ-NH1	-7.59	116.51	120.30
1	C	100	ARG	NE-CZ-NH2	7.58	124.09	120.30
1	E	123	TYR	CG-CD2-CE2	-7.58	115.24	121.30
3	I	304	ASP	CB-CG-OD1	-7.58	111.48	118.30
3	L	52	ARG	NE-CZ-NH1	-7.58	116.51	120.30
1	E	185	PHE	CB-CG-CD2	7.57	126.10	120.80
2	k	199	TYR	CB-CG-CD1	-7.56	116.46	121.00
2	4	103	TYR	N-CA-CB	7.56	124.21	110.60
3	M	70	ASP	CB-CG-OD1	-7.56	111.50	118.30
1	c	180	ARG	NE-CZ-NH1	7.56	124.08	120.30
2	4	36	PHE	CB-CG-CD1	-7.56	115.51	120.80
3	M	236	SER	C-N-CA	7.56	140.59	121.70
1	E	239	ARG	NE-CZ-NH1	7.55	124.08	120.30
3	K	59	ARG	NE-CZ-NH1	-7.54	116.53	120.30
2	k	139	ALA	C-N-CA	7.54	140.54	121.70
3	K	249	ARG	NE-CZ-NH2	-7.53	116.54	120.30
2	2	101	TYR	CZ-CE2-CD2	7.53	126.57	119.80
1	c	148	TYR	CB-CG-CD2	7.52	125.51	121.00
2	4	154	ARG	NE-CZ-NH2	7.52	124.06	120.30
1	A	168	ARG	NE-CZ-NH1	7.51	124.06	120.30
3	I	191	LEU	CB-CG-CD1	7.51	123.77	111.00
2	m	31	ALA	N-CA-CB	7.51	120.61	110.10
3	K	263	ARG	NE-CZ-NH1	7.51	124.05	120.30
1	B	119	PHE	CB-CG-CD1	7.50	126.05	120.80
3	I	397	PHE	CB-CG-CD2	-7.50	115.55	120.80
2	l	184	ASP	CB-CG-OD2	-7.49	111.56	118.30
2	2	25	MET	CG-SD-CE	-7.48	88.23	100.20
2	i	104	PHE	CB-CG-CD2	7.48	126.03	120.80
1	D	217	ASP	CB-CG-OD1	-7.46	111.58	118.30
1	A	103	TYR	CB-CG-CD1	7.46	125.47	121.00
3	I	317	ARG	NE-CZ-NH2	7.46	124.03	120.30
1	a	103	TYR	CB-CG-CD2	-7.45	116.53	121.00
3	K	205	ARG	NE-CZ-NH2	-7.44	116.58	120.30
2	3	101	TYR	CB-CG-CD1	7.43	125.46	121.00
1	A	135	SER	N-CA-CB	7.43	121.64	110.50
1	g	100	ARG	NE-CZ-NH1	-7.42	116.59	120.30
2	4	101	TYR	CG-CD2-CE2	-7.42	115.36	121.30
1	c	174	PHE	CB-CG-CD1	7.41	125.99	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	68	TYR	CB-CG-CD2	-7.41	116.55	121.00
2	6	178	ARG	NE-CZ-NH2	-7.41	116.59	120.30
3	M	303	PHE	CB-CG-CD2	-7.40	115.62	120.80
3	L	291	ASP	CB-CG-OD2	7.40	124.96	118.30
3	K	281	VAL	C-N-CA	7.39	140.18	121.70
2	4	116	ASP	CB-CG-OD1	7.39	124.95	118.30
2	j	178	ARG	NE-CZ-NH2	-7.39	116.61	120.30
1	d	217	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	G	151	ASP	CB-CG-OD2	-7.38	111.66	118.30
1	e	84	ASP	CB-CG-OD1	7.37	124.94	118.30
1	g	175	PHE	CB-CG-CD1	7.37	125.96	120.80
2	j	62	ASP	CB-CG-OD1	-7.37	111.67	118.30
1	E	182	ASP	CB-CG-OD2	7.37	124.93	118.30
2	6	77	TYR	CG-CD1-CE1	7.37	127.19	121.30
2	1	154	ARG	NE-CZ-NH2	-7.36	116.62	120.30
1	a	150	THR	CA-CB-CG2	-7.36	102.09	112.40
2	7	65	PHE	CB-CG-CD2	7.35	125.95	120.80
1	E	235	ARG	NE-CZ-NH2	7.34	123.97	120.30
2	n	51	ARG	NE-CZ-NH2	-7.34	116.63	120.30
3	H	314	PHE	CB-CG-CD1	7.34	125.94	120.80
3	M	326	ARG	NE-CZ-NH2	-7.34	116.63	120.30
2	n	103	TYR	CG-CD2-CE2	-7.33	115.44	121.30
1	A	132	PHE	CB-CG-CD2	-7.33	115.67	120.80
1	A	159	TYR	CB-CG-CD1	7.32	125.39	121.00
2	4	123	TYR	CB-CG-CD1	-7.32	116.61	121.00
1	f	91	ARG	CD-NE-CZ	-7.31	113.36	123.60
2	n	211	PHE	CB-CG-CD1	-7.31	115.68	120.80
3	M	273	ASP	CB-CG-OD1	7.31	124.88	118.30
2	7	211	PHE	CB-CG-CD2	7.30	125.91	120.80
3	M	326	ARG	NE-CZ-NH1	7.30	123.95	120.30
2	2	77	TYR	CD1-CE1-CZ	-7.29	113.23	119.80
1	d	185	PHE	CB-CG-CD2	-7.29	115.70	120.80
1	D	22	PHE	CB-CG-CD1	-7.28	115.71	120.80
2	5	23	VAL	CA-CB-CG2	-7.27	99.99	110.90
1	c	21	LEU	CB-CA-C	-7.27	96.39	110.20
2	7	178	ARG	NE-CZ-NH1	-7.26	116.67	120.30
1	c	239	ARG	NE-CZ-NH1	7.25	123.93	120.30
1	G	235	ARG	NE-CZ-NH1	-7.25	116.67	120.30
3	K	211	PHE	CB-CG-CD1	7.24	125.87	120.80
3	J	341	ARG	NE-CZ-NH2	7.23	123.92	120.30
1	G	218	ASP	CB-CG-OD1	-7.22	111.80	118.30
2	j	65	PHE	CB-CG-CD1	-7.22	115.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	F	10	ARG	NE-CZ-NH2	-7.21	116.69	120.30
3	M	131	GLU	C-N-CA	7.21	139.73	121.70
2	1	80	ARG	NE-CZ-NH2	7.20	123.90	120.30
2	m	176	MET	CG-SD-CE	-7.19	88.69	100.20
2	7	176	MET	CB-CA-C	-7.19	96.02	110.40
1	A	185	PHE	CB-CG-CD2	-7.18	115.77	120.80
1	E	166	MET	N-CA-CB	7.17	123.51	110.60
1	D	139	ALA	N-CA-CB	7.17	120.14	110.10
2	2	187	ASP	CB-CG-OD2	-7.17	111.84	118.30
2	3	187	ASP	CB-CG-OD1	-7.17	111.85	118.30
1	F	28	ARG	NH1-CZ-NH2	7.17	127.29	119.40
2	i	78	GLU	OE1-CD-OE2	-7.17	114.70	123.30
3	H	140	TYR	CB-CG-CD2	-7.16	116.70	121.00
1	E	26	TYR	CB-CG-CD2	7.16	125.30	121.00
1	f	77	ALA	N-CA-CB	-7.16	100.07	110.10
1	g	54	VAL	CA-CB-CG2	-7.16	100.16	110.90
1	E	187	ASP	CB-CG-OD2	-7.14	111.87	118.30
1	b	161	ALA	N-CA-CB	7.14	120.09	110.10
2	1	88	ARG	NE-CZ-NH1	-7.13	116.73	120.30
1	A	26	TYR	CG-CD1-CE1	7.13	127.01	121.30
1	D	241	ARG	NE-CZ-NH2	-7.13	116.73	120.30
1	e	190	VAL	CA-CB-CG2	-7.12	100.21	110.90
3	L	29	ARG	NE-CZ-NH2	7.12	123.86	120.30
1	E	186	ASP	CB-CG-OD1	-7.12	111.89	118.30
2	1	197	TYR	CB-CG-CD2	7.12	125.27	121.00
3	H	397	PHE	CB-CG-CD1	7.11	125.78	120.80
1	e	132	PHE	CB-CG-CD1	-7.10	115.83	120.80
1	B	10	ARG	NE-CZ-NH2	-7.09	116.75	120.30
2	l	162	ASP	CB-CG-OD1	7.09	124.68	118.30
2	5	211	PHE	CB-CG-CD1	7.08	125.76	120.80
2	h	199	TYR	CB-CG-CD1	-7.07	116.76	121.00
2	6	83	ARG	NE-CZ-NH1	-7.07	116.77	120.30
3	M	303	PHE	CB-CG-CD1	7.07	125.75	120.80
2	h	81	ARG	NE-CZ-NH1	-7.07	116.77	120.30
1	e	241	ARG	NE-CZ-NH2	7.07	123.83	120.30
1	a	219	ARG	NE-CZ-NH1	-7.06	116.77	120.30
2	3	102	ARG	NE-CZ-NH1	-7.06	116.77	120.30
3	I	333	ASP	CB-CG-OD2	7.06	124.66	118.30
2	4	103	TYR	CB-CG-CD2	7.05	125.23	121.00
1	D	175	PHE	CB-CG-CD1	7.04	125.73	120.80
1	D	232	TYR	CG-CD1-CE1	-7.04	115.67	121.30
3	H	57	ARG	NE-CZ-NH1	7.04	123.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	20	TYR	CD1-CE1-CZ	-7.04	113.47	119.80
2	i	139	ALA	N-CA-CB	7.04	119.95	110.10
2	6	136	ASP	CB-CG-OD1	-7.04	111.97	118.30
2	3	154	ARG	NE-CZ-NH2	7.03	123.82	120.30
1	c	15	PHE	CB-CG-CD1	7.03	125.72	120.80
1	D	179	TYR	CG-CD2-CE2	-7.03	115.68	121.30
2	n	46	TYR	CG-CD1-CE1	-7.03	115.68	121.30
1	C	218	ASP	CB-CG-OD1	-7.03	111.98	118.30
1	d	118	ASP	CB-CG-OD1	-7.03	111.97	118.30
1	a	27	ALA	CB-CA-C	-7.02	99.56	110.10
3	I	142	ASP	CB-CG-OD1	-7.02	111.98	118.30
1	e	184	SER	N-CA-CB	7.02	121.03	110.50
3	H	50	ARG	NE-CZ-NH1	7.01	123.80	120.30
2	l	101	TYR	CB-CG-CD2	-7.00	116.80	121.00
2	2	126	ASP	CB-CG-OD2	-7.00	112.00	118.30
2	k	154	ARG	CD-NE-CZ	-7.00	113.80	123.60
1	G	26	TYR	CB-CG-CD1	-6.99	116.81	121.00
2	m	156	THR	CA-CB-CG2	-6.99	102.61	112.40
2	h	139	ALA	N-CA-CB	6.99	119.89	110.10
1	b	93	ARG	NE-CZ-NH2	-6.98	116.81	120.30
1	a	232	TYR	CB-CG-CD1	-6.98	116.81	121.00
1	F	159	TYR	CB-CG-CD1	-6.98	116.81	121.00
1	F	218	ASP	CB-CG-OD2	-6.97	112.03	118.30
3	M	105	ARG	NH1-CZ-NH2	-6.97	111.73	119.40
3	M	261	VAL	CA-CB-CG1	6.97	121.35	110.90
1	a	103	TYR	CD1-CE1-CZ	-6.96	113.53	119.80
1	d	15	PHE	CB-CG-CD1	6.96	125.67	120.80
3	L	59	ARG	NH1-CZ-NH2	6.95	127.05	119.40
3	J	334	VAL	CA-CB-CG2	-6.94	100.49	110.90
2	7	197	TYR	CG-CD1-CE1	6.94	126.85	121.30
3	H	230	ALA	CB-CA-C	-6.94	99.69	110.10
1	C	141	VAL	CA-CB-CG1	-6.94	100.50	110.90
2	1	139	ALA	N-CA-CB	6.93	119.80	110.10
2	k	55	THR	CA-CB-CG2	-6.93	102.70	112.40
2	7	80	ARG	NE-CZ-NH2	-6.92	116.84	120.30
2	6	146	THR	CA-CB-CG2	-6.92	102.71	112.40
2	7	46	TYR	CB-CG-CD2	6.92	125.15	121.00
3	J	94	TYR	CG-CD2-CE2	-6.92	115.77	121.30
2	i	19	CYS	N-CA-CB	6.91	123.04	110.60
2	n	65	PHE	CB-CG-CD1	6.91	125.64	120.80
2	n	155	PHE	CB-CG-CD2	6.91	125.64	120.80
2	6	65	PHE	CB-CG-CD1	6.91	125.63	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	6	MET	CG-SD-CE	-6.90	89.15	100.20
1	b	159	TYR	CB-CG-CD2	-6.90	116.86	121.00
3	L	289	ARG	NE-CZ-NH2	-6.88	116.86	120.30
2	2	191	ILE	N-CA-C	-6.88	92.44	111.00
1	c	175	PHE	CB-CG-CD1	6.87	125.61	120.80
2	3	12	THR	CA-CB-CG2	-6.87	102.78	112.40
1	E	30	ALA	N-CA-CB	6.87	119.72	110.10
2	1	154	ARG	NE-CZ-NH1	6.87	123.73	120.30
2	m	181	ALA	CB-CA-C	-6.87	99.80	110.10
1	B	168	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	n	52	MET	CG-SD-CE	6.86	111.18	100.20
1	C	10	ARG	NE-CZ-NH1	6.86	123.73	120.30
2	3	106	TYR	CB-CG-CD2	-6.86	116.89	121.00
1	D	130	ARG	NE-CZ-NH2	-6.85	116.87	120.30
2	i	36	PHE	CB-CG-CD1	6.85	125.60	120.80
3	I	128	TYR	CZ-CE2-CD2	6.85	125.96	119.80
3	K	305	ARG	NE-CZ-NH2	-6.84	116.88	120.30
2	5	36	PHE	CB-CG-CD2	-6.84	116.02	120.80
3	I	114	ALA	CB-CA-C	-6.83	99.85	110.10
1	f	15	PHE	CB-CG-CD2	6.83	125.58	120.80
1	E	148	TYR	CG-CD2-CE2	-6.83	115.84	121.30
1	B	132	PHE	CB-CG-CD1	6.83	125.58	120.80
1	F	118	ASP	CB-CG-OD2	-6.82	112.16	118.30
2	2	88	ARG	NE-CZ-NH2	-6.82	116.89	120.30
2	k	178	ARG	NE-CZ-NH1	6.82	123.71	120.30
1	G	103	TYR	CB-CG-CD1	-6.81	116.91	121.00
2	5	153	ASP	CB-CG-OD2	-6.81	112.17	118.30
2	4	123	TYR	CB-CG-CD2	6.81	125.08	121.00
2	n	180	SER	N-CA-CB	6.80	120.71	110.50
2	2	106	TYR	CB-CG-CD2	6.79	125.08	121.00
2	j	154	ARG	CD-NE-CZ	6.79	133.11	123.60
1	A	26	TYR	CB-CG-CD1	-6.79	116.93	121.00
1	e	103	TYR	CB-CG-CD2	-6.78	116.93	121.00
2	7	50	ASP	CB-CG-OD1	6.78	124.41	118.30
3	I	215	TYR	CB-CG-CD2	6.78	125.07	121.00
1	D	26	TYR	CG-CD1-CE1	-6.78	115.88	121.30
3	I	20	TYR	CB-CG-CD1	6.78	125.07	121.00
3	I	250	ARG	NE-CZ-NH2	6.78	123.69	120.30
1	B	83	ALA	O-C-N	-6.77	111.86	122.70
1	a	123	TYR	CB-CG-CD1	6.77	125.06	121.00
2	7	123	TYR	CB-CG-CD2	6.76	125.06	121.00
1	A	93	ARG	NE-CZ-NH1	6.76	123.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	G	118	ASP	CB-CG-OD1	6.76	124.39	118.30
1	f	126	TYR	CG-CD1-CE1	-6.76	115.89	121.30
1	c	84	ASP	CB-CG-OD2	-6.76	112.22	118.30
3	J	50	ARG	NE-CZ-NH2	-6.75	116.93	120.30
1	G	15	PHE	CB-CG-CD2	6.74	125.52	120.80
1	G	174	PHE	CB-CG-CD1	-6.74	116.08	120.80
2	6	123	TYR	CG-CD2-CE2	-6.73	115.91	121.30
1	B	58	LEU	CB-CG-CD1	-6.73	99.56	111.00
1	E	232	TYR	CB-CG-CD1	-6.73	116.96	121.00
3	J	27	TYR	CB-CG-CD1	-6.73	116.96	121.00
2	7	50	ASP	CB-CG-OD2	-6.71	112.26	118.30
2	5	126	ASP	CB-CG-OD1	6.71	124.34	118.30
3	I	341	ARG	NE-CZ-NH1	-6.71	116.94	120.30
3	L	367	ARG	NE-CZ-NH2	-6.71	116.95	120.30
1	a	103	TYR	CG-CD1-CE1	6.70	126.66	121.30
3	J	44	TYR	CG-CD2-CE2	-6.70	115.94	121.30
2	1	81	ARG	NE-CZ-NH2	6.69	123.64	120.30
1	B	132	PHE	CB-CG-CD2	-6.68	116.12	120.80
3	J	265	MET	CG-SD-CE	-6.68	89.51	100.20
1	d	22	PHE	CB-CG-CD1	-6.68	116.12	120.80
2	2	36	PHE	CB-CG-CD2	-6.68	116.12	120.80
2	l	51	ARG	NE-CZ-NH2	-6.68	116.96	120.30
1	g	159	TYR	CB-CG-CD2	-6.68	116.99	121.00
3	I	24	ARG	NE-CZ-NH1	6.68	123.64	120.30
1	d	123	TYR	CB-CG-CD1	-6.68	116.99	121.00
2	j	196	PHE	CB-CG-CD2	6.67	125.47	120.80
1	f	100	ARG	NE-CZ-NH1	6.67	123.64	120.30
3	H	227	PHE	CB-CG-CD1	6.67	125.47	120.80
1	D	179	TYR	CD1-CE1-CZ	-6.67	113.80	119.80
2	m	188	VAL	CA-CB-CG1	6.66	120.89	110.90
3	M	154	ARG	NE-CZ-NH1	6.65	123.63	120.30
1	A	221	PHE	CB-CG-CD2	-6.65	116.14	120.80
1	a	224	VAL	CA-CB-CG2	-6.65	100.93	110.90
2	2	89	ALA	N-CA-CB	6.65	119.41	110.10
3	J	289	ARG	NE-CZ-NH1	6.64	123.62	120.30
1	F	221	PHE	CB-CG-CD1	-6.64	116.15	120.80
1	F	227	GLU	OE1-CD-OE2	6.64	131.27	123.30
1	f	15	PHE	CB-CG-CD1	-6.64	116.15	120.80
3	M	94	TYR	CB-CG-CD2	-6.64	117.02	121.00
1	A	53	ARG	NE-CZ-NH1	-6.63	116.99	120.30
3	L	68	VAL	CA-CB-CG2	-6.63	100.96	110.90
1	c	118	ASP	CB-CG-OD2	-6.63	112.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	46	TYR	CB-CG-CD2	-6.62	117.03	121.00
3	M	227	PHE	CB-CG-CD1	6.62	125.43	120.80
3	J	291	ASP	CB-CG-OD1	-6.62	112.34	118.30
2	3	30	ARG	NE-CZ-NH1	-6.62	116.99	120.30
1	d	79	SER	N-CA-CB	6.62	120.42	110.50
1	F	68	TYR	CB-CG-CD1	-6.61	117.03	121.00
2	2	139	ALA	N-CA-C	-6.61	93.15	111.00
2	k	36	PHE	CB-CG-CD2	-6.61	116.17	120.80
3	I	20	TYR	CB-CG-CD2	-6.61	117.03	121.00
2	5	153	ASP	CB-CG-OD1	6.61	124.25	118.30
1	D	64	ILE	C-N-CA	6.61	138.22	121.70
1	d	187	ASP	CB-CG-OD1	-6.61	112.35	118.30
2	6	101	TYR	CG-CD1-CE1	-6.61	116.01	121.30
1	e	166	MET	CG-SD-CE	6.60	110.77	100.20
3	M	67	VAL	CA-CB-CG2	6.60	120.80	110.90
3	J	321	PHE	CB-CG-CD2	-6.60	116.18	120.80
1	E	93	ARG	NE-CZ-NH2	6.59	123.60	120.30
1	B	203	GLU	OE1-CD-OE2	6.59	131.21	123.30
2	l	173	TYR	CG-CD1-CE1	-6.59	116.03	121.30
1	A	180	ARG	NE-CZ-NH2	-6.59	117.01	120.30
2	k	51	ARG	NE-CZ-NH2	6.59	123.59	120.30
2	7	154	ARG	NE-CZ-NH2	6.58	123.59	120.30
1	G	62	ASP	CB-CG-OD2	-6.58	112.38	118.30
2	j	46	TYR	CB-CG-CD2	-6.58	117.05	121.00
1	c	213	TYR	CB-CG-CD1	6.57	124.94	121.00
3	K	87	PHE	CB-CG-CD2	6.57	125.40	120.80
1	e	71	ASP	CB-CG-OD2	-6.57	112.39	118.30
1	c	33	ARG	NE-CZ-NH2	6.57	123.58	120.30
1	G	86	ARG	NE-CZ-NH2	-6.57	117.02	120.30
3	M	59	ARG	CG-CD-NE	-6.57	98.01	111.80
2	m	88	ARG	NE-CZ-NH2	-6.56	117.02	120.30
3	H	52	ARG	NE-CZ-NH2	6.56	123.58	120.30
3	J	275	PHE	CB-CG-CD1	-6.56	116.21	120.80
1	f	148	TYR	CG-CD2-CE2	-6.56	116.06	121.30
1	a	220	THR	CA-CB-CG2	-6.55	103.23	112.40
3	H	29	ARG	NE-CZ-NH1	6.54	123.57	120.30
3	M	105	ARG	NE-CZ-NH2	6.53	123.57	120.30
1	G	118	ASP	CB-CG-OD2	-6.53	112.42	118.30
3	L	205	ARG	NH1-CZ-NH2	6.53	126.58	119.40
2	j	154	ARG	NE-CZ-NH2	6.53	123.56	120.30
1	A	9	ASP	CB-CG-OD2	6.52	124.17	118.30
1	g	10	ARG	NE-CZ-NH1	-6.52	117.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6	173	TYR	CB-CG-CD1	-6.52	117.09	121.00
3	I	250	ARG	NE-CZ-NH1	6.52	123.56	120.30
1	b	170	ALA	N-CA-CB	6.51	119.22	110.10
1	d	21	LEU	CB-CA-C	-6.51	97.82	110.20
1	b	235	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	c	241	ARG	NE-CZ-NH2	6.51	123.55	120.30
3	K	362	ALA	N-CA-CB	6.50	119.20	110.10
3	M	299	ARG	N-CA-CB	6.50	122.30	110.60
1	e	24	VAL	CG1-CB-CG2	-6.50	100.50	110.90
1	G	213	TYR	CB-CG-CD1	-6.50	117.10	121.00
2	n	103	TYR	CD1-CE1-CZ	-6.50	113.95	119.80
2	7	52	MET	CG-SD-CE	-6.49	89.82	100.20
2	h	196	PHE	N-CA-CB	6.49	122.28	110.60
3	M	28	ARG	NE-CZ-NH1	-6.49	117.06	120.30
2	6	153	ASP	CB-CG-OD2	-6.48	112.47	118.30
3	I	303	PHE	CB-CG-CD1	-6.48	116.27	120.80
1	G	10	ARG	NE-CZ-NH1	-6.48	117.06	120.30
2	n	108	VAL	CG1-CB-CG2	6.48	121.26	110.90
1	C	93	ARG	NE-CZ-NH2	-6.47	117.06	120.30
1	D	196	MET	CG-SD-CE	-6.47	89.85	100.20
2	k	101	TYR	CZ-CE2-CD2	6.47	125.62	119.80
3	K	224	ARG	NE-CZ-NH2	-6.46	117.07	120.30
3	M	50	ARG	NE-CZ-NH1	6.46	123.53	120.30
1	D	86	ARG	NE-CZ-NH2	-6.46	117.07	120.30
1	F	22	PHE	CB-CG-CD1	-6.46	116.28	120.80
1	B	100	ARG	NE-CZ-NH2	6.46	123.53	120.30
1	g	11	ALA	N-CA-CB	6.45	119.13	110.10
3	K	52	ARG	NE-CZ-NH1	6.45	123.52	120.30
2	l	30	ARG	NE-CZ-NH2	6.44	123.52	120.30
3	M	147	ASP	CB-CG-OD2	-6.44	112.50	118.30
2	i	14	THR	CA-CB-CG2	-6.44	103.39	112.40
2	6	21	ASP	CB-CG-OD2	-6.43	112.51	118.30
2	i	148	TYR	CB-CG-CD1	-6.43	117.14	121.00
2	6	170	ARG	NE-CZ-NH2	6.43	123.52	120.30
2	2	74	ALA	N-CA-CB	6.43	119.10	110.10
3	H	378	ALA	CB-CA-C	-6.42	100.47	110.10
1	c	20	ARG	NE-CZ-NH1	6.42	123.51	120.30
3	J	76	ARG	NE-CZ-NH1	6.41	123.51	120.30
3	K	251	THR	CA-CB-CG2	-6.41	103.43	112.40
3	L	109	ASN	N-CA-CB	6.41	122.13	110.60
1	g	213	TYR	CB-CG-CD1	6.41	124.84	121.00
3	K	36	PHE	CG-CD2-CE2	-6.40	113.76	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	i	211	PHE	CB-CG-CD2	-6.40	116.32	120.80
3	K	303	PHE	CB-CG-CD1	-6.39	116.33	120.80
1	C	84	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	f	20	ARG	NE-CZ-NH2	6.39	123.49	120.30
2	1	170	ARG	NE-CZ-NH2	-6.39	117.11	120.30
2	3	77	TYR	CG-CD2-CE2	6.39	126.41	121.30
2	n	38	ALA	CB-CA-C	-6.38	100.53	110.10
3	L	200	ARG	CD-NE-CZ	-6.38	114.67	123.60
1	C	142	ASP	CB-CG-OD2	6.38	124.04	118.30
1	g	232	TYR	CB-CG-CD1	-6.37	117.17	121.00
3	K	35	LYS	N-CA-CB	6.37	122.07	110.60
2	i	65	PHE	CB-CG-CD2	-6.37	116.34	120.80
2	n	196	PHE	N-CA-CB	6.37	122.07	110.60
1	B	179	TYR	CB-CG-CD1	-6.37	117.18	121.00
1	e	180	ARG	NE-CZ-NH1	-6.37	117.12	120.30
1	c	18	ASP	CB-CG-OD1	6.37	124.03	118.30
2	1	24	VAL	CA-CB-CG1	6.37	120.45	110.90
2	j	187	ASP	CB-CG-OD2	-6.36	112.57	118.30
1	D	179	TYR	CB-CG-CD2	-6.36	117.19	121.00
2	2	103	TYR	CB-CG-CD1	-6.36	117.19	121.00
2	6	30	ARG	NE-CZ-NH1	-6.36	117.12	120.30
1	f	51	ASP	CB-CG-OD2	6.35	124.02	118.30
2	h	51	ARG	NE-CZ-NH1	-6.34	117.13	120.30
2	6	88	ARG	NE-CZ-NH2	6.34	123.47	120.30
1	d	11	ALA	CB-CA-C	-6.33	100.60	110.10
1	g	223	GLU	N-CA-CB	6.33	122.00	110.60
1	A	175	PHE	CB-CG-CD2	-6.33	116.37	120.80
3	M	254	ASP	CB-CG-OD2	6.33	124.00	118.30
1	E	10	ARG	NE-CZ-NH2	6.33	123.47	120.30
3	J	110	GLN	N-CA-CB	6.33	122.00	110.60
2	m	87	VAL	CA-CB-CG2	-6.33	101.41	110.90
2	5	74	ALA	N-CA-CB	6.33	118.96	110.10
1	F	232	TYR	CA-CB-CG	-6.32	101.39	113.40
2	2	199	TYR	CG-CD2-CE2	6.32	126.36	121.30
2	n	106	TYR	CG-CD2-CE2	-6.32	116.24	121.30
2	i	50	ASP	CB-CG-OD2	6.32	123.99	118.30
1	F	75	CYS	N-CA-CB	6.32	121.97	110.60
1	a	103	TYR	CG-CD2-CE2	-6.32	116.25	121.30
1	F	159	TYR	CG-CD1-CE1	-6.32	116.25	121.30
2	2	42	ALA	CB-CA-C	-6.32	100.63	110.10
2	j	46	TYR	CZ-CE2-CD2	6.31	125.48	119.80
3	H	326	ARG	NE-CZ-NH1	6.31	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	i	184	ASP	CB-CG-OD2	6.31	123.98	118.30
3	I	251	THR	CA-CB-CG2	-6.30	103.57	112.40
1	D	53	ARG	NE-CZ-NH1	6.29	123.45	120.30
2	2	139	ALA	N-CA-CB	6.29	118.91	110.10
3	L	326	ARG	NE-CZ-NH2	6.29	123.44	120.30
1	F	77	ALA	N-CA-CB	6.29	118.90	110.10
3	K	24	ARG	NE-CZ-NH1	-6.29	117.16	120.30
3	K	181	TYR	CB-CG-CD1	6.29	124.77	121.00
1	D	213	TYR	CB-CG-CD1	-6.28	117.23	121.00
2	h	95	SER	N-CA-CB	6.28	119.92	110.50
2	i	97	LEU	CB-CA-C	-6.28	98.27	110.20
1	A	60	GLU	OE1-CD-OE2	6.27	130.83	123.30
1	a	148	TYR	CG-CD2-CE2	-6.27	116.28	121.30
3	I	78	VAL	CA-CB-CG2	-6.27	101.50	110.90
2	i	46	TYR	CG-CD1-CE1	-6.27	116.29	121.30
3	L	205	ARG	NE-CZ-NH1	-6.27	117.17	120.30
1	D	93	ARG	NE-CZ-NH2	6.26	123.43	120.30
1	A	58	LEU	CB-CG-CD1	6.26	121.64	111.00
1	a	180	ARG	CD-NE-CZ	-6.26	114.84	123.60
1	c	118	ASP	CB-CA-C	-6.26	97.89	110.40
1	d	190	VAL	CG1-CB-CG2	6.25	120.91	110.90
3	M	278	ARG	NE-CZ-NH2	-6.25	117.17	120.30
3	K	226	VAL	CG1-CB-CG2	-6.25	100.91	110.90
1	c	181	ASP	CB-CG-OD2	-6.24	112.69	118.30
2	2	101	TYR	CG-CD2-CE2	-6.24	116.31	121.30
1	F	235	ARG	NE-CZ-NH1	-6.23	117.18	120.30
2	3	80	ARG	NE-CZ-NH1	-6.23	117.19	120.30
3	L	215	TYR	CD1-CE1-CZ	6.23	125.40	119.80
1	g	100	ARG	NE-CZ-NH2	6.22	123.41	120.30
3	I	317	ARG	NH1-CZ-NH2	-6.22	112.55	119.40
2	m	55	THR	CA-CB-CG2	-6.22	103.69	112.40
2	i	77	TYR	CB-CG-CD1	-6.22	117.27	121.00
2	5	18	VAL	CA-CB-CG1	-6.21	101.59	110.90
2	n	184	ASP	CB-CG-OD2	6.21	123.89	118.30
2	2	50	ASP	CB-CG-OD2	-6.21	112.71	118.30
3	K	249	ARG	N-CA-C	-6.20	94.25	111.00
2	n	139	ALA	C-N-CA	6.20	137.20	121.70
2	m	42	ALA	N-CA-CB	6.20	118.78	110.10
1	A	186	ASP	CB-CG-OD1	6.20	123.88	118.30
2	7	77	TYR	CZ-CE2-CD2	6.19	125.37	119.80
3	K	223	VAL	CA-CB-CG1	-6.19	101.61	110.90
3	L	341	ARG	NE-CZ-NH2	6.19	123.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	2	181	ALA	N-CA-CB	6.19	118.76	110.10
3	M	203	PHE	CB-CG-CD1	6.19	125.13	120.80
1	B	86	ARG	NE-CZ-NH1	6.19	123.39	120.30
1	b	232	TYR	CB-CG-CD2	6.18	124.71	121.00
2	7	36	PHE	CB-CG-CD2	-6.17	116.48	120.80
1	b	33	ARG	NE-CZ-NH2	6.17	123.39	120.30
3	I	250	ARG	NH1-CZ-NH2	-6.17	112.61	119.40
3	L	326	ARG	NE-CZ-NH1	-6.17	117.22	120.30
1	g	22	PHE	CG-CD2-CE2	-6.17	114.01	120.80
1	g	130	ARG	NE-CZ-NH2	-6.17	117.22	120.30
2	4	196	PHE	N-CA-C	-6.17	94.35	111.00
1	A	86	ARG	NE-CZ-NH2	-6.16	117.22	120.30
1	d	225	SER	N-CA-CB	6.16	119.74	110.50
2	2	197	TYR	CB-CG-CD1	-6.16	117.30	121.00
2	4	165	VAL	CA-CB-CG2	6.16	120.14	110.90
2	5	212	ARG	NE-CZ-NH1	6.16	123.38	120.30
3	K	282	LYS	N-CA-CB	6.16	121.69	110.60
2	6	153	ASP	CB-CG-OD1	6.16	123.84	118.30
2	m	65	PHE	CD1-CE1-CZ	6.16	127.49	120.10
1	b	22	PHE	CB-CG-CD2	-6.16	116.49	120.80
1	g	142	ASP	CB-CG-OD1	6.16	123.84	118.30
3	H	192	ALA	N-CA-CB	6.16	118.72	110.10
3	I	368	ALA	N-CA-CB	6.16	118.72	110.10
3	J	203	PHE	CB-CA-C	6.15	122.71	110.40
3	M	57	ARG	NE-CZ-NH1	6.15	123.38	120.30
2	l	106	TYR	CB-CG-CD1	-6.15	117.31	121.00
2	m	77	TYR	CB-CG-CD2	-6.15	117.31	121.00
2	n	46	TYR	CB-CG-CD2	-6.15	117.31	121.00
1	E	33	ARG	NH1-CZ-NH2	-6.14	112.64	119.40
1	g	244	LEU	CB-CG-CD1	-6.14	100.56	111.00
2	k	53	ALA	N-CA-CB	-6.14	101.51	110.10
1	D	26	TYR	CD1-CE1-CZ	6.13	125.32	119.80
2	3	106	TYR	CG-CD2-CE2	-6.13	116.39	121.30
3	I	263	ARG	NE-CZ-NH2	-6.13	117.23	120.30
1	G	239	ARG	NH1-CZ-NH2	-6.13	112.66	119.40
2	l	141	GLY	N-CA-C	-6.13	97.78	113.10
1	B	10	ARG	N-CA-CB	-6.13	99.57	110.60
2	n	196	PHE	N-CA-C	-6.12	94.46	111.00
1	B	175	PHE	CB-CG-CD1	6.12	125.09	120.80
1	D	68	TYR	CB-CG-CD1	-6.12	117.33	121.00
2	i	106	TYR	CG-CD2-CE2	-6.12	116.41	121.30
1	A	68	TYR	CG-CD1-CE1	-6.12	116.41	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	232	TYR	CB-CG-CD2	6.12	124.67	121.00
1	c	244	LEU	CB-CG-CD2	6.12	121.39	111.00
2	3	123	TYR	CB-CG-CD1	6.12	124.67	121.00
2	m	55	THR	N-CA-CB	6.12	121.92	110.30
2	n	199	TYR	CG-CD2-CE2	6.12	126.19	121.30
3	I	147	ASP	CB-CG-OD2	6.12	123.80	118.30
1	d	191	LEU	CB-CG-CD1	6.11	121.39	111.00
3	M	382	VAL	CA-CB-CG2	-6.11	101.73	110.90
1	G	10	ARG	NE-CZ-NH2	-6.11	117.25	120.30
3	I	333	ASP	CB-CG-OD1	-6.11	112.80	118.30
3	J	18	GLU	O-C-N	-6.11	112.93	122.70
1	f	174	PHE	CB-CG-CD2	-6.10	116.53	120.80
3	H	180	LEU	CB-CG-CD2	-6.10	100.62	111.00
3	M	239	PHE	CB-CG-CD1	6.10	125.07	120.80
1	C	150	THR	CA-CB-CG2	-6.10	103.86	112.40
1	f	13	THR	CA-CB-CG2	-6.10	103.86	112.40
1	e	188	ALA	CB-CA-C	-6.10	100.95	110.10
1	a	175	PHE	CB-CG-CD1	6.09	125.07	120.80
3	H	281	VAL	C-N-CA	6.09	136.94	121.70
3	L	143	ILE	C-N-CA	6.09	135.09	122.30
3	J	372	MET	CG-SD-CE	-6.09	90.45	100.20
1	D	15	PHE	CB-CG-CD1	6.09	125.06	120.80
1	f	213	TYR	CB-CG-CD2	6.09	124.65	121.00
3	K	74	ASP	CB-CG-OD2	6.09	123.78	118.30
2	4	77	TYR	CG-CD1-CE1	-6.09	116.43	121.30
1	e	151	ASP	CB-CG-OD1	6.08	123.78	118.30
1	f	122	GLN	N-CA-CB	6.08	121.55	110.60
2	4	24	VAL	CA-CB-CG2	-6.08	101.78	110.90
3	M	215	TYR	CB-CG-CD2	6.08	124.65	121.00
1	E	159	TYR	CG-CD2-CE2	-6.07	116.44	121.30
1	B	126	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	d	156	LEU	CB-CG-CD1	6.07	121.32	111.00
1	G	175	PHE	CB-CG-CD2	-6.07	116.55	120.80
3	L	124	ASP	CB-CG-OD2	6.07	123.76	118.30
2	l	46	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	A	136	LEU	N-CA-C	-6.07	94.61	111.00
1	D	90	ASP	CB-CG-OD1	-6.07	112.84	118.30
2	m	46	TYR	CB-CG-CD2	-6.07	117.36	121.00
1	d	218	ASP	CB-CG-OD1	6.06	123.76	118.30
2	5	155	PHE	CB-CG-CD1	-6.06	116.56	120.80
2	6	28	GLU	N-CA-CB	6.06	121.50	110.60
1	g	123	TYR	CD1-CE1-CZ	6.05	125.25	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	n	178	ARG	NE-CZ-NH2	-6.05	117.27	120.30
2	4	33	MET	CG-SD-CE	-6.05	90.52	100.20
3	L	79	VAL	CA-CB-CG2	-6.05	101.82	110.90
2	m	83	ARG	NE-CZ-NH2	6.05	123.32	120.30
2	h	102	ARG	NE-CZ-NH1	-6.04	117.28	120.30
3	M	200	ARG	NE-CZ-NH1	6.04	123.32	120.30
2	h	140	THR	N-CA-CB	6.04	121.78	110.30
2	l	30	ARG	N-CA-CB	6.04	121.47	110.60
2	j	103	TYR	CB-CG-CD2	-6.04	117.38	121.00
3	L	391	ASP	N-CA-CB	6.03	121.46	110.60
2	2	193	GLU	N-CA-CB	6.03	121.45	110.60
3	M	242	GLU	N-CA-C	-6.03	94.72	111.00
2	k	62	ASP	CB-CG-OD1	6.03	123.73	118.30
1	B	104	ASP	N-CA-CB	6.03	121.45	110.60
1	c	179	TYR	CB-CG-CD1	-6.02	117.39	121.00
2	k	140	THR	N-CA-CB	6.02	121.74	110.30
2	5	196	PHE	CB-CG-CD2	6.02	125.02	120.80
1	E	142	ASP	CB-CG-OD1	6.02	123.72	118.30
2	k	80	ARG	NE-CZ-NH1	-6.02	117.29	120.30
1	g	213	TYR	N-CA-CB	6.02	121.43	110.60
1	c	232	TYR	CB-CG-CD1	-6.01	117.39	121.00
1	F	220	THR	CA-CB-CG2	-6.01	103.98	112.40
1	F	20	ARG	CD-NE-CZ	-6.01	115.18	123.60
2	l	153	ASP	N-CA-CB	6.01	121.42	110.60
2	h	170	ARG	CD-NE-CZ	-6.01	115.19	123.60
1	B	222	LYS	N-CA-CB	6.00	121.40	110.60
1	D	218	ASP	CB-CG-OD1	-6.00	112.90	118.30
2	h	154	ARG	NE-CZ-NH2	6.00	123.30	120.30
2	5	200	SER	N-CA-CB	6.00	119.49	110.50
3	L	275	PHE	CB-CG-CD1	5.99	124.99	120.80
2	1	211	PHE	CB-CG-CD1	-5.99	116.61	120.80
3	H	366	GLU	OE1-CD-OE2	5.99	130.48	123.30
3	I	346	ALA	N-CA-CB	5.99	118.48	110.10
1	G	104	ASP	N-CA-CB	5.98	121.37	110.60
1	E	148	TYR	O-C-N	5.98	132.27	122.70
1	e	50	ALA	N-CA-CB	5.98	118.47	110.10
1	b	225	SER	N-CA-CB	5.98	119.47	110.50
1	D	18	ASP	CB-CA-C	-5.98	98.44	110.40
1	g	26	TYR	CD1-CE1-CZ	5.98	125.18	119.80
3	I	281	VAL	C-N-CA	5.98	136.65	121.70
1	d	244	LEU	CB-CG-CD2	5.98	121.16	111.00
2	6	211	PHE	CB-CG-CD1	5.97	124.98	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	81	SER	N-CA-CB	5.97	119.46	110.50
3	H	317	ARG	NE-CZ-NH2	-5.97	117.31	120.30
1	A	20	ARG	NH1-CZ-NH2	5.97	125.97	119.40
2	6	12	THR	N-CA-C	-5.97	94.89	111.00
3	I	317	ARG	NE-CZ-NH1	5.97	123.28	120.30
3	H	298	LEU	CB-CG-CD2	5.96	121.14	111.00
1	e	174	PHE	CD1-CE1-CZ	-5.96	112.95	120.10
2	n	199	TYR	CD1-CG-CD2	-5.96	111.34	117.90
1	B	7	GLY	N-CA-C	-5.96	98.20	113.10
3	H	339	LEU	CB-CG-CD1	5.96	121.13	111.00
2	j	50	ASP	CB-CG-OD1	-5.95	112.94	118.30
2	3	88	ARG	NE-CZ-NH1	-5.95	117.33	120.30
3	L	28	ARG	CD-NE-CZ	-5.95	115.28	123.60
1	b	126	TYR	CG-CD2-CE2	-5.94	116.55	121.30
2	7	116	ASP	CB-CG-OD1	-5.94	112.95	118.30
1	C	126	TYR	CB-CG-CD1	5.94	124.56	121.00
2	i	32	THR	CA-CB-CG2	-5.94	104.09	112.40
2	4	93	LEU	CB-CG-CD1	5.94	121.09	111.00
2	4	123	TYR	CZ-CE2-CD2	5.94	125.14	119.80
2	l	102	ARG	NE-CZ-NH2	5.94	123.27	120.30
1	a	26	TYR	CB-CG-CD1	5.94	124.56	121.00
1	a	103	TYR	CB-CG-CD1	5.93	124.56	121.00
1	g	148	TYR	CB-CG-CD1	-5.93	117.44	121.00
2	j	114	GLY	N-CA-C	-5.93	98.27	113.10
1	g	28	ARG	NE-CZ-NH1	5.93	123.27	120.30
3	J	241	ASP	CB-CG-OD2	5.93	123.64	118.30
1	A	8	TYR	CB-CG-CD1	5.93	124.56	121.00
3	M	259	ARG	NE-CZ-NH2	5.93	123.27	120.30
2	n	200	SER	N-CA-CB	5.93	119.39	110.50
1	g	15	PHE	CB-CG-CD2	5.92	124.95	120.80
3	L	130	PHE	CB-CG-CD2	-5.92	116.66	120.80
3	L	397	PHE	CB-CG-CD1	-5.92	116.66	120.80
1	C	26	TYR	CZ-CE2-CD2	-5.92	114.47	119.80
1	D	168	ARG	NE-CZ-NH2	-5.92	117.34	120.30
1	d	226	PRO	N-CA-CB	5.92	110.40	103.30
2	l	38	ALA	CB-CA-C	-5.92	101.23	110.10
1	c	234	GLU	OE1-CD-OE2	5.91	130.40	123.30
2	m	80	ARG	CB-CA-C	-5.91	98.57	110.40
3	J	391	ASP	CB-CG-OD2	-5.91	112.98	118.30
1	A	162	THR	CA-CB-CG2	5.90	120.66	112.40
1	E	15	PHE	CB-CG-CD1	-5.90	116.67	120.80
2	6	170	ARG	NE-CZ-NH1	-5.90	117.35	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	43	ARG	NE-CZ-NH1	5.90	123.25	120.30
1	b	65	GLU	CB-CG-CD	-5.90	98.28	114.20
2	2	188	VAL	CA-CB-CG2	5.90	119.75	110.90
1	C	190	VAL	CA-CB-CG1	5.90	119.74	110.90
1	c	50	ALA	N-CA-CB	5.89	118.35	110.10
2	3	146	THR	CA-CB-CG2	-5.89	104.15	112.40
1	D	148	TYR	CG-CD1-CE1	-5.89	116.59	121.30
1	d	93	ARG	NE-CZ-NH1	5.89	123.25	120.30
2	6	138	VAL	CA-CB-CG1	5.88	119.73	110.90
1	B	129	VAL	CB-CA-C	5.88	122.57	111.40
1	G	232	TYR	CB-CG-CD1	-5.87	117.47	121.00
2	i	56	THR	CA-CB-CG2	-5.87	104.18	112.40
1	f	213	TYR	CD1-CE1-CZ	-5.87	114.52	119.80
3	L	397	PHE	CB-CG-CD2	5.87	124.91	120.80
1	C	104	ASP	N-CA-CB	5.87	121.16	110.60
1	d	91	ARG	NE-CZ-NH2	5.87	123.23	120.30
1	G	26	TYR	CG-CD1-CE1	-5.87	116.61	121.30
2	l	154	ARG	NE-CZ-NH2	5.86	123.23	120.30
1	g	141	VAL	N-CA-C	-5.86	95.18	111.00
2	n	184	ASP	CB-CG-OD1	-5.86	113.03	118.30
3	H	117	ASN	N-CA-CB	5.86	121.15	110.60
3	I	244	ASP	CB-CG-OD2	-5.86	113.03	118.30
1	f	148	TYR	CG-CD1-CE1	-5.86	116.61	121.30
2	k	81	ARG	NE-CZ-NH1	5.86	123.23	120.30
3	L	180	LEU	N-CA-CB	5.86	122.11	110.40
1	a	22	PHE	CB-CG-CD1	-5.85	116.70	120.80
1	c	241	ARG	NE-CZ-NH1	-5.85	117.38	120.30
1	d	213	TYR	CG-CD2-CE2	-5.85	116.62	121.30
3	H	334	VAL	CA-CB-CG1	5.85	119.67	110.90
3	K	258	ASP	CB-CG-OD1	5.84	123.56	118.30
2	i	196	PHE	CB-CG-CD1	-5.83	116.72	120.80
2	m	140	THR	CA-CB-CG2	-5.83	104.23	112.40
3	H	282	LYS	N-CA-CB	5.83	121.10	110.60
1	C	64	ILE	N-CA-C	-5.83	95.26	111.00
3	M	76	ARG	NE-CZ-NH2	-5.83	117.39	120.30
3	M	77	VAL	N-CA-C	-5.83	95.26	111.00
2	l	88	ARG	NE-CZ-NH2	-5.83	117.39	120.30
3	K	29	ARG	NE-CZ-NH2	5.83	123.21	120.30
1	A	185	PHE	CB-CG-CD1	5.83	124.88	120.80
1	a	174	PHE	CB-CG-CD1	-5.83	116.72	120.80
2	k	21	ASP	CB-CG-OD1	5.83	123.54	118.30
2	j	36	PHE	CB-CG-CD1	-5.82	116.72	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	242	GLU	N-CA-CB	5.82	121.07	110.60
1	e	68	TYR	CB-CG-CD2	5.82	124.49	121.00
3	I	212	VAL	CA-CB-CG2	5.82	119.63	110.90
3	K	349	ALA	N-CA-CB	5.82	118.25	110.10
2	i	187	ASP	CB-CG-OD2	5.82	123.53	118.30
1	b	179	TYR	CB-CG-CD2	-5.81	117.51	121.00
1	b	212	GLY	N-CA-C	-5.81	98.57	113.10
2	7	30	ARG	NE-CZ-NH1	5.81	123.21	120.30
2	n	179	ASP	CB-CG-OD1	5.81	123.53	118.30
3	J	105	ARG	NE-CZ-NH1	5.81	123.21	120.30
2	m	81	ARG	NE-CZ-NH1	5.81	123.20	120.30
1	f	26	TYR	CB-CG-CD2	-5.81	117.52	121.00
1	c	22	PHE	CG-CD2-CE2	-5.80	114.41	120.80
2	2	77	TYR	CB-CG-CD1	-5.80	117.52	121.00
2	2	212	ARG	NE-CZ-NH1	5.80	123.20	120.30
2	1	155	PHE	CB-CG-CD2	-5.80	116.74	120.80
3	J	120	PRO	N-CA-CB	5.80	110.26	103.30
3	I	44	TYR	CZ-CE2-CD2	5.80	125.02	119.80
1	g	212	GLY	N-CA-C	-5.79	98.61	113.10
3	H	94	TYR	CZ-CE2-CD2	-5.79	114.58	119.80
1	f	161	ALA	N-CA-CB	5.79	118.21	110.10
2	7	154	ARG	NE-CZ-NH1	-5.79	117.40	120.30
2	h	196	PHE	N-CA-C	-5.79	95.37	111.00
2	6	31	ALA	N-CA-CB	5.79	118.20	110.10
3	L	336	PHE	CB-CG-CD1	-5.79	116.75	120.80
1	G	68	TYR	CB-CG-CD2	5.79	124.47	121.00
2	j	62	ASP	CB-CG-OD2	5.79	123.51	118.30
3	I	374	ASP	CB-CG-OD1	5.78	123.50	118.30
1	a	33	ARG	NE-CZ-NH2	5.78	123.19	120.30
2	k	106	TYR	CG-CD2-CE2	-5.78	116.68	121.30
1	e	130	ARG	NE-CZ-NH1	5.77	123.19	120.30
3	K	321	PHE	N-CA-CB	5.77	120.99	110.60
1	B	119	PHE	CB-CG-CD2	-5.77	116.76	120.80
1	A	68	TYR	CD1-CE1-CZ	5.77	124.99	119.80
3	M	27	TYR	CB-CA-C	-5.77	98.86	110.40
1	C	53	ARG	NE-CZ-NH1	-5.76	117.42	120.30
2	l	165	VAL	CA-CB-CG1	5.76	119.55	110.90
2	6	65	PHE	CB-CG-CD2	-5.76	116.77	120.80
2	6	139	ALA	C-N-CA	5.76	136.11	121.70
2	k	183	GLY	N-CA-C	-5.76	98.69	113.10
3	M	29	ARG	NE-CZ-NH2	-5.76	117.42	120.30
1	B	213	TYR	CG-CD1-CE1	-5.76	116.69	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	b	86	ARG	NH1-CZ-NH2	-5.75	113.07	119.40
3	K	49	ARG	NE-CZ-NH1	5.75	123.18	120.30
1	B	123	TYR	CZ-CE2-CD2	-5.75	114.62	119.80
1	a	241	ARG	NE-CZ-NH2	5.75	123.17	120.30
3	L	324	HIS	CA-CB-CG	-5.75	103.83	113.60
1	F	187	ASP	CB-CG-OD2	-5.75	113.13	118.30
3	I	304	ASP	N-CA-CB	5.75	120.94	110.60
1	F	125	GLN	CG-CD-OE1	5.74	133.09	121.60
1	f	148	TYR	CD1-CG-CD2	5.74	124.22	117.90
3	H	265	MET	CG-SD-CE	-5.74	91.01	100.20
3	H	289	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	f	100	ARG	NE-CZ-NH2	-5.74	117.43	120.30
1	G	28	ARG	NE-CZ-NH2	5.74	123.17	120.30
2	h	101	TYR	CB-CG-CD2	-5.74	117.56	121.00
2	6	50	ASP	CB-CG-OD1	5.73	123.46	118.30
1	B	18	ASP	CB-CA-C	-5.73	98.94	110.40
1	g	142	ASP	CB-CG-OD2	-5.73	113.14	118.30
1	c	185	PHE	CB-CG-CD1	-5.73	116.79	120.80
1	f	119	PHE	CB-CG-CD1	5.73	124.81	120.80
1	c	126	TYR	CB-CG-CD2	5.72	124.44	121.00
2	n	106	TYR	CB-CG-CD1	-5.72	117.57	121.00
1	C	20	ARG	NE-CZ-NH1	5.72	123.16	120.30
2	2	65	PHE	CB-CG-CD1	-5.72	116.80	120.80
2	7	65	PHE	CG-CD1-CE1	5.72	127.10	120.80
3	K	36	PHE	CZ-CE2-CD2	5.72	126.97	120.10
3	J	20	TYR	CB-CG-CD1	-5.72	117.57	121.00
3	J	174	PRO	N-CA-CB	5.72	110.16	103.30
2	j	197	TYR	CZ-CE2-CD2	-5.71	114.66	119.80
1	A	159	TYR	CD1-CE1-CZ	5.71	124.94	119.80
1	F	179	TYR	CB-CG-CD2	-5.71	117.58	121.00
2	3	104	PHE	CB-CG-CD2	5.71	124.80	120.80
3	I	387	THR	N-CA-CB	5.71	121.15	110.30
3	M	229	LEU	N-CA-CB	5.71	121.81	110.40
3	L	19	ASP	CB-CG-OD1	-5.71	113.16	118.30
1	d	126	TYR	CG-CD1-CE1	-5.71	116.74	121.30
1	a	51	ASP	CB-CG-OD1	5.70	123.43	118.30
1	C	11	ALA	N-CA-CB	5.70	118.08	110.10
1	g	86	ARG	NE-CZ-NH1	5.70	123.15	120.30
1	G	15	PHE	CB-CG-CD1	-5.70	116.81	120.80
1	g	145	PRO	N-CA-CB	5.70	110.14	103.30
1	a	84	ASP	CB-CG-OD1	-5.70	113.17	118.30
3	M	364	ARG	NE-CZ-NH1	-5.70	117.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	57	ARG	NE-CZ-NH2	-5.69	117.45	120.30
1	c	217	ASP	CB-CG-OD1	-5.69	113.18	118.30
1	C	67	ILE	N-CA-C	-5.68	95.65	111.00
1	f	232	TYR	CB-CG-CD1	-5.68	117.59	121.00
2	n	77	TYR	CD1-CG-CD2	-5.68	111.65	117.90
2	6	154	ARG	NE-CZ-NH2	5.68	123.14	120.30
2	3	41	ALA	N-CA-CB	5.68	118.05	110.10
1	E	144	VAL	CA-CB-CG1	-5.68	102.38	110.90
1	A	67	ILE	N-CA-C	-5.67	95.68	111.00
1	A	136	LEU	N-CA-CB	5.67	121.75	110.40
3	J	28	ARG	NE-CZ-NH1	5.67	123.14	120.30
2	l	123	TYR	CB-CG-CD2	5.67	124.40	121.00
3	J	391	ASP	CB-CG-OD1	5.67	123.40	118.30
1	F	168	ARG	NE-CZ-NH1	-5.67	117.47	120.30
3	I	273	ASP	CB-CG-OD1	5.67	123.40	118.30
2	1	36	PHE	CG-CD1-CE1	5.67	127.03	120.80
3	H	140	TYR	CG-CD1-CE1	5.66	125.83	121.30
3	H	317	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	n	139	ALA	N-CA-CB	5.66	118.02	110.10
2	l	184	ASP	N-CA-CB	5.66	120.78	110.60
3	L	170	VAL	CG1-CB-CG2	5.65	119.95	110.90
1	b	92	ALA	CB-CA-C	-5.65	101.62	110.10
1	E	99	ASN	N-CA-CB	-5.65	100.43	110.60
3	L	302	ARG	NE-CZ-NH2	5.65	123.12	120.30
2	1	204	VAL	CG1-CB-CG2	-5.65	101.86	110.90
2	5	104	PHE	CB-CG-CD2	-5.65	116.85	120.80
1	F	141	VAL	N-CA-C	-5.65	95.76	111.00
1	f	180	ARG	N-CA-CB	5.64	120.76	110.60
2	1	123	TYR	CB-CG-CD2	-5.64	117.61	121.00
3	H	205	ARG	NE-CZ-NH2	-5.64	117.48	120.30
1	E	241	ARG	NE-CZ-NH1	-5.64	117.48	120.30
2	7	116	ASP	CB-CG-OD2	5.64	123.38	118.30
1	g	232	TYR	CB-CG-CD2	5.63	124.38	121.00
1	A	141	VAL	CB-CA-C	-5.63	100.70	111.40
2	h	46	TYR	CG-CD1-CE1	-5.63	116.80	121.30
3	K	61	PRO	N-CA-C	5.63	126.74	112.10
1	b	13	THR	CA-CB-CG2	-5.63	104.52	112.40
1	b	40	ILE	N-CA-C	-5.63	95.80	111.00
2	k	197	TYR	CG-CD1-CE1	5.63	125.80	121.30
1	f	126	TYR	CB-CG-CD2	5.63	124.38	121.00
2	6	57	ALA	N-CA-CB	5.63	117.98	110.10
3	K	203	PHE	CB-CG-CD2	-5.62	116.86	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	J	248	ALA	N-CA-CB	5.62	117.97	110.10
2	3	153	ASP	CB-CG-OD1	5.62	123.36	118.30
2	n	60	VAL	CA-CB-CG2	-5.62	102.47	110.90
1	B	6	MET	CG-SD-CE	-5.62	91.21	100.20
2	h	36	PHE	CB-CG-CD1	-5.62	116.87	120.80
2	6	39	SER	N-CA-CB	5.62	118.92	110.50
1	E	203	GLU	OE1-CD-OE2	5.61	130.04	123.30
1	E	235	ARG	C-N-CA	5.61	135.72	121.70
3	L	233	LYS	N-CA-CB	5.60	120.69	110.60
2	2	173	TYR	CB-CG-CD1	5.60	124.36	121.00
2	6	188	VAL	CA-CB-CG2	-5.60	102.50	110.90
3	J	140	TYR	CG-CD2-CE2	-5.60	116.82	121.30
1	A	119	PHE	CB-CG-CD2	-5.60	116.88	120.80
3	M	280	ASP	N-CA-C	-5.60	95.88	111.00
3	I	190	LEU	CB-CG-CD1	5.60	120.52	111.00
1	a	148	TYR	CB-CG-CD2	-5.60	117.64	121.00
1	C	74	ILE	CA-CB-CG1	5.60	121.64	111.00
2	i	48	ILE	CA-CB-CG1	-5.60	100.36	111.00
3	J	336	PHE	CB-CG-CD2	-5.60	116.88	120.80
1	f	115	LYS	CB-CA-C	-5.59	99.21	110.40
3	L	27	TYR	CB-CG-CD1	-5.59	117.64	121.00
2	6	55	THR	CA-CB-CG2	-5.59	104.57	112.40
1	b	159	TYR	CB-CG-CD1	5.59	124.35	121.00
1	C	92	ALA	N-CA-CB	5.59	117.92	110.10
2	1	182	SER	N-CA-CB	5.59	118.88	110.50
1	E	190	VAL	CA-CB-CG1	5.58	119.28	110.90
1	E	142	ASP	N-CA-CB	5.58	120.65	110.60
2	k	107	LEU	CB-CG-CD2	-5.58	101.51	111.00
3	H	46	ARG	NE-CZ-NH1	-5.58	117.51	120.30
1	c	148	TYR	CB-CG-CD1	-5.58	117.65	121.00
2	1	182	SER	C-N-CA	5.58	134.02	122.30
2	6	176	MET	CG-SD-CE	5.58	109.13	100.20
3	K	227	PHE	CB-CG-CD2	5.58	124.71	120.80
1	e	235	ARG	NE-CZ-NH2	-5.58	117.51	120.30
1	E	103	TYR	CB-CG-CD1	5.58	124.35	121.00
3	M	364	ARG	NE-CZ-NH2	5.58	123.09	120.30
1	F	186	ASP	CB-CG-OD2	5.57	123.32	118.30
2	6	74	ALA	CB-CA-C	-5.57	101.75	110.10
3	M	207	VAL	O-C-N	-5.57	113.73	123.20
1	f	205	VAL	N-CA-C	-5.57	95.97	111.00
2	2	202	GLU	N-CA-CB	5.57	120.62	110.60
2	k	166	GLU	OE1-CD-OE2	5.57	129.98	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	6	179	ASP	CB-CG-OD1	-5.57	113.29	118.30
2	k	205	GLU	CA-CB-CG	5.57	125.64	113.40
3	H	139	SER	CB-CA-C	5.57	120.67	110.10
1	G	180	ARG	NE-CZ-NH2	-5.56	117.52	120.30
2	6	193	GLU	N-CA-CB	5.56	120.61	110.60
2	1	199	TYR	CG-CD2-CE2	5.56	125.75	121.30
2	7	155	PHE	CZ-CE2-CD2	5.56	126.77	120.10
3	L	250	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	B	159	TYR	CB-CG-CD1	-5.56	117.67	121.00
1	b	129	VAL	CB-CA-C	5.56	121.96	111.40
2	2	148	TYR	CB-CG-CD2	5.56	124.33	121.00
3	I	326	ARG	NE-CZ-NH1	-5.56	117.52	120.30
1	E	18	ASP	CB-CG-OD1	5.55	123.30	118.30
2	6	83	ARG	NE-CZ-NH2	5.55	123.08	120.30
1	E	119	PHE	CB-CG-CD2	-5.55	116.92	120.80
2	3	28	GLU	N-CA-CB	5.55	120.58	110.60
2	2	179	ASP	N-CA-CB	5.54	120.58	110.60
3	I	142	ASP	N-CA-CB	5.54	120.58	110.60
2	l	28	GLU	OE1-CD-OE2	5.54	129.95	123.30
2	m	101	TYR	CB-CG-CD1	5.54	124.33	121.00
2	7	41	ALA	CB-CA-C	-5.54	101.79	110.10
1	F	148	TYR	CB-CG-CD1	-5.54	117.68	121.00
1	b	53	ARG	NH1-CZ-NH2	-5.54	113.31	119.40
3	I	283	VAL	CA-CB-CG1	-5.54	102.59	110.90
3	I	350	ASP	CB-CG-OD1	5.54	123.28	118.30
1	G	219	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	h	176	MET	CG-SD-CE	-5.54	91.34	100.20
1	g	159	TYR	CB-CG-CD1	5.53	124.32	121.00
1	b	103	TYR	CZ-CE2-CD2	-5.53	114.82	119.80
3	H	275	PHE	CZ-CE2-CD2	-5.53	113.46	120.10
3	K	302	ARG	NE-CZ-NH2	-5.53	117.53	120.30
3	M	76	ARG	NE-CZ-NH1	5.53	123.06	120.30
1	B	157	LEU	N-CA-CB	5.53	121.46	110.40
1	d	104	ASP	N-CA-CB	5.53	120.55	110.60
2	n	117	SER	N-CA-CB	5.53	118.79	110.50
1	b	213	TYR	N-CA-CB	5.53	120.55	110.60
3	I	257	GLY	C-N-CA	5.53	135.51	121.70
3	M	387	THR	CA-C-N	5.53	132.57	117.10
2	1	104	PHE	CB-CA-C	-5.52	99.35	110.40
2	4	81	ARG	NE-CZ-NH2	-5.52	117.54	120.30
3	L	247	ALA	N-CA-CB	5.52	117.82	110.10
3	J	286	ALA	N-CA-CB	5.52	117.83	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	C	213	TYR	CB-CG-CD2	-5.52	117.69	121.00
1	d	143	GLU	N-CA-C	-5.52	96.11	111.00
3	H	245	ALA	N-CA-CB	5.52	117.82	110.10
1	B	10	ARG	NE-CZ-NH1	-5.51	117.54	120.30
2	l	123	TYR	CB-CG-CD1	-5.51	117.69	121.00
1	c	136	LEU	N-CA-CB	5.51	121.42	110.40
1	f	135	SER	N-CA-CB	5.51	118.77	110.50
2	j	77	TYR	CG-CD2-CE2	-5.51	116.89	121.30
2	5	52	MET	CG-SD-CE	5.51	109.02	100.20
2	l	212	ARG	NE-CZ-NH1	5.51	123.06	120.30
2	j	88	ARG	NE-CZ-NH1	-5.51	117.55	120.30
1	d	159	TYR	CD1-CE1-CZ	-5.51	114.84	119.80
3	L	317	ARG	NE-CZ-NH1	5.51	123.05	120.30
1	A	91	ARG	NE-CZ-NH2	5.50	123.05	120.30
1	B	8	TYR	CB-CG-CD1	-5.50	117.70	121.00
3	J	321	PHE	CB-CG-CD1	5.50	124.65	120.80
1	A	223	GLU	CA-CB-CG	5.50	125.50	113.40
2	k	106	TYR	CB-CG-CD2	-5.50	117.70	121.00
1	B	28	ARG	CD-NE-CZ	-5.50	115.90	123.60
1	D	60	GLU	N-CA-CB	5.50	120.50	110.60
1	c	22	PHE	CZ-CE2-CD2	5.49	126.69	120.10
1	d	61	ALA	N-CA-CB	5.49	117.78	110.10
2	3	175	ALA	N-CA-CB	5.48	117.78	110.10
3	I	132	VAL	N-CA-C	-5.48	96.20	111.00
3	L	29	ARG	CB-CA-C	-5.48	99.44	110.40
2	k	57	ALA	CB-CA-C	-5.48	101.88	110.10
3	L	41	ARG	NE-CZ-NH2	-5.48	117.56	120.30
1	A	130	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	C	203	GLU	C-N-CA	5.47	135.39	121.70
1	B	63	THR	C-N-CA	5.47	135.37	121.70
1	e	219	ARG	N-CA-CB	5.47	120.44	110.60
3	J	225	GLU	N-CA-CB	5.47	120.44	110.60
3	K	211	PHE	CB-CG-CD2	-5.46	116.97	120.80
3	L	104	ALA	N-CA-CB	5.46	117.75	110.10
2	h	139	ALA	C-N-CA	5.46	135.35	121.70
3	I	266	MET	CG-SD-CE	-5.46	91.46	100.20
3	K	364	ARG	NE-CZ-NH2	-5.46	117.57	120.30
1	d	151	ASP	CB-CG-OD1	-5.46	113.39	118.30
2	5	196	PHE	CB-CG-CD1	-5.46	116.98	120.80
2	m	81	ARG	NE-CZ-NH2	-5.46	117.57	120.30
2	n	184	ASP	N-CA-CB	5.45	120.42	110.60
2	1	148	TYR	CB-CG-CD1	5.45	124.27	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	101	TYR	CD1-CE1-CZ	-5.45	114.89	119.80
1	G	10	ARG	NH1-CZ-NH2	5.45	125.39	119.40
3	L	44	TYR	CB-CG-CD2	5.45	124.27	121.00
3	J	81	SER	CB-CA-C	5.45	120.45	110.10
1	F	130	ARG	NH1-CZ-NH2	5.45	125.39	119.40
3	L	291	ASP	CB-CA-C	-5.45	99.51	110.40
2	n	38	ALA	N-CA-CB	5.44	117.72	110.10
2	j	51	ARG	NE-CZ-NH1	-5.44	117.58	120.30
2	4	155	PHE	CB-CG-CD2	5.44	124.61	120.80
2	k	123	TYR	CB-CG-CD2	5.44	124.27	121.00
1	C	232	TYR	CG-CD1-CE1	5.44	125.65	121.30
2	m	104	PHE	CB-CG-CD1	-5.44	116.99	120.80
2	n	118	GLU	N-CA-CB	5.44	120.39	110.60
1	f	20	ARG	NE-CZ-NH1	-5.44	117.58	120.30
1	C	67	ILE	N-CA-CB	5.44	123.30	110.80
2	m	113	GLY	N-CA-C	-5.43	99.51	113.10
3	K	17	GLU	OE1-CD-OE2	5.43	129.82	123.30
1	g	100	ARG	CD-NE-CZ	-5.43	115.99	123.60
2	5	17	LEU	N-CA-CB	5.43	121.27	110.40
1	g	198	LEU	CB-CG-CD2	5.43	120.23	111.00
3	I	59	ARG	CA-CB-CG	5.43	125.35	113.40
1	b	141	VAL	N-CA-C	-5.43	96.34	111.00
1	e	100	ARG	CD-NE-CZ	-5.43	116.00	123.60
1	e	33	ARG	NE-CZ-NH1	-5.42	117.59	120.30
1	f	212	GLY	N-CA-C	-5.42	99.55	113.10
2	j	155	PHE	N-CA-CB	5.42	120.36	110.60
2	m	153	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	e	100	ARG	NE-CZ-NH1	-5.42	117.59	120.30
3	L	204	ILE	N-CA-C	-5.42	96.37	111.00
1	G	229	LEU	CB-CG-CD1	5.42	120.21	111.00
1	g	245	LYS	CB-CA-C	-5.42	99.57	110.40
1	b	214	VAL	N-CA-C	-5.41	96.39	111.00
2	6	150	VAL	CA-CB-CG1	5.41	119.02	110.90
3	L	74	ASP	CB-CG-OD1	-5.41	113.43	118.30
3	L	91	THR	CA-CB-CG2	5.41	119.97	112.40
1	e	74	ILE	N-CA-C	-5.41	96.40	111.00
1	G	163	ALA	N-CA-CB	5.41	117.67	110.10
2	3	170	ARG	NE-CZ-NH2	5.41	123.00	120.30
3	K	186	THR	CA-CB-CG2	5.41	119.97	112.40
2	k	56	THR	CA-CB-CG2	-5.41	104.83	112.40
1	C	161	ALA	N-CA-CB	5.40	117.66	110.10
1	b	145	PRO	O-C-N	-5.40	114.06	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	L	53	SER	N-CA-CB	5.40	118.60	110.50
3	H	350	ASP	CB-CG-OD1	5.40	123.16	118.30
3	I	168	ALA	CB-CA-C	-5.40	102.01	110.10
2	2	30	ARG	N-CA-CB	5.39	120.31	110.60
2	l	134	GLU	N-CA-CB	5.39	120.31	110.60
3	M	87	PHE	CD1-CE1-CZ	-5.39	113.63	120.10
1	d	175	PHE	N-CA-CB	5.39	120.30	110.60
2	7	171	ALA	CB-CA-C	-5.39	102.02	110.10
3	M	119	LEU	O-C-N	-5.39	110.86	121.10
1	E	80	GLY	N-CA-C	-5.39	99.63	113.10
2	j	162	ASP	CB-CG-OD1	5.39	123.15	118.30
1	d	113	ALA	N-CA-CB	5.38	117.64	110.10
1	F	217	ASP	N-CA-CB	5.38	120.29	110.60
2	1	141	GLY	N-CA-C	-5.38	99.64	113.10
1	a	27	ALA	N-CA-CB	5.38	117.64	110.10
1	B	68	TYR	CG-CD1-CE1	-5.38	116.99	121.30
1	f	67	ILE	N-CA-C	-5.38	96.47	111.00
1	d	20	ARG	NE-CZ-NH2	-5.38	117.61	120.30
1	d	130	ARG	NE-CZ-NH1	5.38	122.99	120.30
2	i	170	ARG	NE-CZ-NH1	5.38	122.99	120.30
3	L	50	ARG	N-CA-CB	5.38	120.29	110.60
1	B	174	PHE	CB-CG-CD2	-5.38	117.03	120.80
2	k	23	VAL	CA-CB-CG1	5.38	118.97	110.90
2	4	64	GLN	O-C-N	5.38	131.31	122.70
2	4	101	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	a	68	TYR	CB-CG-CD2	-5.38	117.77	121.00
1	a	211	VAL	CG1-CB-CG2	-5.38	102.30	110.90
2	4	23	VAL	N-CA-C	-5.38	96.48	111.00
2	k	89	ALA	N-CA-CB	5.38	117.63	110.10
1	b	130	ARG	NE-CZ-NH2	5.38	122.99	120.30
2	j	87	VAL	CA-CB-CG1	5.38	118.96	110.90
2	3	94	THR	CA-CB-CG2	-5.37	104.88	112.40
2	k	194	ASP	CB-CA-C	-5.37	99.66	110.40
1	c	88	LEU	CB-CG-CD1	5.37	120.13	111.00
3	I	255	THR	O-C-N	-5.37	114.11	122.70
2	1	68	ARG	NE-CZ-NH1	-5.37	117.62	120.30
2	7	176	MET	N-CA-CB	5.36	120.25	110.60
3	K	305	ARG	NE-CZ-NH1	5.36	122.98	120.30
3	L	282	LYS	N-CA-CB	5.36	120.25	110.60
2	5	136	ASP	N-CA-C	5.36	125.48	111.00
3	J	387	THR	N-CA-CB	5.36	120.49	110.30
2	7	196	PHE	CZ-CE2-CD2	-5.36	113.67	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	I	196	ALA	CB-CA-C	-5.36	102.06	110.10
2	k	104	PHE	N-CA-C	-5.36	96.53	111.00
3	H	212	VAL	CA-CB-CG2	5.36	118.94	110.90
3	H	343	THR	CA-CB-CG2	-5.36	104.90	112.40
1	C	190	VAL	CA-CB-CG2	-5.36	102.87	110.90
1	D	148	TYR	CD1-CE1-CZ	5.36	124.62	119.80
2	n	140	THR	CA-CB-CG2	-5.36	104.90	112.40
3	L	150	ILE	O-C-N	-5.36	114.13	122.70
3	M	21	TYR	CB-CG-CD1	5.36	124.21	121.00
3	M	337	LYS	N-CA-CB	5.36	120.24	110.60
2	4	35	ASN	N-CA-CB	5.35	120.23	110.60
1	E	8	TYR	CZ-CE2-CD2	-5.35	114.98	119.80
1	a	53	ARG	NE-CZ-NH1	-5.35	117.63	120.30
1	g	185	PHE	CB-CG-CD1	5.35	124.55	120.80
2	1	39	SER	CB-CA-C	-5.35	99.94	110.10
2	k	154	ARG	NE-CZ-NH1	5.35	122.97	120.30
1	b	123	TYR	CG-CD2-CE2	-5.35	117.02	121.30
2	3	123	TYR	CG-CD1-CE1	5.35	125.58	121.30
2	k	103	TYR	CB-CG-CD1	-5.35	117.79	121.00
3	L	300	PRO	N-CA-CB	5.35	109.72	103.30
1	c	159	TYR	CB-CG-CD1	5.34	124.21	121.00
2	4	103	TYR	CZ-CE2-CD2	5.34	124.61	119.80
1	f	112	LEU	CB-CG-CD1	5.34	120.08	111.00
2	m	116	ASP	CB-CG-OD2	-5.34	113.49	118.30
1	b	142	ASP	CB-CG-OD1	-5.34	113.49	118.30
2	1	80	ARG	CD-NE-CZ	-5.34	116.12	123.60
3	I	86	LYS	N-CA-CB	5.34	120.21	110.60
1	D	126	TYR	N-CA-CB	5.34	120.21	110.60
1	B	37	ALA	N-CA-CB	5.34	117.57	110.10
2	3	41	ALA	CB-CA-C	-5.33	102.10	110.10
2	m	49	ALA	N-CA-C	-5.33	96.60	111.00
1	c	104	ASP	CB-CG-OD2	-5.33	113.50	118.30
2	6	173	TYR	CB-CG-CD2	5.33	124.20	121.00
3	L	181	TYR	CA-CB-CG	5.33	123.52	113.40
1	F	84	ASP	CB-CG-OD2	-5.33	113.51	118.30
2	n	77	TYR	CG-CD1-CE1	5.33	125.56	121.30
1	e	28	ARG	NE-CZ-NH1	-5.32	117.64	120.30
2	m	36	PHE	N-CA-C	-5.32	96.62	111.00
1	D	181	ASP	CB-CG-OD2	-5.32	113.51	118.30
1	d	79	SER	CB-CA-C	-5.32	99.99	110.10
2	2	136	ASP	CB-CG-OD1	-5.32	113.51	118.30
2	k	116	ASP	CB-CG-OD1	-5.32	113.51	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	68	TYR	CA-CB-CG	-5.32	103.30	113.40
3	I	211	PHE	CA-CB-CG	-5.32	101.14	113.90
1	D	160	LYS	O-C-N	5.32	131.21	122.70
1	G	180	ARG	NE-CZ-NH1	5.31	122.96	120.30
2	j	63	ALA	N-CA-CB	5.31	117.54	110.10
3	H	152	GLU	CG-CD-OE1	5.31	128.93	118.30
3	K	205	ARG	NE-CZ-NH1	5.31	122.96	120.30
1	F	54	VAL	O-C-N	-5.31	114.17	123.20
1	D	94	ILE	O-C-N	-5.31	114.21	122.70
1	d	51	ASP	CB-CG-OD1	5.31	123.08	118.30
2	7	189	VAL	CA-C-N	-5.31	105.53	117.20
3	H	167	PHE	CB-CG-CD1	-5.31	117.08	120.80
3	M	289	ARG	CD-NE-CZ	-5.31	116.17	123.60
2	2	55	THR	N-CA-C	-5.30	96.69	111.00
2	3	28	GLU	N-CA-C	-5.30	96.69	111.00
3	M	398	VAL	CA-C-O	-5.30	108.97	120.10
1	E	205	VAL	CA-CB-CG1	-5.30	102.95	110.90
1	G	212	GLY	N-CA-C	-5.30	99.85	113.10
2	k	192	THR	CA-CB-CG2	5.30	119.82	112.40
3	K	52	ARG	CD-NE-CZ	-5.30	116.18	123.60
1	f	193	LEU	CB-CG-CD1	5.30	120.01	111.00
3	K	398	VAL	CA-C-O	-5.30	108.98	120.10
1	f	28	ARG	NE-CZ-NH2	5.29	122.95	120.30
3	I	16	LEU	C-N-CA	5.29	134.94	121.70
2	4	46	TYR	N-CA-CB	5.29	120.13	110.60
3	L	398	VAL	CA-C-O	-5.29	108.98	120.10
3	I	350	ASP	CB-CG-OD2	-5.29	113.54	118.30
3	K	76	ARG	NE-CZ-NH2	-5.29	117.66	120.30
3	J	398	VAL	CA-C-O	-5.29	108.99	120.10
1	D	28	ARG	NH1-CZ-NH2	5.29	125.22	119.40
1	a	31	VAL	CA-CB-CG1	-5.29	102.97	110.90
1	f	137	LEU	N-CA-CB	5.29	120.97	110.40
2	1	88	ARG	NE-CZ-NH2	5.29	122.94	120.30
2	i	199	TYR	CB-CG-CD2	5.29	124.17	121.00
3	H	398	VAL	CA-C-O	-5.29	109.00	120.10
1	G	219	ARG	N-CA-CB	5.28	120.11	110.60
2	6	191	ILE	N-CA-C	-5.28	96.73	111.00
3	L	247	ALA	CB-CA-C	-5.28	102.17	110.10
2	l	198	GLN	N-CA-C	-5.28	96.74	111.00
3	H	258	ASP	CB-CG-OD2	5.28	123.05	118.30
1	C	8	TYR	CB-CG-CD1	5.28	124.17	121.00
1	c	161	ALA	N-CA-CB	5.28	117.49	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	3	207	ILE	CA-CB-CG1	-5.28	100.97	111.00
3	M	355	CYS	CA-CB-SG	-5.28	104.50	114.00
2	5	56	THR	CA-CB-CG2	-5.28	105.01	112.40
2	5	78	GLU	OE1-CD-OE2	-5.28	116.97	123.30
3	I	398	VAL	CA-C-O	-5.28	109.02	120.10
3	J	314	PHE	CB-CG-CD2	-5.28	117.11	120.80
1	a	191	LEU	CB-CG-CD1	5.27	119.96	111.00
1	b	130	ARG	N-CA-CB	5.27	120.09	110.60
2	2	155	PHE	CB-CG-CD1	5.27	124.49	120.80
2	6	139	ALA	N-CA-C	-5.27	96.77	111.00
3	I	156	ALA	N-CA-CB	5.27	117.48	110.10
3	M	202	THR	N-CA-CB	5.27	120.32	110.30
1	F	68	TYR	CB-CG-CD2	5.27	124.16	121.00
1	f	39	GLY	N-CA-C	-5.27	99.93	113.10
3	H	19	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	A	190	VAL	CG1-CB-CG2	-5.27	102.47	110.90
1	C	62	ASP	CB-CG-OD2	-5.27	113.56	118.30
1	D	180	ARG	NE-CZ-NH1	-5.27	117.67	120.30
1	g	235	ARG	NE-CZ-NH2	5.27	122.93	120.30
2	5	199	TYR	CB-CG-CD1	5.27	124.16	121.00
2	i	102	ARG	NE-CZ-NH1	-5.26	117.67	120.30
3	H	126	MET	CG-SD-CE	-5.26	91.78	100.20
1	b	21	LEU	CB-CG-CD2	-5.26	102.05	111.00
1	C	37	ALA	N-CA-C	-5.26	96.79	111.00
2	3	88	ARG	CD-NE-CZ	5.26	130.97	123.60
3	H	181	TYR	CB-CG-CD1	-5.26	117.84	121.00
3	L	383	LEU	CB-CG-CD1	5.26	119.95	111.00
1	b	165	GLY	N-CA-C	-5.26	99.95	113.10
1	a	159	TYR	CB-CG-CD2	-5.26	117.85	121.00
1	B	65	GLU	N-CA-CB	5.26	120.06	110.60
2	6	140	THR	N-CA-CB	5.26	120.29	110.30
2	k	81	ARG	CD-NE-CZ	-5.25	116.24	123.60
1	a	119	PHE	CB-CG-CD1	-5.25	117.12	120.80
1	e	159	TYR	CA-CB-CG	-5.25	103.42	113.40
2	1	18	VAL	CA-CB-CG1	5.25	118.78	110.90
2	l	103	TYR	CB-CG-CD1	5.25	124.15	121.00
2	7	156	THR	N-CA-C	-5.25	96.83	111.00
2	3	193	GLU	N-CA-CB	5.25	120.05	110.60
3	H	386	THR	C-N-CA	5.25	134.82	121.70
1	G	181	ASP	CB-CG-OD2	-5.24	113.58	118.30
2	m	68	ARG	CB-CA-C	-5.24	99.91	110.40
2	1	35	ASN	N-CA-CB	5.24	120.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	j	158	GLU	CB-CG-CD	-5.24	100.05	114.20
2	l	173	TYR	CB-CG-CD2	-5.24	117.86	121.00
2	n	30	ARG	N-CA-CB	5.24	120.03	110.60
1	D	53	ARG	NE-CZ-NH2	-5.24	117.68	120.30
2	k	105	PRO	N-CA-CB	5.24	109.59	103.30
2	5	169	VAL	CA-CB-CG2	-5.24	103.04	110.90
1	g	225	SER	CA-C-O	-5.24	109.10	120.10
2	j	81	ARG	CD-NE-CZ	-5.24	116.27	123.60
1	F	12	ILE	CA-CB-CG1	5.24	120.95	111.00
2	j	63	ALA	CB-CA-C	-5.24	102.25	110.10
2	l	50	ASP	N-CA-CB	5.24	120.03	110.60
3	M	84	GLY	CA-C-O	-5.24	111.17	120.60
1	B	123	TYR	CB-CG-CD1	-5.23	117.86	121.00
2	3	21	ASP	CB-CG-OD2	5.23	123.01	118.30
2	6	66	LEU	CB-CG-CD2	5.23	119.90	111.00
3	J	118	VAL	N-CA-C	-5.23	96.87	111.00
1	b	17	PRO	O-C-N	5.23	131.07	122.70
1	E	195	ALA	CB-CA-C	-5.23	102.25	110.10
2	n	186	ILE	N-CA-C	-5.23	96.88	111.00
3	K	397	PHE	N-CA-CB	5.23	120.01	110.60
2	l	156	THR	N-CA-C	-5.23	96.88	111.00
1	C	149	GLU	N-CA-C	-5.23	96.89	111.00
1	A	30	ALA	CB-CA-C	-5.22	102.26	110.10
2	j	187	ASP	CB-CG-OD1	5.22	123.00	118.30
2	6	77	TYR	CD1-CG-CD2	-5.22	112.15	117.90
2	m	19	CYS	N-CA-CB	5.22	120.00	110.60
2	n	178	ARG	CD-NE-CZ	-5.22	116.29	123.60
3	K	349	ALA	CB-CA-C	-5.22	102.27	110.10
2	j	213	LYS	N-CA-CB	5.22	120.00	110.60
2	i	31	ALA	CB-CA-C	5.22	117.93	110.10
2	3	17	LEU	CB-CG-CD2	5.22	119.87	111.00
3	L	259	ARG	O-C-N	5.22	131.05	122.70
1	D	166	MET	CG-SD-CE	5.22	108.55	100.20
1	A	196	MET	CG-SD-CE	-5.22	91.85	100.20
2	7	173	TYR	CB-CG-CD2	-5.21	117.87	121.00
1	e	123	TYR	CB-CG-CD1	5.21	124.13	121.00
1	d	37	ALA	O-C-N	5.21	131.04	122.70
1	F	126	TYR	CB-CG-CD1	5.21	124.13	121.00
3	H	29	ARG	CD-NE-CZ	-5.21	116.31	123.60
3	H	362	ALA	CB-CA-C	5.21	117.92	110.10
3	J	386	THR	N-CA-CB	5.21	120.20	110.30
2	4	39	SER	N-CA-CB	5.21	118.31	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	K	104	ALA	N-CA-CB	5.21	117.39	110.10
3	L	250	ARG	NE-CZ-NH1	5.21	122.91	120.30
1	c	163	ALA	CB-CA-C	-5.21	102.29	110.10
2	1	77	TYR	CB-CG-CD1	-5.21	117.88	121.00
2	5	170	ARG	CD-NE-CZ	5.21	130.89	123.60
1	g	59	LEU	CB-CG-CD1	5.20	119.85	111.00
2	j	80	ARG	NE-CZ-NH2	-5.20	117.70	120.30
3	M	368	ALA	CB-CA-C	5.20	117.90	110.10
1	f	119	PHE	CG-CD2-CE2	5.20	126.52	120.80
1	g	137	LEU	CB-CA-C	-5.20	100.32	110.20
1	A	42	CYS	N-CA-C	-5.20	96.97	111.00
2	i	155	PHE	CB-CG-CD1	-5.20	117.16	120.80
1	D	177	LYS	CB-CA-C	-5.20	100.01	110.40
2	h	172	ILE	O-C-N	-5.20	114.39	122.70
2	k	41	ALA	CB-CA-C	-5.20	102.31	110.10
1	c	168	ARG	NE-CZ-NH1	-5.19	117.70	120.30
2	m	208	LEU	N-CA-CB	5.19	120.79	110.40
3	J	105	ARG	N-CA-CB	5.19	119.95	110.60
1	C	141	VAL	N-CA-C	-5.19	96.98	111.00
1	d	73	HIS	CA-CB-CG	5.19	122.43	113.60
2	h	49	ALA	O-C-N	-5.19	114.39	122.70
1	e	123	TYR	CD1-CE1-CZ	5.19	124.47	119.80
3	H	387	THR	CA-CB-CG2	-5.19	105.13	112.40
1	A	183	LEU	CB-CA-C	-5.19	100.34	110.20
1	E	186	ASP	CB-CG-OD2	5.19	122.97	118.30
2	2	101	TYR	CD1-CE1-CZ	5.18	124.47	119.80
2	6	123	TYR	CD1-CG-CD2	5.18	123.60	117.90
2	1	156	THR	N-CA-CB	5.18	120.15	110.30
3	L	221	ARG	CD-NE-CZ	-5.18	116.35	123.60
1	B	77	ALA	N-CA-CB	5.18	117.35	110.10
1	g	174	PHE	O-C-N	-5.18	114.41	122.70
1	E	159	TYR	CG-CD1-CE1	-5.18	117.16	121.30
3	K	194	ALA	CB-CA-C	-5.18	102.33	110.10
2	h	33	MET	N-CA-C	-5.18	97.02	111.00
3	L	21	TYR	CG-CD1-CE1	5.18	125.44	121.30
1	D	151	ASP	CA-CB-CG	-5.17	102.02	113.40
1	F	196	MET	O-C-N	-5.17	114.41	123.20
1	f	179	TYR	N-CA-CB	5.17	119.91	110.60
1	g	144	VAL	CB-CA-C	-5.17	101.57	111.40
2	m	156	THR	CA-CB-OG1	5.17	119.86	109.00
1	c	103	TYR	CB-CG-CD1	-5.17	117.90	121.00
2	h	88	ARG	NE-CZ-NH1	-5.17	117.71	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	k	106	TYR	N-CA-C	-5.17	97.04	111.00
1	C	218	ASP	CA-CB-CG	-5.17	102.03	113.40
2	l	90	ILE	O-C-N	-5.17	114.43	122.70
3	K	331	ALA	N-CA-CB	5.17	117.33	110.10
1	e	64	ILE	N-CA-C	-5.17	97.05	111.00
3	I	90	ASN	C-N-CA	5.17	134.62	121.70
3	I	224	ARG	N-CA-CB	5.17	119.90	110.60
3	K	397	PHE	CB-CG-CD2	5.17	124.42	120.80
1	e	100	ARG	NE-CZ-NH2	5.16	122.88	120.30
3	K	356	THR	N-CA-CB	5.16	120.11	110.30
2	m	33	MET	N-CA-C	-5.16	97.06	111.00
3	L	52	ARG	NE-CZ-NH2	5.16	122.88	120.30
3	M	77	VAL	CA-CB-CG2	-5.16	103.16	110.90
1	C	46	VAL	CG1-CB-CG2	5.16	119.15	110.90
2	k	189	VAL	O-C-N	-5.16	114.45	122.70
2	5	212	ARG	NE-CZ-NH2	-5.16	117.72	120.30
1	F	185	PHE	CB-CG-CD2	-5.15	117.19	120.80
1	f	145	PRO	O-C-N	5.15	130.94	122.70
1	G	187	ASP	CB-CG-OD2	-5.15	113.66	118.30
2	2	136	ASP	CB-CG-OD2	5.15	122.94	118.30
1	d	28	ARG	NE-CZ-NH2	5.15	122.88	120.30
1	F	166	MET	CG-SD-CE	-5.15	91.97	100.20
1	d	209	ILE	N-CA-CB	5.14	122.63	110.80
2	n	46	TYR	CD1-CG-CD2	5.14	123.56	117.90
3	K	140	TYR	CB-CG-CD2	5.14	124.09	121.00
3	L	142	ASP	CB-CG-OD1	-5.14	113.67	118.30
1	a	40	ILE	N-CA-C	-5.14	97.11	111.00
2	3	184	ASP	CB-CG-OD2	-5.14	113.67	118.30
3	I	334	VAL	CB-CA-C	5.14	121.17	111.40
1	b	31	VAL	CA-CB-CG1	-5.14	103.19	110.90
2	n	170	ARG	NE-CZ-NH2	5.14	122.87	120.30
3	K	248	ALA	CB-CA-C	5.14	117.81	110.10
2	7	33	MET	CG-SD-CE	-5.14	91.98	100.20
1	c	129	VAL	CA-CB-CG1	-5.14	103.20	110.90
3	M	221	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	3	27	THR	CA-CB-CG2	-5.13	105.21	112.40
2	5	199	TYR	CG-CD1-CE1	-5.13	117.19	121.30
3	I	140	TYR	CB-CG-CD2	5.13	124.08	121.00
1	B	134	VAL	CA-CB-CG2	-5.13	103.21	110.90
1	c	92	ALA	CB-CA-C	-5.13	102.41	110.10
2	2	203	GLU	CG-CD-OE1	-5.13	108.04	118.30
3	J	382	VAL	CA-CB-CG2	-5.13	103.21	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	D	243	LEU	O-C-N	5.13	130.90	122.70
3	K	151	GLU	OE1-CD-OE2	5.13	129.45	123.30
2	2	101	TYR	CE1-CZ-CE2	-5.12	111.60	119.80
1	d	132	PHE	CG-CD2-CE2	5.12	126.43	120.80
1	e	126	TYR	CB-CG-CD1	-5.12	117.93	121.00
1	F	73	HIS	CA-CB-CG	5.12	122.31	113.60
1	D	150	THR	CA-CB-CG2	-5.12	105.23	112.40
1	G	78	THR	CA-C-N	-5.12	105.94	117.20
1	D	180	ARG	NE-CZ-NH2	5.12	122.86	120.30
2	2	24	VAL	N-CA-C	-5.12	97.19	111.00
1	f	132	PHE	CG-CD2-CE2	-5.11	115.17	120.80
2	k	83	ARG	N-CA-CB	5.11	119.81	110.60
3	M	25	GLU	N-CA-CB	-5.11	101.40	110.60
1	D	10	ARG	CD-NE-CZ	-5.11	116.44	123.60
1	e	104	ASP	N-CA-CB	5.11	119.80	110.60
3	M	163	LYS	N-CA-CB	5.11	119.80	110.60
1	G	163	ALA	CB-CA-C	-5.11	102.44	110.10
3	H	130	PHE	N-CA-CB	5.11	119.80	110.60
3	M	43	ARG	CG-CD-NE	-5.11	101.07	111.80
1	b	90	ASP	CB-CG-OD2	-5.11	113.70	118.30
1	B	221	PHE	CB-CG-CD1	-5.11	117.23	120.80
2	3	155	PHE	CB-CG-CD1	-5.11	117.23	120.80
2	5	80	ARG	CD-NE-CZ	-5.11	116.45	123.60
3	L	140	TYR	CG-CD1-CE1	5.11	125.38	121.30
3	H	146	LEU	O-C-N	-5.10	114.53	122.70
1	A	26	TYR	CZ-CE2-CD2	5.10	124.39	119.80
1	d	43	LYS	CB-CA-C	-5.10	100.19	110.40
1	G	82	VAL	CG1-CB-CG2	5.10	119.06	110.90
2	n	121	SER	CB-CA-C	-5.10	100.41	110.10
3	M	12	LYS	CA-C-O	-5.10	109.39	120.10
2	2	77	TYR	CZ-CE2-CD2	5.10	124.39	119.80
1	C	139	ALA	CB-CA-C	-5.10	102.45	110.10
1	F	63	THR	CA-CB-CG2	-5.10	105.26	112.40
3	H	41	ARG	N-CA-CB	5.10	119.78	110.60
3	K	245	ALA	CB-CA-C	-5.10	102.45	110.10
2	3	140	THR	N-CA-CB	5.10	119.98	110.30
3	H	375	PHE	CG-CD2-CE2	-5.10	115.19	120.80
2	k	88	ARG	NE-CZ-NH2	5.09	122.85	120.30
2	m	200	SER	N-CA-CB	5.09	118.14	110.50
3	I	107	ALA	N-CA-CB	5.09	117.23	110.10
1	a	130	ARG	NE-CZ-NH2	5.09	122.85	120.30
1	b	182	ASP	CB-CA-C	-5.09	100.22	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	i	101	TYR	CB-CG-CD2	-5.09	117.94	121.00
2	j	106	TYR	CB-CG-CD1	-5.09	117.94	121.00
1	a	15	PHE	CB-CG-CD1	-5.09	117.24	120.80
2	i	105	PRO	N-CD-CG	5.09	110.84	103.20
2	m	173	TYR	CG-CD2-CE2	5.09	125.37	121.30
2	7	83	ARG	NE-CZ-NH1	-5.09	117.75	120.30
3	I	186	THR	CA-C-N	-5.09	106.02	116.20
1	F	82	VAL	CB-CA-C	-5.09	101.74	111.40
2	2	83	ARG	NH1-CZ-NH2	5.08	124.99	119.40
2	1	190	LYS	N-CA-C	-5.08	97.27	111.00
2	k	104	PHE	CB-CG-CD1	-5.08	117.24	120.80
2	6	136	ASP	CB-CG-OD2	5.08	122.88	118.30
3	L	382	VAL	CG1-CB-CG2	-5.08	102.77	110.90
1	C	211	VAL	N-CA-CB	5.08	122.68	111.50
3	I	255	THR	CA-CB-CG2	-5.08	105.29	112.40
3	J	140	TYR	CG-CD1-CE1	-5.08	117.23	121.30
1	G	100	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	D	123	TYR	CZ-CE2-CD2	5.08	124.37	119.80
2	1	155	PHE	CB-CG-CD1	5.08	124.35	120.80
3	J	200	ARG	NE-CZ-NH2	5.08	122.84	120.30
2	l	68	ARG	NE-CZ-NH2	-5.07	117.76	120.30
3	K	161	LEU	CB-CG-CD2	-5.07	102.38	111.00
3	K	377	LYS	CB-CG-CD	5.07	124.79	111.60
2	h	46	TYR	N-CA-C	-5.07	97.31	111.00
1	B	6	MET	CA-CB-CG	5.07	121.92	113.30
1	d	205	VAL	N-CA-C	-5.07	97.31	111.00
1	F	62	ASP	CB-CA-C	-5.07	100.26	110.40
2	3	212	ARG	NE-CZ-NH2	-5.07	117.77	120.30
1	c	10	ARG	N-CA-CB	-5.07	101.47	110.60
3	L	331	ALA	N-CA-CB	5.07	117.20	110.10
2	h	138	VAL	CB-CA-C	5.07	121.03	111.40
3	L	94	TYR	CA-CB-CG	-5.07	103.77	113.40
3	J	94	TYR	CZ-CE2-CD2	5.07	124.36	119.80
2	3	67	ALA	N-CA-CB	5.07	117.19	110.10
3	L	41	ARG	O-C-N	-5.07	114.59	122.70
3	J	122	SER	N-CA-CB	5.06	118.10	110.50
1	d	219	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	4	170	ARG	NE-CZ-NH1	-5.06	117.77	120.30
2	l	197	TYR	CB-CG-CD2	-5.06	117.96	121.00
2	h	197	TYR	CB-CG-CD2	5.06	124.04	121.00
2	3	187	ASP	CB-CA-C	5.06	120.52	110.40
2	k	139	ALA	N-CA-C	-5.06	97.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	7	107	LEU	N-CA-CB	5.06	120.52	110.40
2	7	123	TYR	CB-CG-CD1	-5.06	117.96	121.00
1	d	126	TYR	CB-CG-CD1	-5.06	117.96	121.00
2	1	155	PHE	CZ-CE2-CD2	5.06	126.17	120.10
2	2	76	LEU	CB-CG-CD2	5.06	119.60	111.00
2	k	191	ILE	N-CA-CB	5.06	122.44	110.80
2	5	63	ALA	CB-CA-C	-5.06	102.51	110.10
3	I	25	GLU	N-CA-CB	5.06	119.71	110.60
3	J	122	SER	N-CA-C	-5.06	97.34	111.00
3	I	378	ALA	CB-CA-C	-5.06	102.51	110.10
2	k	57	ALA	N-CA-CB	5.06	117.18	110.10
1	c	26	TYR	CB-CG-CD1	-5.05	117.97	121.00
1	D	241	ARG	NE-CZ-NH1	-5.05	117.77	120.30
2	2	119	GLY	O-C-N	-5.05	114.61	122.70
3	H	275	PHE	CB-CG-CD2	-5.05	117.26	120.80
3	M	295	PRO	O-C-N	5.05	130.78	122.70
2	m	30	ARG	NE-CZ-NH2	5.05	122.83	120.30
2	m	46	TYR	CD1-CE1-CZ	-5.05	115.26	119.80
3	H	159	LEU	CA-C-N	5.05	131.24	117.10
1	C	121	GLN	CG-CD-OE1	5.05	131.70	121.60
1	g	77	ALA	N-CA-CB	5.05	117.17	110.10
2	5	111	LEU	N-CA-C	-5.05	97.37	111.00
3	I	259	ARG	C-N-CA	5.05	134.32	121.70
1	E	146	LYS	CB-CA-C	-5.05	100.31	110.40
2	3	148	TYR	CG-CD1-CE1	-5.05	117.26	121.30
2	n	56	THR	CA-CB-CG2	-5.05	105.33	112.40
3	L	263	ARG	NE-CZ-NH2	5.05	122.82	120.30
3	M	10	LEU	CB-CA-C	-5.05	100.61	110.20
1	C	15	PHE	CB-CG-CD2	5.04	124.33	120.80
1	D	241	ARG	NH1-CZ-NH2	5.04	124.95	119.40
3	K	101	LYS	N-CA-C	-5.04	97.38	111.00
1	G	74	ILE	N-CA-C	-5.04	97.39	111.00
1	g	33	ARG	CG-CD-NE	5.04	122.39	111.80
2	k	154	ARG	CB-CA-C	-5.04	100.32	110.40
3	M	350	ASP	CB-CG-OD1	-5.04	113.76	118.30
1	B	175	PHE	CB-CG-CD2	-5.04	117.27	120.80
1	F	164	ILE	N-CA-C	-5.04	97.39	111.00
1	c	202	SER	N-CA-CB	5.04	118.06	110.50
2	6	211	PHE	CB-CG-CD2	-5.04	117.27	120.80
3	H	215	TYR	CG-CD2-CE2	-5.04	117.27	121.30
3	M	311	LEU	CB-CG-CD1	5.04	119.56	111.00
1	D	205	VAL	N-CA-C	-5.04	97.40	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	E	189	MET	CG-SD-CE	-5.04	92.14	100.20
2	i	77	TYR	CG-CD1-CE1	-5.04	117.27	121.30
3	H	344	GLU	CB-CG-CD	-5.04	100.61	114.20
3	J	211	PHE	CB-CG-CD2	5.04	124.33	120.80
2	k	136	ASP	CB-CG-OD1	-5.03	113.77	118.30
2	k	62	ASP	CB-CG-OD2	-5.03	113.77	118.30
2	6	77	TYR	CB-CG-CD2	-5.03	117.98	121.00
1	a	20	ARG	NE-CZ-NH2	-5.03	117.79	120.30
1	e	196	MET	CB-CA-C	-5.03	100.34	110.40
2	4	32	THR	OG1-CB-CG2	-5.03	98.43	110.00
1	F	149	GLU	N-CA-CB	5.03	119.65	110.60
1	f	240	ILE	O-C-N	5.03	130.75	122.70
2	l	24	VAL	CA-CB-CG2	-5.03	103.36	110.90
1	B	54	VAL	CG1-CB-CG2	-5.02	102.86	110.90
1	E	148	TYR	CZ-CE2-CD2	5.02	124.32	119.80
3	M	242	GLU	N-CA-CB	5.02	119.64	110.60
3	H	16	LEU	CB-CG-CD1	-5.02	102.46	111.00
1	A	20	ARG	NE-CZ-NH2	-5.02	117.79	120.30
1	A	174	PHE	O-C-N	-5.02	114.67	122.70
1	d	131	PRO	N-CD-CG	5.02	110.73	103.20
2	4	184	ASP	CB-CG-OD2	5.02	122.82	118.30
1	B	106	PRO	CA-N-CD	-5.02	104.47	111.50
1	G	77	ALA	N-CA-CB	5.02	117.12	110.10
1	G	168	ARG	NE-CZ-NH1	5.02	122.81	120.30
2	4	108	VAL	N-CA-C	-5.02	97.45	111.00
2	6	102	ARG	NE-CZ-NH1	-5.02	117.79	120.30
2	n	159	ILE	C-N-CA	5.02	132.84	122.30
3	M	276	ASP	CB-CG-OD2	-5.02	113.78	118.30
3	K	128	TYR	CG-CD2-CE2	-5.02	117.29	121.30
1	A	201	GLU	N-CA-CB	5.01	119.63	110.60
1	C	186	ASP	CB-CG-OD1	-5.01	113.79	118.30
2	5	191	ILE	N-CA-C	-5.01	97.46	111.00
3	I	87	PHE	CZ-CE2-CD2	-5.01	114.08	120.10
3	K	85	PRO	N-CD-CG	5.01	110.72	103.20
3	L	281	VAL	CA-CB-CG1	5.01	118.42	110.90
3	J	140	TYR	CB-CG-CD2	-5.01	117.99	121.00
1	e	205	VAL	N-CA-C	-5.01	97.46	111.00
1	b	77	ALA	N-CA-CB	5.01	117.12	110.10
2	h	25	MET	O-C-N	-5.01	114.68	122.70
2	3	133	GLU	C-N-CA	5.01	134.23	121.70
3	I	289	ARG	NE-CZ-NH1	5.01	122.81	120.30
3	L	224	ARG	NH1-CZ-NH2	-5.01	113.89	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	M	167	PHE	CB-CG-CD2	5.01	124.31	120.80
1	F	201	GLU	OE1-CD-OE2	5.01	129.31	123.30
1	B	123	TYR	CB-CG-CD2	5.01	124.00	121.00
2	j	118	GLU	N-CA-CB	-5.01	101.59	110.60
3	L	178	VAL	CA-CB-CG2	-5.01	103.39	110.90
2	2	41	ALA	CB-CA-C	-5.00	102.59	110.10
1	a	161	ALA	CB-CA-C	-5.00	102.59	110.10
2	j	115	ILE	CB-CA-C	5.00	121.61	111.60
2	n	88	ARG	NE-CZ-NH1	-5.00	117.80	120.30
2	2	17	LEU	CB-CA-C	5.00	119.70	110.20
3	H	200	ARG	NH1-CZ-NH2	5.00	124.90	119.40

There are no chirality outliers.

All (306) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	103	TYR	Sidechain
2	1	173	TYR	Sidechain
2	1	211	PHE	Sidechain
2	1	83	ARG	Sidechain
2	2	103	TYR	Sidechain
2	2	123	TYR	Sidechain
2	2	139	ALA	Peptide,Mainchain
2	2	178	ARG	Sidechain
2	2	212	ARG	Sidechain
2	2	46	TYR	Sidechain
2	2	68	ARG	Sidechain
2	3	123	TYR	Sidechain
2	3	199	TYR	Sidechain
2	3	211	PHE	Sidechain
2	3	51	ARG	Sidechain
2	3	80	ARG	Sidechain
2	3	81	ARG	Sidechain
2	4	139	ALA	Peptide
2	4	154	ARG	Sidechain
2	4	155	PHE	Sidechain
2	4	178	ARG	Sidechain
2	4	77	TYR	Sidechain
2	4	81	ARG	Sidechain
2	4	88	ARG	Sidechain
2	5	102	ARG	Sidechain
2	5	154	ARG	Sidechain

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Mol	Chain	Res	Type	Group
2	5	170	ARG	Sidechain
2	5	173	TYR	Sidechain
2	5	178	ARG	Sidechain
2	5	197	TYR	Sidechain
2	5	46	TYR	Sidechain
2	5	68	ARG	Sidechain
2	5	83	ARG	Sidechain
2	6	197	TYR	Sidechain
2	6	30	ARG	Sidechain
2	6	51	ARG	Sidechain
2	7	102	ARG	Sidechain
2	7	103	TYR	Sidechain
2	7	106	TYR	Sidechain
2	7	123	TYR	Sidechain
2	7	132	ILE	Peptide
2	7	139	ALA	Peptide
2	7	173	TYR	Sidechain
2	7	81	ARG	Sidechain
1	A	123	TYR	Sidechain
1	A	130	ARG	Sidechain
1	A	159	TYR	Sidechain
1	A	160	LYS	Peptide
1	A	168	ARG	Sidechain
1	A	213	TYR	Sidechain
1	A	65	GLU	Peptide
1	B	130	ARG	Sidechain
1	B	14	VAL	Peptide
1	B	159	TYR	Sidechain
1	B	185	PHE	Sidechain
1	B	213	TYR	Sidechain
1	B	220	THR	Peptide
1	B	232	TYR	Sidechain
1	B	68	TYR	Sidechain
1	B	91	ARG	Sidechain
1	C	126	TYR	Sidechain
1	C	179	TYR	Sidechain
1	C	65	GLU	Peptide
1	C	66	LYS	Peptide
1	D	126	TYR	Sidechain
1	D	150	THR	Peptide
1	D	159	TYR	Sidechain
1	D	179	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	D	180	ARG	Sidechain
1	D	213	TYR	Sidechain
1	D	22	PHE	Sidechain
1	D	220	THR	Peptide
1	D	239	ARG	Sidechain
1	D	8	TYR	Sidechain
1	D	93	ARG	Sidechain
1	E	123	TYR	Sidechain
1	E	215	LYS	Mainchain
1	E	220	THR	Peptide
1	E	241	ARG	Sidechain
1	E	93	ARG	Sidechain
1	F	15	PHE	Sidechain
1	F	179	TYR	Sidechain
1	F	213	TYR	Sidechain
1	F	220	THR	Peptide
1	F	235	ARG	Sidechain
1	F	8	TYR	Sidechain
1	F	86	ARG	Sidechain
1	F	93	ARG	Sidechain
1	G	123	TYR	Sidechain
1	G	130	ARG	Sidechain
1	G	179	TYR	Sidechain
1	G	180	ARG	Sidechain
1	G	220	THR	Peptide
1	G	28	ARG	Sidechain
1	G	35	ALA	Peptide
1	G	5	GLN	Peptide
1	G	53	ARG	Sidechain
3	H	119	LEU	Peptide
3	H	140	TYR	Sidechain
3	H	154	ARG	Sidechain
3	H	181	TYR	Peptide,Sidechain
3	H	211	PHE	Sidechain
3	H	224	ARG	Sidechain
3	H	249	ARG	Sidechain
3	H	250	ARG	Sidechain
3	H	254	ASP	Peptide
3	H	269	LEU	Peptide
3	H	27	TYR	Sidechain
3	H	275	PHE	Sidechain
3	H	278	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	H	28	ARG	Sidechain
3	H	303	PHE	Peptide
3	H	317	ARG	Sidechain
3	H	367	ARG	Sidechain
3	H	371	THR	Peptide
3	H	387	THR	Peptide
3	H	50	ARG	Sidechain
3	H	94	TYR	Sidechain
3	I	119	LEU	Peptide
3	I	120	PRO	Peptide
3	I	186	THR	Peptide
3	I	205	ARG	Sidechain
3	I	207	VAL	Peptide
3	I	211	PHE	Sidechain
3	I	224	ARG	Sidechain
3	I	24	ARG	Sidechain
3	I	250	ARG	Sidechain
3	I	263	ARG	Sidechain
3	I	289	ARG	Sidechain
3	I	29	ARG	Sidechain
3	I	321	PHE	Sidechain
3	I	324	HIS	Sidechain
3	I	326	ARG	Sidechain
3	I	385	LYS	Peptide
3	I	386	THR	Peptide
3	I	387	THR	Peptide
3	I	46	ARG	Sidechain
3	J	201	ALA	Peptide,Mainchain
3	J	215	TYR	Sidechain
3	J	24	ARG	Sidechain
3	J	269	LEU	Peptide,Mainchain
3	J	277	PRO	Peptide
3	J	289	ARG	Sidechain
3	J	302	ARG	Sidechain
3	J	305	ARG	Sidechain
3	J	386	THR	Peptide
3	J	44	TYR	Sidechain
3	J	57	ARG	Sidechain
3	J	87	PHE	Sidechain
3	K	20	TYR	Sidechain
3	K	205	ARG	Sidechain
3	K	215	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	K	221	ARG	Sidechain
3	K	250	ARG	Sidechain
3	K	289	ARG	Sidechain
3	K	317	ARG	Sidechain
3	K	385	LYS	Peptide
3	K	50	ARG	Sidechain
3	K	57	ARG	Sidechain
3	K	94	TYR	Sidechain
3	L	128	TYR	Sidechain
3	L	130	PHE	Sidechain
3	L	140	TYR	Sidechain
3	L	200	ARG	Sidechain
3	L	205	ARG	Sidechain
3	L	21	TYR	Sidechain
3	L	214	LYS	Peptide
3	L	215	TYR	Sidechain
3	L	221	ARG	Sidechain
3	L	227	PHE	Sidechain
3	L	254	ASP	Peptide
3	L	259	ARG	Sidechain
3	L	263	ARG	Sidechain
3	L	28	ARG	Sidechain
3	L	29	ARG	Sidechain
3	L	317	ARG	Sidechain
3	L	371	THR	Peptide
3	L	386	THR	Peptide
3	L	387	THR	Peptide
3	L	46	ARG	Sidechain
3	L	49	ARG	Sidechain
3	M	154	ARG	Sidechain
3	M	215	TYR	Peptide,Mainchain
3	M	217	GLY	Peptide
3	M	218	GLU	Peptide
3	M	236	SER	Peptide
3	M	240	ILE	Peptide
3	M	249	ARG	Sidechain
3	M	250	ARG	Sidechain
3	M	254	ASP	Peptide
3	M	276	ASP	Peptide
3	M	28	ARG	Sidechain
3	M	302	ARG	Sidechain
3	M	311	LEU	Peptide

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Mol	Chain	Res	Type	Group
3	M	321	PHE	Sidechain
3	M	326	ARG	Sidechain
3	M	341	ARG	Sidechain
3	M	43	ARG	Sidechain
3	M	59	ARG	Sidechain
1	a	159	TYR	Sidechain
1	a	179	TYR	Sidechain
1	a	20	ARG	Sidechain
1	a	213	TYR	Sidechain
1	a	220	THR	Peptide
1	a	232	TYR	Sidechain
1	a	26	TYR	Sidechain
1	a	28	ARG	Sidechain
1	a	86	ARG	Sidechain
1	b	10	ARG	Sidechain
1	b	103	TYR	Sidechain
1	b	119	PHE	Sidechain
1	b	213	TYR	Sidechain
1	b	220	THR	Peptide
1	b	91	ARG	Sidechain
1	c	126	TYR	Sidechain
1	c	179	TYR	Sidechain
1	c	219	ARG	Sidechain
1	c	232	TYR	Sidechain
1	c	235	ARG	Sidechain
1	c	28	ARG	Sidechain
1	c	53	ARG	Sidechain
1	c	86	ARG	Sidechain
1	d	103	TYR	Sidechain
1	d	119	PHE	Sidechain
1	d	123	TYR	Sidechain
1	d	175	PHE	Sidechain
1	d	179	TYR	Sidechain
1	d	220	THR	Peptide
1	d	221	PHE	Sidechain
1	d	232	TYR	Sidechain
1	d	26	TYR	Sidechain
1	d	86	ARG	Sidechain
1	e	10	ARG	Sidechain
1	e	103	TYR	Sidechain
1	e	123	TYR	Sidechain
1	e	220	THR	Peptide

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Mol	Chain	Res	Type	Group
1	e	53	ARG	Sidechain
1	e	73	HIS	Sidechain
1	e	93	ARG	Sidechain
1	f	132	PHE	Sidechain
1	f	179	TYR	Sidechain
1	f	219	ARG	Sidechain
1	f	220	THR	Peptide,Mainchain
1	f	239	ARG	Sidechain
1	f	93	ARG	Sidechain
1	g	100	ARG	Sidechain
1	g	103	TYR	Sidechain
1	g	130	ARG	Sidechain
1	g	159	TYR	Sidechain
1	g	179	TYR	Sidechain
1	g	219	ARG	Sidechain
1	g	220	THR	Peptide
1	g	68	TYR	Sidechain
2	h	101	TYR	Sidechain
2	h	102	ARG	Sidechain
2	h	106	TYR	Sidechain
2	h	123	TYR	Sidechain
2	h	139	ALA	Peptide
2	h	170	ARG	Sidechain
2	h	81	ARG	Sidechain
2	i	101	TYR	Sidechain
2	i	102	ARG	Sidechain
2	i	123	TYR	Sidechain
2	i	139	ALA	Peptide
2	i	30	ARG	Sidechain
2	i	77	TYR	Sidechain
2	j	106	TYR	Sidechain
2	j	148	TYR	Sidechain
2	j	197	TYR	Sidechain
2	j	80	ARG	Sidechain
2	k	102	ARG	Sidechain
2	k	103	TYR	Sidechain
2	k	106	TYR	Sidechain
2	k	148	TYR	Sidechain
2	k	173	TYR	Sidechain
2	k	211	PHE	Sidechain
2	k	36	PHE	Sidechain
2	k	46	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	k	68	ARG	Sidechain
2	k	88	ARG	Sidechain
2	l	101	TYR	Sidechain
2	l	123	TYR	Sidechain
2	l	154	ARG	Sidechain
2	l	170	ARG	Sidechain
2	l	199	TYR	Sidechain
2	l	51	ARG	Sidechain
2	l	65	PHE	Sidechain
2	l	77	TYR	Sidechain
2	m	148	TYR	Sidechain
2	m	155	PHE	Sidechain
2	m	173	TYR	Sidechain
2	m	178	ARG	Sidechain
2	m	30	ARG	Sidechain
2	m	68	ARG	Sidechain
2	n	102	ARG	Sidechain
2	n	132	ILE	Peptide
2	n	139	ALA	Peptide
2	n	173	TYR	Sidechain
2	n	68	ARG	Sidechain
2	n	83	ARG	Sidechain

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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%)	228 (95%)	10 (4%)	2 (1%)	19 60
1	B	240/242 (99%)	225 (94%)	10 (4%)	5 (2%)	7 36

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	C	240/242 (99%)	222 (92%)	12 (5%)	6 (2%)	5	32
1	D	240/242 (99%)	222 (92%)	11 (5%)	7 (3%)	4	29
1	E	240/242 (99%)	228 (95%)	11 (5%)	1 (0%)	34	72
1	F	240/242 (99%)	228 (95%)	9 (4%)	3 (1%)	12	48
1	G	240/242 (99%)	227 (95%)	9 (4%)	4 (2%)	9	42
1	a	235/242 (97%)	220 (94%)	10 (4%)	5 (2%)	7	36
1	b	235/242 (97%)	219 (93%)	14 (6%)	2 (1%)	17	57
1	c	235/242 (97%)	220 (94%)	12 (5%)	3 (1%)	12	48
1	d	235/242 (97%)	223 (95%)	7 (3%)	5 (2%)	7	36
1	e	235/242 (97%)	218 (93%)	15 (6%)	2 (1%)	17	57
1	f	235/242 (97%)	222 (94%)	10 (4%)	3 (1%)	12	48
1	g	235/242 (97%)	221 (94%)	8 (3%)	6 (3%)	5	31
2	1	200/202 (99%)	189 (94%)	8 (4%)	3 (2%)	10	46
2	2	200/202 (99%)	181 (90%)	13 (6%)	6 (3%)	4	28
2	3	200/202 (99%)	180 (90%)	18 (9%)	2 (1%)	15	54
2	4	200/202 (99%)	182 (91%)	16 (8%)	2 (1%)	15	54
2	5	200/202 (99%)	182 (91%)	13 (6%)	5 (2%)	5	32
2	6	200/202 (99%)	181 (90%)	13 (6%)	6 (3%)	4	28
2	7	200/202 (99%)	179 (90%)	15 (8%)	6 (3%)	4	28
2	h	200/202 (99%)	180 (90%)	14 (7%)	6 (3%)	4	28
2	i	200/202 (99%)	188 (94%)	10 (5%)	2 (1%)	15	54
2	j	200/202 (99%)	186 (93%)	13 (6%)	1 (0%)	29	69
2	k	200/202 (99%)	183 (92%)	13 (6%)	4 (2%)	7	38
2	l	200/202 (99%)	184 (92%)	13 (6%)	3 (2%)	10	46
2	m	200/202 (99%)	190 (95%)	8 (4%)	2 (1%)	15	54
2	n	200/202 (99%)	181 (90%)	9 (4%)	10 (5%)	2	20
3	H	388/390 (100%)	342 (88%)	27 (7%)	19 (5%)	2	20
3	I	388/390 (100%)	346 (89%)	27 (7%)	15 (4%)	3	23
3	J	388/390 (100%)	353 (91%)	28 (7%)	7 (2%)	8	40
3	K	388/390 (100%)	355 (92%)	22 (6%)	11 (3%)	5	30
3	L	388/390 (100%)	349 (90%)	26 (7%)	13 (3%)	3	26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
3	M	388/390 (100%)	351 (90%)	24 (6%)	13 (3%)	3 26
All	All	8453/8556 (99%)	7785 (92%)	478 (6%)	190 (2%)	10 35

All (190) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ILE
1	a	35	ALA
1	B	64	ILE
1	C	67	ILE
1	D	65	GLU
1	E	221	PHE
1	F	9	ASP
1	f	12	ILE
1	G	54	VAL
1	g	218	ASP
2	h	140	THR
2	2	41	ALA
2	2	212	ARG
2	l	137	ILE
2	l	212	ARG
2	n	131	ALA
2	n	139	ALA
2	n	140	THR
3	H	92	SER
3	H	109	ASN
3	H	212	VAL
3	H	270	ALA
3	H	292	ILE
3	I	120	PRO
3	I	190	LEU
3	I	191	LEU
3	I	387	THR
3	K	282	LYS
3	L	212	VAL
3	L	244	ASP
3	M	119	LEU
3	M	163	LYS
3	M	237	ILE
3	M	248	ALA
3	M	255	THR
3	M	366	GLU

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Mol	Chain	Res	Type
3	M	387	THR
3	J	122	SER
3	J	269	LEU
3	J	270	ALA
3	J	387	THR
1	a	54	VAL
1	a	161	ALA
1	b	73	HIS
1	C	20	ARG
1	D	161	ALA
1	d	35	ALA
1	d	54	VAL
1	d	161	ALA
1	d	221	PHE
1	F	221	PHE
1	G	221	PHE
1	g	217	ASP
2	h	35	ASN
2	h	137	ILE
2	h	139	ALA
2	2	30	ARG
2	2	106	TYR
2	3	139	ALA
2	j	136	ASP
2	k	193	GLU
2	5	193	GLU
2	5	212	ARG
2	6	139	ALA
2	6	193	GLU
2	m	193	GLU
2	n	35	ASN
2	n	132	ILE
3	H	221	ARG
3	H	246	ILE
3	H	255	THR
3	H	282	LYS
3	H	310	PRO
3	I	282	LYS
3	I	304	ASP
3	I	331	ALA
3	K	242	GLU
3	K	245	ALA

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Mol	Chain	Res	Type
3	K	273	ASP
3	L	187	GLY
3	L	246	ILE
3	L	389	ILE
3	L	391	ASP
3	M	242	GLU
3	M	290	ILE
3	J	212	VAL
1	B	143	GLU
1	B	221	PHE
1	C	221	PHE
1	C	245	LYS
1	c	179	TYR
1	c	219	ARG
1	e	73	HIS
1	e	161	ALA
1	f	183	LEU
1	G	73	HIS
1	G	143	GLU
1	g	201	GLU
1	g	221	PHE
2	1	136	ASP
2	2	139	ALA
2	i	44	LYS
2	3	181	ALA
2	4	136	ASP
2	5	200	SER
2	6	19	CYS
2	6	40	LYS
2	7	34	GLY
2	7	35	ASN
2	7	133	GLU
3	H	247	ALA
3	H	280	ASP
3	I	134	GLU
3	I	214	LYS
3	I	394	GLY
3	K	275	PHE
3	M	135	LYS
3	M	296	ALA
3	M	333	ASP
3	J	258	ASP

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Mol	Chain	Res	Type
1	a	182	ASP
1	a	221	PHE
1	C	154	GLY
1	c	17	PRO
2	h	41	ALA
2	4	193	GLU
2	k	182	SER
2	5	35	ASN
2	l	40	LYS
2	6	20	LYS
2	6	136	ASP
2	m	136	ASP
2	7	83	ARG
2	7	184	ASP
2	n	181	ALA
2	n	194	ASP
3	H	146	LEU
3	H	269	LEU
3	H	391	ASP
3	I	273	ASP
3	I	388	PRO
3	K	135	LYS
3	K	211	PHE
3	K	284	ILE
3	K	330	LEU
3	L	214	LYS
3	L	388	PRO
3	L	396	MET
1	B	65	GLU
1	D	73	HIS
1	d	143	GLU
1	f	179	TYR
1	g	106	PRO
2	1	39	SER
2	h	191	ILE
2	2	193	GLU
2	7	105	PRO
2	n	137	ILE
3	H	110	GLN
3	H	202	THR
3	H	275	PHE
3	I	368	ALA

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Mol	Chain	Res	Type
3	K	389	ILE
3	L	217	GLY
3	L	310	PRO
3	J	271	GLU
1	B	12	ILE
1	C	36	THR
1	D	6	MET
1	F	105	GLU
1	g	203	GLU
2	1	21	ASP
2	i	210	LYS
2	k	30	ARG
2	k	135	LYS
3	L	303	PHE
3	M	280	ASP
1	A	106	PRO
1	D	64	ILE
1	D	106	PRO
2	5	191	ILE
3	I	297	ILE
1	b	54	VAL
3	H	68	VAL
1	D	14	VAL
3	I	212	VAL
2	n	200	SER
3	K	334	VAL
3	L	395	VAL
2	n	129	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	203/203 (100%)	195 (96%)	8 (4%)	32 56
1	B	203/203 (100%)	198 (98%)	5 (2%)	47 68
1	C	203/203 (100%)	192 (95%)	11 (5%)	22 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	D	203/203 (100%)	194 (96%)	9 (4%)	28 53
1	E	203/203 (100%)	192 (95%)	11 (5%)	22 47
1	F	203/203 (100%)	199 (98%)	4 (2%)	55 74
1	G	203/203 (100%)	194 (96%)	9 (4%)	28 53
1	a	199/203 (98%)	193 (97%)	6 (3%)	41 63
1	b	199/203 (98%)	192 (96%)	7 (4%)	36 59
1	c	199/203 (98%)	195 (98%)	4 (2%)	55 74
1	d	199/203 (98%)	193 (97%)	6 (3%)	41 63
1	e	199/203 (98%)	188 (94%)	11 (6%)	21 47
1	f	199/203 (98%)	190 (96%)	9 (4%)	27 52
1	g	199/203 (98%)	191 (96%)	8 (4%)	31 55
2	1	164/164 (100%)	157 (96%)	7 (4%)	29 53
2	2	164/164 (100%)	153 (93%)	11 (7%)	16 41
2	3	164/164 (100%)	163 (99%)	1 (1%)	86 92
2	4	164/164 (100%)	161 (98%)	3 (2%)	59 77
2	5	164/164 (100%)	159 (97%)	5 (3%)	41 63
2	6	164/164 (100%)	155 (94%)	9 (6%)	21 47
2	7	164/164 (100%)	160 (98%)	4 (2%)	49 69
2	h	164/164 (100%)	158 (96%)	6 (4%)	34 58
2	i	164/164 (100%)	155 (94%)	9 (6%)	21 47
2	j	164/164 (100%)	160 (98%)	4 (2%)	49 69
2	k	164/164 (100%)	160 (98%)	4 (2%)	49 69
2	l	164/164 (100%)	157 (96%)	7 (4%)	29 53
2	m	164/164 (100%)	159 (97%)	5 (3%)	41 63
2	n	164/164 (100%)	154 (94%)	10 (6%)	18 44
3	H	338/338 (100%)	330 (98%)	8 (2%)	49 69
3	I	338/338 (100%)	324 (96%)	14 (4%)	30 55
3	J	338/338 (100%)	322 (95%)	16 (5%)	26 51
3	K	338/338 (100%)	329 (97%)	9 (3%)	44 65
3	L	338/338 (100%)	326 (96%)	12 (4%)	35 59
3	M	338/338 (100%)	325 (96%)	13 (4%)	33 57

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
All	All	7138/7166 (100%)	6873 (96%)	265 (4%)	37 58

All (265) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	86	ARG
1	A	108	THR
1	A	121	GLN
1	A	162	THR
1	A	169	ASN
1	A	208	ASN
1	A	209	ILE
1	A	225	SER
1	a	21	LEU
1	a	28	ARG
1	a	33	ARG
1	a	189	MET
1	a	210	GLU
1	a	234	GLU
1	B	6	MET
1	B	142	ASP
1	B	152	PRO
1	B	207	GLU
1	B	229	LEU
1	b	15	PHE
1	b	28	ARG
1	b	91	ARG
1	b	121	GLN
1	b	143	GLU
1	b	144	VAL
1	b	182	ASP
1	C	57	LYS
1	C	69	LYS
1	C	73	HIS
1	C	98	ILE
1	C	104	ASP
1	C	131	PRO
1	C	134	VAL
1	C	151	ASP
1	C	166	MET
1	C	234	GLU
1	C	239	ARG

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Mol	Chain	Res	Type
1	c	75	CYS
1	c	166	MET
1	c	180	ARG
1	c	213	TYR
1	D	57	LYS
1	D	84	ASP
1	D	99	ASN
1	D	106	PRO
1	D	121	GLN
1	D	129	VAL
1	D	196	MET
1	D	218	ASP
1	D	229	LEU
1	d	15	PHE
1	d	21	LEU
1	d	40	ILE
1	d	117	CYS
1	d	124	THR
1	d	230	LYS
1	E	33	ARG
1	E	40	ILE
1	E	43	LYS
1	E	54	VAL
1	E	99	ASN
1	E	144	VAL
1	E	187	ASP
1	E	205	VAL
1	E	213	TYR
1	E	217	ASP
1	E	220	THR
1	e	18	ASP
1	e	21	LEU
1	e	40	ILE
1	e	62	ASP
1	e	90	ASP
1	e	94	ILE
1	e	121	GLN
1	e	144	VAL
1	e	208	ASN
1	e	217	ASP
1	e	220	THR
1	F	121	GLN

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Mol	Chain	Res	Type
1	F	182	ASP
1	F	217	ASP
1	F	229	LEU
1	f	21	LEU
1	f	22	PHE
1	f	33	ARG
1	f	57	LYS
1	f	121	GLN
1	f	129	VAL
1	f	134	VAL
1	f	178	GLU
1	f	181	ASP
1	G	5	GLN
1	G	21	LEU
1	G	42	CYS
1	G	57	LYS
1	G	115	LYS
1	G	176	GLU
1	G	181	ASP
1	G	209	ILE
1	G	242	GLU
1	g	20	ARG
1	g	59	LEU
1	g	102	THR
1	g	117	CYS
1	g	121	GLN
1	g	151	ASP
1	g	221	PHE
1	g	229	LEU
2	1	17	LEU
2	1	28	GLU
2	1	45	ILE
2	1	102	ARG
2	1	150	VAL
2	1	179	ASP
2	1	202	GLU
2	h	52	MET
2	h	56	THR
2	h	104	PHE
2	h	107	LEU
2	h	126	ASP
2	h	205	GLU

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Mol	Chain	Res	Type
2	2	14	THR
2	2	17	LEU
2	2	27	THR
2	2	28	GLU
2	2	35	ASN
2	2	45	ILE
2	2	46	TYR
2	2	148	TYR
2	2	156	THR
2	2	161	VAL
2	2	211	PHE
2	i	45	ILE
2	i	60	VAL
2	i	122	ILE
2	i	136	ASP
2	i	137	ILE
2	i	140	THR
2	i	153	ASP
2	i	156	THR
2	i	161	VAL
2	3	128	ILE
2	j	33	MET
2	j	136	ASP
2	j	148	TYR
2	j	162	ASP
2	4	45	ILE
2	4	128	ILE
2	4	188	VAL
2	k	32	THR
2	k	107	LEU
2	k	170	ARG
2	k	188	VAL
2	5	43	LYS
2	5	45	ILE
2	5	72	ILE
2	5	198	GLN
2	5	205	GLU
2	l	17	LEU
2	l	27	THR
2	l	28	GLU
2	l	33	MET
2	l	40	LYS

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Mol	Chain	Res	Type
2	l	45	ILE
2	l	104	PHE
2	6	28	GLU
2	6	33	MET
2	6	45	ILE
2	6	120	LYS
2	6	136	ASP
2	6	146	THR
2	6	161	VAL
2	6	202	GLU
2	6	205	GLU
2	m	55	THR
2	m	136	ASP
2	m	161	VAL
2	m	170	ARG
2	m	187	ASP
2	7	45	ILE
2	7	50	ASP
2	7	64	GLN
2	7	161	VAL
2	n	13	THR
2	n	17	LEU
2	n	27	THR
2	n	87	VAL
2	n	106	TYR
2	n	116	ASP
2	n	136	ASP
2	n	170	ARG
2	n	208	LEU
2	n	212	ARG
3	H	73	GLU
3	H	93	GLN
3	H	122	SER
3	H	132	VAL
3	H	161	LEU
3	H	250	ARG
3	H	252	ASN
3	H	299	ARG
3	I	37	ILE
3	I	59	ARG
3	I	92	SER
3	I	161	LEU

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Mol	Chain	Res	Type
3	I	165	GLU
3	I	190	LEU
3	I	205	ARG
3	I	207	VAL
3	I	250	ARG
3	I	265	MET
3	I	302	ARG
3	I	337	LYS
3	I	380	GLU
3	I	392	LEU
3	K	73	GLU
3	K	116	VAL
3	K	173	GLU
3	K	197	ASN
3	K	214	LYS
3	K	269	LEU
3	K	283	VAL
3	K	334	VAL
3	K	352	LYS
3	L	85	PRO
3	L	93	GLN
3	L	101	LYS
3	L	137	GLU
3	L	140	TYR
3	L	160	PRO
3	L	181	TYR
3	L	206	VAL
3	L	207	VAL
3	L	242	GLU
3	L	313	THR
3	L	332	GLU
3	M	88	VAL
3	M	89	VAL
3	M	102	PRO
3	M	125	PRO
3	M	133	GLU
3	M	139	SER
3	M	165	GLU
3	M	250	ARG
3	M	260	GLU
3	M	302	ARG
3	M	311	LEU

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Mol	Chain	Res	Type
3	M	333	ASP
3	M	386	THR
3	J	15	LYS
3	J	41	ARG
3	J	97	GLU
3	J	105	ARG
3	J	110	GLN
3	J	137	GLU
3	J	165	GLU
3	J	203	PHE
3	J	224	ARG
3	J	241	ASP
3	J	251	THR
3	J	255	THR
3	J	266	MET
3	J	289	ARG
3	J	330	LEU
3	J	350	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (35) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	169	ASN
1	b	237	ASN
1	C	5	GLN
1	C	97	GLN
1	C	237	ASN
1	c	23	GLN
1	c	97	GLN
1	c	99	ASN
1	D	73	HIS
1	D	121	GLN
1	D	125	GLN
1	d	97	GLN
1	d	122	GLN
1	d	237	ASN
1	E	237	ASN
1	f	73	HIS
1	f	237	ASN
1	G	97	GLN
1	G	121	GLN
1	g	97	GLN

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Mol	Chain	Res	Type
1	g	121	GLN
2	1	206	GLN
2	i	64	GLN
2	k	75	ASN
2	5	47	GLN
2	5	64	GLN
2	m	75	ASN
2	7	75	ASN
2	7	99	ASN
3	K	111	GLN
3	K	262	GLN
3	M	90	ASN
3	M	93	GLN
3	M	319	GLN
3	J	324	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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	$\#\|Z\|>2$
6	ADP	K	401	4	24,29,29	1.65	2 (8%)	29,45,45	2.33	8 (27%)
5	ATP	J	401	4	26,33,33	1.32	3 (11%)	31,52,52	2.73	5 (16%)
5	ATP	M	401	4	26,33,33	1.35	3 (11%)	31,52,52	2.09	7 (22%)
5	ATP	I	401	4	26,33,33	1.31	4 (15%)	31,52,52	3.18	9 (29%)
5	ATP	I	402	4	26,33,33	1.09	2 (7%)	31,52,52	2.46	10 (32%)

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
6	ADP	K	401	4	-	1/12/32/32	0/3/3/3
5	ATP	J	401	4	-	4/18/38/38	0/3/3/3
5	ATP	M	401	4	-	4/18/38/38	0/3/3/3
5	ATP	I	401	4	-	7/18/38/38	0/3/3/3
5	ATP	I	402	4	-	1/18/38/38	0/3/3/3

All (14) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	K	401	ADP	O4'-C1'	6.26	1.49	1.41
5	J	401	ATP	C8-N7	-4.10	1.27	1.34
5	I	401	ATP	C8-N7	-3.58	1.28	1.34
5	M	401	ATP	C4-N3	-3.54	1.30	1.35
5	J	401	ATP	C2'-C1'	-3.30	1.48	1.53
6	K	401	ADP	C2'-C1'	-3.14	1.49	1.53
5	I	402	ATP	C8-N7	-2.94	1.29	1.34
5	M	401	ATP	C8-N7	-2.69	1.29	1.34
5	I	401	ATP	C2'-C1'	-2.65	1.49	1.53
5	M	401	ATP	O4'-C4'	2.54	1.50	1.45
5	I	402	ATP	PA-O2A	-2.41	1.44	1.55
5	I	401	ATP	C2-N3	-2.22	1.28	1.32
5	J	401	ATP	O4'-C4'	-2.22	1.40	1.45
5	I	401	ATP	C5'-C4'	2.18	1.58	1.51

All (39) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	I	401	ATP	PB-O3B-PG	11.12	170.97	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	J	401	ATP	PB-O3B-PG	10.79	169.84	132.83
5	I	401	ATP	PA-O3A-PB	10.22	167.89	132.83
5	I	402	ATP	PB-O3B-PG	8.78	162.94	132.83
5	J	401	ATP	PA-O3A-PB	8.18	160.90	132.83
5	M	401	ATP	PA-O3A-PB	7.13	157.29	132.83
6	K	401	ADP	PA-O3A-PB	7.10	157.20	132.83
6	K	401	ADP	N6-C6-N1	6.67	132.41	118.57
5	I	402	ATP	PA-O3A-PB	6.39	154.75	132.83
5	M	401	ATP	N6-C6-N1	4.65	128.22	118.57
5	M	401	ATP	PB-O3B-PG	4.43	148.04	132.83
5	I	401	ATP	N3-C2-N1	3.77	134.57	128.68
6	K	401	ADP	C5-C6-N1	-3.77	111.80	120.35
5	I	401	ATP	N6-C6-N1	3.71	126.28	118.57
5	J	401	ATP	N6-C6-N1	3.64	126.13	118.57
5	I	402	ATP	N6-C6-N1	3.58	126.01	118.57
5	I	401	ATP	C5-C6-N1	-3.32	112.82	120.35
5	I	401	ATP	C3'-C2'-C1'	-3.21	96.14	100.98
5	I	402	ATP	C5-C6-N1	-3.18	113.15	120.35
6	K	401	ADP	C5-C6-N6	-3.02	115.77	120.35
6	K	401	ADP	C3'-C2'-C1'	2.85	105.27	100.98
5	M	401	ATP	O4'-C4'-C3'	-2.69	99.79	105.11
5	M	401	ATP	C5-C6-N1	-2.69	114.25	120.35
5	I	402	ATP	O5'-C5'-C4'	2.53	117.70	108.99
5	I	401	ATP	O3G-PG-O2G	2.42	116.88	107.64
5	J	401	ATP	C1'-N9-C4	2.34	130.75	126.64
6	K	401	ADP	O3A-PB-O1B	-2.32	98.33	111.19
5	J	401	ATP	C5-C6-N1	-2.31	115.11	120.35
5	M	401	ATP	C5-C6-N6	-2.26	116.91	120.35
5	I	402	ATP	C2'-C3'-C4'	2.24	106.99	102.64
5	I	402	ATP	N3-C2-N1	2.15	132.03	128.68
5	I	402	ATP	O3G-PG-O2G	2.12	115.75	107.64
6	K	401	ADP	N3-C2-N1	2.11	131.98	128.68
5	I	402	ATP	C3'-C2'-C1'	-2.08	97.85	100.98
5	M	401	ATP	O5'-C5'-C4'	2.08	116.14	108.99
6	K	401	ADP	O3B-PB-O1B	2.05	118.71	110.68
5	I	402	ATP	C4-C5-N7	-2.04	107.28	109.40
5	I	401	ATP	O2G-PG-O3B	-2.03	97.82	104.64
5	I	401	ATP	C4-C5-N7	2.02	111.50	109.40

There are no chirality outliers.

All (17) torsion outliers are listed below:

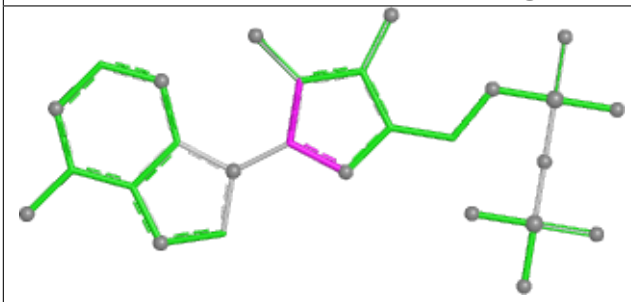
Mol	Chain	Res	Type	Atoms
5	I	401	ATP	PB-O3B-PG-O2G
5	I	401	ATP	C5'-O5'-PA-O1A
6	K	401	ADP	PA-O3A-PB-O2B
5	I	402	ATP	C4'-C5'-O5'-PA
5	M	401	ATP	C3'-C4'-C5'-O5'
5	I	401	ATP	PG-O3B-PB-O1B
5	I	401	ATP	C5'-O5'-PA-O2A
5	J	401	ATP	C5'-O5'-PA-O2A
5	M	401	ATP	PA-O3A-PB-O2B
5	M	401	ATP	O4'-C4'-C5'-O5'
5	I	401	ATP	PB-O3B-PG-O3G
5	J	401	ATP	PB-O3B-PG-O2G
5	I	401	ATP	C5'-O5'-PA-O3A
5	J	401	ATP	C5'-O5'-PA-O3A
5	I	401	ATP	PG-O3B-PB-O2B
5	M	401	ATP	PA-O3A-PB-O1B
5	J	401	ATP	PB-O3A-PA-O2A

There are no ring outliers.

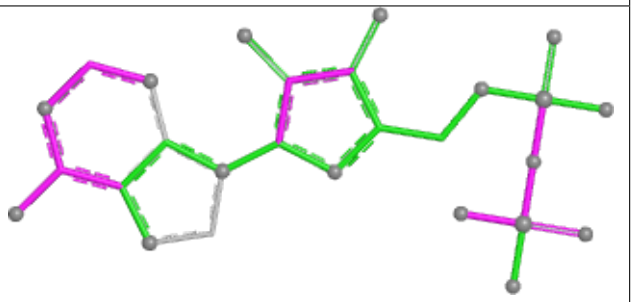
No monomer is involved in short contacts.

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 then 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.

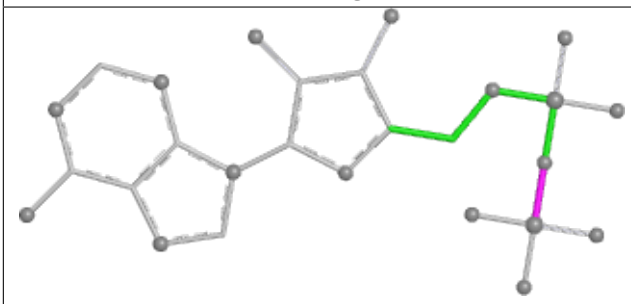
Ligand ADP K 401



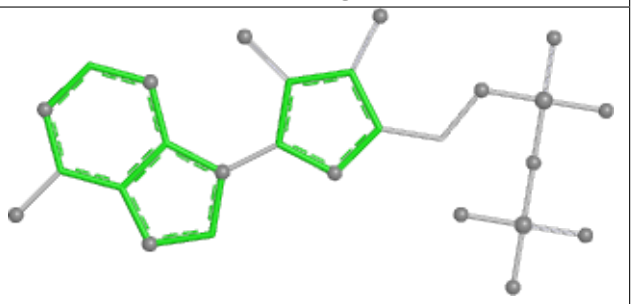
Bond lengths



Bond angles

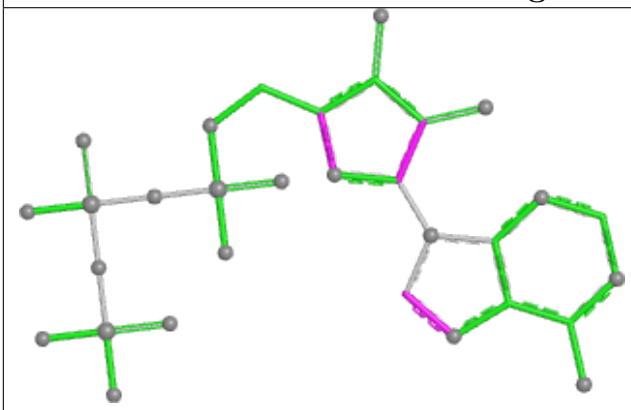


Torsions

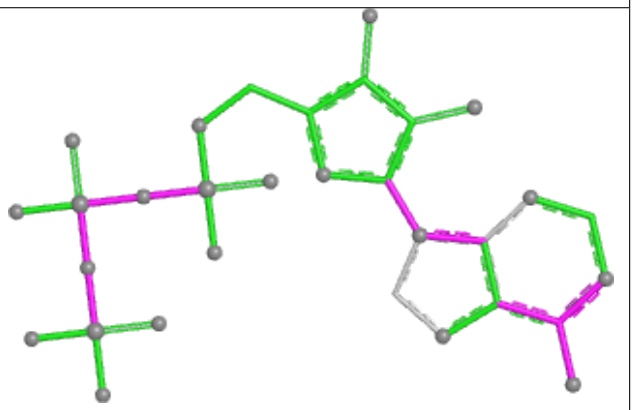


Rings

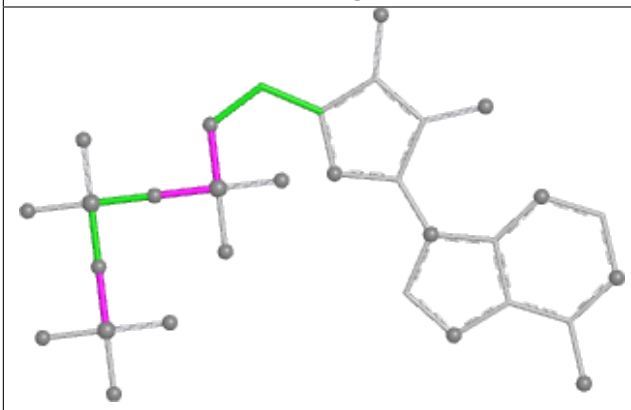
Ligand ATP J 401



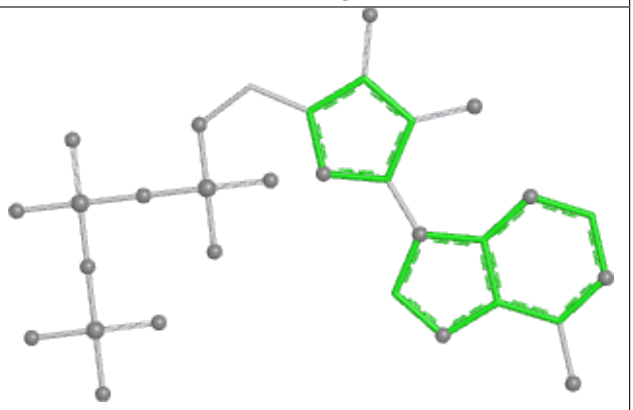
Bond lengths



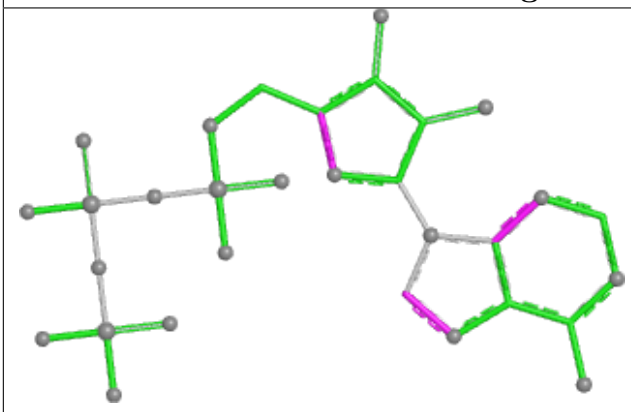
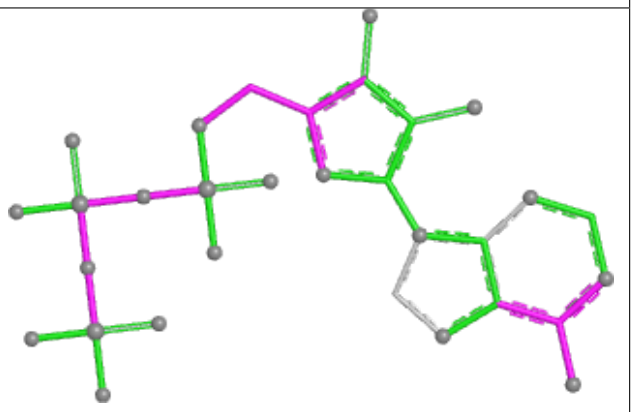
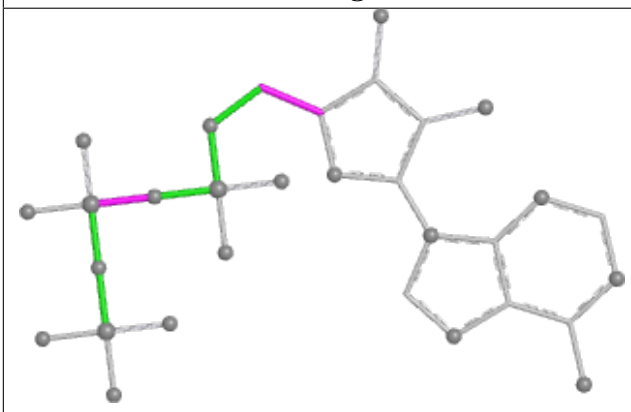
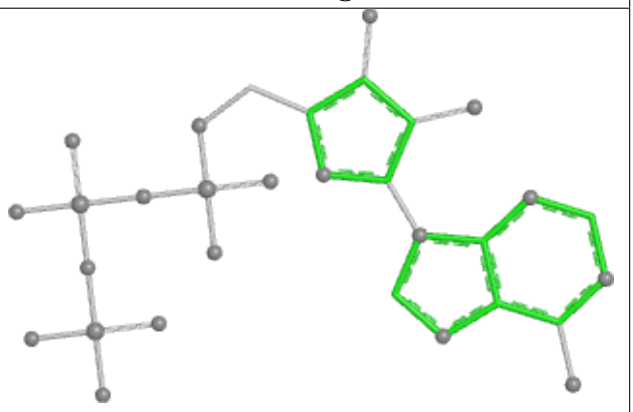
Bond angles



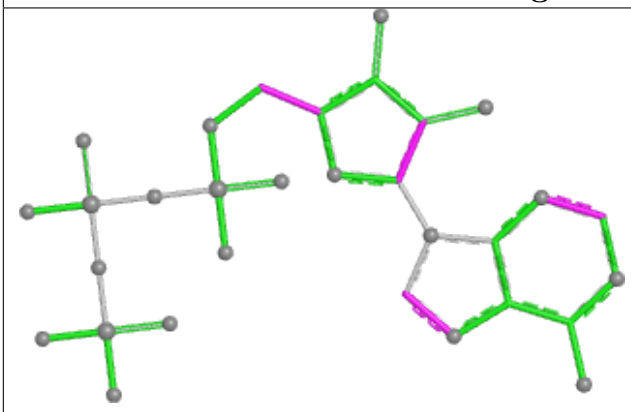
Torsions



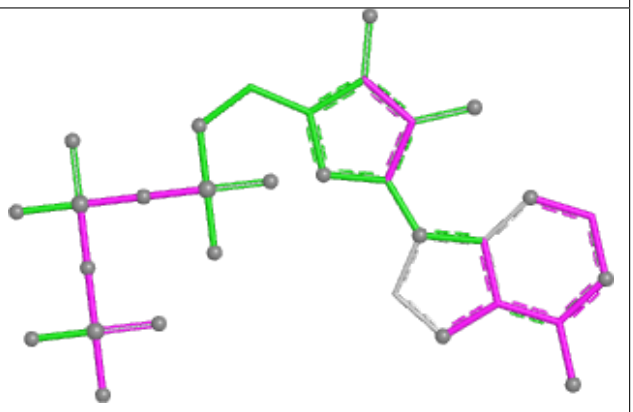
Rings

Ligand ATP M 401	
 Bond lengths	 Bond angles
 Torsions	 Rings

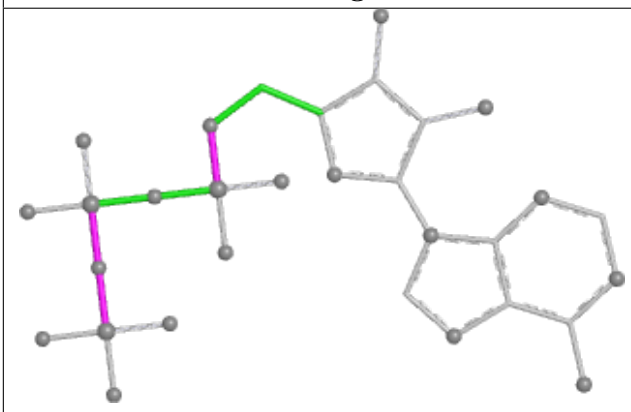
Ligand ATP I 401



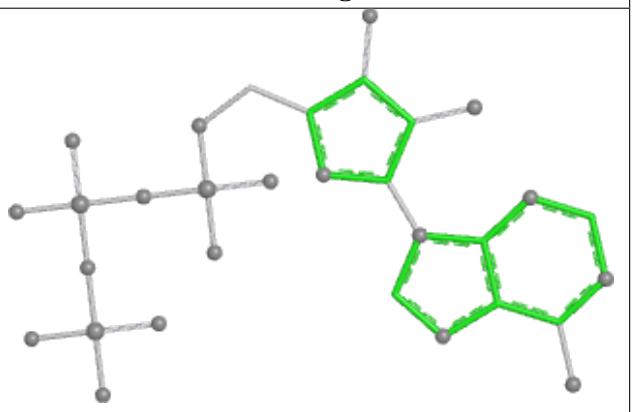
Bond lengths



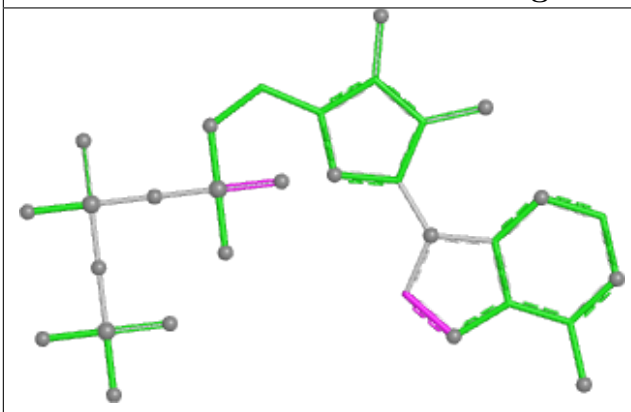
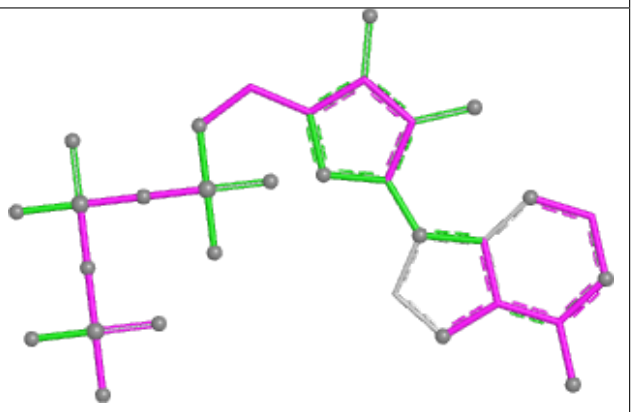
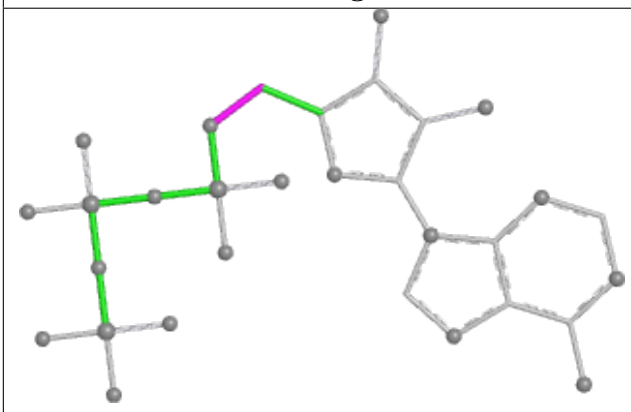
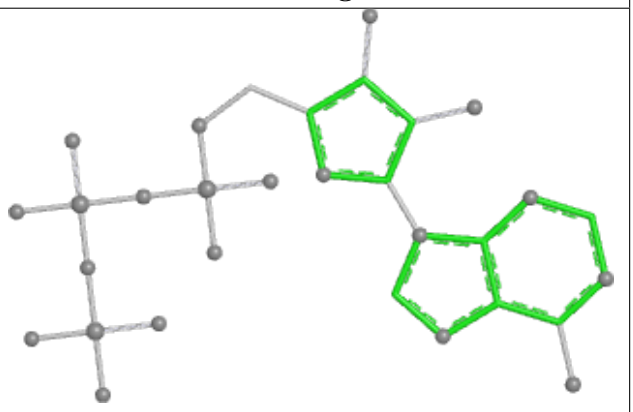
Bond angles



Torsions



Rings

Ligand ATP I 402	
 Bond lengths	 Bond angles
 Torsions	 Rings

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

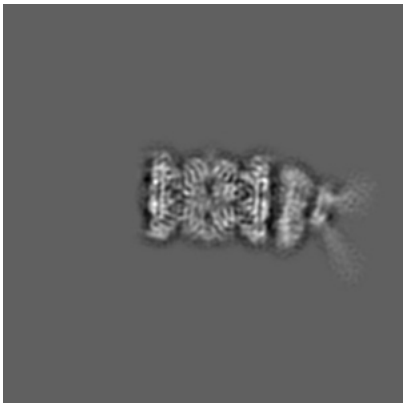
This section contains visualisations of the EMDB entry EMD-0214. These allow visual inspection of the internal detail of the map and identification of artifacts.

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.

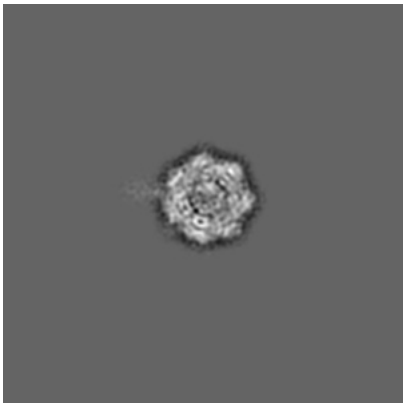
6.1 Orthogonal projections

6.1.1 Primary map

X



Y



Z

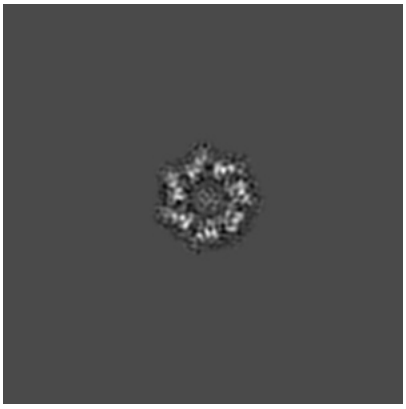
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map

X Index: 192

Y Index: 192



Z Index: 192

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

6.3 Largest variance slices (i)

6.3.1 Primary map

X Index: 179

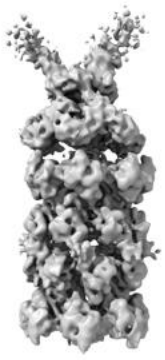
Y Index: 181

Z Index: 250

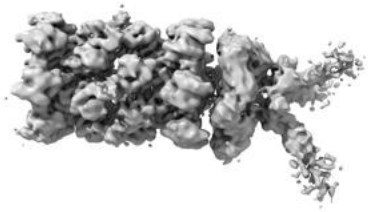
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

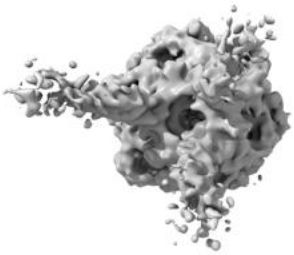
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0072. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

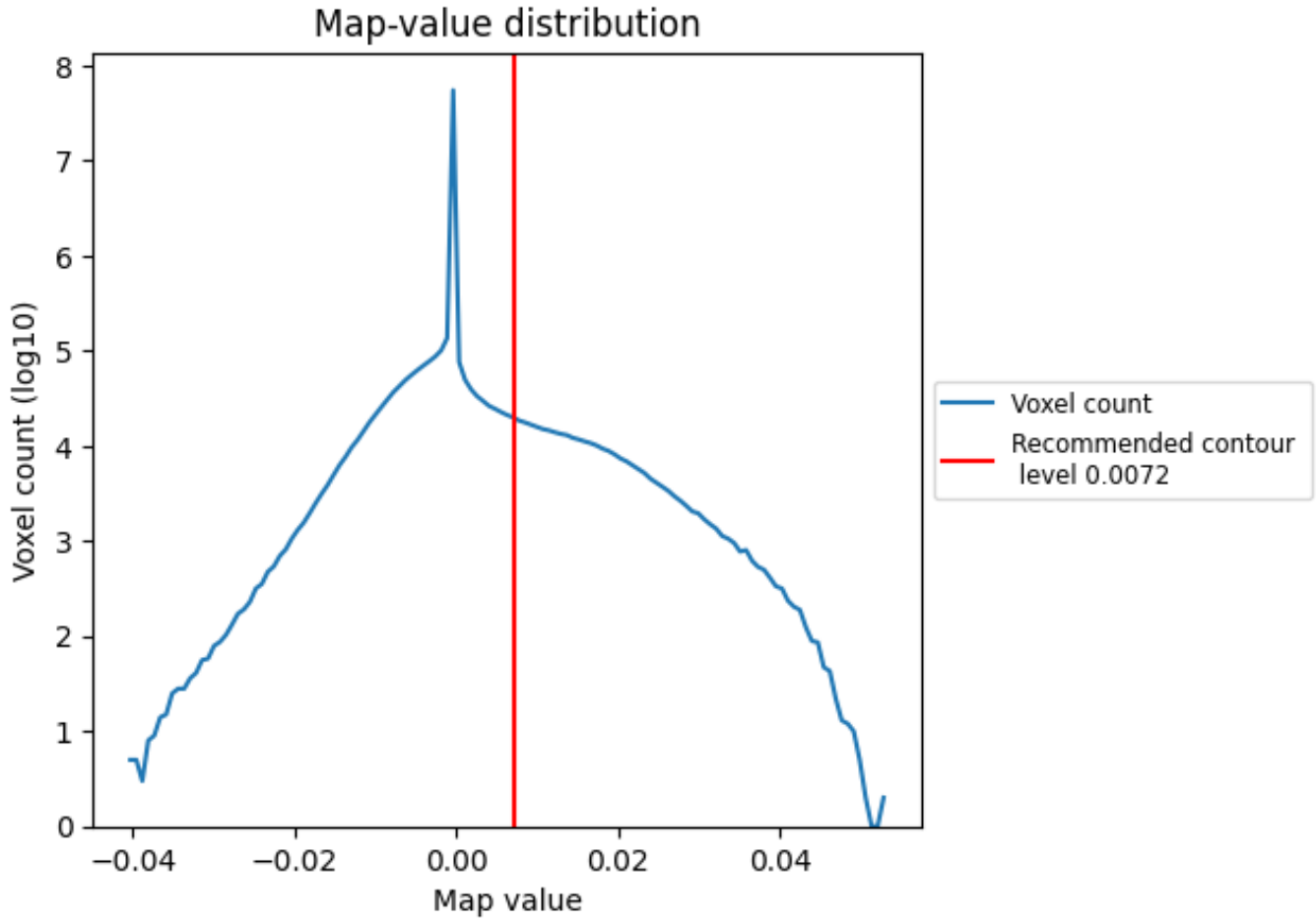
6.5 Mask visualisation (i)

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

7 Map analysis

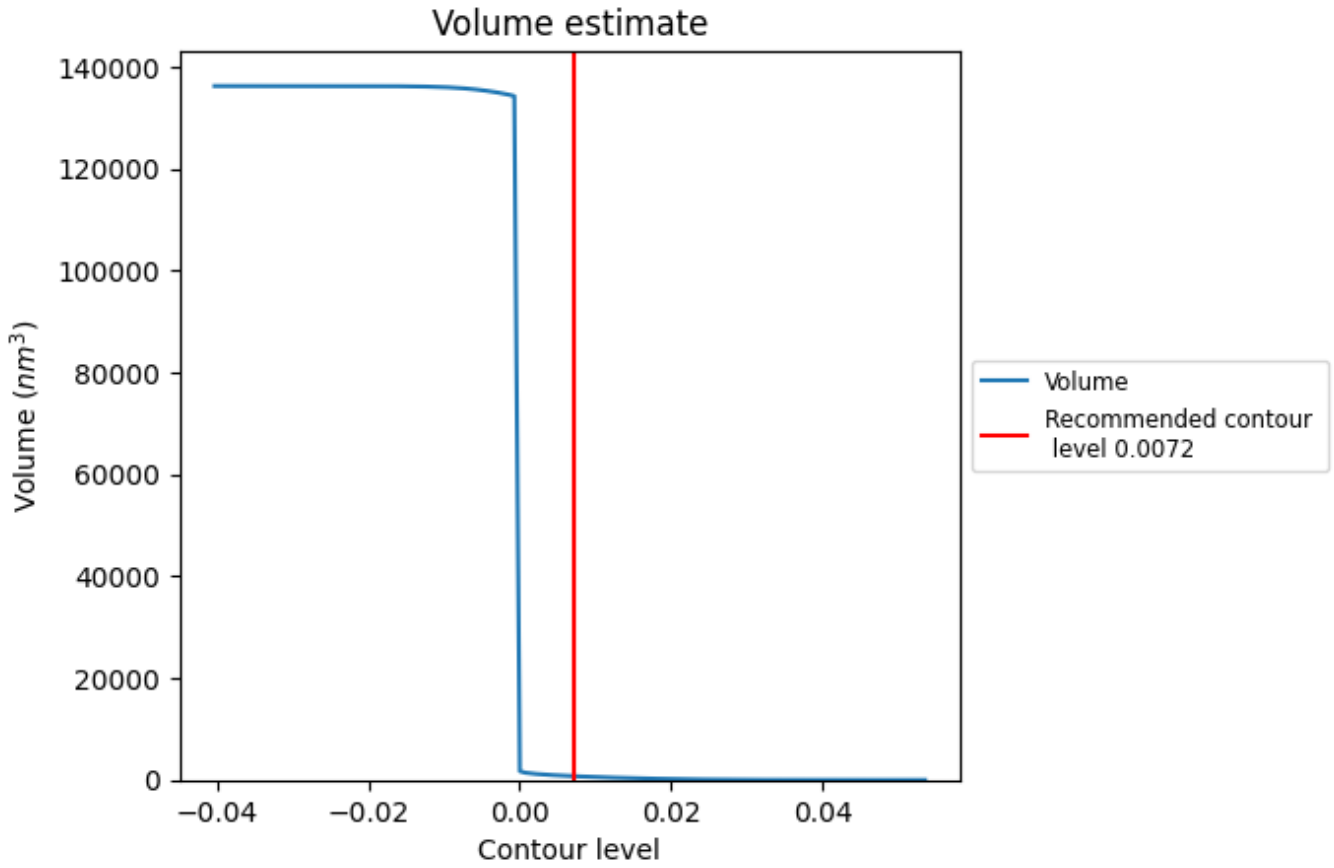
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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.

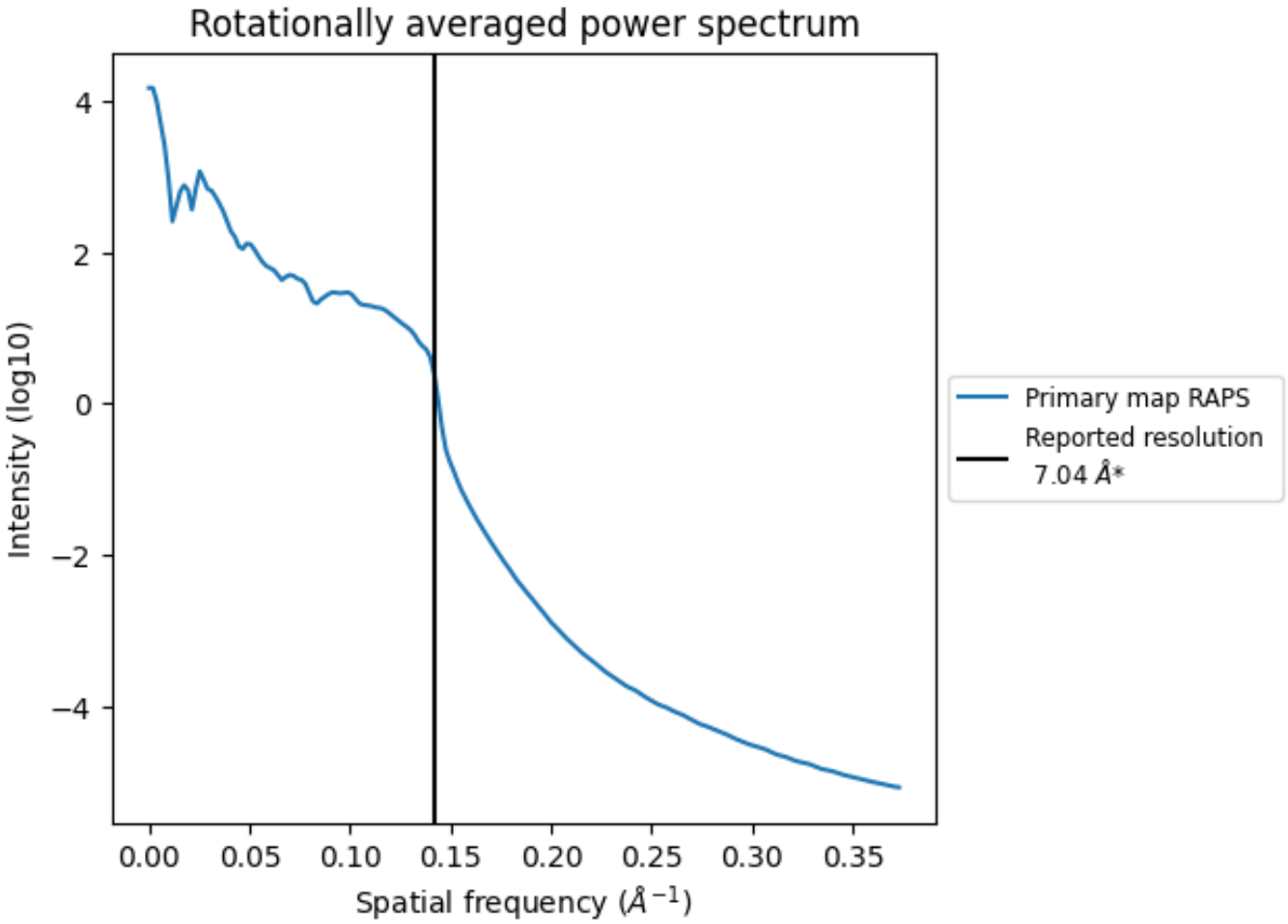
7.2 Volume estimate



The volume at the recommended contour level is 742 nm^3; this corresponds to an approximate mass of 670 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 0.142 Å^{-1}

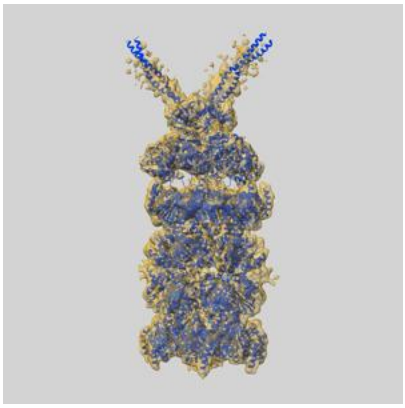
8 Fourier-Shell correlation

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

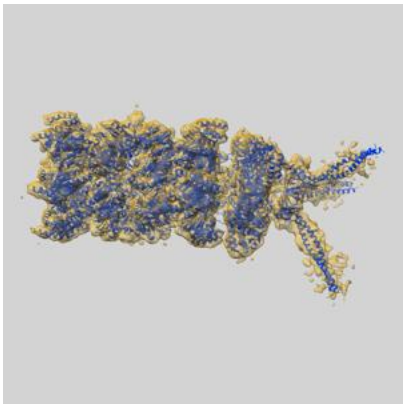
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-0214 and PDB model 6HEA. Per-residue inclusion information can be found in section 3 on page 8.

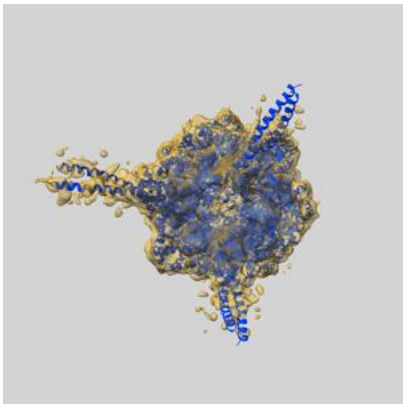
9.1 Map-model overlay



X



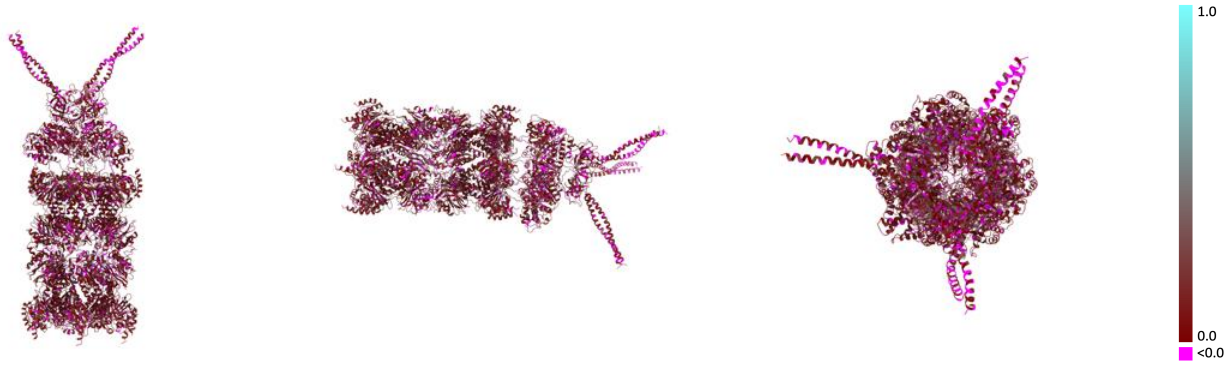
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0072 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.

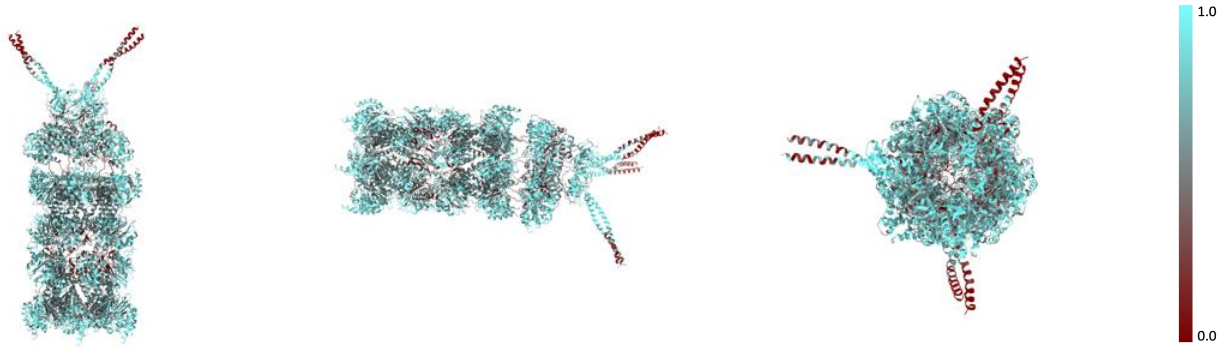
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according 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.

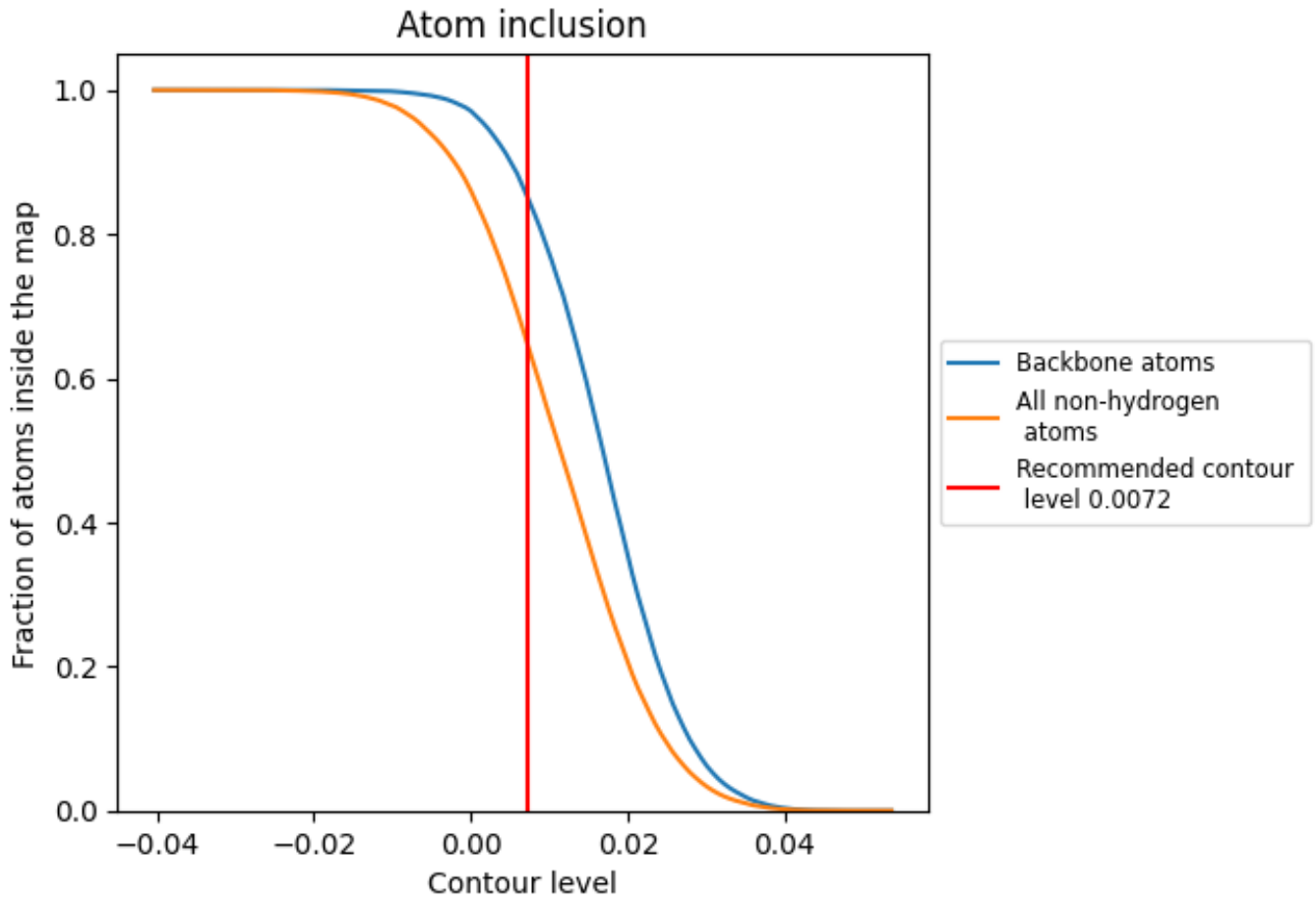
9.3 Atom inclusion mapped to coordinate model



X Y Z

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 (0.0072).

9.4 Atom inclusion (i)



At the recommended contour level, 85% 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 (0.0072) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6487	0.1140
1	0.6149	0.1140
2	0.6215	0.1250
3	0.6136	0.1170
4	0.6208	0.1240
5	0.6182	0.1200
6	0.6228	0.1150
7	0.6406	0.1110
A	0.6770	0.1260
B	0.6765	0.1320
C	0.6803	0.1260
D	0.6776	0.1340
E	0.6840	0.1250
F	0.6845	0.1240
G	0.6845	0.1240
H	0.6314	0.1010
I	0.6498	0.1000
J	0.6705	0.1110
K	0.6697	0.1060
L	0.6224	0.0890
M	0.6077	0.0880
a	0.6941	0.1220
b	0.6875	0.1260
c	0.6711	0.1180
d	0.6678	0.1180
e	0.6820	0.1220
f	0.6727	0.1140
g	0.6743	0.1220
h	0.6149	0.1160
i	0.6201	0.1120
j	0.6149	0.1180
k	0.6142	0.1170
l	0.6116	0.1130
m	0.6063	0.1020
n	0.6050	0.1090