Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 12:57 am GMT

PDB ID	:	6FVU
EMDB ID	:	EMD-3535
Title	:	26S proteasome, s2 state
Authors	:	Eisele, M.R.; Reed, R.G.; Rudack, T.; Schweitzer, A.; Beck, F.; Nagy, I.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Tomko, R.J.; Sakata, E.
Deposited on	:	2018-03-05
Resolution	:	4.50 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:

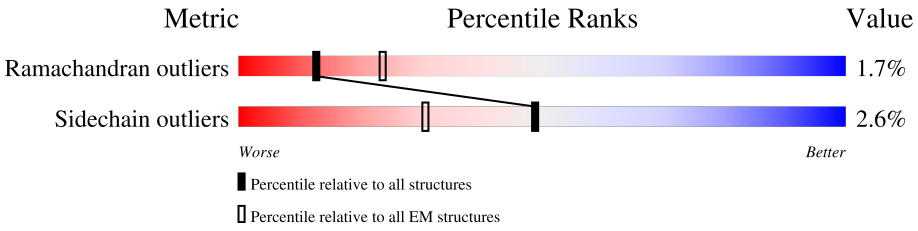
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.50 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	29% 77% 20% ·
1	a	242	67% 80% 17% ·
2	B	249	42% 77% 20% ·
2	b	249	67% 78% 20% ·
3	C	244	48% 81% 17% ·
3	c	244	59% 79% 18% ·
4	D	251	26% 75% 17% · 6%
4	d	251	65% 78% 19% ·
5	E	249	34% 83% 13% ·

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Mol	Chain	Length	Quality of chain
5	e	249	71% 79% 16%
6	F	231	52% 78% 17% 5%
6	f	231	68% 78% 20%
7	G	242	48% 79% 18%
7	g	242	65% 78% 20%
8	1	196	35% 76% 22%
8	h	196	65% 73% 24%
9	2	226	61% 84% 15%
9	i	226	62% 81% 19%
10	3	204	62% 78% 19%
10	j	204	66% 78% 19%
11	4	195	37% 74% 24%
11	k	195	64% 80% 16%
12	5	212	51% 72% 26%
12	l	212	63% 72% 25%
13	6	222	57% 77% 20%
13	m	222	64% 73% 24%
14	7	232	57% 75% 21%
14	n	232	63% 82% 15%
15	W	197	86% 77% 20%
16	V	289	85% 78% 19%
17	T	266	90% 77% 21%
18	X	127	100% 73% 23%
19	Y	89	73% 80% 18%
20	Z	970	91% 86% 7% 7%

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Mol	Chain	Length	Quality of chain
21	N	922	82% 81% 17%
22	S	475	87% 78% 19%
23	P	440	70% 82% 17%
24	Q	434	78% 77% 18%
25	R	405	82% 78% 18%
26	U	304	81% 82% 16%
27	O	388	80% 78% 20%
28	H	426	78% 78% 18%
29	I	384	80% 76% 21%
30	K	394	73% 76% 21%
31	L	388	78% 78% 18%
32	M	421	78% 78% 20%
33	J	405	81% 79% 17%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 110592 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 type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	242	Total	C	N	O	S	0	0
			1913	1217	321	367	8		
1	A	242	Total	C	N	O	S	0	0
			1913	1217	321	367	8		

- Molecule 2 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		
2	B	249	Total	C	N	O	S	0	0
			1907	1214	314	376	3		

- Molecule 3 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	244	Total	C	N	O	S	0	0
			1905	1201	321	380	3		
3	C	244	Total	C	N	O	S	0	0
			1905	1201	321	380	3		

- Molecule 4 is a protein called Proteasome subunit alpha type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	251	Total	C	N	O	S	0	0
			1982	1235	350	393	4		
4	D	237	Total	C	N	O	S	0	0
			1859	1164	325	366	4		

- Molecule 5 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	249	Total	C	N	O	S	0	0
			1926	1204	324	391	7		
5	E	249	Total	C	N	O	S	0	0
			1926	1204	324	391	7		

- Molecule 6 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		
6	F	231	Total	C	N	O	S	0	0
			1773	1114	307	348	4		

- Molecule 7 is a protein called Probable proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	242	Total	C	N	O	S	0	0
			1886	1199	328	355	4		
7	G	242	Total	C	N	O	S	0	0
			1886	1199	328	355	4		

- Molecule 8 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	h	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		
8	1	196	Total	C	N	O	S	0	0
			1512	955	250	300	7		

- Molecule 9 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1720	1082	298	333	7		
9	2	226	Total	C	N	O	S	0	0
			1720	1082	298	333	7		

- Molecule 10 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	j	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

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Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	204	Total	C	N	O	S	0	0
			1581	1010	258	305	8		

- Molecule 11 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	k	195	Total	C	N	O	S	0	0
			1562	992	264	300	6		
11	4	195	Total	C	N	O	S	0	0
			1562	992	264	300	6		

- Molecule 12 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	l	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		
12	5	212	Total	C	N	O	S	0	0
			1644	1045	280	312	7		

- Molecule 13 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	m	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		
13	6	222	Total	C	N	O	S	0	0
			1757	1115	303	335	4		

- Molecule 14 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	232	Total	C	N	O	S	0	0
			1816	1148	311	350	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

- Molecule 15 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	197	Total	C	N	O	S	0	0
			1535	962	269	301	3		

- Molecule 16 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	289	Total	C	N	O	S	0	0
			2274	1425	389	446	14		

- Molecule 17 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	266	Total	C	N	O	S	0	0
			2193	1405	349	433	6		

- Molecule 18 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	X	127	Total	C	N	O	S	0	0
			1033	664	169	196	4		

- Molecule 19 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Y	89	Total	C	N	O	S	0	0
			731	447	119	164	1		

- Molecule 20 is a protein called 26S proteasome regulatory subunit RPN1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	Z	906	Total	C	N	O	S	0	0
			7006	4416	1150	1410	30		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	N	922	Total	C	N	O	S	0	0
			7158	4536	1205	1389	28		

- Molecule 22 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	S	475	Total	C	N	O	S	0	0
			3895	2488	653	739	15		

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	P	440	Total	C	N	O	S	0	0
			3609	2297	604	698	10		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Q	434	Total	C	N	O	S	0	0
			3499	2225	577	681	16		

- Molecule 25 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	R	405	Total	C	N	O	S	0	0
			3259	2077	535	637	10		

- Molecule 26 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	304	Total	C	N	O	S	0	0
			2427	1529	414	477	7		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN9.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	O	388	Total	C	N	O	S	0	0
			3186	2051	519	608	8		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	H	426	Total	C	N	O	S	0	0
			3313	2056	592	648	17		

- Molecule 29 is a protein called 26S proteasome regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	I	384	Total	C	N	O	S	0	0
			3015	1895	507	596	17		

- Molecule 30 is a protein called 26S proteasome regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K	394	Total	C	N	O	S	0	0
			3113	1951	548	604	10		

- Molecule 31 is a protein called 26S proteasome subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	L	388	Total	C	N	O	S	0	0
			3083	1942	548	581	12		

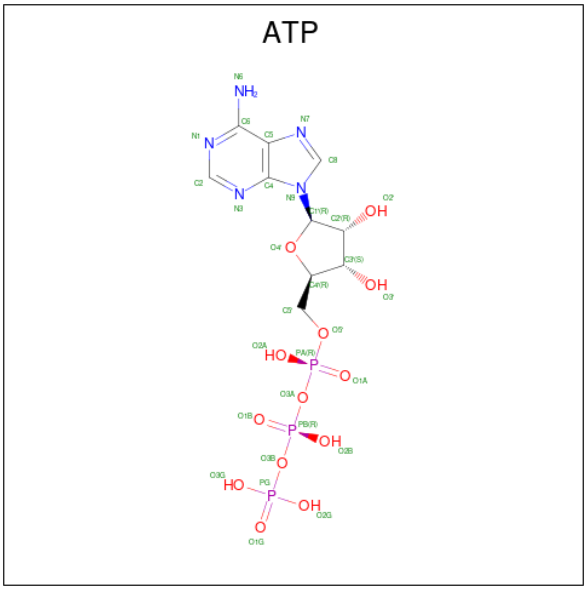
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	M	421	Total	C	N	O	S	0	0
			3285	2043	573	656	13		

- Molecule 33 is a protein called 26S proteasome regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	405	Total	C	N	O	S	0	0
			3171	1995	565	593	18		

- Molecule 34 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



Mol	Chain	Residues	Atoms					AltConf
34	H	1	Total	C	N	O	P	0
			31	10	5	13	3	

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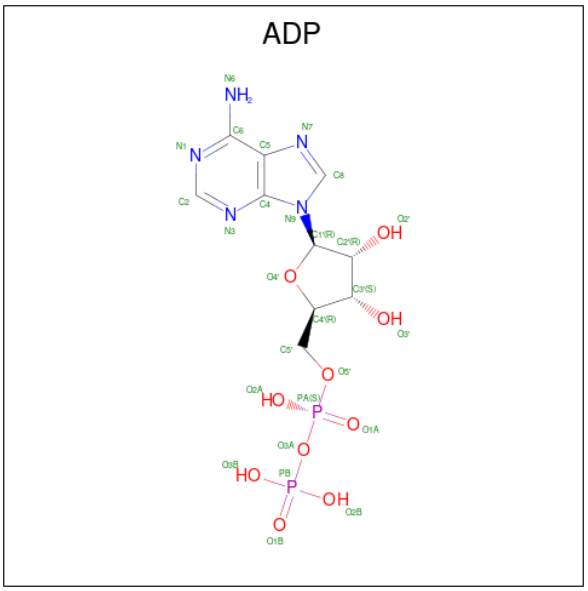
Mol	Chain	Residues	Atoms					AltConf
34	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 35 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 36 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



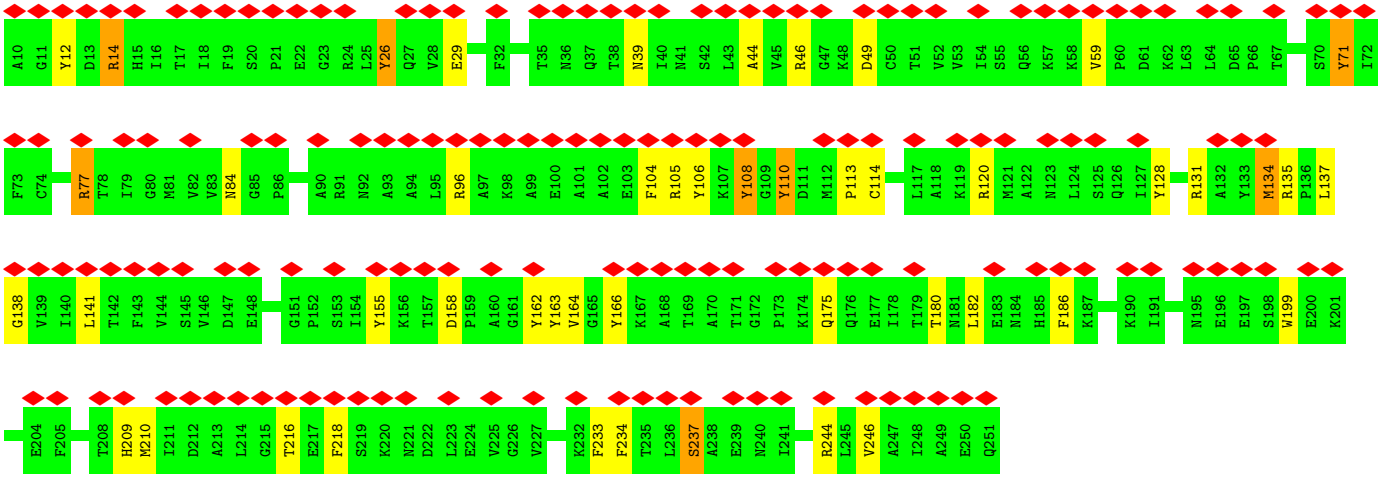
Mol	Chain	Residues	Atoms					AltConf
36	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

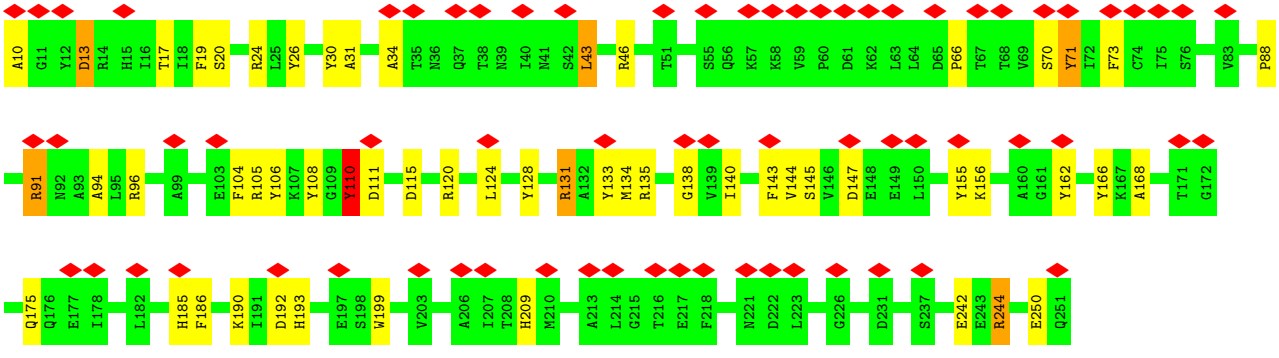
• Molecule 1: Proteasome subunit alpha type-1

Chain a:



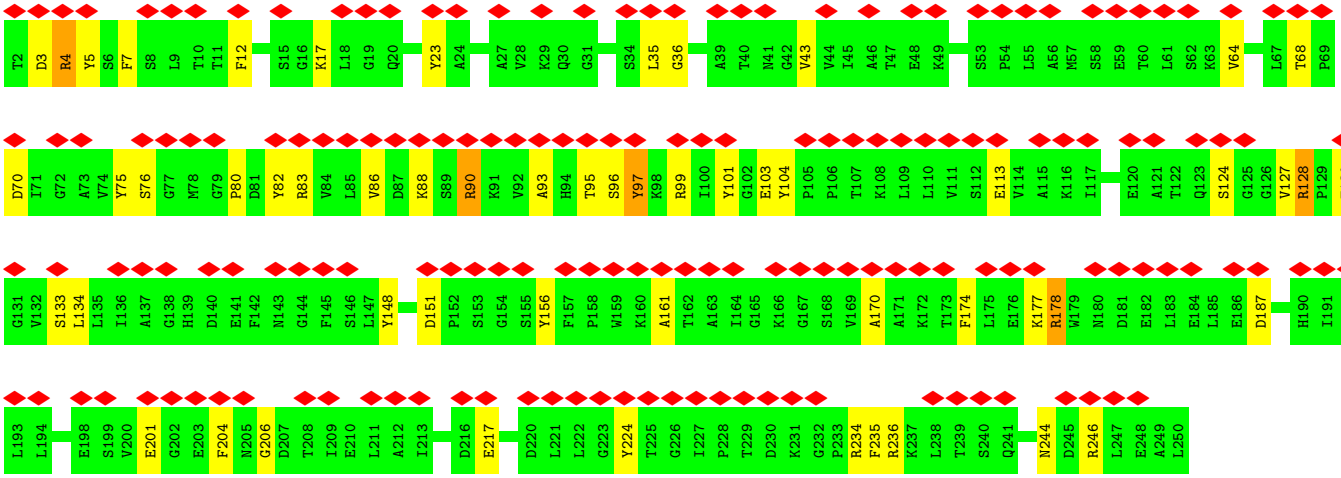
• Molecule 1: Proteasome subunit alpha type-1

Chain A:



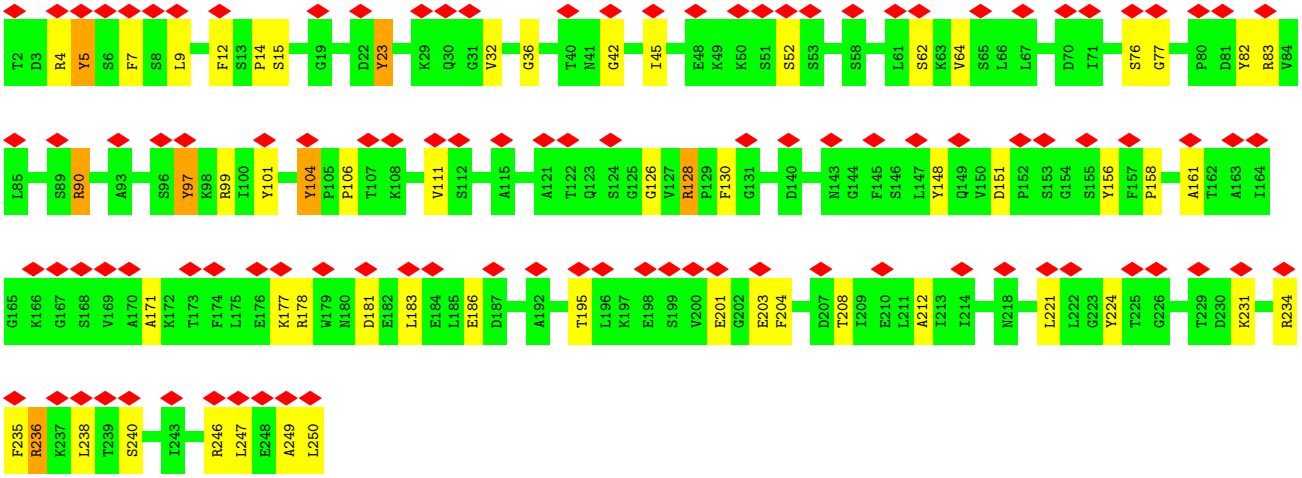
• Molecule 2: Proteasome subunit alpha type-2

Chain b:



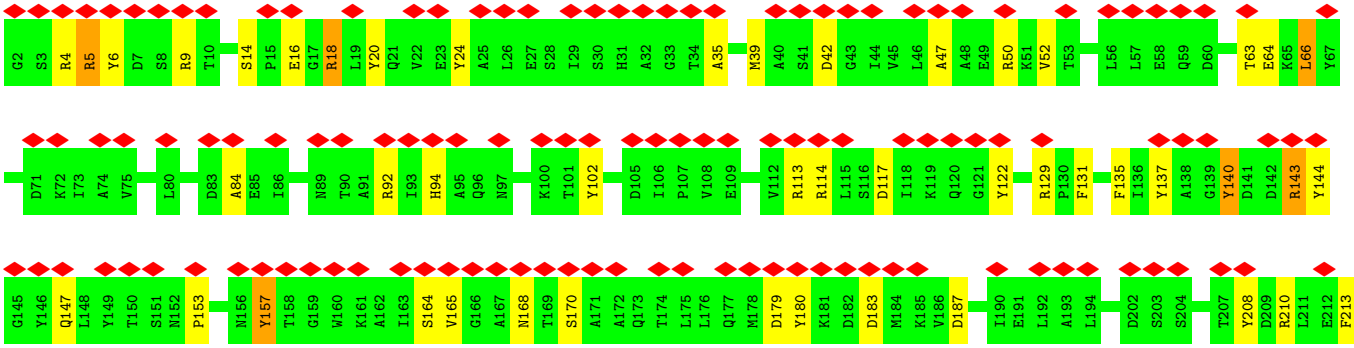
• Molecule 2: Proteasome subunit alpha type-2

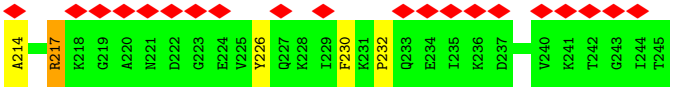
Chain B:



• Molecule 3: Proteasome subunit alpha type-3

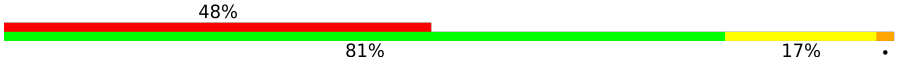
Chain c:

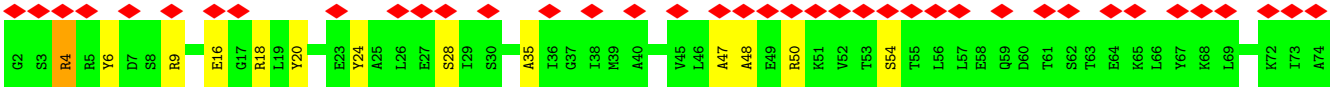


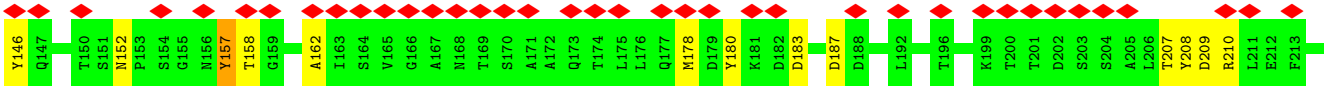


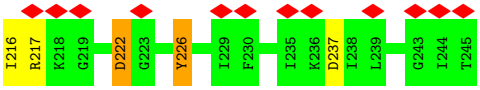
• Molecule 3: Proteasome subunit alpha type-3

Chain C:



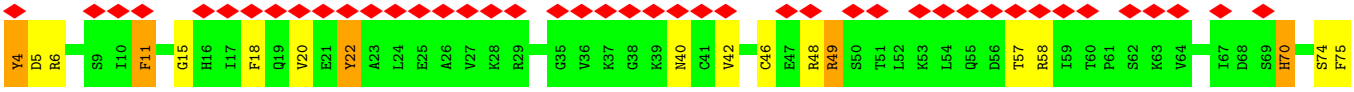


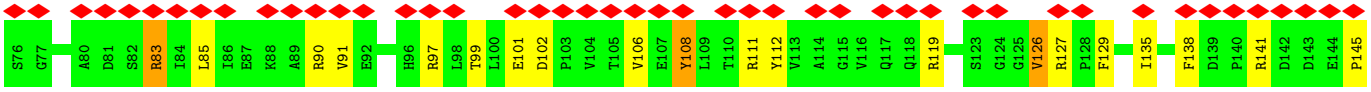


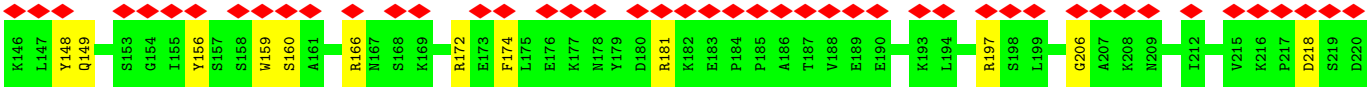


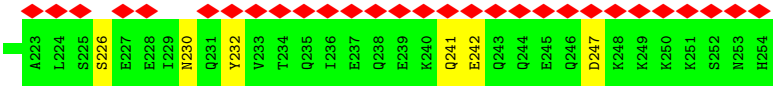
• Molecule 4: Proteasome subunit alpha type-4

Chain d:



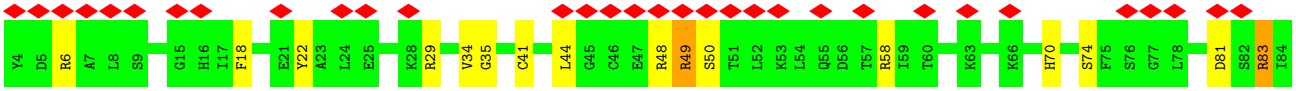


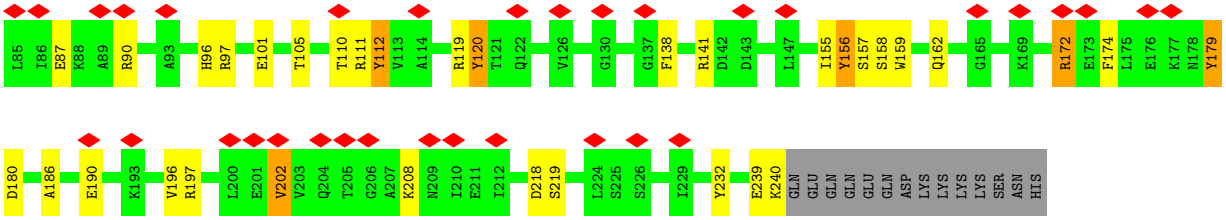




• Molecule 4: Proteasome subunit alpha type-4

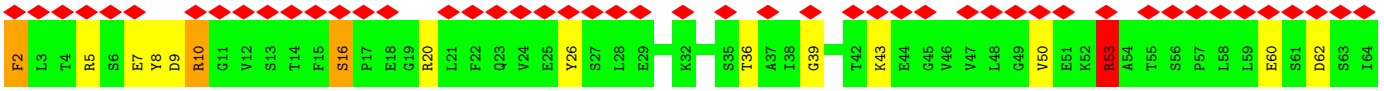
Chain D:

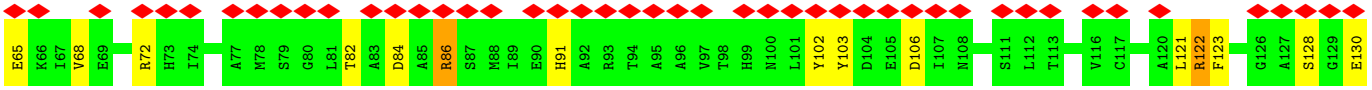


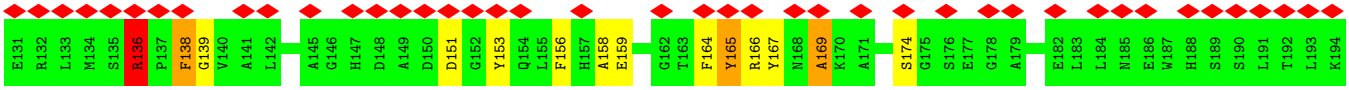


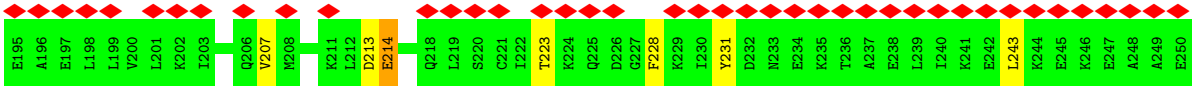
• Molecule 5: Proteasome subunit alpha type-5

Chain e:



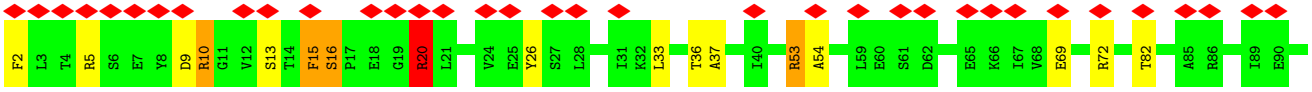


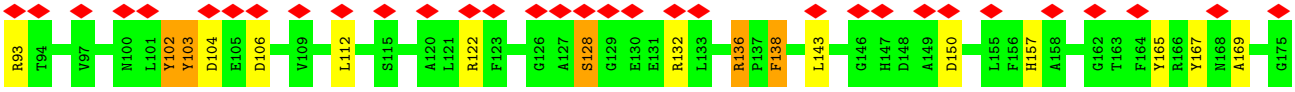


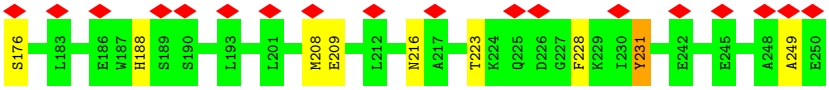


• Molecule 5: Proteasome subunit alpha type-5

Chain E:

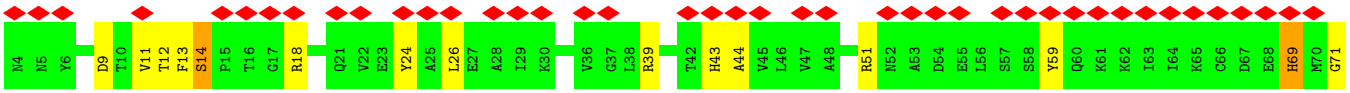


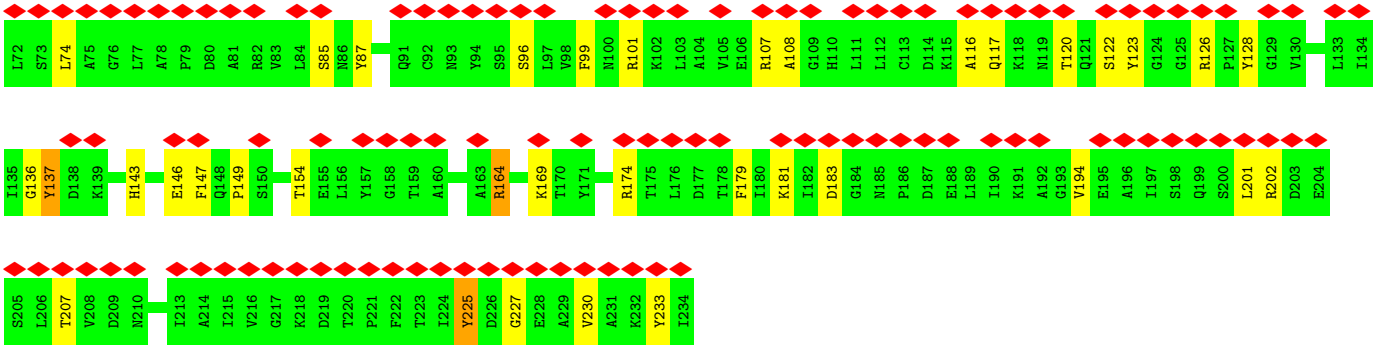




• Molecule 6: Proteasome subunit alpha type-6

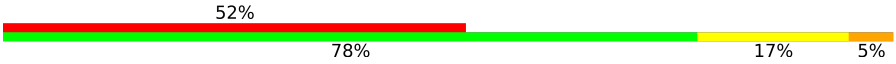
Chain f:

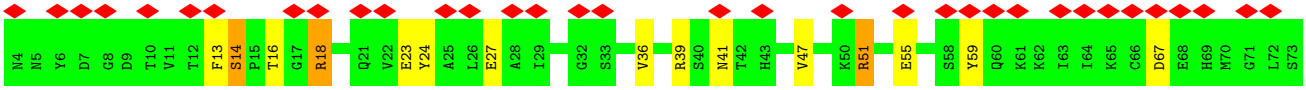


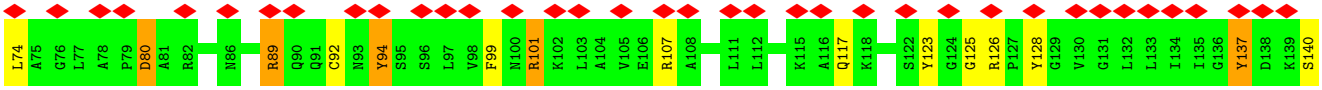


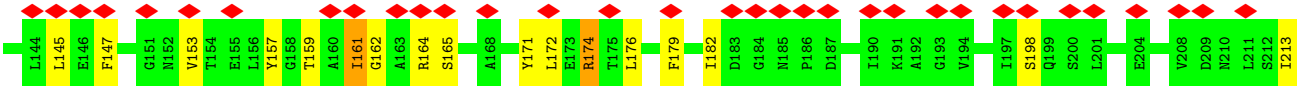
• Molecule 6: Proteasome subunit alpha type-6

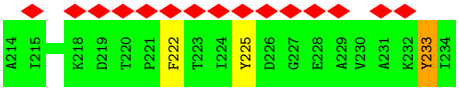
Chain F:





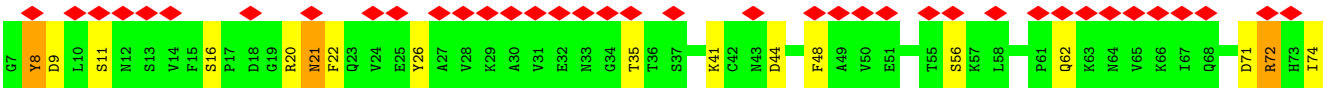


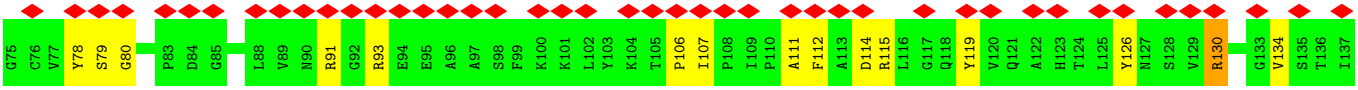


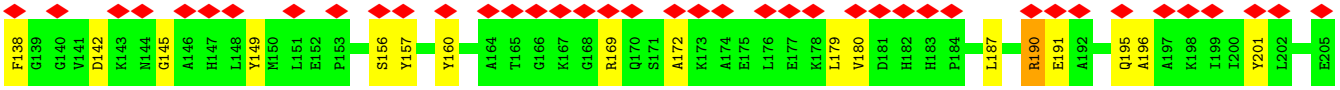


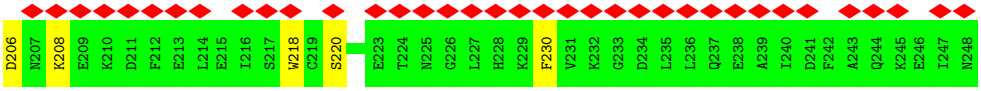
• Molecule 7: Probable proteasome subunit alpha type-7

Chain g:



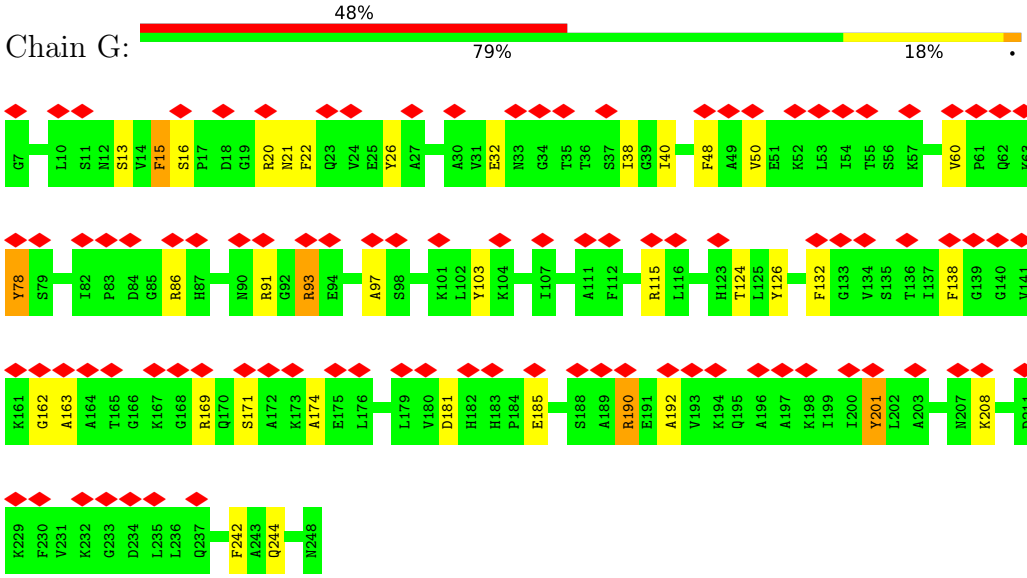






• Molecule 7: Probable proteasome subunit alpha type-7

Chain G:

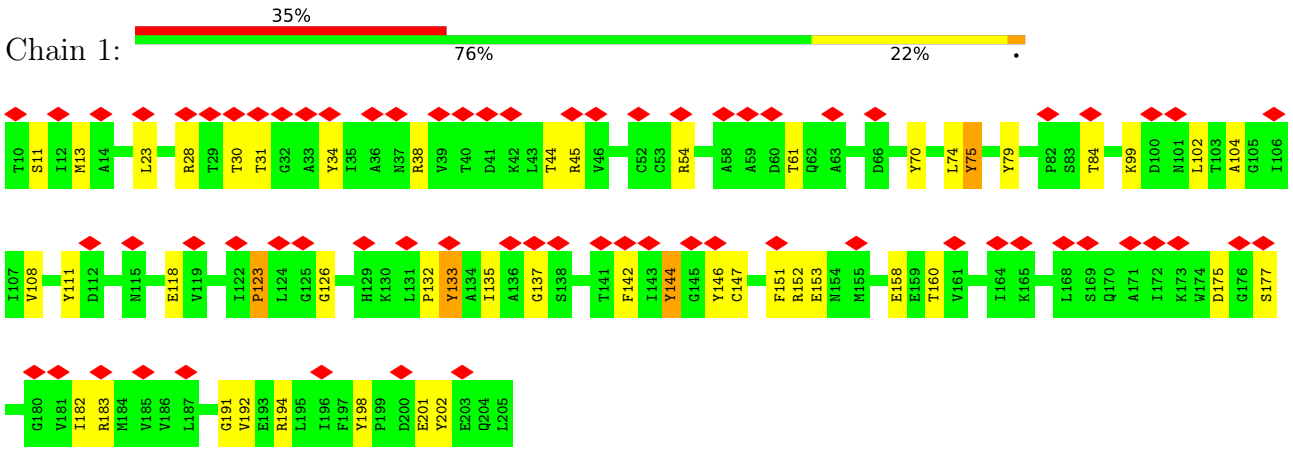


• Molecule 8: Proteasome subunit beta type-1

Chain h:

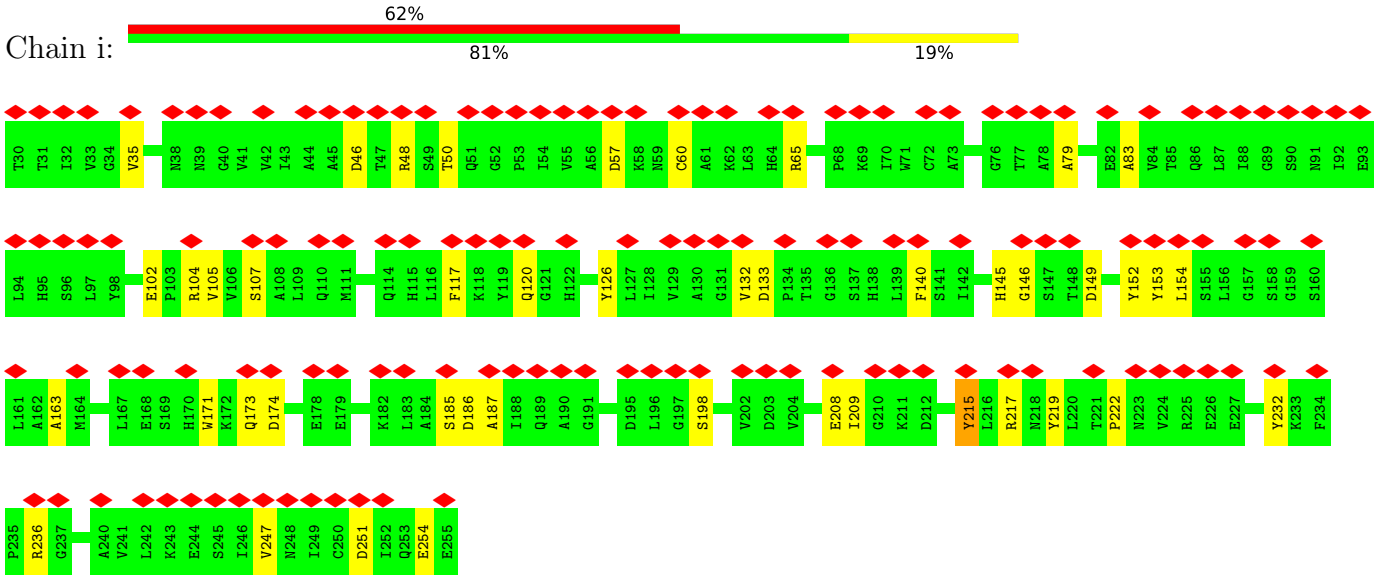
• Molecule 8: Proteasome subunit beta type-1

Chain 1:



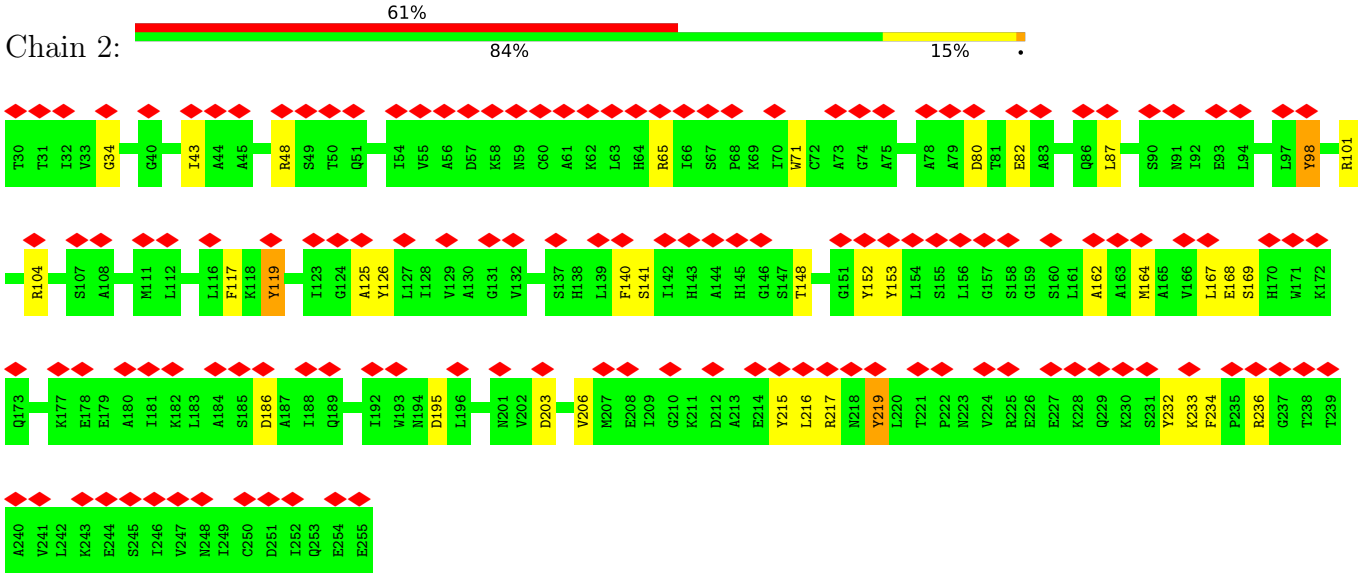
• Molecule 9: Proteasome subunit beta type-2

Chain i:



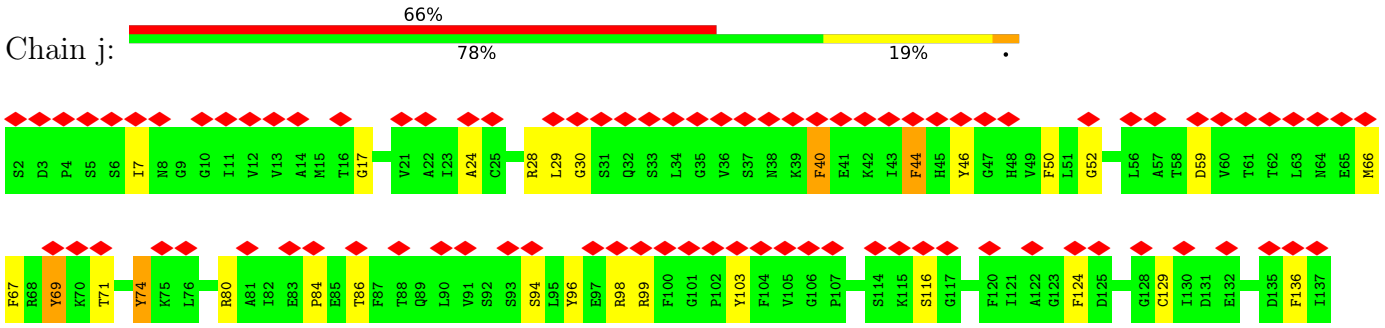
• Molecule 9: Proteasome subunit beta type-2

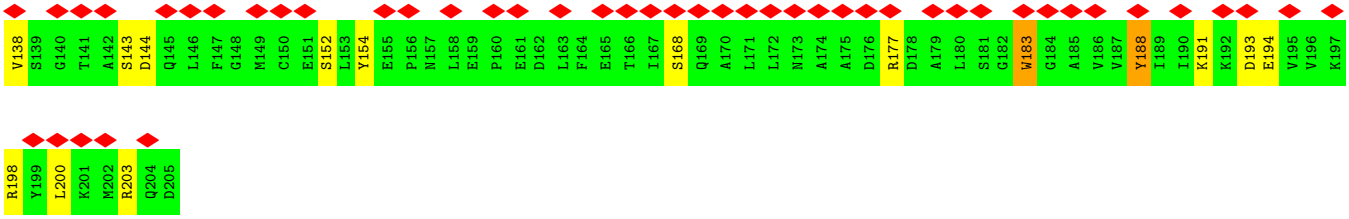
Chain 2:



• Molecule 10: Proteasome subunit beta type-3

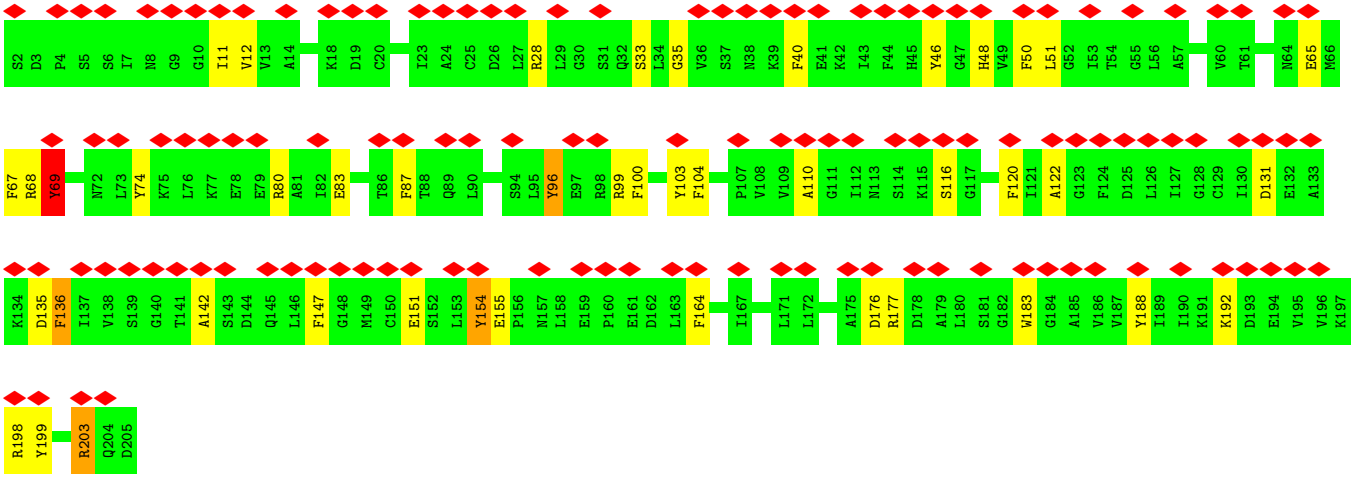
Chain j:





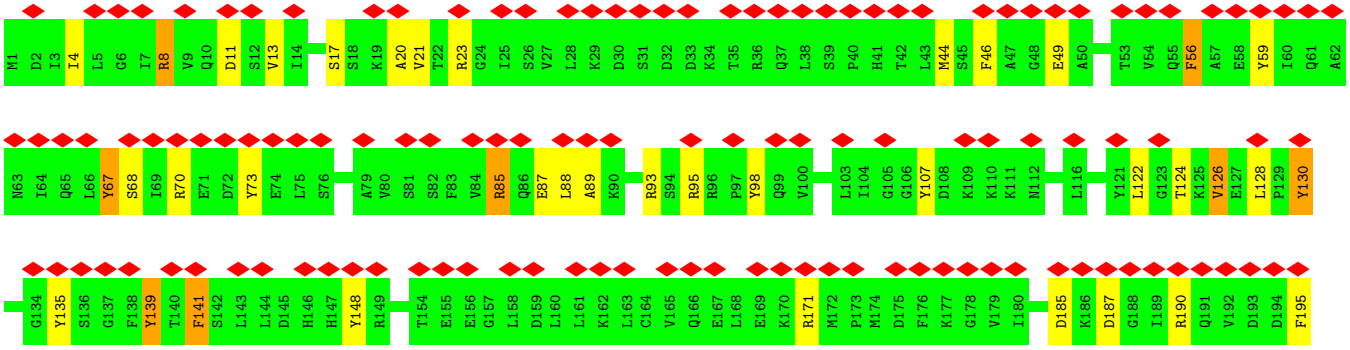
• Molecule 10: Proteasome subunit beta type-3

Chain 3:



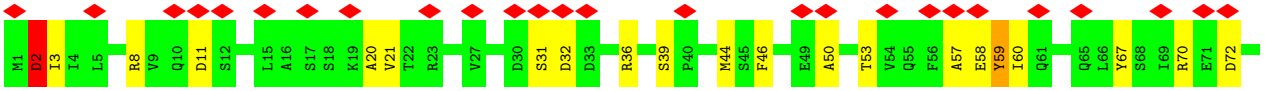
• Molecule 11: Proteasome subunit beta type-4

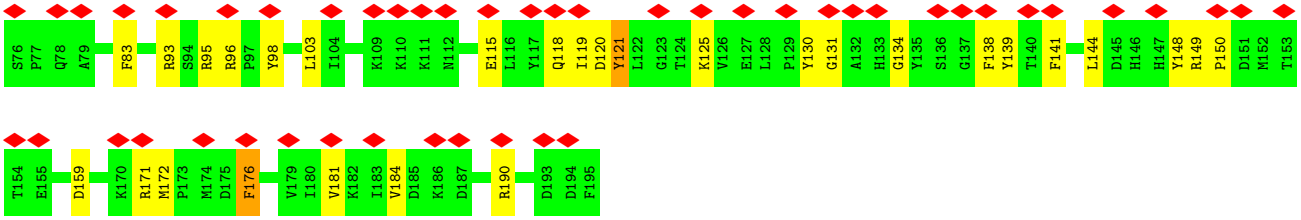
Chain k:



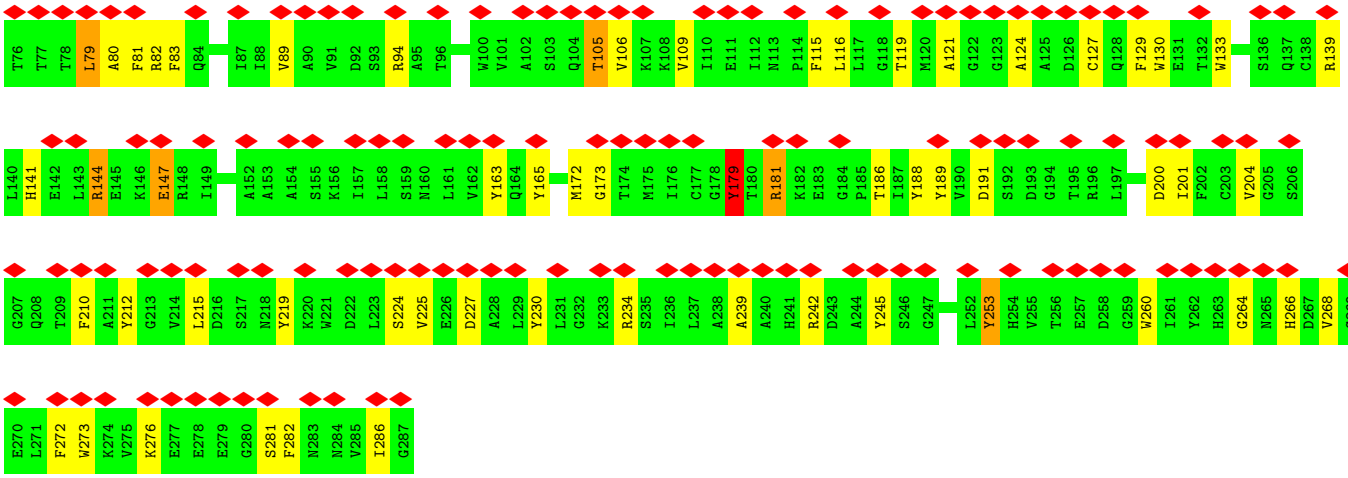
• Molecule 11: Proteasome subunit beta type-4

Chain 4:

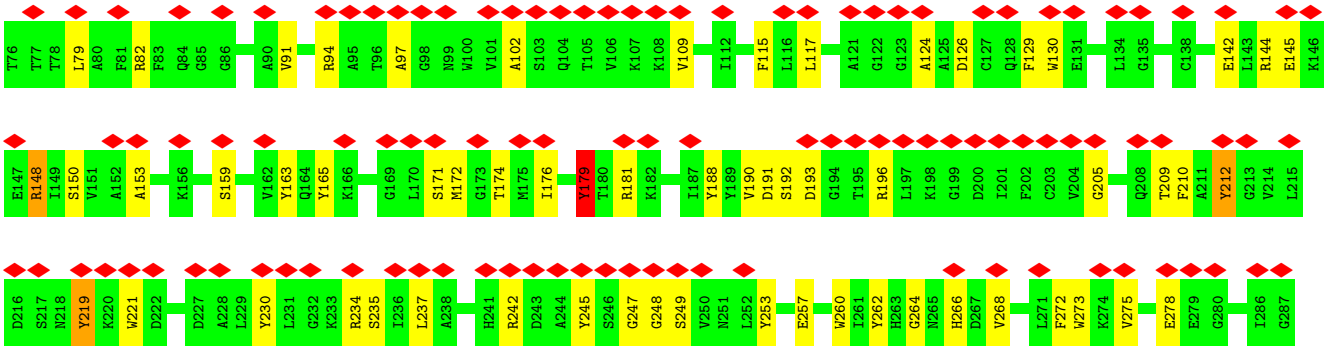




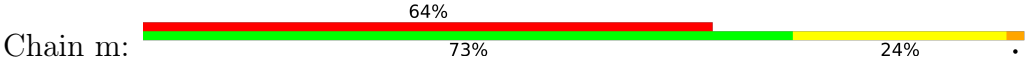
• Molecule 12: Proteasome subunit beta type-5

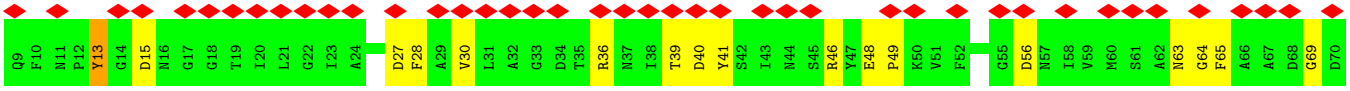


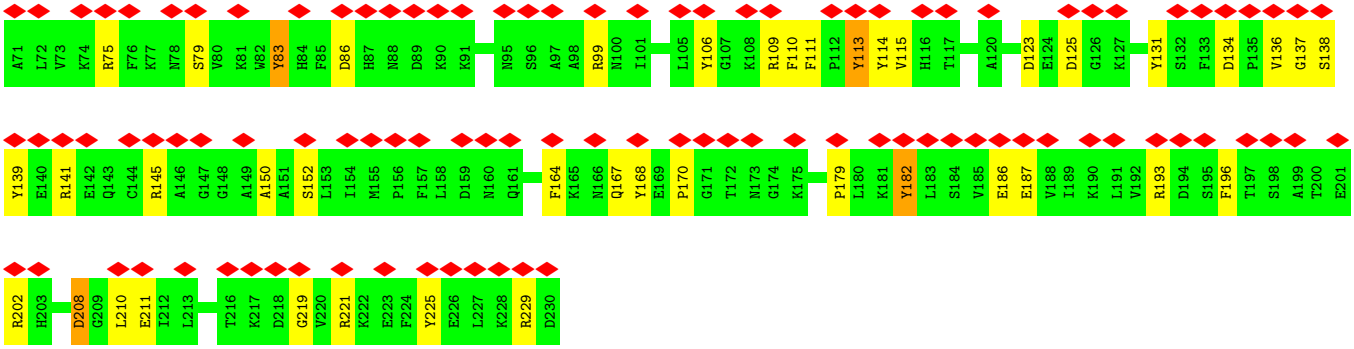
• Molecule 12: Proteasome subunit beta type-5



• Molecule 13: Proteasome subunit beta type-6

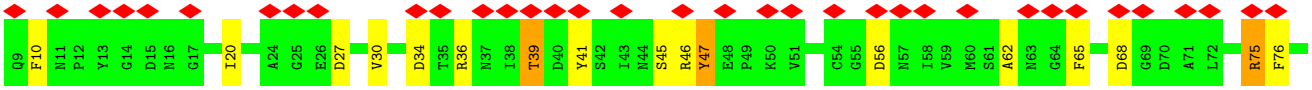


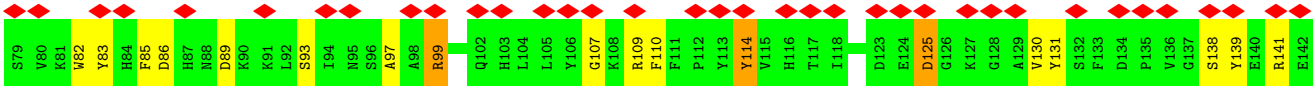


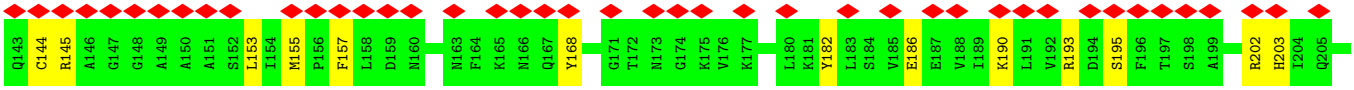


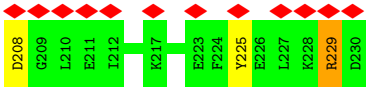
• Molecule 13: Proteasome subunit beta type-6

Chain 6:



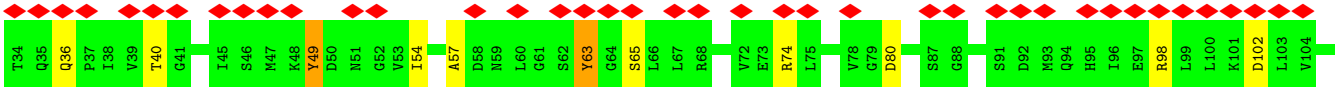


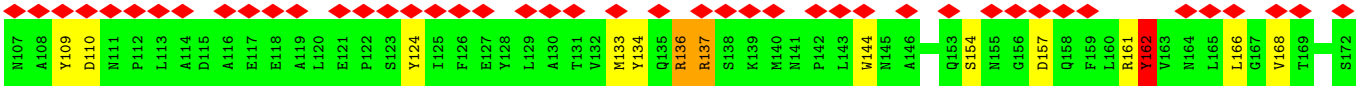


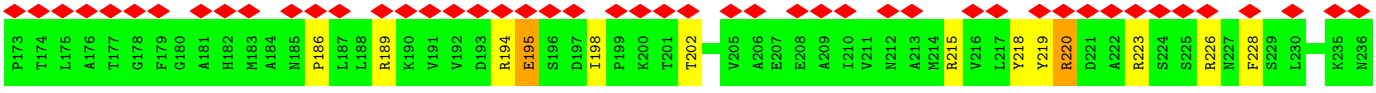


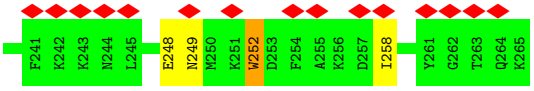
• Molecule 14: Proteasome subunit beta type-7

Chain n:



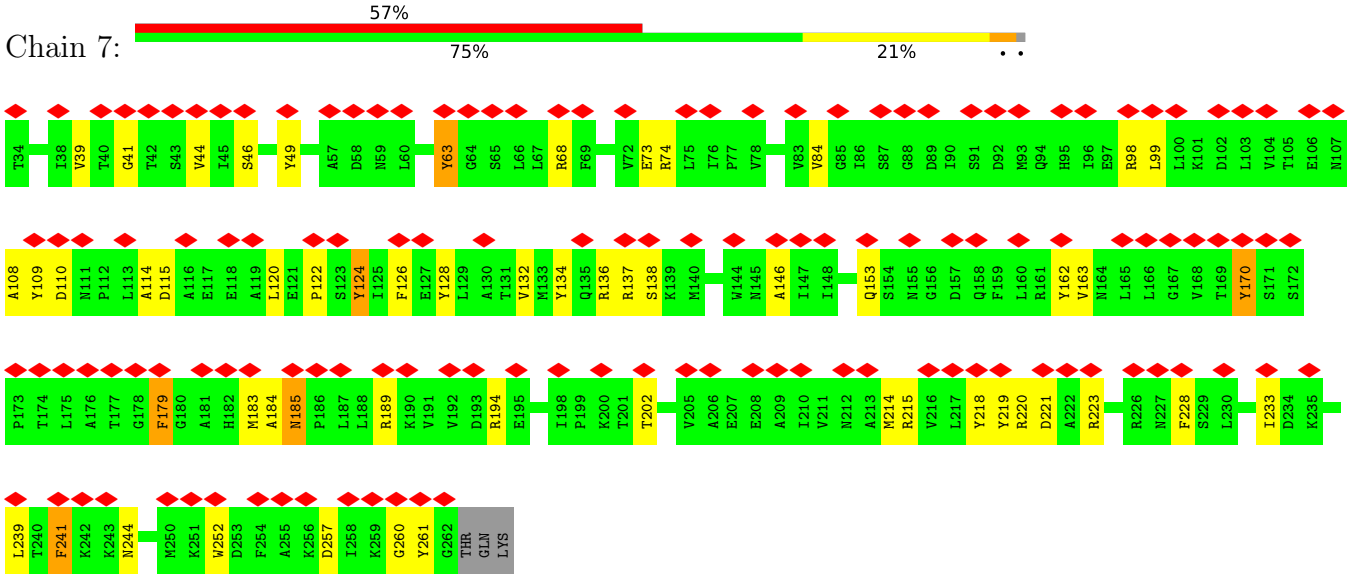






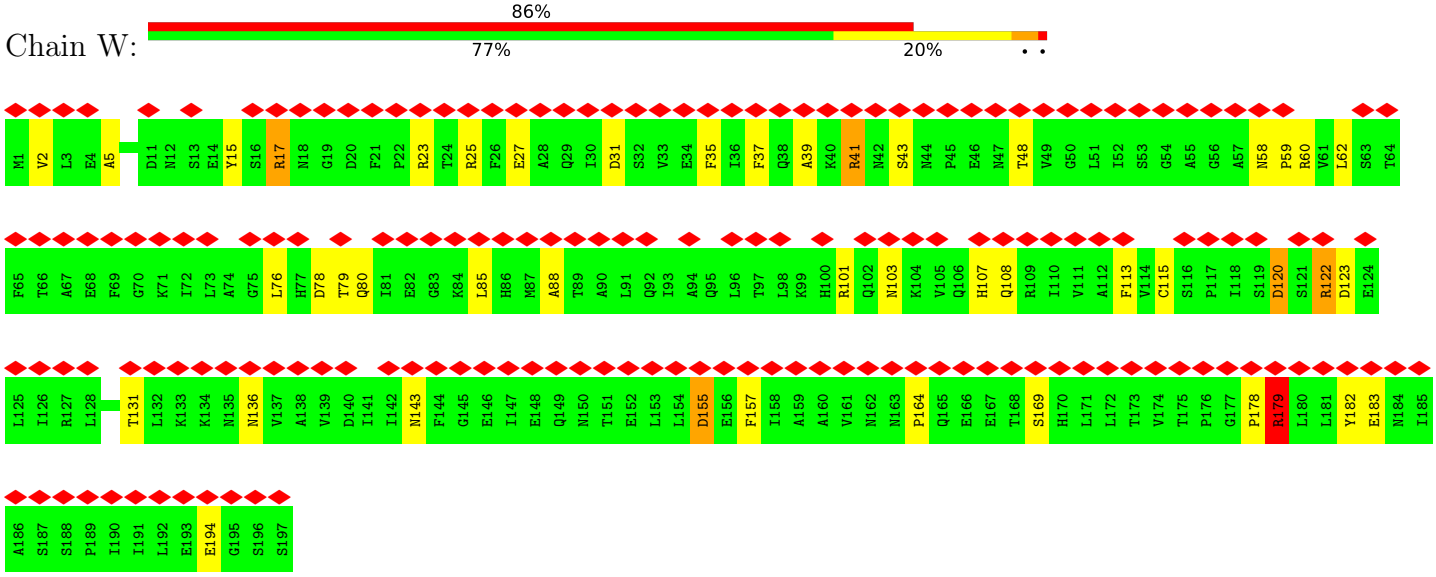
• Molecule 14: Proteasome subunit beta type-7

Chain 7:



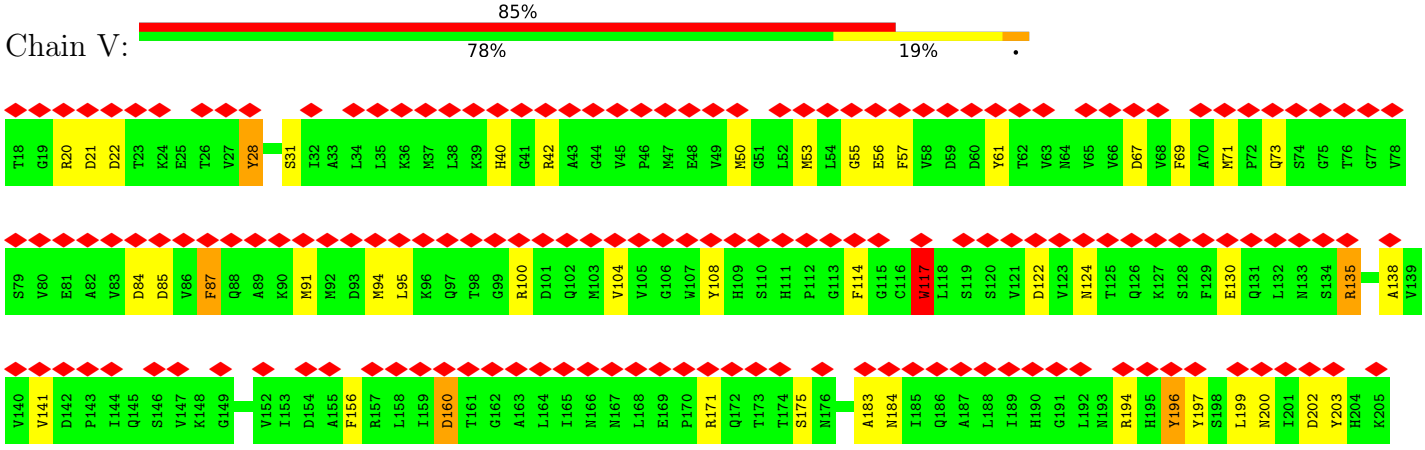
• Molecule 15: 26S proteasome regulatory subunit RPN10

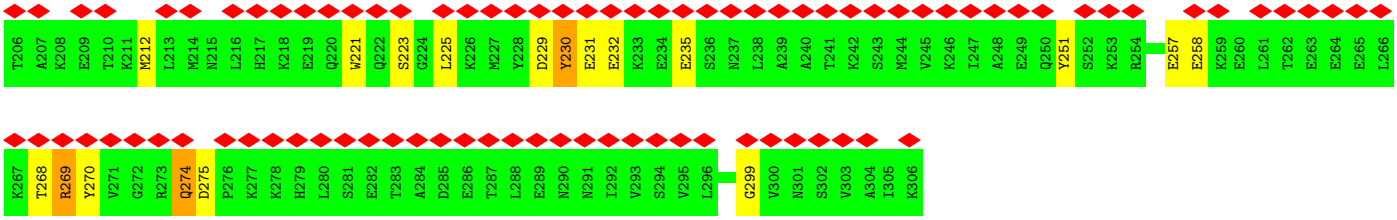
Chain W:



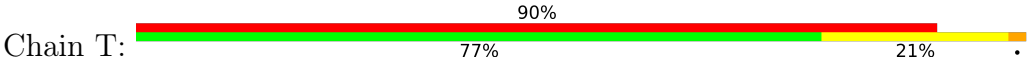
• Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

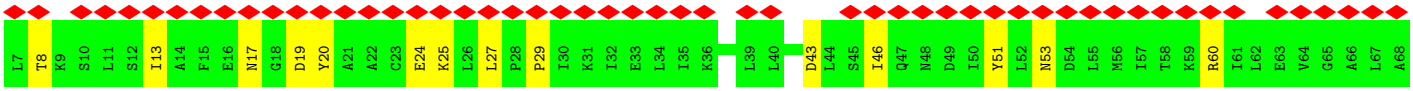
Chain V:

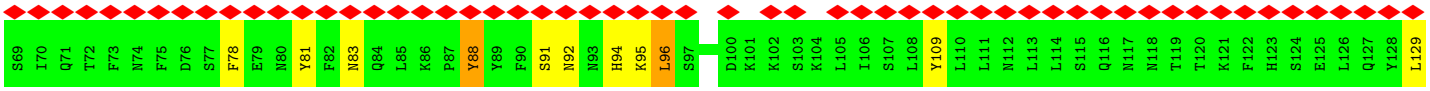


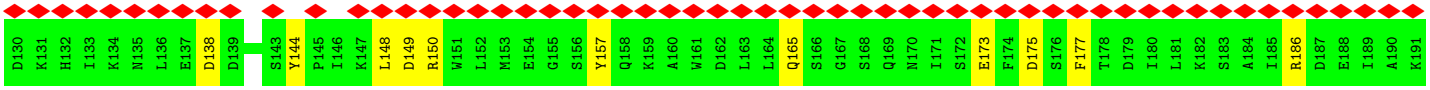


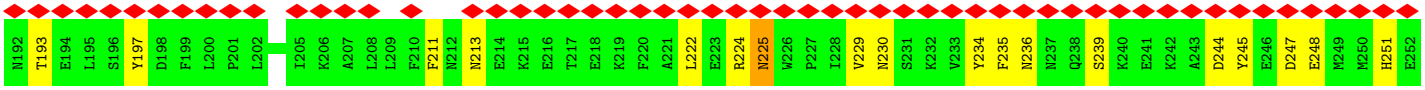
• Molecule 17: 26S proteasome regulatory subunit RPN12

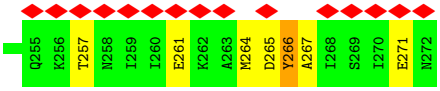




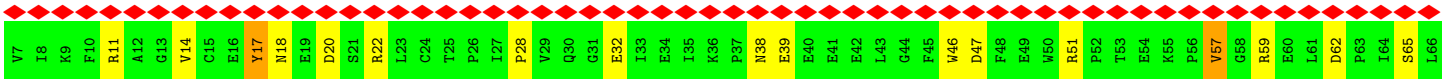


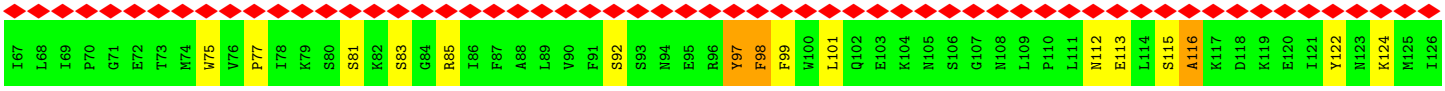


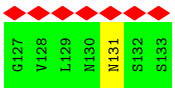




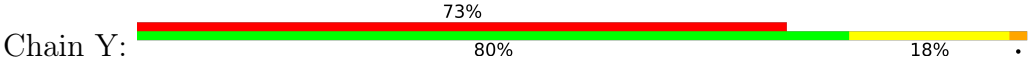
• Molecule 18: 26S proteasome regulatory subunit RPN13

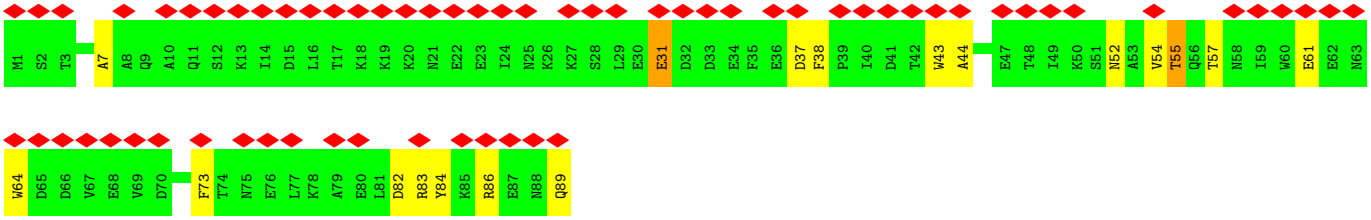






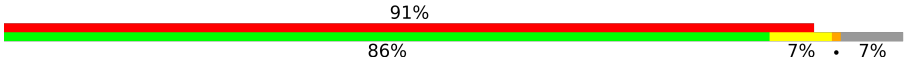
• Molecule 19: 26S proteasome complex subunit SEM1

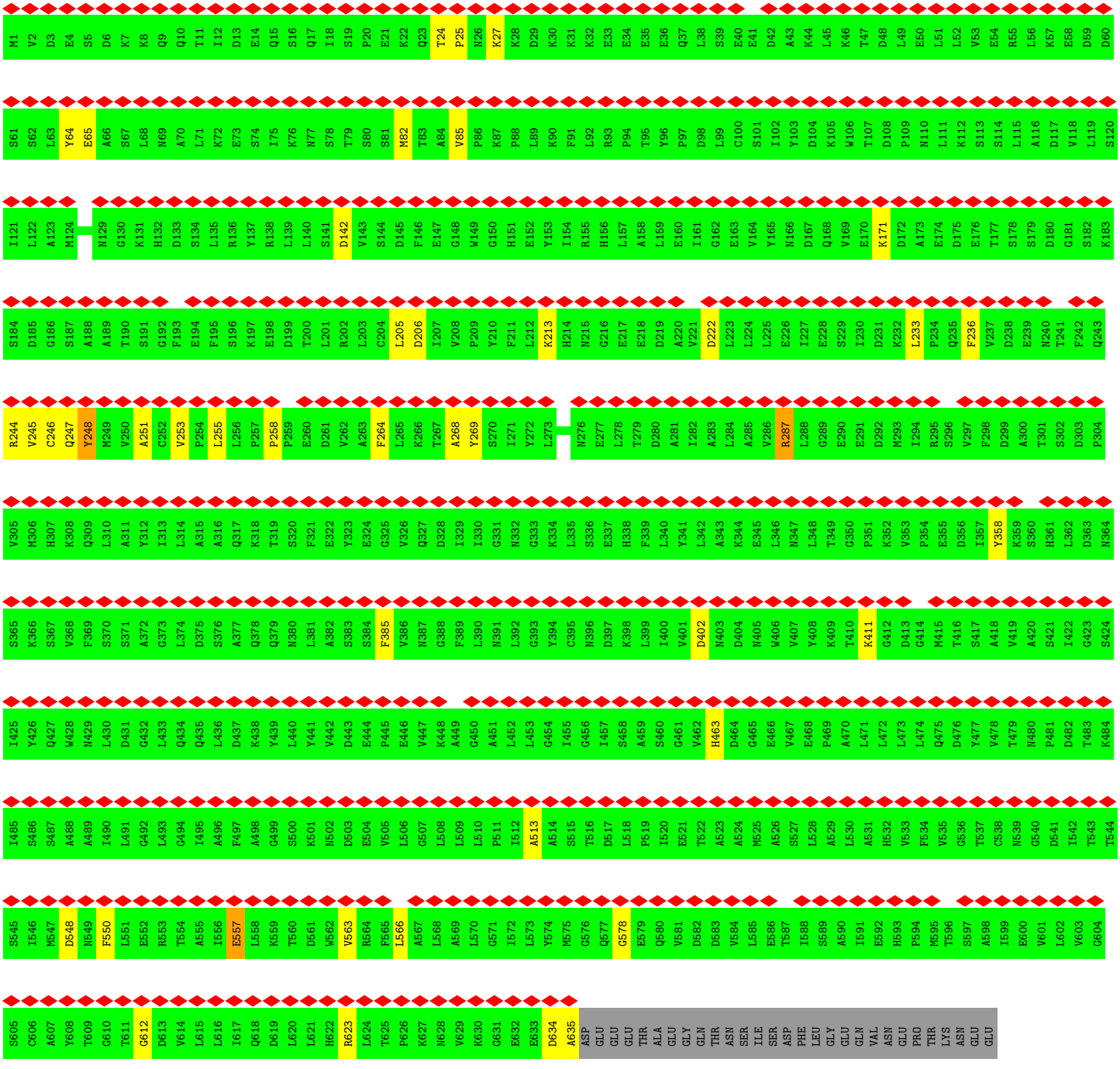


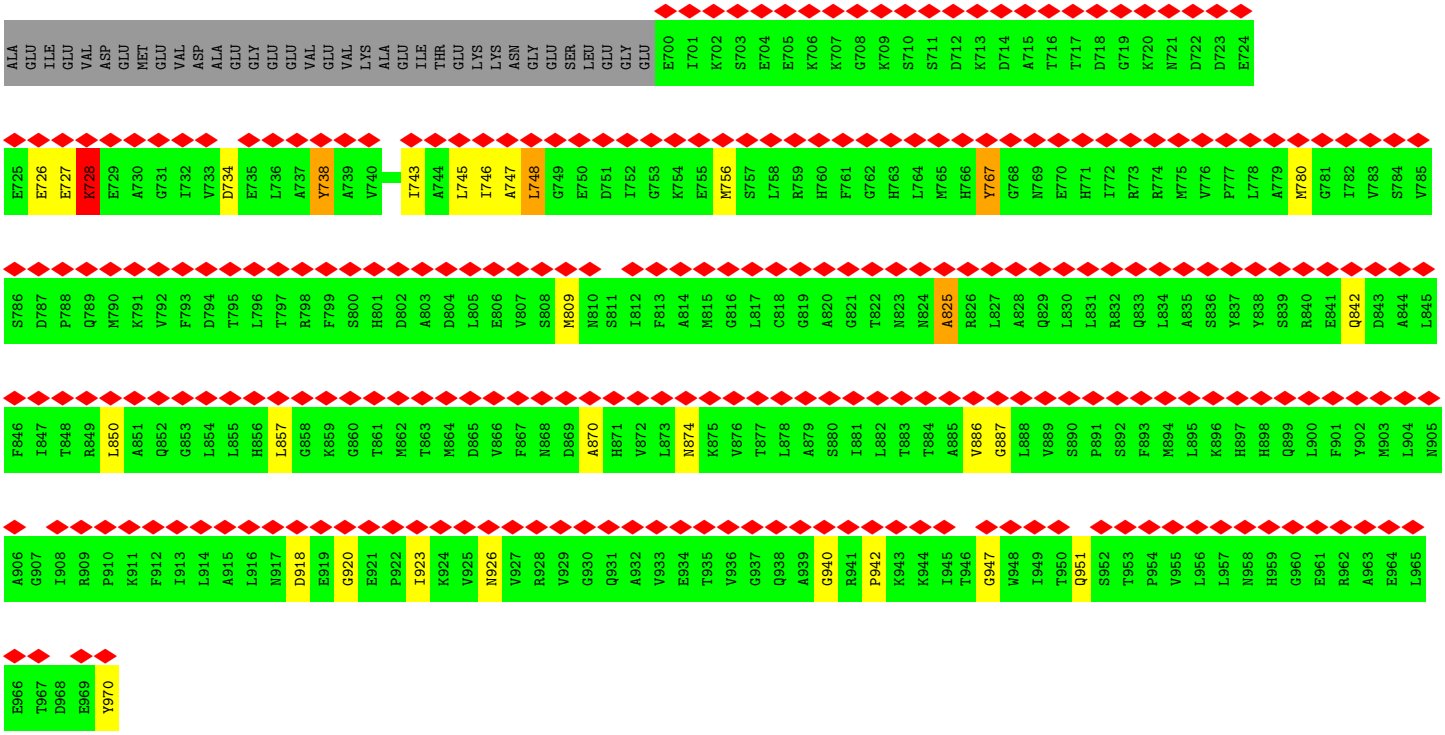


• Molecule 20: 26S proteasome regulatory subunit RPN1

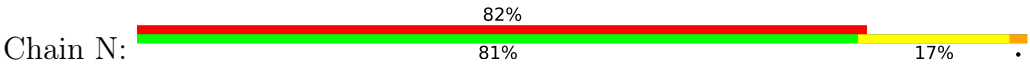
Chain Z:

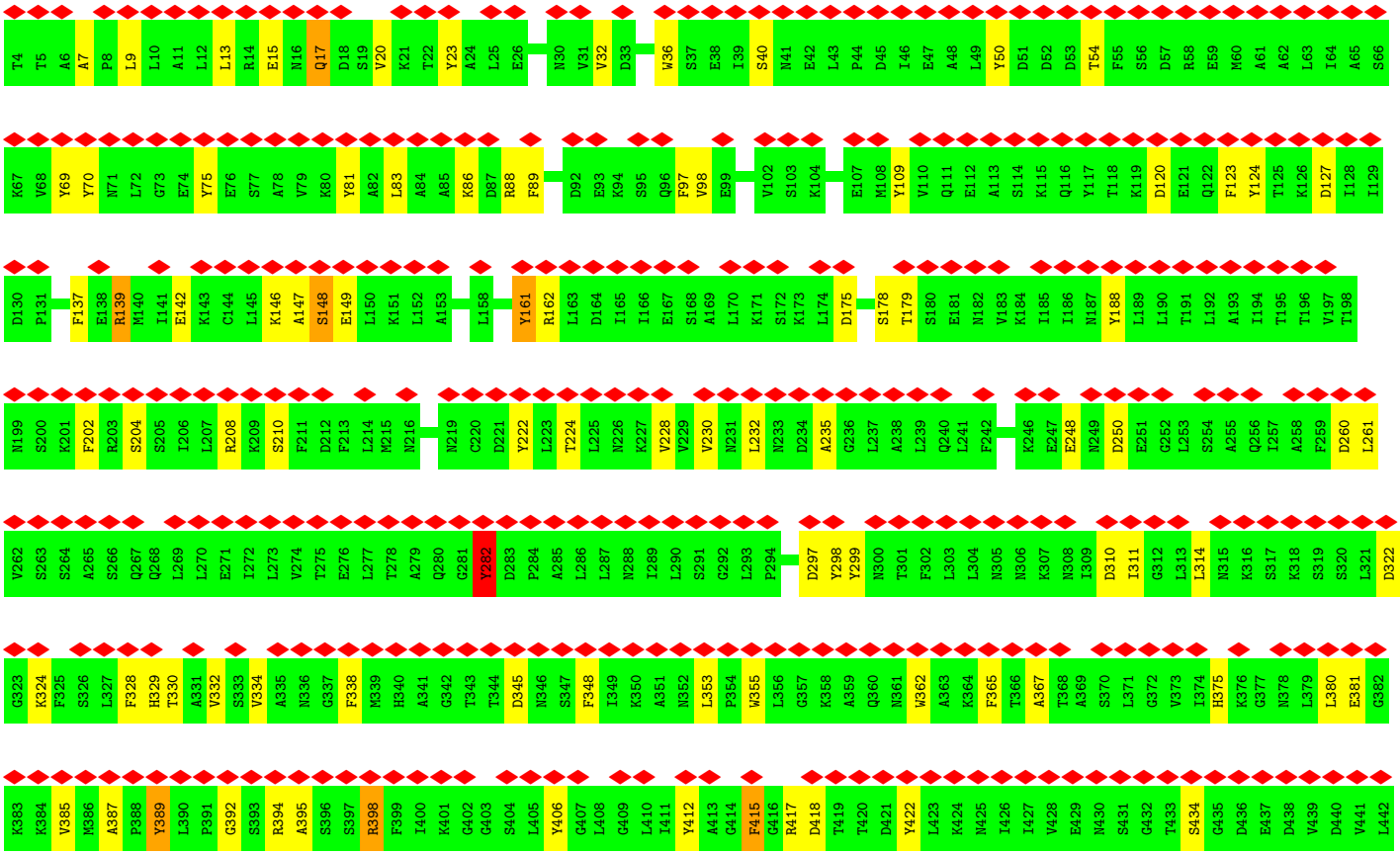


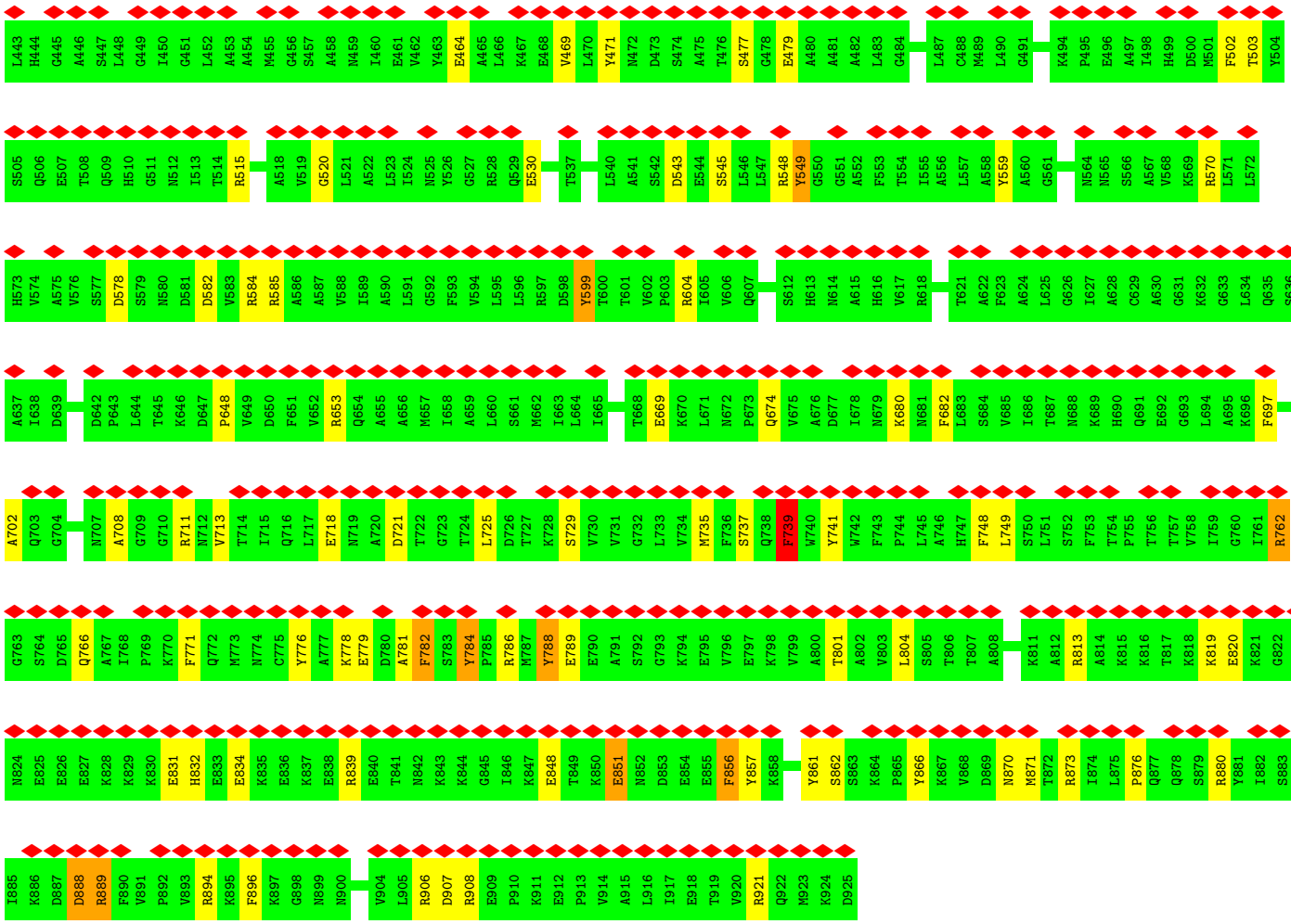




• Molecule 21: 26S proteasome regulatory subunit RPN2

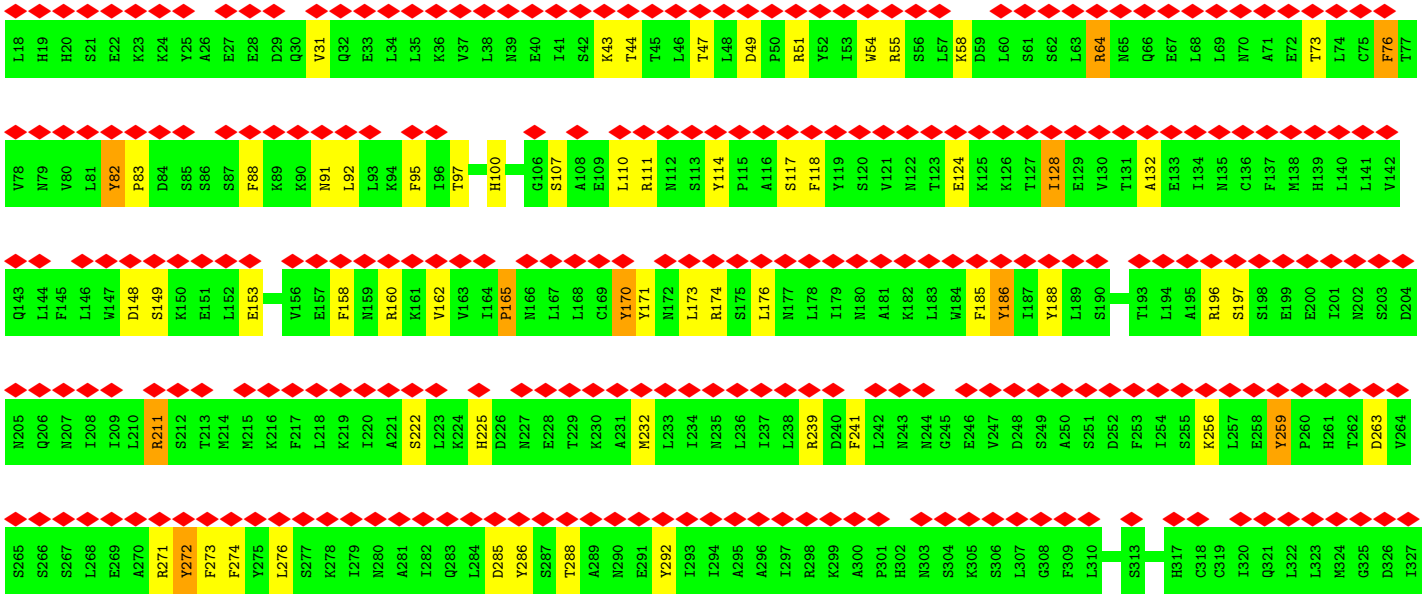


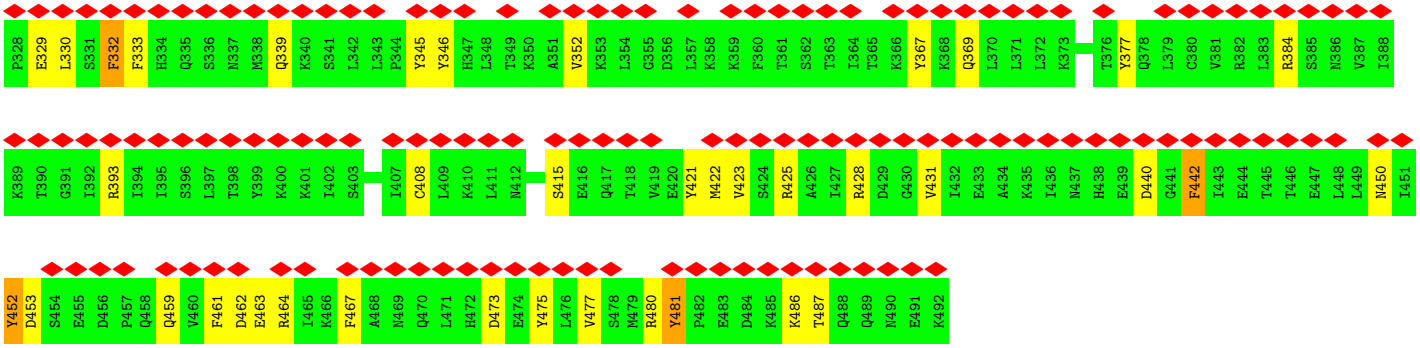




• Molecule 22: 26S proteasome regulatory subunit RPN3

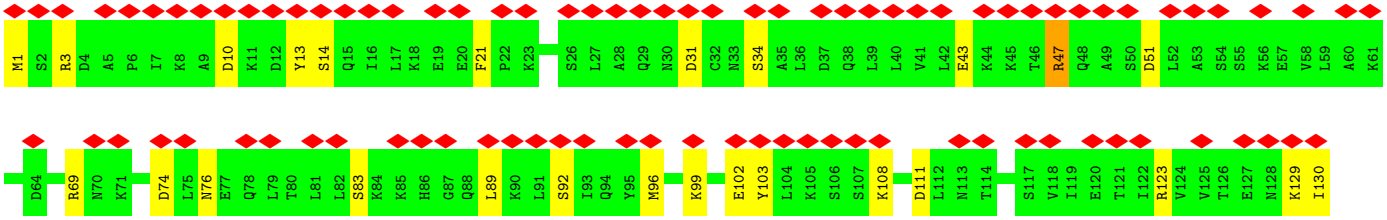
Chain S:





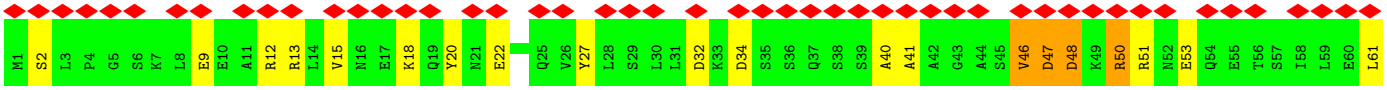
• Molecule 23: 26S proteasome regulatory subunit RPN5

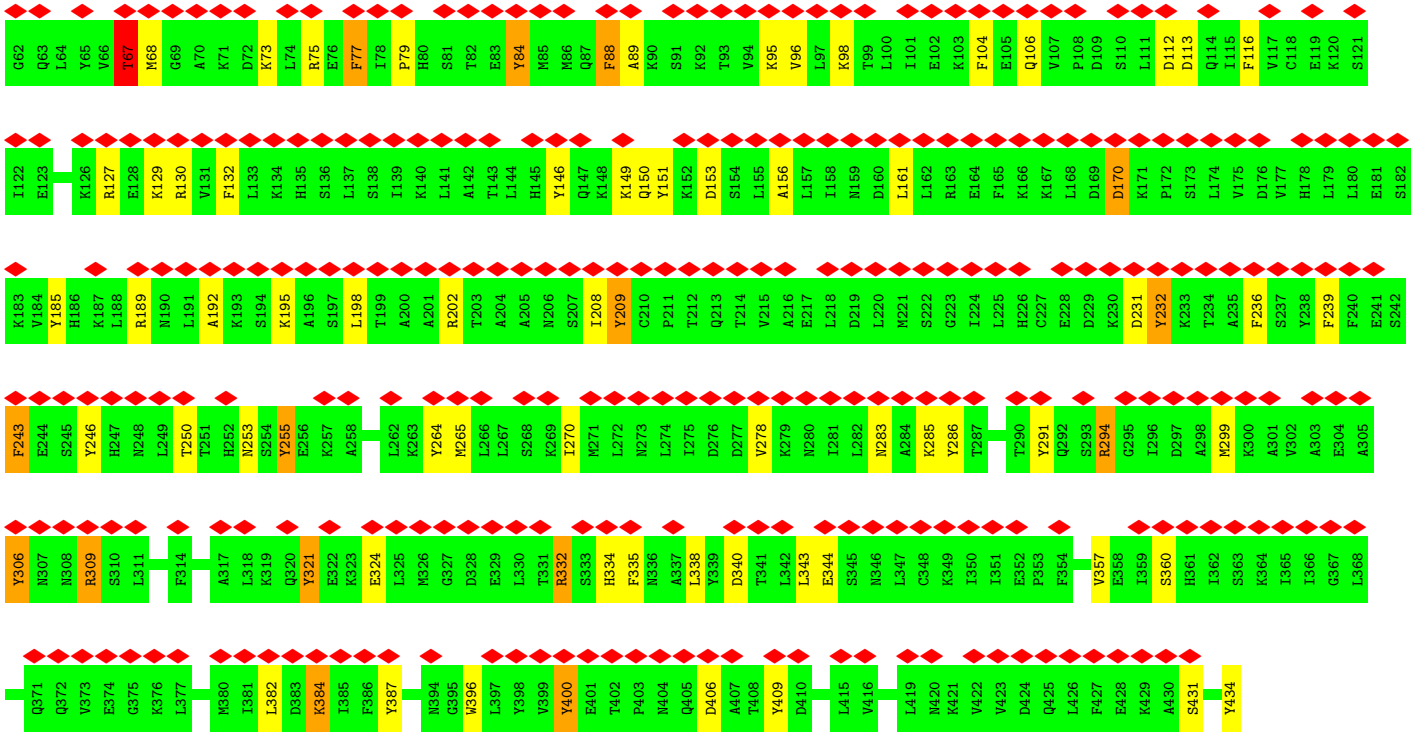
Chain P:



• Molecule 24: 26S proteasome regulatory subunit RPN6

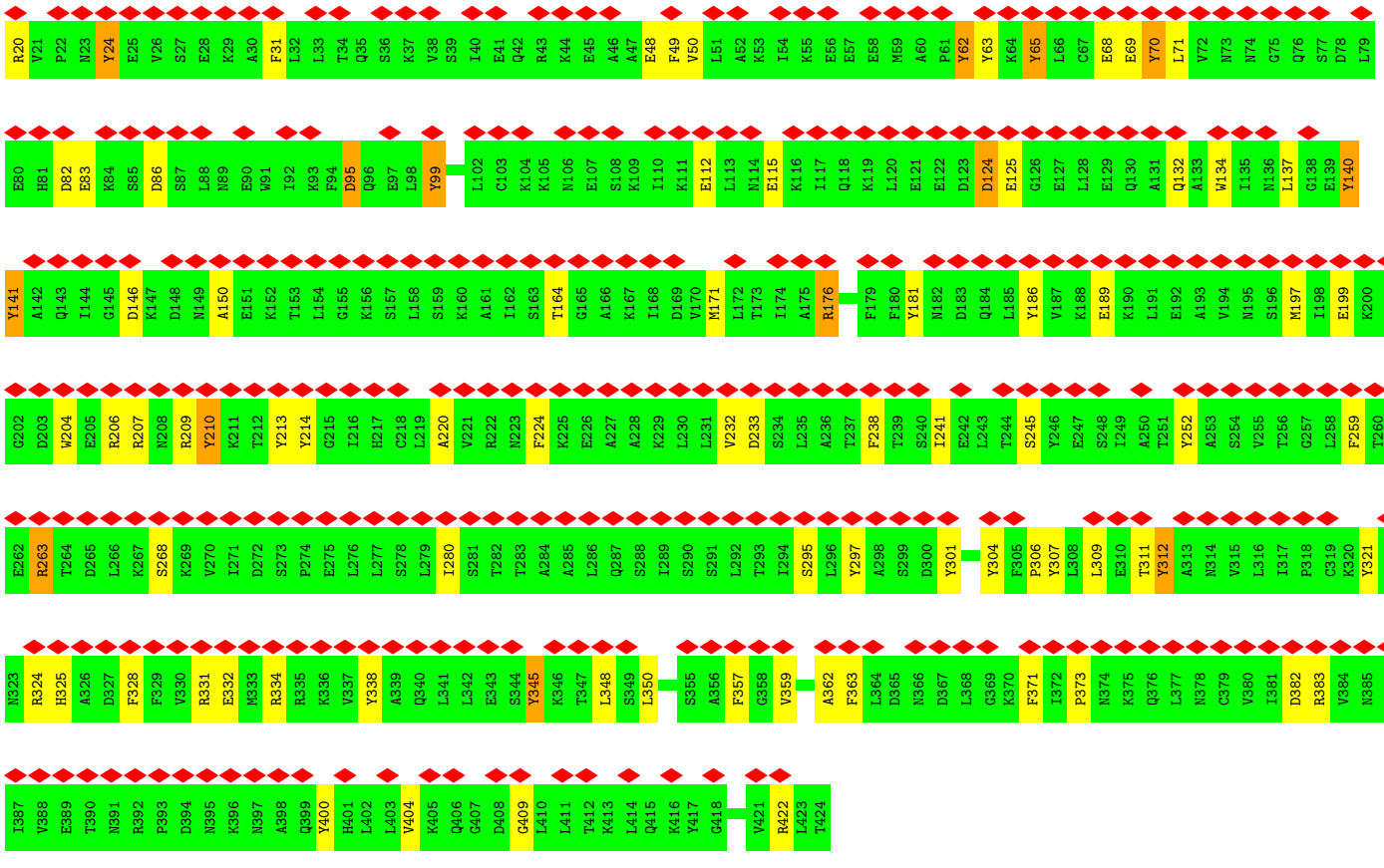
Chain Q:





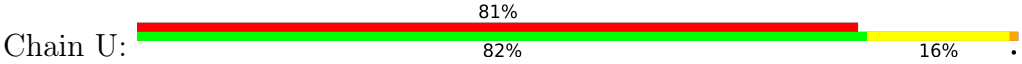
• Molecule 25: 26S proteasome regulatory subunit RPN7

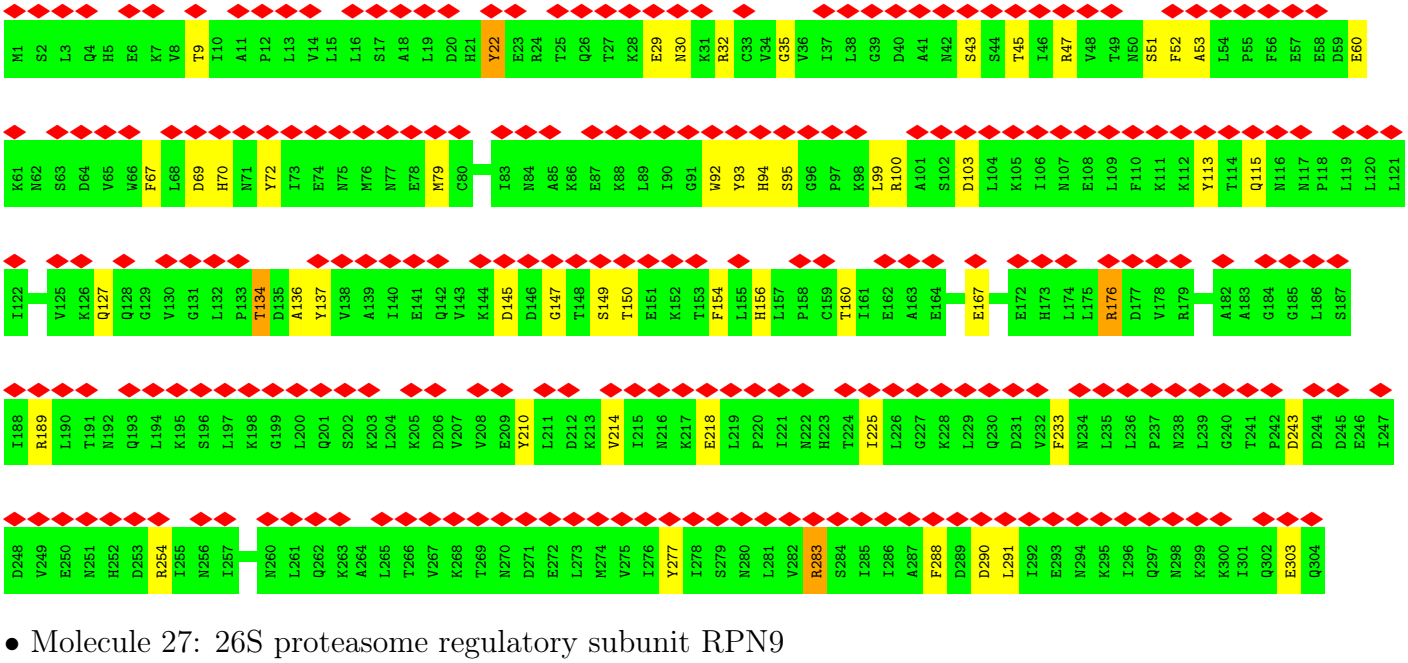
Chain R:



• Molecule 26: 26S proteasome regulatory subunit RPN8

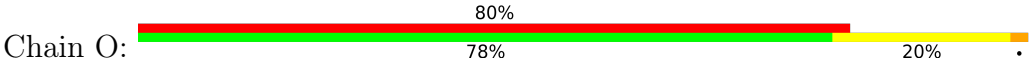
Chain U:

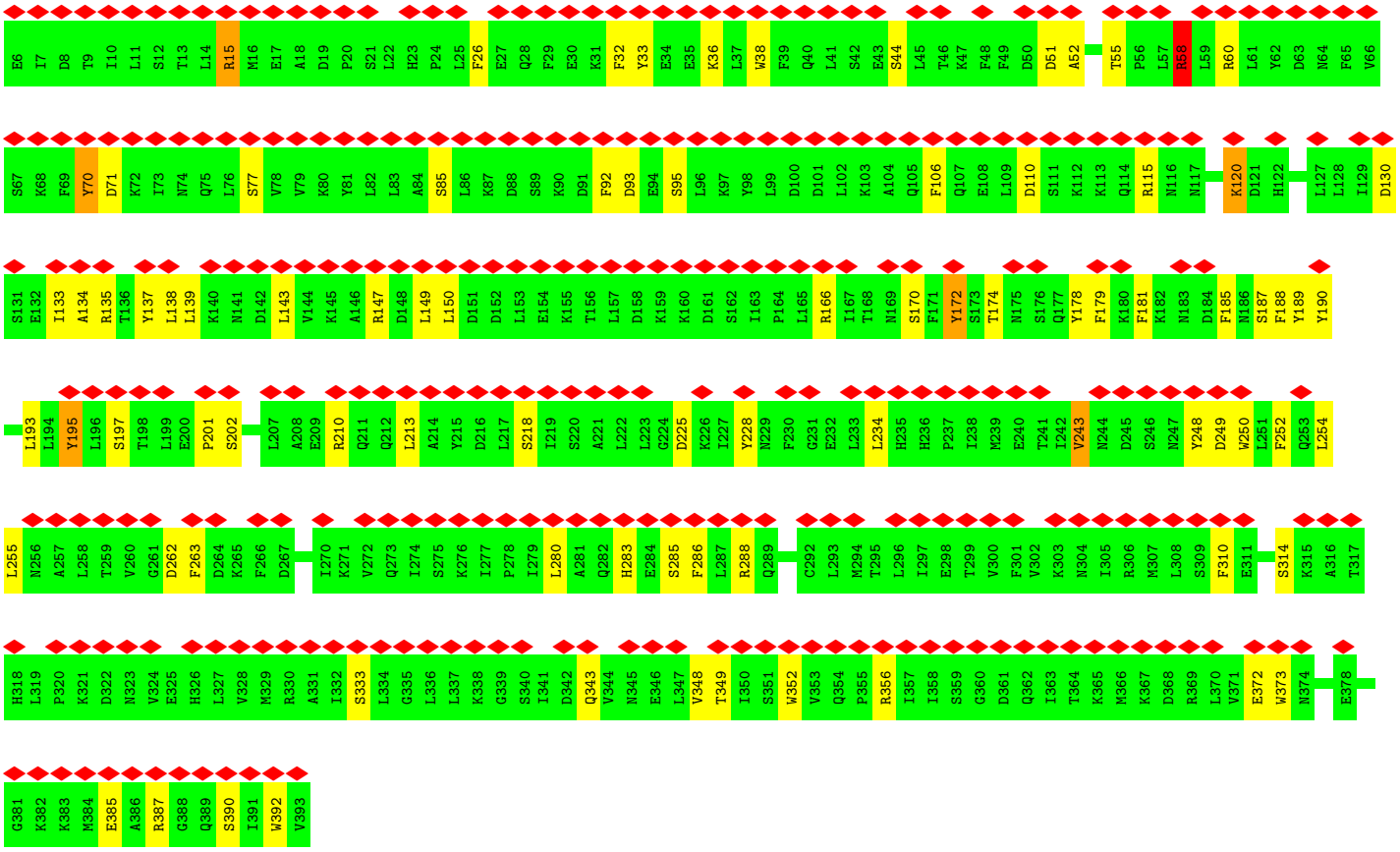




• Molecule 27: 26S proteasome regulatory subunit RPN9

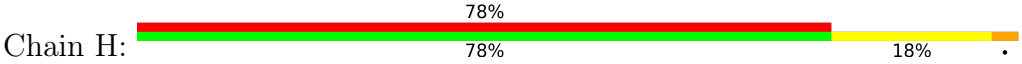
Chain O:

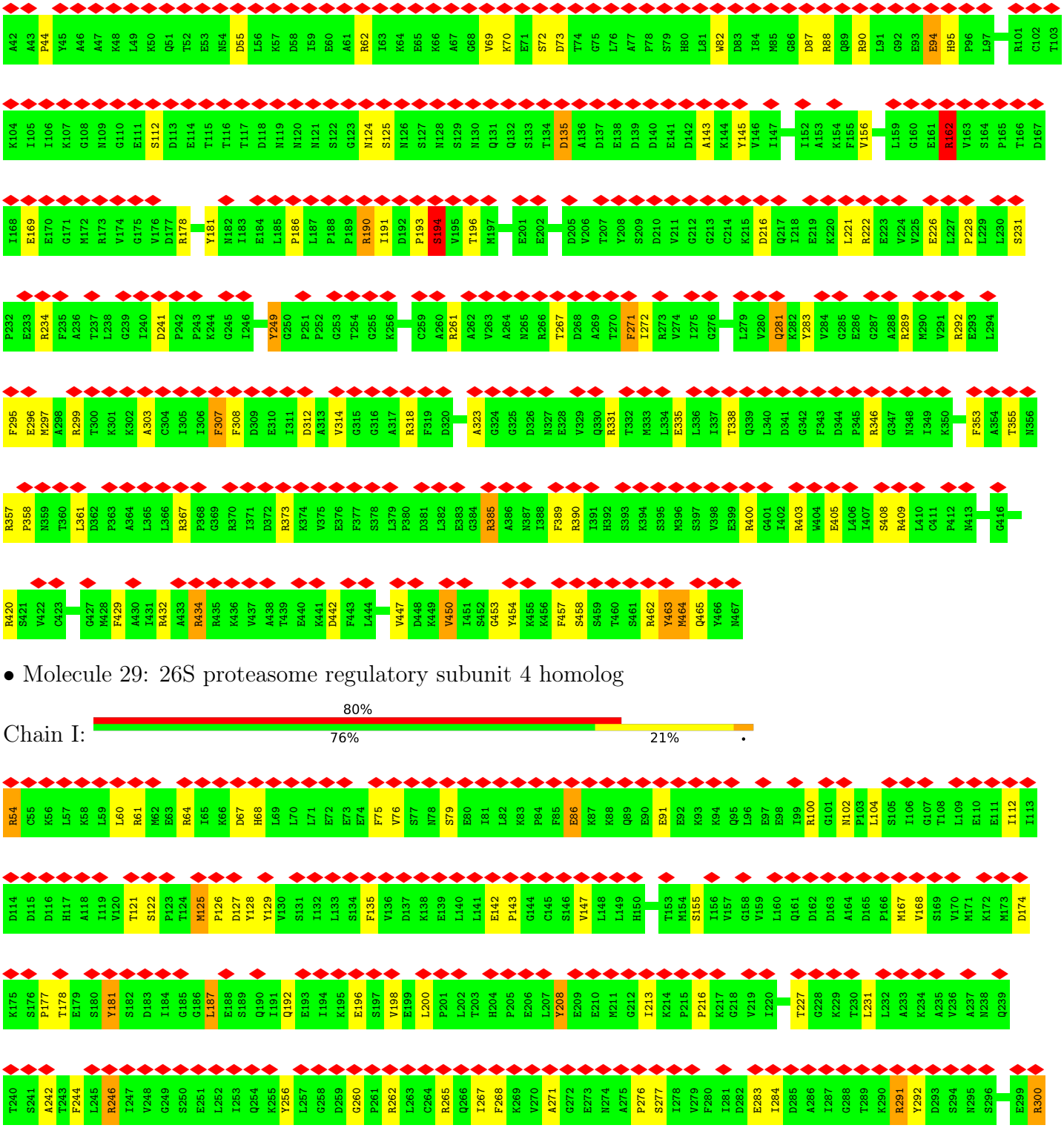




• Molecule 28: 26S proteasome regulatory subunit 7 homolog

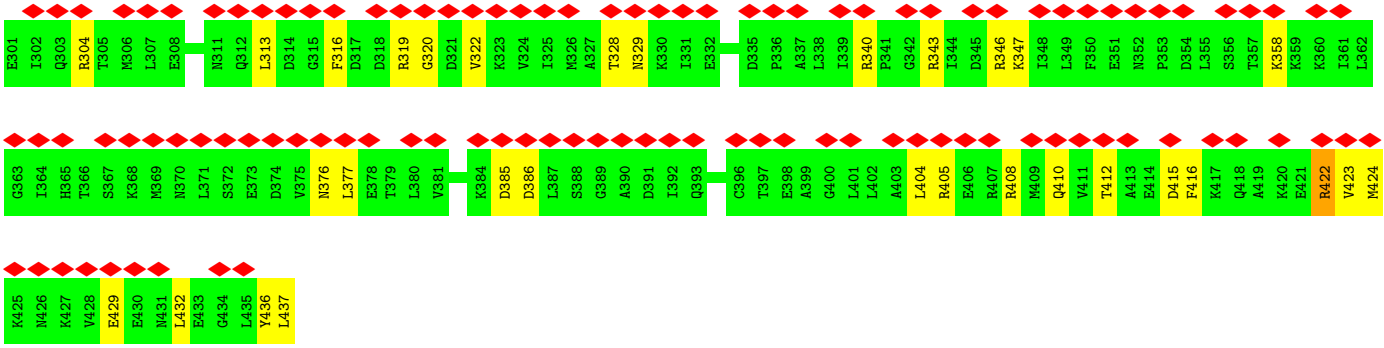
Chain H:





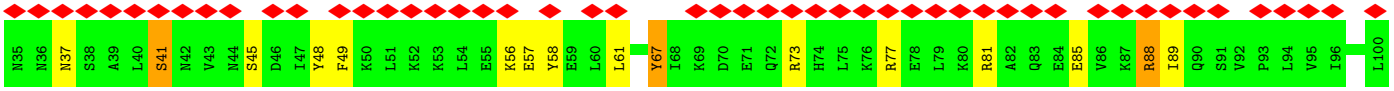
• Molecule 29: 26S proteasome regulatory subunit 4 homolog

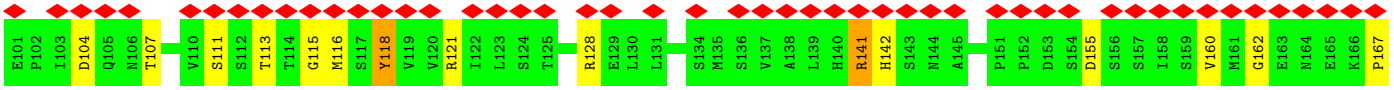
Chain I:

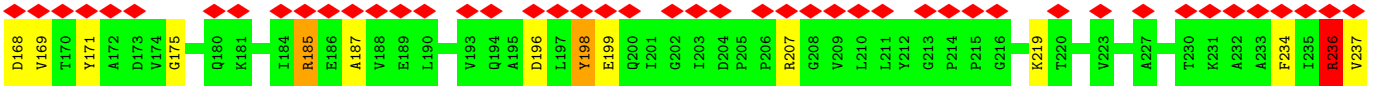


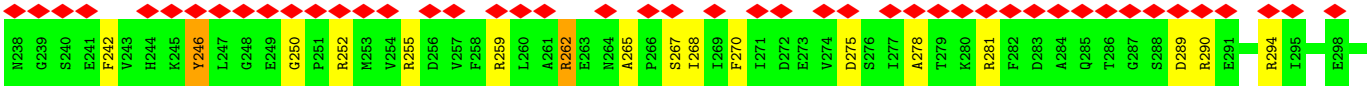
• Molecule 30: 26S proteasome regulatory subunit 6B homolog

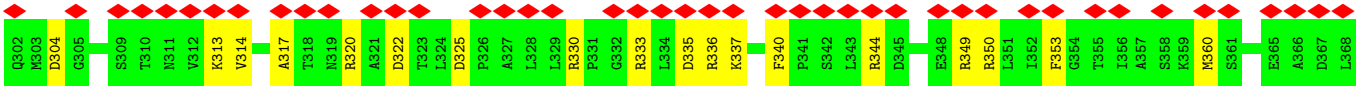
Chain K:

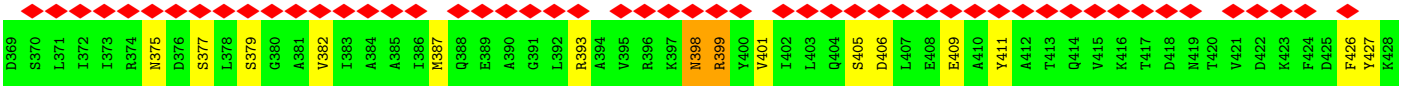






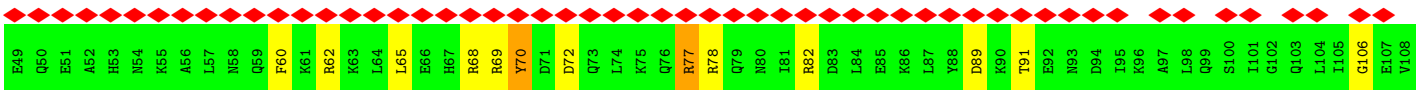


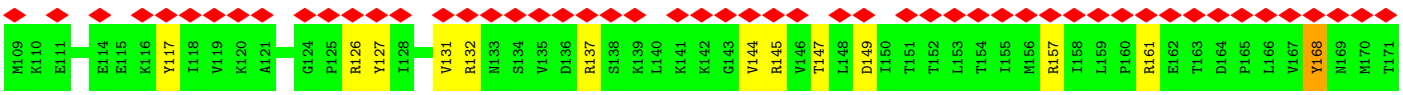


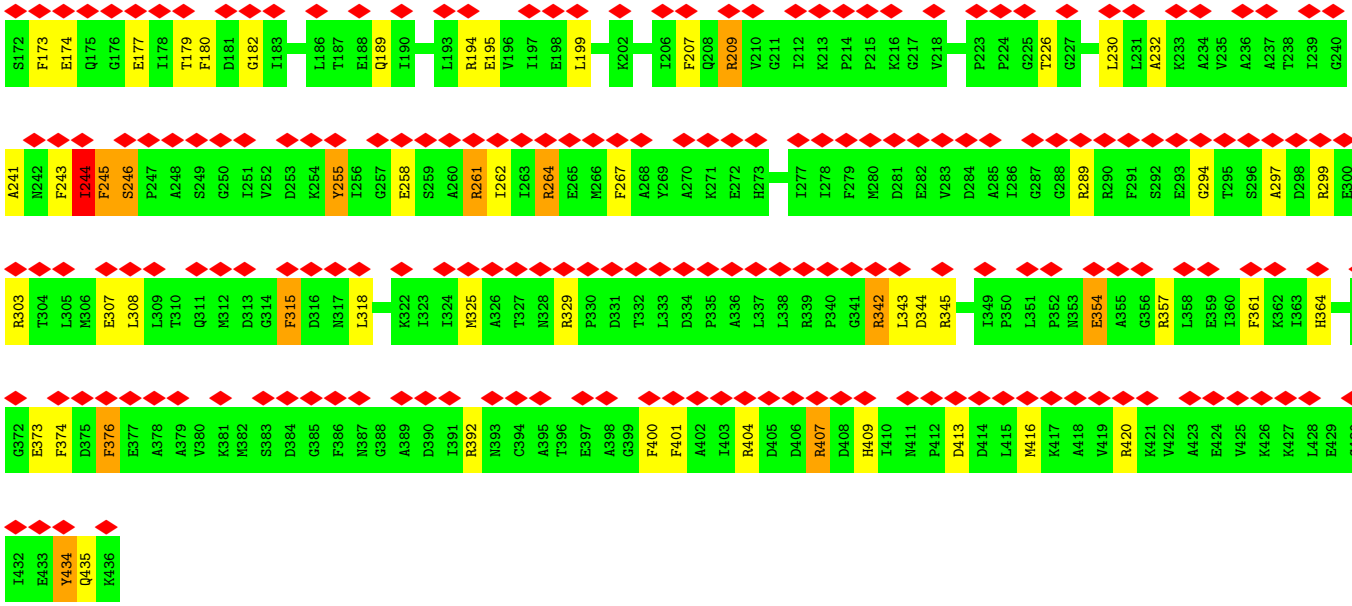


• Molecule 31: 26S proteasome subunit RPT4

Chain L:

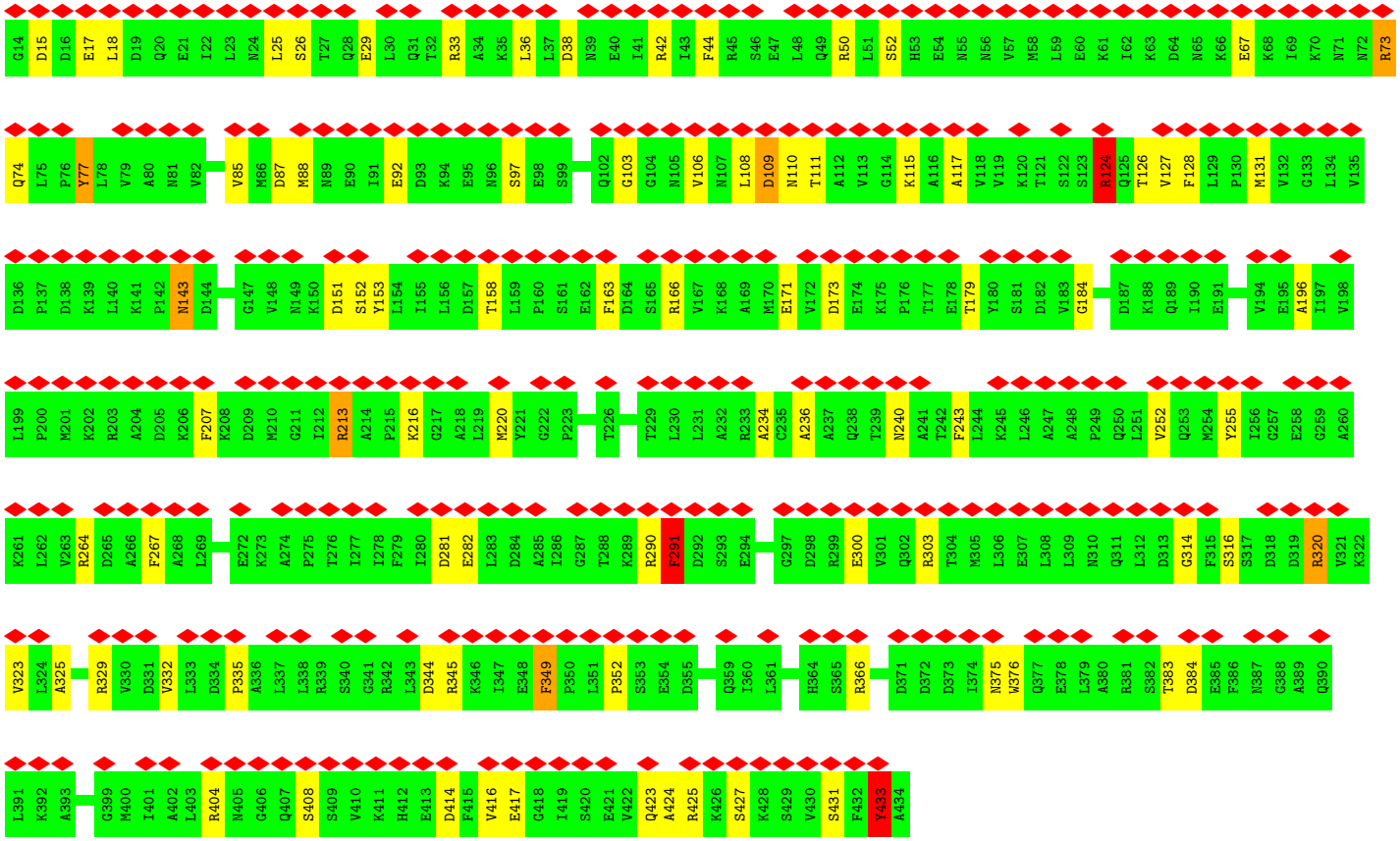






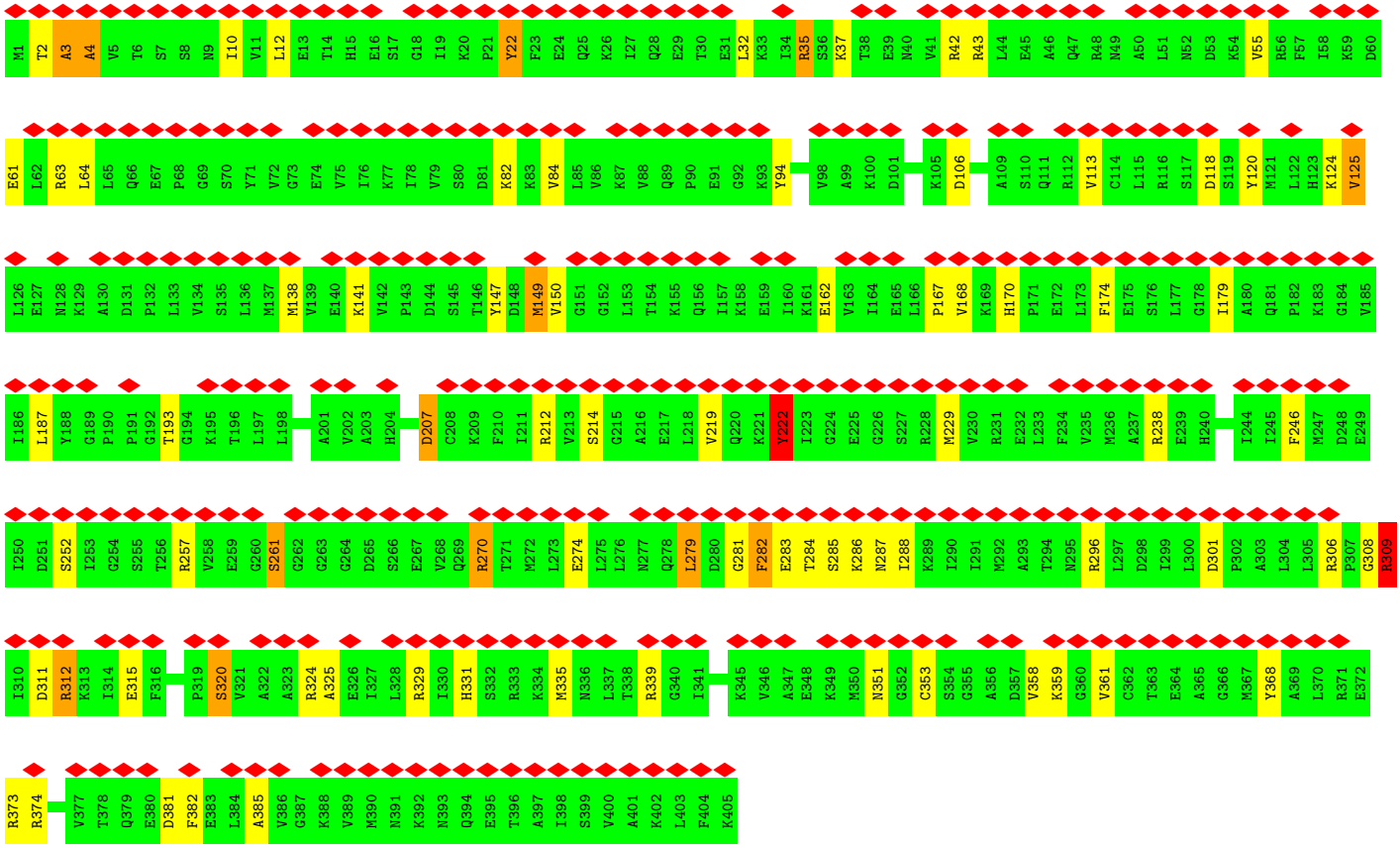
• Molecule 32: 26S proteasome regulatory subunit 6A

Chain M:



• Molecule 33: 26S proteasome regulatory subunit 8 homolog

Chain J:


M1 T2 A3 A4 W5 T6 S7 S8 N9 I10 V11 L12 E13 T14 H15 E16 S17 G18 I19 K20 P21 Y22 F23 E24 Q25 K26 I27 Q28 E29 T30 E31 L32 K33 I34 R35 S36 K37 T38 E39 N40 V41 R42 R43 L44 E45 A46 Q47 R48 N49 A50 L51 N52 D53 K54 V55 R56 F57 I58 K59 D60
E61 L62 R63 L64 L65 Q66 E67 P68 G69 S70 Y71 V72 G73 E74 V75 I76 K77 I78 V79 S80 D81 K82 K83 V84 L85 V86 K87 V88 Q89 P90 E91 G92 K93 Y94 V98 A99 K100 D101 K105 D106 A109 S110 Q111 R112 V113 C114 L115 R116 S117 D118 S119 Y120 M121 L122 H123 K124 V125
L126 E127 N128 K129 A130 D131 P132 L133 V134 S135 L136 M137 M138 V139 E140 K141 V142 P143 D144 S145 T146 Y147 D148 M149 V150 G151 G152 L153 T154 K155 Q156 I157 K158 E159 I160 K161 E162 V163 I164 E165 L166 P167 V168 K169 H170 P171 E172 L173 F174 E175 S176 L177 G178 I179 A180 Q181 P182 K183 G184 V185
I186 L187 Y188 G189 P190 P191 G192 T193 G194 K195 T196 L197 L198 A201 V202 A203 H204 D207 C208 K209 F210 I211 R212 V213 S214 G215 A216 E217 L218 V219 Q220 K221 Y222 I223 G224 E225 G226 S227 R228 M229 V230 R231 E232 L233 F234 V235 M236 A237 R238 E239 H240 I244 I245 F246 M247 D248 E249
I250 D251 S252 I253 G254 S255 T256 R257 V258 E259 G260 S261 G262 G263 G264 D265 S266 E267 V268 Q269 R270 T271 M272 L273 E274 L275 L276 N277 Q278 L279 D280 G281 F282 E283 T284 S285 K286 N287 I288 K289 I290 I291 M292 A293 T294 N295 R296 L297 D298 I299 L300 D301 P302 A303 L304 L305 R306 P307 G308 R309
I310 D311 R312 K313 I314 E315 F316 P319 S320 V321 A322 A323 R324 A325 E326 I327 L328 R329 I330 H331 S332 R333 K334 M335 N336 L337 T338 R339 G340 I341 K345 V346 A347 E348 K349 M350 N351 G352 C353 S354 G355 A356 D357 V358 K359 G360 V361 C362 T363 E364 A365 G366 M367 Y368 A369 L370 R371 E372
R373 R374 V377 T378 Q379 E380 D381 F382 E383 L384 A385 V386 G387 K388 V389 M390 N391 K392 N393 Q394 E395 T396 A397 I398 S399 V400 A401 K402 L403 F404 K405

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	193337	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 ($e^-/Å^2$)	45	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	0.131	Depositor
Minimum map value	-0.092	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.017	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.77	22/1951 (1.1%)	2.03	57/2641 (2.2%)
1	a	1.68	17/1951 (0.9%)	2.04	47/2641 (1.8%)
2	B	1.74	18/1944 (0.9%)	1.91	49/2632 (1.9%)
2	b	1.71	14/1944 (0.7%)	1.96	53/2632 (2.0%)
3	C	1.74	19/1935 (1.0%)	2.00	51/2618 (1.9%)
3	c	1.73	16/1935 (0.8%)	2.02	56/2618 (2.1%)
4	D	1.76	21/1888 (1.1%)	1.84	39/2557 (1.5%)
4	d	1.76	22/2012 (1.1%)	1.96	54/2718 (2.0%)
5	E	1.72	12/1953 (0.6%)	1.86	32/2630 (1.2%)
5	e	1.72	18/1953 (0.9%)	1.97	45/2630 (1.7%)
6	F	1.65	12/1800 (0.7%)	1.96	46/2433 (1.9%)
6	f	1.74	16/1800 (0.9%)	1.84	35/2433 (1.4%)
7	G	2.10	15/1926 (0.8%)	2.17	54/2599 (2.1%)
7	g	2.22	19/1926 (1.0%)	2.18	49/2599 (1.9%)
8	1	1.75	14/1541 (0.9%)	2.06	49/2087 (2.3%)
8	h	1.78	28/1541 (1.8%)	1.89	39/2087 (1.9%)
9	2	1.69	14/1751 (0.8%)	1.92	39/2373 (1.6%)
9	i	1.73	17/1751 (1.0%)	1.88	33/2373 (1.4%)
10	3	1.74	14/1611 (0.9%)	1.94	38/2174 (1.7%)
10	j	1.77	13/1611 (0.8%)	1.91	35/2174 (1.6%)
11	4	1.78	18/1590 (1.1%)	1.98	49/2142 (2.3%)
11	k	1.75	15/1590 (0.9%)	2.06	45/2142 (2.1%)
12	5	1.85	25/1681 (1.5%)	2.00	55/2274 (2.4%)
12	l	1.74	11/1681 (0.7%)	1.99	54/2274 (2.4%)
13	6	1.72	13/1795 (0.7%)	2.02	49/2420 (2.0%)
13	m	1.77	22/1795 (1.2%)	1.96	51/2420 (2.1%)
14	7	3.35	23/1821 (1.3%)	2.02	51/2470 (2.1%)
14	n	3.30	20/1847 (1.1%)	1.89	39/2503 (1.6%)
15	W	1.69	12/1558 (0.8%)	1.86	35/2111 (1.7%)
16	V	1.72	25/2309 (1.1%)	1.93	53/3115 (1.7%)
17	T	1.67	17/2236 (0.8%)	1.91	48/3017 (1.6%)
18	X	1.75	14/1059 (1.3%)	1.92	25/1432 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	Y	1.58	2/741 (0.3%)	1.93	18/1000 (1.8%)
20	Z	1.88	20/7123 (0.3%)	1.25	59/9645 (0.6%)
21	N	1.70	54/7273 (0.7%)	1.88	156/9822 (1.6%)
22	S	1.69	35/3967 (0.9%)	1.88	82/5355 (1.5%)
23	P	1.68	29/3664 (0.8%)	1.89	72/4940 (1.5%)
24	Q	1.71	33/3556 (0.9%)	1.88	76/4787 (1.6%)
25	R	1.70	30/3314 (0.9%)	1.95	72/4469 (1.6%)
26	U	1.66	13/2461 (0.5%)	1.81	48/3327 (1.4%)
27	O	1.70	26/3247 (0.8%)	1.96	86/4380 (2.0%)
28	H	1.85	39/3363 (1.2%)	1.90	62/4532 (1.4%)
29	I	1.72	23/3054 (0.8%)	2.06	74/4111 (1.8%)
30	K	1.76	30/3156 (1.0%)	1.99	87/4261 (2.0%)
31	L	1.71	25/3129 (0.8%)	2.00	76/4204 (1.8%)
32	M	1.67	25/3323 (0.8%)	1.91	70/4478 (1.6%)
33	J	1.72	26/3212 (0.8%)	1.86	64/4316 (1.5%)
All	All	1.83	966/112269 (0.9%)	1.91	2556/151596 (1.7%)

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	5
1	a	0	6
2	B	0	8
2	b	0	3
3	C	0	6
3	c	0	8
4	D	0	8
4	d	0	5
5	E	0	10
5	e	0	7
6	F	0	10
6	f	0	8
7	G	0	7
7	g	0	7
8	1	0	4
8	h	0	7
9	2	0	5
9	i	0	3
10	3	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	j	0	7
11	4	0	3
11	k	0	4
12	5	0	5
12	l	0	5
13	6	0	7
13	m	0	8
14	7	0	7
14	n	0	6
15	W	0	4
16	V	0	6
17	T	0	5
18	X	0	3
20	Z	1	5
21	N	0	24
22	S	0	12
23	P	0	8
24	Q	0	14
25	R	0	17
26	U	0	4
27	O	0	5
28	H	0	8
29	I	0	8
30	K	0	10
31	L	0	23
32	M	0	9
33	J	0	10
All	All	1	350

All (966) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	728	LYS	CG-CD	72.36	3.98	1.52
20	Z	635	ALA	CA-CB	69.47	2.98	1.52
20	Z	748	LEU	CG-CD2	67.40	4.01	1.51
7	g	93	ARG	CZ-NH2	61.09	2.12	1.33
14	7	109	TYR	CG-CD2	57.76	2.14	1.39
7	G	93	ARG	CZ-NH2	57.37	2.07	1.33
14	n	109	TYR	CG-CD1	55.52	2.11	1.39
14	7	109	TYR	CE1-CZ	54.91	2.10	1.38
14	n	109	TYR	CE2-CZ	54.78	2.09	1.38
14	n	109	TYR	CG-CD2	52.77	2.07	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	109	TYR	CG-CD1	52.12	2.06	1.39
14	7	109	TYR	CE2-CZ	49.28	2.02	1.38
14	n	109	TYR	CE1-CZ	48.82	2.02	1.38
14	7	109	TYR	CD2-CE2	43.08	2.04	1.39
20	Z	738	TYR	CZ-OH	42.12	2.09	1.37
14	n	109	TYR	CD2-CE2	41.92	2.02	1.39
14	7	109	TYR	CD1-CE1	41.14	2.01	1.39
14	n	109	TYR	CD1-CE1	40.09	1.99	1.39
20	Z	748	LEU	CG-CD1	28.45	2.57	1.51
28	H	307	PHE	C-N	25.13	1.91	1.34
20	Z	728	LYS	CD-CE	24.31	2.12	1.51
29	I	322	VAL	C-N	21.18	1.82	1.34
28	H	308	PHE	C-N	20.80	1.81	1.34
20	Z	748	LEU	CB-CG	19.80	2.10	1.52
20	Z	728	LYS	CA-CB	14.24	1.85	1.53
20	Z	728	LYS	CB-CG	13.01	1.87	1.52
20	Z	748	LEU	CA-CB	12.12	1.81	1.53
2	b	124	SER	CA-CB	10.25	1.68	1.52
20	Z	728	LYS	N-CA	9.87	1.66	1.46
31	L	82	ARG	CZ-NH2	9.36	1.45	1.33
32	M	431	SER	CA-CB	9.23	1.66	1.52
13	m	229	ARG	NE-CZ	8.91	1.44	1.33
28	H	385	ARG	CD-NE	8.58	1.61	1.46
3	c	129	ARG	CZ-NH2	8.51	1.44	1.33
9	i	198	SER	CA-CB	8.30	1.65	1.52
31	L	357	ARG	CZ-NH1	8.16	1.43	1.33
2	B	42	GLY	N-CA	-8.11	1.33	1.46
10	3	28	ARG	CZ-NH2	8.05	1.43	1.33
29	I	181	TYR	CG-CD2	8.04	1.49	1.39
22	S	64	ARG	NE-CZ	8.03	1.43	1.33
20	Z	728	LYS	CE-NZ	8.01	1.69	1.49
26	U	32	ARG	NE-CZ	8.01	1.43	1.33
28	H	226	GLU	CD-OE2	7.96	1.34	1.25
21	N	839	ARG	CD-NE	7.88	1.59	1.46
11	k	95	ARG	CD-NE	7.85	1.59	1.46
11	4	95	ARG	CZ-NH1	7.84	1.43	1.33
29	I	313	LEU	C-N	7.80	1.51	1.34
23	P	179	PHE	CG-CD2	7.78	1.50	1.38
33	J	312	ARG	CZ-NH1	7.76	1.43	1.33
22	S	464	ARG	NE-CZ	7.75	1.43	1.33
31	L	407	ARG	CD-NE	7.73	1.59	1.46
2	B	203	GLU	CG-CD	7.70	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	51	ARG	CZ-NH1	7.69	1.43	1.33
8	h	198	TYR	CG-CD1	7.67	1.49	1.39
2	B	246	ARG	CZ-NH2	7.65	1.43	1.33
7	G	22	PHE	CG-CD2	7.64	1.50	1.38
4	D	87	GLU	CG-CD	7.62	1.63	1.51
20	Z	635	ALA	N-CA	7.62	1.61	1.46
20	Z	748	LEU	CA-C	7.62	1.72	1.52
10	3	46	TYR	CG-CD1	7.61	1.49	1.39
20	Z	635	ALA	CA-C	7.60	1.72	1.52
3	c	140	TYR	CG-CD2	7.56	1.49	1.39
21	N	362	TRP	NE1-CE2	7.54	1.47	1.37
21	N	422	TYR	CE1-CZ	7.47	1.48	1.38
10	j	44	PHE	CG-CD1	7.44	1.50	1.38
27	O	195	TYR	CE1-CZ	7.42	1.48	1.38
4	d	4	TYR	CE1-CZ	7.41	1.48	1.38
21	N	23	TYR	CG-CD2	7.41	1.48	1.39
23	P	339	GLU	CD-OE2	7.40	1.33	1.25
33	J	257	ARG	CD-NE	7.39	1.59	1.46
33	J	61	GLU	CD-OE2	7.37	1.33	1.25
9	i	217	ARG	NE-CZ	7.37	1.42	1.33
2	B	158	PRO	N-CD	-7.37	1.37	1.47
3	C	98	TYR	CZ-OH	7.34	1.50	1.37
30	K	207	ARG	CD-NE	7.33	1.58	1.46
23	P	103	TYR	CE2-CZ	7.31	1.48	1.38
10	3	99	ARG	NE-CZ	7.30	1.42	1.33
26	U	137	TYR	CG-CD2	7.28	1.48	1.39
10	j	143	SER	CA-CB	7.27	1.63	1.52
1	A	31	ALA	CA-CB	7.27	1.67	1.52
12	l	144	ARG	CZ-NH2	7.26	1.42	1.33
2	b	201	GLU	CD-OE1	7.24	1.33	1.25
23	P	395	ARG	CZ-NH1	7.24	1.42	1.33
31	L	299	ARG	NE-CZ	7.24	1.42	1.33
12	5	171	SER	CA-CB	7.24	1.63	1.52
12	5	192	SER	CA-CB	7.21	1.63	1.52
2	B	99	ARG	CD-NE	7.18	1.58	1.46
10	j	30	GLY	CA-C	-7.16	1.40	1.51
31	L	255	TYR	CG-CD2	7.16	1.48	1.39
13	m	79	SER	CA-CB	7.14	1.63	1.52
8	h	198	TYR	CZ-OH	7.12	1.50	1.37
5	e	166	ARG	CZ-NH2	7.11	1.42	1.33
28	H	88	ARG	CZ-NH1	7.11	1.42	1.33
17	T	51	TYR	CG-CD1	7.08	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	78	ARG	CZ-NH2	7.06	1.42	1.33
25	R	210	TYR	CE2-CZ	7.06	1.47	1.38
14	n	124	TYR	CE1-CZ	7.05	1.47	1.38
8	h	70	TYR	CE2-CZ	7.01	1.47	1.38
33	J	270	ARG	CZ-NH1	6.99	1.42	1.33
4	d	172	ARG	NE-CZ	6.99	1.42	1.33
5	E	20	ARG	CZ-NH1	6.98	1.42	1.33
27	O	333	SER	CA-CB	6.97	1.63	1.52
3	C	9	ARG	NE-CZ	6.96	1.42	1.33
9	2	236	ARG	NE-CZ	6.96	1.42	1.33
9	2	152	TYR	CE2-CZ	6.95	1.47	1.38
7	g	126	TYR	CE2-CZ	6.94	1.47	1.38
24	Q	202	ARG	CZ-NH1	6.93	1.42	1.33
30	K	67	TYR	CG-CD2	6.91	1.48	1.39
23	P	194	SER	CA-CB	6.86	1.63	1.52
28	H	358	PRO	N-CD	-6.86	1.38	1.47
6	f	69	HIS	CB-CG	-6.85	1.37	1.50
14	n	215	ARG	NE-CZ	6.85	1.42	1.33
14	7	134	TYR	CE1-CZ	6.84	1.47	1.38
4	D	157	SER	CA-CB	6.84	1.63	1.52
19	Y	83	ARG	NE-CZ	6.84	1.42	1.33
21	N	208	ARG	CZ-NH2	6.82	1.42	1.33
25	R	83	GLU	CD-OE1	-6.81	1.18	1.25
6	f	128	TYR	CG-CD2	6.80	1.48	1.39
27	O	218	SER	CA-CB	6.80	1.63	1.52
26	U	303	GLU	CB-CG	6.80	1.65	1.52
27	O	228	TYR	CE1-CZ	6.79	1.47	1.38
8	h	163	PHE	CG-CD2	6.79	1.49	1.38
8	1	201	GLU	CD-OE1	6.78	1.33	1.25
22	S	118	PHE	CG-CD1	6.77	1.49	1.38
9	2	169	SER	CA-CB	6.76	1.63	1.52
21	N	89	PHE	CE2-CZ	6.75	1.50	1.37
8	1	153	GLU	CD-OE1	6.74	1.33	1.25
13	m	170	PRO	N-CD	-6.74	1.38	1.47
8	1	202	TYR	CB-CG	6.73	1.61	1.51
1	a	131	ARG	CZ-NH1	6.73	1.41	1.33
3	C	144	TYR	CG-CD2	6.72	1.47	1.39
2	B	201	GLU	CB-CG	6.70	1.64	1.52
15	W	60	ARG	CD-NE	6.69	1.57	1.46
3	C	24	TYR	CB-CG	6.69	1.61	1.51
8	1	194	ARG	NE-CZ	6.68	1.41	1.33
13	6	195	SER	CA-CB	6.68	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	29	PRO	N-CD	-6.67	1.38	1.47
6	F	89	ARG	NE-CZ	6.66	1.41	1.33
21	N	208	ARG	NE-CZ	6.65	1.41	1.33
29	I	246	ARG	CZ-NH2	6.65	1.41	1.33
16	V	196	TYR	CG-CD2	6.64	1.47	1.39
8	h	38	ARG	CD-NE	6.63	1.57	1.46
10	j	28	ARG	NE-CZ	6.63	1.41	1.33
25	R	112	GLU	CA-CB	6.63	1.68	1.53
22	S	55	ARG	CZ-NH2	6.63	1.41	1.33
1	A	46	ARG	CZ-NH1	6.62	1.41	1.33
3	C	50	ARG	CD-NE	6.62	1.57	1.46
24	Q	53	GLU	CD-OE2	6.62	1.32	1.25
29	I	405	ARG	CZ-NH1	6.62	1.41	1.33
32	M	404	ARG	CZ-NH1	6.62	1.41	1.33
23	P	162	GLU	CD-OE2	6.60	1.32	1.25
8	h	28	ARG	CD-NE	6.60	1.57	1.46
8	1	28	ARG	CZ-NH1	6.59	1.41	1.33
32	M	166	ARG	CZ-NH2	6.59	1.41	1.33
25	R	259	PHE	CG-CD1	6.59	1.48	1.38
28	H	408	SER	CA-CB	6.59	1.62	1.52
24	Q	12	ARG	CZ-NH1	6.59	1.41	1.33
4	D	58	ARG	CZ-NH1	6.59	1.41	1.33
15	W	25	ARG	CZ-NH1	6.58	1.41	1.33
20	Z	727	GLU	C-N	6.58	1.49	1.34
12	l	224	SER	CA-CB	6.58	1.62	1.52
1	A	193	HIS	CA-CB	6.57	1.68	1.53
3	c	114	ARG	CD-NE	6.56	1.57	1.46
6	f	71	GLY	N-CA	-6.55	1.36	1.46
11	4	134	GLY	N-CA	-6.55	1.36	1.46
16	V	232	GLU	CG-CD	6.55	1.61	1.51
1	A	250	GLU	CD-OE1	6.54	1.32	1.25
10	j	52	GLY	N-CA	-6.53	1.36	1.46
3	c	4	ARG	CD-NE	6.53	1.57	1.46
6	f	107	ARG	CD-NE	6.53	1.57	1.46
21	N	839	ARG	CZ-NH2	6.53	1.41	1.33
30	K	393	ARG	NE-CZ	6.53	1.41	1.33
14	7	41	GLY	CA-C	-6.52	1.41	1.51
4	D	49	ARG	CD-NE	6.51	1.57	1.46
3	c	164	SER	CA-CB	6.51	1.62	1.52
21	N	559	TYR	CE1-CZ	6.51	1.47	1.38
3	c	143	ARG	NE-CZ	6.51	1.41	1.33
9	i	215	TYR	CE1-CZ	6.50	1.47	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	161	ARG	CZ-NH1	6.48	1.41	1.33
21	N	873	ARG	CD-NE	6.47	1.57	1.46
28	H	190	ARG	NE-CZ	6.47	1.41	1.33
31	L	357	ARG	CD-NE	6.46	1.57	1.46
18	X	85	ARG	CZ-NH1	6.46	1.41	1.33
28	H	292	ARG	CZ-NH1	6.44	1.41	1.33
4	D	49	ARG	CZ-NH1	6.44	1.41	1.33
1	A	110	TYR	CB-CG	6.43	1.61	1.51
2	b	236	ARG	NE-CZ	6.43	1.41	1.33
21	N	394	ARG	NE-CZ	6.43	1.41	1.33
32	M	300	GLU	CD-OE1	6.43	1.32	1.25
22	S	480	ARG	CD-NE	6.42	1.57	1.46
27	O	390	SER	CB-OG	6.42	1.50	1.42
8	1	133	TYR	CB-CG	6.42	1.61	1.51
25	R	49	PHE	CG-CD1	6.41	1.48	1.38
9	2	217	ARG	CZ-NH1	6.41	1.41	1.33
12	5	144	ARG	CZ-NH1	6.41	1.41	1.33
27	O	106	PHE	CG-CD1	6.40	1.48	1.38
16	V	251	TYR	CZ-OH	6.40	1.48	1.37
24	Q	291	TYR	CZ-OH	6.39	1.48	1.37
30	K	41	SER	CA-CB	6.39	1.62	1.52
22	S	475	TYR	CE1-CZ	6.39	1.46	1.38
13	6	41	TYR	CD2-CE2	6.38	1.49	1.39
4	d	49	ARG	CZ-NH2	6.38	1.41	1.33
12	5	94	ARG	CD-NE	6.38	1.57	1.46
21	N	204	SER	CA-CB	6.38	1.62	1.52
13	6	141	ARG	CZ-NH1	6.37	1.41	1.33
30	K	350	ARG	NE-CZ	6.37	1.41	1.33
4	d	111	ARG	CZ-NH2	6.37	1.41	1.33
4	D	50	SER	CB-OG	6.37	1.50	1.42
3	C	208	TYR	CG-CD1	6.37	1.47	1.39
9	2	217	ARG	CZ-NH2	6.37	1.41	1.33
4	D	239	GLU	CD-OE1	6.36	1.32	1.25
5	e	139	GLY	CA-C	-6.35	1.41	1.51
11	k	68	SER	CA-CB	6.35	1.62	1.52
3	c	64	GLU	CD-OE1	6.34	1.32	1.25
12	5	196	ARG	CZ-NH2	6.33	1.41	1.33
25	R	263	ARG	CZ-NH2	6.33	1.41	1.33
17	T	20	TYR	CE2-CZ	6.33	1.46	1.38
6	F	99	PHE	CG-CD1	6.32	1.48	1.38
30	K	88	ARG	CZ-NH1	6.32	1.41	1.33
14	n	161	ARG	CD-NE	6.32	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	20	ARG	NE-CZ	6.31	1.41	1.33
14	n	195	GLU	CD-OE1	6.31	1.32	1.25
1	A	120	ARG	CD-NE	6.30	1.57	1.46
21	N	604	ARG	NE-CZ	6.30	1.41	1.33
8	1	158	GLU	CD-OE2	6.30	1.32	1.25
4	d	22	TYR	CB-CG	6.28	1.61	1.51
6	f	96	SER	CA-CB	6.28	1.62	1.52
18	X	97	TYR	CE2-CZ	6.28	1.46	1.38
20	Z	738	TYR	CE2-CZ	6.27	1.46	1.38
21	N	545	SER	CA-CB	6.27	1.62	1.52
10	j	28	ARG	CD-NE	6.26	1.57	1.46
11	4	98	TYR	CZ-OH	6.26	1.48	1.37
21	N	298	TYR	CZ-OH	6.26	1.48	1.37
13	m	141	ARG	CD-NE	6.26	1.57	1.46
15	W	23	ARG	CD-NE	6.26	1.57	1.46
24	Q	387	TYR	CE1-CZ	6.26	1.46	1.38
7	g	201	TYR	CE1-CZ	6.25	1.46	1.38
28	H	400	ARG	NE-CZ	6.25	1.41	1.33
27	O	283	HIS	CB-CG	6.24	1.61	1.50
16	V	171	ARG	NE-CZ	6.24	1.41	1.33
6	f	51	ARG	NE-CZ	6.24	1.41	1.33
9	i	132	VAL	N-CA	-6.24	1.33	1.46
7	G	72	ARG	NE-CZ	6.23	1.41	1.33
30	K	379	SER	CA-C	-6.23	1.36	1.52
10	j	96	TYR	CD2-CE2	6.22	1.48	1.39
12	l	234	ARG	CZ-NH2	6.22	1.41	1.33
3	c	24	TYR	CE2-CZ	6.22	1.46	1.38
21	N	149	GLU	CB-CG	6.21	1.64	1.52
17	T	248	GLU	CG-CD	6.21	1.61	1.51
5	E	176	SER	CA-CB	6.20	1.62	1.52
21	N	784	TYR	CE1-CZ	6.20	1.46	1.38
11	4	190	ARG	CZ-NH1	6.19	1.41	1.33
29	I	61	ARG	NE-CZ	6.19	1.41	1.33
12	5	82	ARG	CZ-NH2	6.18	1.41	1.33
22	S	464	ARG	CZ-NH2	6.18	1.41	1.33
31	L	264	ARG	CZ-NH2	6.17	1.41	1.33
21	N	866	TYR	CD1-CE1	6.17	1.48	1.39
31	L	161	ARG	NE-CZ	6.17	1.41	1.33
28	H	90	ARG	NE-CZ	6.17	1.41	1.33
1	A	106	TYR	CE2-CZ	6.17	1.46	1.38
16	V	100	ARG	NE-CZ	6.16	1.41	1.33
1	a	128	TYR	CE1-CZ	6.16	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	133	TRP	CD2-CE2	-6.16	1.33	1.41
21	N	776	TYR	CG-CD2	6.15	1.47	1.39
23	P	149	GLU	CD-OE2	6.15	1.32	1.25
2	b	75	TYR	CE2-CZ	6.15	1.46	1.38
32	M	417	GLU	CG-CD	6.14	1.61	1.51
3	C	158	THR	N-CA	-6.14	1.34	1.46
21	N	479	GLU	CG-CD	6.13	1.61	1.51
13	6	141	ARG	NE-CZ	6.12	1.41	1.33
5	e	128	SER	CA-CB	6.12	1.62	1.52
14	7	194	ARG	CD-NE	6.12	1.56	1.46
28	H	434	ARG	CZ-NH1	6.12	1.41	1.33
16	V	231	GLU	CD-OE2	6.12	1.32	1.25
4	d	226	SER	CA-CB	6.11	1.62	1.52
9	i	120	GLN	C-N	6.11	1.44	1.33
26	U	113	TYR	CE2-CZ	6.10	1.46	1.38
6	F	162	GLY	CA-C	-6.10	1.42	1.51
21	N	873	ARG	NE-CZ	6.10	1.41	1.33
2	b	4	ARG	CD-NE	6.09	1.56	1.46
24	Q	299	MET	N-CA	-6.09	1.34	1.46
31	L	329	ARG	CZ-NH2	6.08	1.41	1.33
12	l	253	TYR	CD2-CE2	6.08	1.48	1.39
21	N	142	GLU	CD-OE2	6.08	1.32	1.25
2	b	217	GLU	CD-OE1	-6.07	1.19	1.25
15	W	194	GLU	C-N	6.07	1.44	1.33
8	h	56	GLY	N-CA	-6.07	1.36	1.46
25	R	69	GLU	CD-OE1	6.07	1.32	1.25
29	I	262	ARG	CZ-NH2	6.06	1.41	1.33
30	K	85	GLU	CD-OE2	6.06	1.32	1.25
13	6	114	TYR	CD2-CE2	6.06	1.48	1.39
13	m	145	ARG	CZ-NH2	6.05	1.41	1.33
11	4	70	ARG	CD-NE	6.05	1.56	1.46
29	I	91	GLU	CG-CD	6.04	1.61	1.51
21	N	299	TYR	CE1-CZ	6.03	1.46	1.38
1	a	46	ARG	CZ-NH1	6.03	1.40	1.33
3	C	18	ARG	NE-CZ	6.02	1.40	1.33
7	G	13	SER	N-CA	-6.02	1.34	1.46
15	W	17	ARG	NE-CZ	6.01	1.40	1.33
25	R	334	ARG	CZ-NH1	6.01	1.40	1.33
3	C	146	TYR	CG-CD1	6.01	1.47	1.39
24	Q	209	TYR	CE1-CZ	6.01	1.46	1.38
28	H	403	ARG	CZ-NH2	6.01	1.40	1.33
28	H	145	TYR	CB-CG	-6.01	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	215	ARG	CZ-NH2	6.00	1.40	1.33
28	H	231	SER	CA-CB	6.00	1.61	1.52
28	H	361	LEU	CA-CB	6.00	1.67	1.53
7	G	86	ARG	CZ-NH1	6.00	1.40	1.33
6	F	165	SER	CA-CB	5.99	1.61	1.52
33	J	120	TYR	CB-CG	5.98	1.60	1.51
12	l	141	HIS	CB-CG	5.98	1.60	1.50
31	L	294	GLY	CA-C	-5.98	1.42	1.51
32	M	349	PHE	CE1-CZ	5.98	1.48	1.37
33	J	308	GLY	CA-C	-5.97	1.42	1.51
9	i	140	PHE	CG-CD1	5.97	1.47	1.38
32	M	171	GLU	CG-CD	5.97	1.60	1.51
21	N	880	ARG	NE-CZ	5.97	1.40	1.33
13	6	157	PHE	CB-CG	5.96	1.61	1.51
2	B	148	TYR	CE1-CZ	5.96	1.46	1.38
31	L	325	MET	CA-CB	5.96	1.67	1.53
27	O	356	ARG	CZ-NH1	5.95	1.40	1.33
16	V	117	TRP	CE3-CZ3	5.95	1.48	1.38
16	V	175	SER	CA-CB	5.94	1.61	1.52
13	6	47	TYR	CZ-OH	5.94	1.48	1.37
23	P	123	ARG	CZ-NH2	5.94	1.40	1.33
25	R	409	GLY	CA-C	-5.94	1.42	1.51
32	M	345	ARG	CZ-NH1	5.94	1.40	1.33
11	k	148	TYR	CD1-CE1	-5.93	1.30	1.39
5	E	10	ARG	CZ-NH2	5.93	1.40	1.33
1	a	96	ARG	CZ-NH1	5.93	1.40	1.33
5	e	10	ARG	CZ-NH1	5.93	1.40	1.33
25	R	206	ARG	NE-CZ	5.93	1.40	1.33
14	7	257	ASP	N-CA	-5.93	1.34	1.46
17	T	51	TYR	CE1-CZ	5.93	1.46	1.38
7	G	20	ARG	CZ-NH1	5.92	1.40	1.33
9	i	208	GLU	CD-OE1	-5.92	1.19	1.25
4	D	172	ARG	CZ-NH1	5.92	1.40	1.33
8	h	51	TRP	NE1-CE2	5.92	1.45	1.37
30	K	58	TYR	CE1-CZ	5.92	1.46	1.38
28	H	357	ARG	NE-CZ	5.91	1.40	1.33
21	N	365	PHE	CG-CD1	5.91	1.47	1.38
13	6	107	GLY	N-CA	-5.91	1.37	1.46
4	d	83	ARG	CZ-NH2	5.90	1.40	1.33
8	h	10	THR	N-CA	5.90	1.58	1.46
8	h	24	GLY	N-CA	-5.89	1.37	1.46
15	W	43	SER	CA-CB	5.89	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	V	235	GLU	CG-CD	5.89	1.60	1.51
14	n	215	ARG	CZ-NH1	5.88	1.40	1.33
24	Q	409	TYR	CE1-CZ	5.88	1.46	1.38
25	R	213	TYR	CG-CD2	5.88	1.46	1.39
33	J	61	GLU	CG-CD	-5.88	1.43	1.51
4	D	111	ARG	CZ-NH1	5.88	1.40	1.33
21	N	906	ARG	CZ-NH2	5.88	1.40	1.33
1	A	145	SER	CA-CB	5.88	1.61	1.52
23	P	359	ARG	CD-NE	5.88	1.56	1.46
7	g	160	TYR	CB-CG	-5.87	1.42	1.51
10	3	28	ARG	CD-NE	5.87	1.56	1.46
10	j	80	ARG	NE-CZ	5.87	1.40	1.33
12	5	245	TYR	CE2-CZ	5.87	1.46	1.38
33	J	285	SER	CA-CB	5.87	1.61	1.52
23	P	168	TYR	CZ-OH	5.86	1.47	1.37
8	h	77	SER	CA-CB	5.86	1.61	1.52
30	K	141	ARG	CZ-NH2	5.86	1.40	1.33
23	P	136	ARG	NE-CZ	5.86	1.40	1.33
7	g	160	TYR	CE1-CZ	5.85	1.46	1.38
17	T	261	GLU	CG-CD	5.85	1.60	1.51
23	P	102	GLU	CB-CG	5.85	1.63	1.52
24	Q	232	TYR	CE1-CZ	5.84	1.46	1.38
13	6	45	SER	CA-CB	5.83	1.61	1.52
18	X	122	TYR	CG-CD2	5.83	1.46	1.39
6	f	179	PHE	CE2-CZ	5.83	1.48	1.37
18	X	51	ARG	CZ-NH2	5.82	1.40	1.33
24	Q	151	TYR	CB-CG	-5.82	1.43	1.51
5	e	231	TYR	CE2-CZ	5.82	1.46	1.38
32	M	213	ARG	NE-CZ	5.81	1.40	1.33
30	K	118	TYR	CZ-OH	5.81	1.47	1.37
24	Q	13	ARG	NE-CZ	5.80	1.40	1.33
7	g	16	SER	CB-OG	-5.80	1.34	1.42
14	n	248	GLU	CG-CD	5.80	1.60	1.51
16	V	257	GLU	CD-OE1	5.80	1.32	1.25
24	Q	77	PHE	CG-CD1	5.80	1.47	1.38
24	Q	344	GLU	CG-CD	5.80	1.60	1.51
33	J	42	ARG	CZ-NH2	5.80	1.40	1.33
21	N	222	TYR	CE1-CZ	5.79	1.46	1.38
28	H	249	TYR	CB-CG	5.79	1.60	1.51
17	T	266	TYR	CG-CD1	5.78	1.46	1.39
27	O	95	SER	CA-CB	5.78	1.61	1.52
12	5	257	GLU	CD-OE1	5.77	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	392	GLY	CA-C	-5.77	1.42	1.51
5	E	102	TYR	CE1-CZ	5.77	1.46	1.38
11	k	93	ARG	CZ-NH2	5.76	1.40	1.33
18	X	17	TYR	CE2-CZ	5.76	1.46	1.38
4	D	35	GLY	CA-C	-5.75	1.42	1.51
2	b	23	TYR	CG-CD1	5.75	1.46	1.39
12	l	130	TRP	CD2-CE2	5.75	1.48	1.41
4	d	15	GLY	N-CA	-5.74	1.37	1.46
16	V	55	GLY	N-CA	-5.74	1.37	1.46
6	f	227	GLY	N-CA	-5.74	1.37	1.46
3	c	102	TYR	CG-CD2	5.74	1.46	1.39
12	5	266	HIS	CB-CG	-5.74	1.39	1.50
7	g	201	TYR	CE2-CZ	5.74	1.46	1.38
14	n	136	ARG	NE-CZ	5.73	1.40	1.33
5	e	65	GLU	CA-CB	5.73	1.66	1.53
13	m	48	GLU	CD-OE2	5.73	1.31	1.25
11	4	95	ARG	NE-CZ	5.73	1.40	1.33
25	R	332	GLU	CG-CD	5.73	1.60	1.51
30	K	234	PHE	CG-CD2	5.73	1.47	1.38
5	e	7	GLU	CB-CG	5.72	1.63	1.52
22	S	117	SER	CA-CB	5.72	1.61	1.52
4	D	156	TYR	CD2-CE2	5.72	1.48	1.39
30	K	67	TYR	CG-CD1	5.72	1.46	1.39
25	R	186	TYR	CG-CD1	5.72	1.46	1.39
27	O	170	SER	CA-CB	5.72	1.61	1.52
4	D	159	TRP	CE2-CZ2	-5.71	1.30	1.39
9	i	126	TYR	CE2-CZ	5.71	1.46	1.38
27	O	285	SER	CA-CB	5.71	1.61	1.52
10	3	87	PHE	CG-CD1	5.71	1.47	1.38
6	f	39	ARG	NE-CZ	5.71	1.40	1.33
11	k	70	ARG	CD-NE	5.71	1.56	1.46
13	m	28	PHE	CG-CD1	5.71	1.47	1.38
1	a	77	ARG	CZ-NH2	5.71	1.40	1.33
6	F	171	TYR	CG-CD1	5.70	1.46	1.39
30	K	185	ARG	NE-CZ	5.70	1.40	1.33
33	J	162	GLU	CD-OE1	5.70	1.31	1.25
22	S	480	ARG	CZ-NH1	5.70	1.40	1.33
23	P	359	ARG	CZ-NH2	5.70	1.40	1.33
32	M	267	PHE	CE1-CZ	5.70	1.48	1.37
3	c	50	ARG	CD-NE	5.70	1.56	1.46
24	Q	13	ARG	CD-NE	5.70	1.56	1.46
10	j	152	SER	CA-CB	5.70	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	149	PRO	N-CD	-5.70	1.39	1.47
21	N	718	GLU	CG-CD	5.70	1.60	1.51
17	T	25	LYS	CD-CE	5.69	1.65	1.51
4	d	127	ARG	NE-CZ	5.69	1.40	1.33
10	j	94	SER	CA-CB	5.69	1.61	1.52
10	3	183	TRP	CD2-CE2	-5.69	1.34	1.41
23	P	14	SER	CA-CB	5.69	1.61	1.52
27	O	202	SER	CA-CB	5.69	1.61	1.52
4	d	46	CYS	CB-SG	5.69	1.92	1.82
14	7	179	PHE	C-N	5.69	1.43	1.33
23	P	332	GLU	CG-CD	5.68	1.60	1.51
8	1	126	GLY	CA-C	-5.68	1.42	1.51
31	L	68	ARG	CZ-NH1	5.68	1.40	1.33
14	n	220	ARG	CZ-NH2	5.68	1.40	1.33
33	J	43	ARG	CZ-NH1	5.68	1.40	1.33
2	B	201	GLU	CG-CD	5.67	1.60	1.51
4	d	90	ARG	CZ-NH1	5.67	1.40	1.33
31	L	299	ARG	CZ-NH2	5.67	1.40	1.33
32	M	67	GLU	CD-OE1	5.67	1.31	1.25
4	d	74	SER	CA-CB	5.67	1.61	1.52
11	k	67	TYR	CZ-OH	5.67	1.47	1.37
32	M	152	SER	CA-CB	5.67	1.61	1.52
33	J	374	ARG	NE-CZ	5.67	1.40	1.33
13	m	131	TYR	CG-CD1	5.66	1.46	1.39
20	Z	745	LEU	CA-C	-5.66	1.38	1.52
5	E	13	SER	CB-OG	5.65	1.49	1.42
3	c	180	TYR	CZ-OH	5.65	1.47	1.37
29	I	284	ILE	N-CA	-5.65	1.35	1.46
30	K	270	PHE	CG-CD1	5.65	1.47	1.38
11	4	121	TYR	CG-CD2	5.65	1.46	1.39
22	S	292	TYR	CE1-CZ	5.65	1.45	1.38
9	2	71	TRP	NE1-CE2	-5.64	1.30	1.37
29	I	128	TYR	CG-CD2	5.64	1.46	1.39
2	B	234	ARG	CZ-NH1	5.64	1.40	1.33
9	2	168	GLU	CG-CD	5.63	1.60	1.51
7	G	163	ALA	N-CA	-5.63	1.35	1.46
23	P	356	TYR	CZ-OH	5.63	1.47	1.37
1	a	138	GLY	N-CA	5.62	1.54	1.46
13	m	145	ARG	CD-NE	5.62	1.56	1.46
16	V	299	GLY	N-CA	-5.62	1.37	1.46
32	M	103	GLY	N-CA	-5.62	1.37	1.46
11	k	49	GLU	CD-OE1	5.62	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	288	ARG	CZ-NH2	5.62	1.40	1.33
26	U	214	VAL	CA-CB	-5.62	1.43	1.54
33	J	296	ARG	CZ-NH2	5.62	1.40	1.33
18	X	22	ARG	NE-CZ	5.61	1.40	1.33
5	e	214	GLU	CD-OE1	5.61	1.31	1.25
9	2	141	SER	CB-OG	-5.61	1.34	1.42
27	O	387	ARG	NE-CZ	5.61	1.40	1.33
22	S	425	ARG	CD-NE	5.61	1.55	1.46
25	R	48	GLU	CD-OE1	5.61	1.31	1.25
17	T	150	ARG	CD-NE	5.61	1.55	1.46
14	n	223	ARG	CD-NE	5.60	1.55	1.46
31	L	373	GLU	CG-CD	5.60	1.60	1.51
8	1	137	GLY	N-CA	-5.60	1.37	1.46
22	S	88	PHE	CG-CD1	5.60	1.47	1.38
7	G	78	TYR	CG-CD2	5.60	1.46	1.39
33	J	167	PRO	N-CD	-5.60	1.40	1.47
5	E	128	SER	CA-CB	5.59	1.61	1.52
1	a	131	ARG	NE-CZ	5.59	1.40	1.33
2	b	206	GLY	CA-C	-5.59	1.43	1.51
8	h	79	TYR	CG-CD1	5.59	1.46	1.39
2	B	23	TYR	CB-CG	5.58	1.60	1.51
31	L	342	ARG	CZ-NH2	5.58	1.40	1.33
20	Z	727	GLU	CA-C	5.58	1.67	1.52
2	b	178	ARG	CZ-NH1	5.58	1.40	1.33
28	H	346	ARG	NE-CZ	5.58	1.40	1.33
28	H	390	ARG	CD-NE	5.58	1.55	1.46
30	K	349	ARG	CZ-NH2	5.58	1.40	1.33
6	f	136	GLY	CA-C	-5.57	1.43	1.51
8	h	202	TYR	CB-CG	5.57	1.60	1.51
5	E	37	ALA	CA-CB	5.57	1.64	1.52
12	5	230	TYR	CB-CG	-5.57	1.43	1.51
4	d	148	TYR	CE1-CZ	5.57	1.45	1.38
24	Q	202	ARG	CD-NE	5.57	1.55	1.46
27	O	314	SER	CA-CB	5.57	1.61	1.52
29	I	122	SER	CA-CB	5.57	1.61	1.52
21	N	406	TYR	CZ-OH	5.57	1.47	1.37
21	N	789	GLU	N-CA	-5.57	1.35	1.46
24	Q	46	VAL	CB-CG1	5.57	1.64	1.52
1	A	24	ARG	CZ-NH1	5.56	1.40	1.33
8	1	31	THR	C-N	5.56	1.43	1.33
22	S	428	ARG	CD-NE	5.56	1.55	1.46
26	U	145	ASP	CB-CG	5.56	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	U	189	ARG	NE-CZ	5.56	1.40	1.33
14	7	189	ARG	CZ-NH2	5.56	1.40	1.33
22	S	58	LYS	CA-CB	5.55	1.66	1.53
10	3	151	GLU	CG-CD	5.55	1.60	1.51
5	E	69	GLU	CD-OE1	5.55	1.31	1.25
21	N	729	SER	CA-CB	5.55	1.61	1.52
4	D	156	TYR	CD1-CE1	5.55	1.47	1.39
13	m	211	GLU	CG-CD	5.55	1.60	1.51
4	D	174	PHE	CG-CD2	5.54	1.47	1.38
21	N	813	ARG	CZ-NH1	5.54	1.40	1.33
25	R	204	TRP	CG-CD2	5.54	1.53	1.43
10	3	104	PHE	CG-CD2	5.54	1.47	1.38
22	S	274	PHE	CE1-CZ	5.54	1.47	1.37
10	j	99	ARG	NE-CZ	5.53	1.40	1.33
1	a	233	PHE	CG-CD1	5.53	1.47	1.38
1	A	185	HIS	CA-CB	5.53	1.66	1.53
28	H	373	ARG	CZ-NH2	5.53	1.40	1.33
32	M	303	ARG	CZ-NH1	5.53	1.40	1.33
18	X	46	TRP	CB-CG	5.53	1.60	1.50
22	S	124	GLU	CA-CB	5.53	1.66	1.53
13	m	40	ASP	CA-CB	5.52	1.66	1.53
1	A	242	GLU	CD-OE1	5.52	1.31	1.25
22	S	393	ARG	CD-NE	5.52	1.55	1.46
25	R	207	ARG	CZ-NH1	5.52	1.40	1.33
6	F	140	SER	CA-CB	5.52	1.61	1.52
2	b	103	GLU	CG-CD	5.52	1.60	1.51
7	g	190	ARG	CD-NE	5.52	1.55	1.46
11	4	70	ARG	NE-CZ	5.52	1.40	1.33
16	V	203	TYR	CZ-OH	5.51	1.47	1.37
22	S	51	ARG	CZ-NH1	5.51	1.40	1.33
7	G	174	ALA	CA-CB	5.51	1.64	1.52
28	H	389	PHE	CG-CD2	5.51	1.47	1.38
7	g	11	SER	N-CA	-5.51	1.35	1.46
7	G	132	PHE	CG-CD1	5.50	1.47	1.38
10	3	28	ARG	NE-CZ	5.50	1.40	1.33
16	V	28	TYR	CB-CG	-5.50	1.43	1.51
13	m	137	GLY	CA-C	-5.50	1.43	1.51
14	n	154	SER	CB-OG	-5.50	1.35	1.42
16	V	50	MET	C-N	5.50	1.43	1.33
33	J	229	MET	N-CA	-5.50	1.35	1.46
12	l	230	TYR	CZ-OH	5.50	1.47	1.37
28	H	261	ARG	CZ-NH1	5.50	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	228	PRO	N-CD	-5.50	1.40	1.47
32	M	52	SER	CA-CB	5.50	1.61	1.52
23	P	312	PRO	CA-C	-5.50	1.41	1.52
26	U	254	ARG	CD-NE	5.49	1.55	1.46
24	Q	2	SER	CA-CB	5.49	1.61	1.52
9	2	219	TYR	CD1-CE1	5.49	1.47	1.39
17	T	20	TYR	CE1-CZ	5.49	1.45	1.38
21	N	15	GLU	CD-OE1	5.49	1.31	1.25
23	P	409	SER	N-CA	-5.49	1.35	1.46
6	F	107	ARG	CZ-NH2	5.49	1.40	1.33
5	E	209	GLU	CD-OE2	5.48	1.31	1.25
7	G	215	GLU	CD-OE2	-5.48	1.19	1.25
27	O	286	PHE	CB-CG	-5.48	1.42	1.51
28	H	186	PRO	N-CD	-5.48	1.40	1.47
21	N	520	GLY	CA-C	5.48	1.60	1.51
4	d	112	TYR	CB-CG	-5.48	1.43	1.51
3	C	28	SER	CB-OG	-5.48	1.35	1.42
23	P	373	GLU	CG-CD	5.48	1.60	1.51
24	Q	189	ARG	NE-CZ	5.47	1.40	1.33
26	U	35	GLY	CA-C	-5.47	1.43	1.51
26	U	127	GLN	CA-CB	5.47	1.66	1.53
11	k	85	ARG	CZ-NH2	5.47	1.40	1.33
23	P	166	GLU	CD-OE1	5.47	1.31	1.25
3	C	107	PRO	CA-C	-5.46	1.42	1.52
27	O	188	PHE	CG-CD1	5.46	1.47	1.38
29	I	54	ARG	NE-CZ	5.46	1.40	1.33
1	a	155	TYR	CE1-CZ	5.46	1.45	1.38
13	m	182	TYR	CG-CD1	5.46	1.46	1.39
8	1	191	GLY	CA-C	-5.46	1.43	1.51
11	4	149	ARG	CZ-NH2	5.46	1.40	1.33
30	K	115	GLY	CA-C	-5.46	1.43	1.51
14	n	137	ARG	CZ-NH2	5.45	1.40	1.33
3	c	217	ARG	N-CA	-5.45	1.35	1.46
1	a	84	ASN	N-CA	-5.45	1.35	1.46
22	S	149	SER	CA-CB	5.45	1.61	1.52
6	F	164	ARG	CZ-NH2	5.45	1.40	1.33
14	7	98	ARG	CZ-NH1	5.45	1.40	1.33
16	V	31	SER	CA-CB	5.45	1.61	1.52
17	T	8	THR	CA-C	-5.45	1.38	1.52
12	5	142	GLU	CD-OE2	-5.45	1.19	1.25
30	K	81	ARG	CZ-NH2	5.45	1.40	1.33
31	L	182	GLY	CA-C	-5.45	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	141	ARG	CD-NE	5.44	1.55	1.46
21	N	417	ARG	CZ-NH2	5.44	1.40	1.33
4	d	242	GLU	CG-CD	5.44	1.60	1.51
24	Q	324	GLU	CD-OE2	5.44	1.31	1.25
3	c	170	SER	CA-CB	5.43	1.61	1.52
23	P	390	TYR	CB-CG	5.43	1.59	1.51
10	3	188	TYR	CE2-CZ	5.43	1.45	1.38
5	e	102	TYR	CZ-OH	5.43	1.47	1.37
21	N	389	TYR	CZ-OH	5.43	1.47	1.37
29	I	260	GLY	CA-C	-5.43	1.43	1.51
11	k	98	TYR	CZ-OH	5.42	1.47	1.37
24	Q	130	ARG	CA-CB	5.42	1.65	1.53
17	T	24	GLU	CA-CB	5.42	1.65	1.53
7	g	106	PRO	N-CD	-5.42	1.40	1.47
18	X	11	ARG	CZ-NH2	5.42	1.40	1.33
12	5	262	TYR	CD2-CE2	5.42	1.47	1.39
15	W	27	GLU	CG-CD	5.42	1.60	1.51
18	X	59	ARG	CZ-NH2	5.42	1.40	1.33
32	M	433	TYR	CZ-OH	5.42	1.47	1.37
2	B	224	TYR	CG-CD1	5.42	1.46	1.39
6	F	51	ARG	NE-CZ	5.42	1.40	1.33
2	b	80	PRO	CA-C	-5.41	1.42	1.52
5	e	136	ARG	NE-CZ	5.41	1.40	1.33
22	S	239	ARG	CD-NE	5.41	1.55	1.46
27	O	250	TRP	CB-CG	5.41	1.59	1.50
30	K	255	ARG	NE-CZ	5.41	1.40	1.33
33	J	324	ARG	NE-CZ	5.41	1.40	1.33
9	2	126	TYR	CG-CD1	5.41	1.46	1.39
22	S	64	ARG	CZ-NH2	5.41	1.40	1.33
12	5	174	THR	CB-OG1	-5.41	1.32	1.43
4	d	106	VAL	CB-CG2	5.40	1.64	1.52
9	i	153	TYR	CA-CB	5.40	1.65	1.53
29	I	181	TYR	CE2-CZ	5.40	1.45	1.38
32	M	349	PHE	C-N	-5.39	1.24	1.34
1	a	14	ARG	CZ-NH1	5.39	1.40	1.33
8	h	161	VAL	CB-CG1	5.39	1.64	1.52
11	4	96	ARG	N-CA	-5.39	1.35	1.46
14	7	189	ARG	NE-CZ	5.39	1.40	1.33
4	d	145	PRO	N-CA	-5.39	1.38	1.47
4	D	141	ARG	CZ-NH2	5.39	1.40	1.33
29	I	405	ARG	CZ-NH2	5.39	1.40	1.33
8	h	152	ARG	CD-NE	5.38	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	115	ARG	CZ-NH2	5.38	1.40	1.33
6	F	27	GLU	CD-OE2	5.38	1.31	1.25
17	T	271	GLU	CB-CG	5.38	1.62	1.52
33	J	324	ARG	CD-NE	5.38	1.55	1.46
10	3	188	TYR	CZ-OH	5.38	1.47	1.37
21	N	415	PHE	CB-CG	-5.38	1.42	1.51
1	a	114	CYS	CB-SG	5.38	1.91	1.82
12	5	248	GLY	N-CA	-5.37	1.38	1.46
30	K	198	TYR	CE1-CZ	5.37	1.45	1.38
7	g	78	TYR	CE1-CZ	5.37	1.45	1.38
13	6	75	ARG	CD-NE	5.37	1.55	1.46
1	a	105	ARG	CZ-NH2	5.37	1.40	1.33
24	Q	22	GLU	CD-OE1	5.37	1.31	1.25
3	C	122	TYR	CG-CD2	5.37	1.46	1.39
12	5	212	TYR	C-N	5.37	1.42	1.33
15	W	88	ALA	CA-CB	5.37	1.63	1.52
13	m	186	GLU	CD-OE2	5.36	1.31	1.25
22	S	158	PHE	CG-CD2	5.36	1.46	1.38
30	K	67	TYR	CE1-CZ	5.36	1.45	1.38
31	L	255	TYR	CB-CG	-5.36	1.43	1.51
30	K	128	ARG	NE-CZ	5.36	1.40	1.33
4	d	159	TRP	CB-CG	5.35	1.59	1.50
22	S	463	GLU	CD-OE2	5.35	1.31	1.25
8	h	20	GLY	CA-C	-5.35	1.43	1.51
13	6	186	GLU	CD-OE2	5.35	1.31	1.25
5	e	174	SER	CB-OG	-5.35	1.35	1.42
1	A	133	TYR	CE2-CZ	5.35	1.45	1.38
3	C	114	ARG	CZ-NH1	5.35	1.40	1.33
22	S	346	TYR	CZ-OH	5.35	1.47	1.37
1	A	26	TYR	CG-CD1	5.34	1.46	1.39
12	5	247	GLY	N-CA	-5.34	1.38	1.46
24	Q	84	TYR	CE2-CZ	5.34	1.45	1.38
12	5	221	TRP	CZ2-CH2	5.34	1.47	1.37
22	S	481	TYR	CE2-CZ	5.34	1.45	1.38
8	h	54	ARG	CZ-NH1	5.34	1.40	1.33
11	4	67	TYR	CG-CD1	5.34	1.46	1.39
9	i	140	PHE	CE2-CZ	5.33	1.47	1.37
32	M	163	PHE	CE2-CZ	5.33	1.47	1.37
1	a	106	TYR	CG-CD2	5.33	1.46	1.39
14	7	153	GLN	CG-CD	5.33	1.63	1.51
31	L	144	VAL	CA-CB	-5.33	1.43	1.54
6	f	107	ARG	NE-CZ	5.33	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	36	GLY	N-CA	-5.33	1.38	1.46
5	E	165	TYR	CG-CD2	5.33	1.46	1.39
8	1	104	ALA	N-CA	-5.32	1.35	1.46
21	N	375	HIS	CB-CG	-5.32	1.40	1.50
21	N	776	TYR	CZ-OH	5.32	1.47	1.37
1	a	135	ARG	NE-CZ	5.32	1.40	1.33
14	n	137	ARG	NE-CZ	5.32	1.40	1.33
4	D	87	GLU	CD-OE2	5.32	1.31	1.25
12	5	278	GLU	CB-CG	5.32	1.62	1.52
15	W	122	ARG	CZ-NH1	5.32	1.40	1.33
9	i	107	SER	CA-CB	5.32	1.60	1.52
11	4	8	ARG	CD-NE	5.32	1.55	1.46
14	7	218	TYR	CE2-CZ	5.32	1.45	1.38
22	S	165	PRO	N-CD	-5.32	1.40	1.47
27	O	372	GLU	CG-CD	5.32	1.59	1.51
33	J	120	TYR	CE2-CZ	5.32	1.45	1.38
18	X	32	GLU	CB-CG	5.31	1.62	1.52
3	C	94	HIS	CB-CG	5.31	1.59	1.50
33	J	22	TYR	CZ-OH	5.31	1.46	1.37
26	U	218	GLU	CB-CG	5.31	1.62	1.52
31	L	209	ARG	CZ-NH2	5.31	1.40	1.33
5	e	43	LYS	N-CA	-5.31	1.35	1.46
9	i	104	ARG	CZ-NH1	5.31	1.40	1.33
1	A	135	ARG	CG-CD	5.31	1.65	1.51
12	5	150	SER	CA-CB	5.31	1.60	1.52
15	W	85	LEU	N-CA	-5.31	1.35	1.46
28	H	181	TYR	CG-CD2	5.31	1.46	1.39
3	c	52	VAL	CB-CG2	5.31	1.64	1.52
23	P	379	TYR	CZ-OH	5.31	1.46	1.37
17	T	235	PHE	CG-CD2	5.30	1.46	1.38
20	Z	255	LEU	N-CA	-5.30	1.35	1.46
27	O	185	PHE	CG-CD1	5.30	1.46	1.38
32	M	67	GLU	CD-OE2	5.30	1.31	1.25
21	N	570	ARG	CZ-NH1	5.30	1.40	1.33
23	P	170	SER	CA-CB	-5.30	1.45	1.52
18	X	11	ARG	CD-NE	5.30	1.55	1.46
23	P	168	TYR	CG-CD2	5.30	1.46	1.39
25	R	204	TRP	CD2-CE2	-5.30	1.34	1.41
3	C	35	ALA	CA-C	-5.30	1.39	1.52
28	H	222	ARG	CZ-NH2	5.30	1.40	1.33
32	M	73	ARG	CZ-NH1	5.30	1.40	1.33
2	B	62	SER	CB-OG	-5.29	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	105	ARG	CZ-NH2	5.29	1.40	1.33
8	h	194	ARG	CZ-NH2	5.29	1.40	1.33
13	6	130	VAL	CB-CG1	5.29	1.64	1.52
6	f	183	ASP	C-N	5.29	1.42	1.33
31	L	68	ARG	CZ-NH2	5.29	1.40	1.33
21	N	40	SER	CA-CB	5.29	1.60	1.52
11	4	8	ARG	CZ-NH2	5.28	1.40	1.33
4	D	120	TYR	CG-CD2	5.28	1.46	1.39
7	g	191	GLU	CB-CG	5.28	1.62	1.52
12	l	127	CYS	CB-SG	5.28	1.91	1.82
7	g	149	TYR	CZ-OH	5.28	1.46	1.37
12	l	264	GLY	N-CA	-5.28	1.38	1.46
16	V	230	TYR	CE1-CZ	5.28	1.45	1.38
33	J	270	ARG	CZ-NH2	5.27	1.40	1.33
23	P	168	TYR	CB-CG	5.27	1.59	1.51
14	7	122	PRO	CA-C	-5.27	1.42	1.52
28	H	299	ARG	CD-NE	5.27	1.55	1.46
30	K	399	ARG	NE-CZ	5.27	1.39	1.33
33	J	329	ARG	CZ-NH1	5.27	1.39	1.33
3	C	107	PRO	N-CD	5.26	1.55	1.47
24	Q	309	ARG	CZ-NH2	5.26	1.39	1.33
5	e	159	GLU	CG-CD	5.26	1.59	1.51
21	N	820	GLU	CG-CD	5.26	1.59	1.51
2	B	83	ARG	CZ-NH1	5.26	1.39	1.33
21	N	248	GLU	CD-OE1	5.26	1.31	1.25
30	K	333	ARG	CD-NE	5.26	1.55	1.46
7	g	72	ARG	NE-CZ	5.26	1.39	1.33
1	A	88	PRO	CA-CB	5.25	1.64	1.53
11	k	195	PHE	CB-CG	-5.25	1.42	1.51
2	B	231	LYS	N-CA	-5.25	1.35	1.46
27	O	135	ARG	CZ-NH2	5.25	1.39	1.33
30	K	262	ARG	CG-CD	5.25	1.65	1.51
4	d	83	ARG	CZ-NH1	5.25	1.39	1.33
15	W	131	THR	C-N	5.25	1.46	1.34
2	b	7	PHE	CE2-CZ	5.25	1.47	1.37
1	A	20	SER	N-CA	-5.25	1.35	1.46
6	f	202	ARG	CZ-NH2	5.25	1.39	1.33
9	2	216	LEU	CA-CB	-5.25	1.41	1.53
14	n	65	SER	CA-CB	5.24	1.60	1.52
25	R	331	ARG	CZ-NH2	5.24	1.39	1.33
28	H	162	ARG	CZ-NH1	5.24	1.39	1.33
33	J	315	GLU	CB-CG	5.24	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	45	ARG	CZ-NH2	5.24	1.39	1.33
9	2	152	TYR	CD1-CE1	5.24	1.47	1.39
29	I	155	SER	CA-CB	5.24	1.60	1.52
8	h	91	PHE	CG-CD2	5.24	1.46	1.38
13	m	229	ARG	CZ-NH1	5.24	1.39	1.33
23	P	379	TYR	CG-CD1	5.23	1.46	1.39
7	g	72	ARG	CZ-NH2	5.23	1.39	1.33
11	k	171	ARG	CZ-NH1	5.23	1.39	1.33
21	N	299	TYR	CG-CD1	5.23	1.46	1.39
5	e	60	GLU	CB-CG	5.23	1.62	1.52
18	X	98	PHE	CG-CD1	5.23	1.46	1.38
10	3	69	TYR	CG-CD1	-5.22	1.32	1.39
14	7	220	ARG	NE-CZ	5.22	1.39	1.33
30	K	73	ARG	CZ-NH1	5.22	1.39	1.33
31	L	194	ARG	CD-NE	5.22	1.55	1.46
4	d	11	PHE	CE1-CZ	5.22	1.47	1.37
7	g	145	GLY	CA-C	-5.22	1.43	1.51
30	K	45	SER	CA-CB	5.22	1.60	1.52
24	Q	20	TYR	CE2-CZ	5.22	1.45	1.38
7	g	157	TYR	CZ-OH	5.22	1.46	1.37
24	Q	132	PHE	CB-CG	5.22	1.60	1.51
24	Q	195	LYS	N-CA	-5.22	1.35	1.46
27	O	385	GLU	CB-CG	5.22	1.62	1.52
22	S	174	ARG	CZ-NH2	5.22	1.39	1.33
21	N	282	TYR	CZ-OH	5.21	1.46	1.37
11	4	44	MET	CA-C	-5.21	1.39	1.52
5	E	72	ARG	CZ-NH1	5.21	1.39	1.33
24	Q	270	ILE	C-N	5.21	1.46	1.34
6	f	71	GLY	CA-C	-5.21	1.43	1.51
8	h	174	TRP	NE1-CE2	5.21	1.44	1.37
16	V	194	ARG	CZ-NH1	5.21	1.39	1.33
21	N	228	VAL	N-CA	5.21	1.56	1.46
2	B	126	GLY	N-CA	-5.21	1.38	1.46
16	V	117	TRP	NE1-CE2	5.21	1.44	1.37
11	k	93	ARG	NE-CZ	5.20	1.39	1.33
27	O	15	ARG	CZ-NH2	5.20	1.39	1.33
7	g	195	GLN	CG-CD	5.20	1.63	1.51
25	R	295	SER	CB-OG	5.20	1.49	1.42
27	O	137	TYR	CZ-OH	5.20	1.46	1.37
32	M	115	LYS	CD-CE	5.20	1.64	1.51
26	U	147	GLY	N-CA	-5.20	1.38	1.46
9	2	48	ARG	CZ-NH1	5.20	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	X	113	GLU	CG-CD	5.20	1.59	1.51
21	N	739	PHE	CA-CB	5.20	1.65	1.53
22	S	415	SER	CA-CB	5.20	1.60	1.52
7	G	71	ASP	CB-CG	5.19	1.62	1.51
4	d	230	ASN	CB-CG	5.19	1.62	1.51
14	7	194	ARG	NE-CZ	5.19	1.39	1.33
29	I	79	SER	CA-CB	5.19	1.60	1.52
16	V	197	TYR	CZ-OH	5.19	1.46	1.37
1	A	91	ARG	CD-NE	5.18	1.55	1.46
1	A	110	TYR	CE1-CZ	5.18	1.45	1.38
3	C	129	ARG	CZ-NH2	5.18	1.39	1.33
7	G	242	PHE	N-CA	-5.18	1.35	1.46
32	M	196	ALA	CA-C	-5.18	1.39	1.52
13	m	219	GLY	N-CA	-5.18	1.38	1.46
25	R	65	TYR	CE1-CZ	5.18	1.45	1.38
11	4	96	ARG	CZ-NH1	5.18	1.39	1.33
16	V	42	ARG	CZ-NH2	5.18	1.39	1.33
25	R	115	GLU	CD-OE2	-5.18	1.20	1.25
10	j	29	LEU	C-N	5.18	1.42	1.33
13	m	48	GLU	CD-OE1	5.18	1.31	1.25
10	j	191	LYS	CA-CB	5.17	1.65	1.53
13	6	99	ARG	NE-CZ	5.17	1.39	1.33
22	S	82	TYR	CZ-OH	5.17	1.46	1.37
5	e	174	SER	CA-CB	5.17	1.60	1.52
11	4	171	ARG	CZ-NH1	5.17	1.39	1.33
24	Q	9	GLU	CG-CD	5.17	1.59	1.51
1	A	156	LYS	CD-CE	5.17	1.64	1.51
8	1	38	ARG	CZ-NH2	5.17	1.39	1.33
21	N	381	GLU	CB-CG	5.17	1.61	1.52
31	L	180	PHE	CG-CD1	5.17	1.46	1.38
32	M	33	ARG	CD-NE	5.16	1.55	1.46
32	M	110	ASN	N-CA	-5.16	1.36	1.46
16	V	20	ARG	CZ-NH1	5.16	1.39	1.33
22	S	196	ARG	NE-CZ	5.16	1.39	1.33
31	L	195	GLU	CG-CD	5.16	1.59	1.51
1	A	138	GLY	N-CA	-5.16	1.38	1.46
10	3	203	ARG	NE-CZ	5.16	1.39	1.33
25	R	213	TYR	CD2-CE2	5.16	1.47	1.39
31	L	157	ARG	CZ-NH2	5.16	1.39	1.33
7	G	190	ARG	NE-CZ	5.16	1.39	1.33
28	H	234	ARG	NE-CZ	5.16	1.39	1.33
1	a	29	GLU	CB-CG	5.16	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	97	PHE	CG-CD1	5.16	1.46	1.38
25	R	199	GLU	CG-CD	5.15	1.59	1.51
16	V	268	THR	N-CA	-5.15	1.36	1.46
23	P	356	TYR	CA-CB	5.15	1.65	1.53
29	I	196	GLU	CG-CD	5.15	1.59	1.51
7	g	91	ARG	CD-NE	5.15	1.55	1.46
13	m	69	GLY	CA-C	5.15	1.60	1.51
32	M	433	TYR	CE1-CZ	5.14	1.45	1.38
29	I	291	ARG	CZ-NH1	5.14	1.39	1.33
8	h	32	GLY	N-CA	-5.13	1.38	1.46
15	W	107	HIS	CG-CD2	5.13	1.44	1.35
13	m	202	ARG	NE-CZ	5.13	1.39	1.33
13	m	182	TYR	CB-CG	-5.13	1.44	1.51
24	Q	236	PHE	CG-CD2	5.13	1.46	1.38
3	C	210	ARG	CD-NE	5.12	1.55	1.46
11	4	184	VAL	CA-CB	-5.12	1.44	1.54
22	S	428	ARG	NE-CZ	5.12	1.39	1.33
25	R	186	TYR	CE2-CZ	5.12	1.45	1.38
29	I	276	PRO	N-CA	-5.12	1.38	1.47
12	5	145	GLU	N-CA	-5.12	1.36	1.46
2	b	101	TYR	CZ-OH	5.12	1.46	1.37
29	I	262	ARG	CZ-NH1	5.12	1.39	1.33
3	C	54	SER	CA-CB	5.11	1.60	1.52
11	k	23	ARG	NE-CZ	5.11	1.39	1.33
11	k	141	PHE	CE2-CZ	5.11	1.47	1.37
13	m	63	ASN	CB-CG	5.11	1.62	1.51
1	A	46	ARG	CZ-NH2	5.11	1.39	1.33
1	a	104	PHE	CD2-CE2	5.11	1.49	1.39
12	5	264	GLY	CA-C	-5.10	1.43	1.51
28	H	162	ARG	NE-CZ	5.10	1.39	1.33
11	k	93	ARG	CG-CD	5.10	1.64	1.51
12	5	102	ALA	CA-CB	5.10	1.63	1.52
17	T	83	ASN	CB-CG	5.10	1.62	1.51
25	R	334	ARG	CZ-NH2	5.10	1.39	1.33
27	O	310	PHE	CG-CD1	5.10	1.46	1.38
28	H	453	GLY	CA-C	-5.10	1.43	1.51
33	J	246	PHE	CG-CD1	5.10	1.46	1.38
14	7	74	ARG	CZ-NH2	5.10	1.39	1.33
6	F	89	ARG	CZ-NH2	5.09	1.39	1.33
24	Q	106	GLN	CA-CB	5.09	1.65	1.53
30	K	409	GLU	CA-CB	5.09	1.65	1.53
9	i	65	ARG	CZ-NH2	5.09	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	185	SER	CA-CB	5.09	1.60	1.52
22	S	162	VAL	CB-CG2	5.09	1.63	1.52
30	K	168	ASP	CB-CG	5.09	1.62	1.51
33	J	170	HIS	CG-CD2	5.09	1.44	1.35
12	l	94	ARG	CZ-NH1	5.09	1.39	1.33
14	7	98	ARG	CD-NE	5.09	1.55	1.46
14	7	73	GLU	CD-OE2	5.08	1.31	1.25
8	h	19	ASP	C-N	5.08	1.42	1.33
26	U	95	SER	CA-CB	5.08	1.60	1.52
2	B	240	SER	CB-OG	-5.08	1.35	1.42
21	N	737	SER	CA-CB	5.08	1.60	1.52
30	K	199	GLU	N-CA	-5.08	1.36	1.46
25	R	238	PHE	N-CA	-5.08	1.36	1.46
8	h	142	PHE	CG-CD2	5.08	1.46	1.38
25	R	321	TYR	CB-CG	-5.08	1.44	1.51
6	f	230	VAL	CA-CB	-5.07	1.44	1.54
22	S	170	TYR	CE2-CZ	5.07	1.45	1.38
22	S	332	PHE	CG-CD2	5.07	1.46	1.38
6	F	164	ARG	CD-NE	5.07	1.55	1.46
21	N	88	ARG	NE-CZ	5.07	1.39	1.33
28	H	72	SER	CA-CB	5.07	1.60	1.52
5	e	72	ARG	NE-CZ	5.07	1.39	1.33
8	h	51	TRP	CZ3-CH2	-5.07	1.31	1.40
8	1	70	TYR	CB-CG	-5.07	1.44	1.51
16	V	100	ARG	CD-NE	5.06	1.55	1.46
23	P	310	ARG	CD-NE	5.06	1.55	1.46
29	I	100	ARG	CD-NE	5.06	1.55	1.46
10	3	65	GLU	CD-OE1	5.05	1.31	1.25
22	S	91	ASN	CB-CG	5.05	1.62	1.51
28	H	296	GLU	CA-CB	5.05	1.65	1.53
4	D	172	ARG	CD-NE	5.05	1.55	1.46
5	E	15	PHE	CG-CD1	5.05	1.46	1.38
17	T	94	HIS	N-CA	-5.05	1.36	1.46
28	H	261	ARG	CD-NE	5.05	1.55	1.46
9	i	48	ARG	CZ-NH1	5.05	1.39	1.33
21	N	36	TRP	NE1-CE2	5.05	1.44	1.37
4	D	22	TYR	CD2-CE2	5.05	1.47	1.39
9	2	82	GLU	CG-CD	5.05	1.59	1.51
29	I	422	ARG	NE-CZ	5.05	1.39	1.33
2	B	77	GLY	CA-C	-5.04	1.43	1.51
23	P	92	SER	CA-CB	5.04	1.60	1.52
21	N	162	ARG	CZ-NH2	5.04	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	324	ARG	CD-NE	5.04	1.55	1.46
28	H	281	GLN	CA-CB	5.04	1.65	1.53
13	m	179	PRO	CA-CB	5.04	1.63	1.53
3	c	143	ARG	CZ-NH2	5.04	1.39	1.33
28	H	70	LYS	CA-C	-5.04	1.39	1.52
5	e	122	ARG	NE-CZ	5.04	1.39	1.33
11	4	58	GLU	CB-CG	5.04	1.61	1.52
28	H	335	GLU	CD-OE1	-5.04	1.20	1.25
8	h	28	ARG	CZ-NH1	5.03	1.39	1.33
2	B	186	GLU	CG-CD	5.03	1.59	1.51
8	h	167	SER	CA-CB	5.03	1.60	1.52
18	X	75	TRP	CB-CG	5.03	1.59	1.50
24	Q	357	VAL	CB-CG1	5.03	1.63	1.52
3	c	5	ARG	NE-CZ	5.02	1.39	1.33
25	R	189	GLU	CD-OE2	5.02	1.31	1.25
12	5	205	GLY	CA-C	-5.02	1.43	1.51
17	T	19	ASP	CB-CG	5.02	1.62	1.51
12	5	234	ARG	NE-CZ	5.02	1.39	1.33
19	Y	61	GLU	CG-CD	5.02	1.59	1.51
24	Q	127	ARG	NE-CZ	5.02	1.39	1.33
8	h	147	CYS	CB-SG	5.02	1.90	1.82
25	R	363	PHE	CE1-CZ	5.01	1.46	1.37
27	O	197	SER	CB-OG	5.01	1.48	1.42
9	i	247	VAL	CB-CG2	5.01	1.63	1.52
12	5	212	TYR	CE2-CZ	5.01	1.45	1.38
4	D	138	PHE	CA-C	-5.01	1.40	1.52
9	i	102	GLU	CD-OE1	5.01	1.31	1.25
16	V	258	GLU	CA-CB	5.01	1.65	1.53
33	J	219	VAL	CB-CG1	5.01	1.63	1.52
4	d	4	TYR	CG-CD1	5.00	1.45	1.39
28	H	405	GLU	CG-CD	5.00	1.59	1.51
33	J	306	ARG	CZ-NH2	5.00	1.39	1.33

All (2556) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	93	ARG	NE-CZ-NH1	-44.71	97.95	120.30
7	G	93	ARG	NE-CZ-NH1	-44.55	98.03	120.30
29	I	313	LEU	C-N-CA	-35.90	31.95	121.70
29	I	313	LEU	CA-C-N	-30.88	49.27	117.20
29	I	313	LEU	O-C-N	26.17	164.58	122.70
20	Z	635	ALA	CB-CA-C	24.05	146.17	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	93	ARG	NE-CZ-NH2	23.02	131.81	120.30
11	k	93	ARG	NE-CZ-NH2	-21.57	109.52	120.30
31	L	404	ARG	NE-CZ-NH2	-20.92	109.84	120.30
25	R	338	TYR	CB-CG-CD1	20.63	133.38	121.00
21	N	422	TYR	CB-CG-CD2	-19.85	109.09	121.00
23	P	13	TYR	CB-CG-CD2	-17.96	110.22	121.00
7	g	93	ARG	NE-CZ-NH2	17.96	129.28	120.30
31	L	117	TYR	CB-CG-CD2	-17.68	110.39	121.00
31	L	69	ARG	NE-CZ-NH1	17.36	128.98	120.30
1	a	106	TYR	CB-CG-CD2	-17.05	110.77	121.00
17	T	60	ARG	NE-CZ-NH2	-17.05	111.77	120.30
13	6	202	ARG	NE-CZ-NH2	-17.00	111.80	120.30
7	g	115	ARG	NE-CZ-NH1	16.67	128.64	120.30
7	g	22	PHE	CB-CG-CD1	-16.43	109.30	120.80
5	e	20	ARG	NE-CZ-NH2	-16.36	112.12	120.30
13	6	139	TYR	CB-CG-CD1	-16.33	111.20	121.00
30	K	320	ARG	NE-CZ-NH2	-16.27	112.17	120.30
30	K	350	ARG	NE-CZ-NH1	16.25	128.42	120.30
1	A	19	PHE	CB-CG-CD2	16.20	132.14	120.80
27	O	172	TYR	CB-CG-CD1	16.05	130.63	121.00
25	R	263	ARG	NE-CZ-NH1	16.02	128.31	120.30
3	C	157	TYR	CB-CG-CD2	-15.98	111.41	121.00
22	S	273	PHE	CB-CG-CD1	15.94	131.96	120.80
1	A	135	ARG	NE-CZ-NH1	15.87	128.23	120.30
17	T	186	ARG	NE-CZ-NH2	-15.75	112.42	120.30
25	R	338	TYR	CB-CG-CD2	-15.50	111.70	121.00
1	a	106	TYR	CB-CG-CD1	15.47	130.28	121.00
8	1	34	TYR	CB-CG-CD2	-15.23	111.86	121.00
7	G	91	ARG	NE-CZ-NH1	15.07	127.83	120.30
11	k	8	ARG	NE-CZ-NH2	-14.96	112.82	120.30
31	L	404	ARG	NE-CZ-NH1	14.94	127.77	120.30
20	Z	738	TYR	CD1-CE1-CZ	14.89	133.20	119.80
1	A	96	ARG	NE-CZ-NH1	14.85	127.73	120.30
13	m	141	ARG	NE-CZ-NH1	-14.85	112.88	120.30
20	Z	738	TYR	CB-CG-CD2	14.62	129.77	121.00
25	R	331	ARG	NE-CZ-NH1	14.49	127.55	120.30
3	C	157	TYR	CB-CG-CD1	14.48	129.69	121.00
22	S	333	PHE	CB-CG-CD1	-14.44	110.69	120.80
20	Z	727	GLU	N-CA-CB	-14.25	84.94	110.60
20	Z	728	LYS	CB-CG-CD	14.10	148.26	111.60
25	R	371	PHE	CB-CG-CD1	13.88	130.51	120.80
21	N	422	TYR	CB-CG-CD1	13.81	129.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	377	TYR	CB-CG-CD2	13.80	129.28	121.00
1	a	71	TYR	CB-CG-CD2	-13.75	112.75	121.00
24	Q	434	TYR	CB-CG-CD2	-13.69	112.79	121.00
31	L	299	ARG	NE-CZ-NH2	-13.66	113.47	120.30
26	U	52	PHE	CB-CG-CD1	-13.60	111.28	120.80
2	B	90	ARG	NE-CZ-NH1	13.59	127.09	120.30
5	E	167	TYR	CB-CG-CD2	-13.59	112.85	121.00
6	F	174	ARG	NE-CZ-NH1	-13.56	113.52	120.30
4	d	232	TYR	CB-CG-CD1	13.54	129.12	121.00
11	4	171	ARG	NE-CZ-NH2	-13.51	113.55	120.30
22	S	273	PHE	CB-CG-CD2	-13.47	111.37	120.80
1	a	244	ARG	NE-CZ-NH2	-13.43	113.59	120.30
23	P	213	TYR	CB-CG-CD2	-13.41	112.95	121.00
1	a	162	TYR	CB-CG-CD2	-13.40	112.96	121.00
7	g	22	PHE	CB-CG-CD2	13.37	130.16	120.80
16	V	269	ARG	NE-CZ-NH2	-13.34	113.63	120.30
2	b	204	PHE	CB-CG-CD1	-13.22	111.55	120.80
27	O	356	ARG	NE-CZ-NH1	13.21	126.91	120.30
3	c	4	ARG	NE-CZ-NH1	13.06	126.83	120.30
21	N	711	ARG	NE-CZ-NH1	13.06	126.83	120.30
20	Z	635	ALA	N-CA-CB	13.02	128.32	110.10
3	C	217	ARG	NE-CZ-NH1	12.99	126.80	120.30
30	K	320	ARG	NE-CZ-NH1	12.97	126.78	120.30
11	4	98	TYR	CB-CG-CD1	12.96	128.78	121.00
7	g	201	TYR	CB-CG-CD1	-12.94	113.24	121.00
3	C	129	ARG	NE-CZ-NH2	-12.90	113.85	120.30
14	7	124	TYR	CB-CG-CD1	12.82	128.69	121.00
13	6	229	ARG	NE-CZ-NH2	-12.77	113.92	120.30
1	a	46	ARG	NE-CZ-NH1	-12.73	113.94	120.30
7	G	20	ARG	NE-CZ-NH1	12.68	126.64	120.30
32	M	425	ARG	NE-CZ-NH1	-12.64	113.98	120.30
22	S	421	TYR	CB-CG-CD1	-12.64	113.42	121.00
30	K	330	ARG	NE-CZ-NH1	12.63	126.61	120.30
8	1	133	TYR	CB-CG-CD2	12.62	128.57	121.00
5	e	53	ARG	NE-CZ-NH1	12.54	126.57	120.30
4	d	119	ARG	NE-CZ-NH1	12.53	126.56	120.30
20	Z	745	LEU	CB-CG-CD1	-12.53	89.70	111.00
20	Z	728	LYS	N-CA-CB	12.47	133.05	110.60
21	N	124	TYR	CB-CG-CD2	-12.46	113.53	121.00
14	n	98	ARG	NE-CZ-NH1	12.42	126.51	120.30
13	6	139	TYR	CB-CG-CD2	12.36	128.41	121.00
17	T	150	ARG	NE-CZ-NH2	-12.35	114.13	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	222	ARG	NE-CZ-NH1	12.35	126.47	120.30
23	P	13	TYR	CB-CG-CD1	12.32	128.39	121.00
1	A	30	TYR	CB-CG-CD2	-12.31	113.61	121.00
4	d	49	ARG	NE-CZ-NH1	12.29	126.44	120.30
16	V	135	ARG	NE-CZ-NH1	12.29	126.44	120.30
27	O	147	ARG	NE-CZ-NH2	12.28	126.44	120.30
27	O	172	TYR	CB-CG-CD2	-12.26	113.64	121.00
27	O	135	ARG	NE-CZ-NH1	12.20	126.40	120.30
3	c	226	TYR	CB-CG-CD2	-12.17	113.70	121.00
30	K	58	TYR	CB-CG-CD1	-12.17	113.70	121.00
12	l	163	TYR	CB-CG-CD1	12.17	128.30	121.00
7	g	93	ARG	NH1-CZ-NH2	12.15	132.77	119.40
14	7	241	PHE	CB-CG-CD2	-12.14	112.30	120.80
28	H	283	TYR	CB-CG-CD2	12.14	128.28	121.00
16	V	194	ARG	NE-CZ-NH2	-12.06	114.27	120.30
8	1	142	PHE	CB-CG-CD2	12.05	129.24	120.80
17	T	78	PHE	CB-CG-CD1	12.05	129.23	120.80
28	H	454	TYR	CB-CG-CD2	-11.99	113.81	121.00
31	L	78	ARG	NE-CZ-NH2	-11.96	114.32	120.30
6	F	123	TYR	CB-CG-CD2	-11.85	113.89	121.00
25	R	382	ASP	CB-CG-OD2	-11.85	107.64	118.30
7	g	26	TYR	CB-CG-CD1	11.79	128.07	121.00
12	5	179	TYR	CB-CG-CD1	11.79	128.07	121.00
3	C	144	TYR	CB-CG-CD1	11.73	128.04	121.00
23	P	201	ARG	NE-CZ-NH2	11.71	126.16	120.30
1	a	12	TYR	CB-CG-CD2	-11.69	113.98	121.00
3	c	226	TYR	CB-CG-CD1	11.69	128.02	121.00
9	2	48	ARG	NE-CZ-NH2	-11.68	114.46	120.30
1	a	244	ARG	NE-CZ-NH1	11.67	126.14	120.30
9	i	217	ARG	NE-CZ-NH2	-11.66	114.47	120.30
13	m	202	ARG	NE-CZ-NH2	-11.65	114.47	120.30
1	A	30	TYR	CB-CG-CD1	11.65	127.99	121.00
6	F	39	ARG	NE-CZ-NH1	11.64	126.12	120.30
5	E	2	PHE	CB-CG-CD2	-11.63	112.66	120.80
33	J	296	ARG	NE-CZ-NH2	-11.62	114.49	120.30
1	a	162	TYR	CB-CG-CD1	11.60	127.96	121.00
12	5	253	TYR	CB-CG-CD2	-11.52	114.09	121.00
14	7	124	TYR	CB-CG-CD2	-11.50	114.10	121.00
19	Y	84	TYR	CB-CG-CD1	11.49	127.89	121.00
1	A	91	ARG	NE-CZ-NH1	11.46	126.03	120.30
31	L	117	TYR	CB-CG-CD1	11.44	127.87	121.00
32	M	42	ARG	NE-CZ-NH2	-11.42	114.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	292	ARG	NE-CZ-NH2	-11.40	114.60	120.30
10	3	154	TYR	CB-CG-CD1	-11.39	114.17	121.00
21	N	786	ARG	NE-CZ-NH2	-11.34	114.63	120.30
7	G	26	TYR	CB-CG-CD1	-11.32	114.21	121.00
14	7	219	TYR	CB-CG-CD2	-11.27	114.24	121.00
28	H	162	ARG	NE-CZ-NH2	-11.27	114.66	120.30
12	5	212	TYR	CB-CG-CD1	11.26	127.75	121.00
6	F	126	ARG	NE-CZ-NH1	11.25	125.93	120.30
3	c	117	ASP	CB-CG-OD2	-11.25	108.17	118.30
2	b	128	ARG	NE-CZ-NH2	-11.21	114.69	120.30
6	F	164	ARG	NE-CZ-NH1	11.20	125.90	120.30
22	S	480	ARG	NE-CZ-NH1	-11.15	114.72	120.30
21	N	906	ARG	NE-CZ-NH1	11.11	125.85	120.30
11	4	98	TYR	CB-CG-CD2	-11.07	114.36	121.00
11	k	148	TYR	CB-CG-CD2	-11.05	114.37	121.00
2	b	235	PHE	CB-CG-CD1	-11.04	113.07	120.80
1	a	105	ARG	NE-CZ-NH2	-11.04	114.78	120.30
5	e	72	ARG	NE-CZ-NH2	-11.02	114.79	120.30
9	i	152	TYR	CB-CG-CD2	-11.00	114.40	121.00
10	j	28	ARG	NE-CZ-NH2	-10.99	114.80	120.30
20	Z	247	GLN	CB-CA-C	10.97	132.34	110.40
28	H	420	ARG	NE-CZ-NH2	-10.95	114.82	120.30
23	P	47	ARG	NE-CZ-NH2	-10.94	114.83	120.30
6	F	164	ARG	NE-CZ-NH2	-10.93	114.83	120.30
17	T	88	TYR	CB-CG-CD2	-10.92	114.45	121.00
22	S	271	ARG	NE-CZ-NH2	-10.92	114.84	120.30
21	N	921	ARG	NE-CZ-NH2	-10.92	114.84	120.30
21	N	813	ARG	NE-CZ-NH1	10.91	125.76	120.30
23	P	47	ARG	NE-CZ-NH1	10.91	125.76	120.30
2	b	104	TYR	CB-CG-CD1	10.89	127.54	121.00
2	B	5	TYR	CB-CG-CD1	-10.85	114.49	121.00
7	g	112	PHE	CB-CG-CD1	-10.82	113.22	120.80
25	R	263	ARG	NE-CZ-NH2	-10.81	114.89	120.30
12	l	179	TYR	CB-CG-CD1	10.81	127.49	121.00
21	N	548	ARG	NE-CZ-NH2	-10.80	114.90	120.30
12	l	272	PHE	CB-CG-CD1	10.80	128.36	120.80
22	S	286	TYR	CB-CG-CD2	-10.75	114.55	121.00
7	G	132	PHE	CB-CG-CD2	-10.75	113.28	120.80
19	Y	38	PHE	CB-CG-CD2	-10.74	113.28	120.80
5	e	231	TYR	CB-CG-CD1	-10.71	114.58	121.00
10	j	28	ARG	NE-CZ-NH1	10.69	125.64	120.30
29	I	64	ARG	NE-CZ-NH1	10.67	125.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	113	TYR	CB-CG-CD2	-10.64	114.62	121.00
5	E	138	PHE	CB-CG-CD2	-10.62	113.37	120.80
23	P	103	TYR	CB-CG-CD1	-10.61	114.63	121.00
12	5	179	TYR	CB-CG-CD2	-10.58	114.65	121.00
2	B	4	ARG	NE-CZ-NH2	-10.56	115.02	120.30
21	N	776	TYR	CB-CG-CD2	10.56	127.34	121.00
3	c	9	ARG	NE-CZ-NH2	-10.50	115.05	120.30
31	L	127	TYR	CB-CG-CD1	-10.47	114.72	121.00
3	C	122	TYR	CB-CG-CD2	-10.46	114.73	121.00
23	P	390	TYR	CB-CG-CD2	-10.45	114.73	121.00
14	n	162	TYR	CB-CG-CD2	10.42	127.25	121.00
9	2	203	ASP	CB-CG-OD2	-10.42	108.92	118.30
11	k	46	PHE	CB-CG-CD2	-10.41	113.51	120.80
32	M	44	PHE	CB-CG-CD1	10.40	128.08	120.80
32	M	42	ARG	NE-CZ-NH1	10.37	125.48	120.30
29	I	262	ARG	NE-CZ-NH2	-10.36	115.12	120.30
12	5	245	TYR	CB-CG-CD1	-10.31	114.81	121.00
20	Z	728	LYS	CA-CB-CG	10.31	136.07	113.40
3	C	122	TYR	CB-CG-CD1	10.29	127.17	121.00
4	d	197	ARG	NE-CZ-NH2	-10.28	115.16	120.30
20	Z	251	ALA	N-CA-CB	10.28	124.49	110.10
17	T	81	TYR	CB-CG-CD1	-10.28	114.83	121.00
29	I	128	TYR	CG-CD2-CE2	-10.20	113.14	121.30
22	S	377	TYR	CB-CG-CD1	-10.18	114.89	121.00
29	I	436	TYR	CB-CG-CD2	-10.12	114.93	121.00
5	E	53	ARG	NE-CZ-NH2	-10.12	115.24	120.30
23	P	356	TYR	CB-CG-CD2	-10.10	114.94	121.00
6	F	233	TYR	CB-CG-CD1	-10.10	114.94	121.00
20	Z	635	ALA	N-CA-C	-10.10	83.74	111.00
23	P	359	ARG	NE-CZ-NH1	10.08	125.34	120.30
12	l	234	ARG	NE-CZ-NH1	10.07	125.33	120.30
14	7	261	TYR	CB-CG-CD2	-10.05	114.97	121.00
24	Q	104	PHE	CB-CG-CD1	10.03	127.82	120.80
31	L	209	ARG	NE-CZ-NH2	-10.03	115.29	120.30
32	M	166	ARG	NE-CZ-NH2	-10.03	115.29	120.30
31	L	72	ASP	CB-CG-OD2	10.02	127.32	118.30
24	Q	202	ARG	NE-CZ-NH1	10.02	125.31	120.30
4	d	108	TYR	CB-CG-CD2	9.99	126.99	121.00
31	L	68	ARG	NE-CZ-NH2	-9.99	115.31	120.30
16	V	42	ARG	NE-CZ-NH1	9.99	125.29	120.30
14	n	74	ARG	NE-CZ-NH2	-9.98	115.31	120.30
6	f	99	PHE	CB-CG-CD1	9.98	127.78	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	34	ASP	CB-CG-OD1	-9.97	109.32	118.30
7	G	91	ARG	NE-CZ-NH2	-9.96	115.32	120.30
1	A	128	TYR	CB-CG-CD2	-9.94	115.04	121.00
12	5	272	PHE	CB-CG-CD1	-9.91	113.86	120.80
22	S	333	PHE	CB-CG-CD2	9.90	127.73	120.80
8	h	111	TYR	CB-CG-CD2	-9.89	115.06	121.00
22	S	464	ARG	NE-CZ-NH2	-9.89	115.35	120.30
11	4	138	PHE	CB-CG-CD2	-9.87	113.89	120.80
21	N	75	TYR	CB-CG-CD1	-9.86	115.08	121.00
32	M	320	ARG	NE-CZ-NH2	-9.84	115.38	120.30
11	4	96	ARG	NE-CZ-NH1	9.82	125.21	120.30
21	N	224	THR	CA-CB-CG2	-9.81	98.66	112.40
8	h	34	TYR	CB-CG-CD1	-9.81	115.12	121.00
21	N	418	ASP	CB-CG-OD1	-9.81	109.47	118.30
2	b	101	TYR	CB-CG-CD2	-9.80	115.12	121.00
20	Z	745	LEU	CB-CA-C	-9.80	91.58	110.20
6	f	87	TYR	CB-CG-CD2	9.78	126.87	121.00
7	G	93	ARG	NH1-CZ-NH2	9.77	130.15	119.40
29	I	67	ASP	CB-CG-OD2	9.76	127.08	118.30
31	L	78	ARG	NE-CZ-NH1	9.76	125.18	120.30
17	T	60	ARG	NE-CZ-NH1	9.72	125.16	120.30
29	I	64	ARG	NE-CZ-NH2	-9.68	115.46	120.30
32	M	366	ARG	NE-CZ-NH2	-9.67	115.47	120.30
29	I	265	ARG	NE-CZ-NH1	9.66	125.13	120.30
3	C	217	ARG	NE-CZ-NH2	-9.66	115.47	120.30
23	P	201	ARG	NH1-CZ-NH2	-9.66	108.78	119.40
3	c	18	ARG	NE-CZ-NH2	-9.61	115.50	120.30
13	m	75	ARG	NE-CZ-NH2	-9.59	115.50	120.30
18	X	22	ARG	NE-CZ-NH2	-9.56	115.52	120.30
12	l	179	TYR	CB-CG-CD2	-9.56	115.27	121.00
9	2	65	ARG	NE-CZ-NH1	9.54	125.07	120.30
2	b	5	TYR	CB-CG-CD2	-9.54	115.28	121.00
1	A	115	ASP	CB-CG-OD1	-9.54	109.71	118.30
28	H	367	ARG	NE-CZ-NH1	9.54	125.07	120.30
17	T	78	PHE	CB-CG-CD2	-9.53	114.13	120.80
13	m	36	ARG	NE-CZ-NH1	-9.51	115.54	120.30
2	B	5	TYR	CB-CG-CD2	9.49	126.70	121.00
21	N	748	PHE	CB-CG-CD2	9.47	127.43	120.80
21	N	549	TYR	CG-CD1-CE1	-9.44	113.75	121.30
26	U	176	ARG	NE-CZ-NH2	-9.44	115.58	120.30
9	i	65	ARG	NE-CZ-NH2	9.43	125.02	120.30
4	d	218	ASP	CB-CG-OD1	-9.42	109.82	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	27	TYR	CB-CG-CD1	9.41	126.65	121.00
7	g	190	ARG	NE-CZ-NH1	9.40	125.00	120.30
12	5	148	ARG	NE-CZ-NH1	9.39	125.00	120.30
16	V	171	ARG	NE-CZ-NH1	9.37	124.99	120.30
30	K	262	ARG	NE-CZ-NH1	9.37	124.98	120.30
12	5	82	ARG	NE-CZ-NH1	9.37	124.98	120.30
5	e	16	SER	N-CA-CB	9.36	124.54	110.50
7	G	86	ARG	NE-CZ-NH1	9.34	124.97	120.30
1	A	244	ARG	NE-CZ-NH1	9.32	124.96	120.30
27	O	387	ARG	NE-CZ-NH2	-9.32	115.64	120.30
32	M	384	ASP	CB-CG-OD1	-9.31	109.92	118.30
27	O	33	TYR	CB-CG-CD2	-9.31	115.41	121.00
5	E	5	ARG	NE-CZ-NH1	9.30	124.95	120.30
9	i	46	ASP	CB-CG-OD1	9.29	126.66	118.30
1	A	104	PHE	CB-CG-CD2	-9.28	114.30	120.80
14	7	228	PHE	CB-CG-CD2	-9.28	114.31	120.80
16	V	212	MET	CG-SD-CE	-9.27	85.36	100.20
11	4	67	TYR	CB-CG-CD2	-9.27	115.44	121.00
8	1	54	ARG	NE-CZ-NH1	9.26	124.93	120.30
23	P	74	ASP	CB-CG-OD1	-9.26	109.96	118.30
11	k	56	PHE	CB-CG-CD2	-9.26	114.32	120.80
6	f	179	PHE	CB-CG-CD2	-9.25	114.32	120.80
10	3	135	ASP	CB-CG-OD2	9.25	126.63	118.30
23	P	201	ARG	NE-CZ-NH1	9.25	124.93	120.30
9	i	232	TYR	CB-CG-CD1	-9.25	115.45	121.00
12	l	272	PHE	CB-CG-CD2	-9.25	114.33	120.80
14	7	126	PHE	CB-CG-CD1	-9.25	114.33	120.80
7	g	230	PHE	CB-CG-CD2	9.24	127.27	120.80
31	L	161	ARG	NE-CZ-NH2	-9.24	115.68	120.30
16	V	138	ALA	N-CA-CB	9.22	123.01	110.10
14	n	223	ARG	NE-CZ-NH1	9.21	124.91	120.30
31	L	132	ARG	NE-CZ-NH2	-9.19	115.70	120.30
31	L	60	PHE	CB-CG-CD2	-9.19	114.36	120.80
31	L	132	ARG	NE-CZ-NH1	9.17	124.89	120.30
15	W	37	PHE	CB-CG-CD1	9.16	127.21	120.80
25	R	324	ARG	NE-CZ-NH1	-9.15	115.72	120.30
23	P	3	ARG	NE-CZ-NH1	-9.14	115.73	120.30
28	H	420	ARG	NE-CZ-NH1	9.14	124.87	120.30
32	M	38	ASP	CB-CG-OD2	-9.14	110.08	118.30
3	c	131	PHE	CB-CG-CD2	9.13	127.19	120.80
23	P	266	TYR	CD1-CE1-CZ	9.13	128.01	119.80
3	C	20	TYR	CB-CG-CD2	-9.11	115.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	99	ARG	NE-CZ-NH2	-9.11	115.75	120.30
13	m	164	PHE	CB-CG-CD2	9.10	127.17	120.80
22	S	367	TYR	CB-CG-CD1	9.10	126.46	121.00
25	R	383	ARG	NE-CZ-NH1	9.07	124.84	120.30
29	I	346	ARG	NE-CZ-NH1	9.07	124.83	120.30
4	D	48	ARG	NE-CZ-NH1	-9.06	115.77	120.30
7	g	115	ARG	NE-CZ-NH2	-9.04	115.78	120.30
9	2	104	ARG	NE-CZ-NH1	-9.03	115.78	120.30
5	e	10	ARG	NE-CZ-NH1	9.03	124.81	120.30
27	O	92	PHE	CB-CG-CD2	-9.02	114.49	120.80
23	P	359	ARG	NE-CZ-NH2	-9.01	115.79	120.30
16	V	100	ARG	NE-CZ-NH2	-9.01	115.80	120.30
11	4	141	PHE	CB-CG-CD2	-9.01	114.50	120.80
3	c	24	TYR	CB-CG-CD2	-9.01	115.60	121.00
25	R	422	ARG	NE-CZ-NH1	8.99	124.80	120.30
9	2	98	TYR	CB-CG-CD2	8.99	126.39	121.00
11	k	56	PHE	CB-CG-CD1	8.98	127.09	120.80
33	J	373	ARG	NE-CZ-NH1	8.98	124.79	120.30
4	D	119	ARG	NE-CZ-NH1	-8.96	115.82	120.30
20	Z	970	TYR	CB-CG-CD1	8.95	126.37	121.00
30	K	242	PHE	CB-CG-CD2	8.95	127.07	120.80
19	Y	86	ARG	NE-CZ-NH2	-8.95	115.83	120.30
28	H	390	ARG	NE-CZ-NH1	8.95	124.77	120.30
13	m	139	TYR	CB-CG-CD2	-8.94	115.63	121.00
1	a	12	TYR	CG-CD2-CE2	-8.94	114.15	121.30
29	I	271	ALA	N-CA-CB	8.94	122.61	110.10
30	K	77	ARG	NE-CZ-NH1	8.94	124.77	120.30
26	U	100	ARG	NE-CZ-NH2	-8.93	115.84	120.30
30	K	198	TYR	CB-CG-CD1	-8.92	115.65	121.00
27	O	228	TYR	CB-CG-CD1	-8.92	115.65	121.00
30	K	349	ARG	NE-CZ-NH1	8.90	124.75	120.30
27	O	356	ARG	NE-CZ-NH2	-8.90	115.85	120.30
10	3	99	ARG	NE-CZ-NH1	-8.89	115.85	120.30
4	d	141	ARG	NE-CZ-NH2	-8.89	115.86	120.30
19	Y	84	TYR	CB-CG-CD2	-8.88	115.67	121.00
4	D	83	ARG	NE-CZ-NH1	8.84	124.72	120.30
2	b	128	ARG	NE-CZ-NH1	8.84	124.72	120.30
6	f	174	ARG	NE-CZ-NH2	-8.84	115.88	120.30
2	B	204	PHE	CB-CG-CD2	-8.84	114.61	120.80
17	T	244	ASP	CB-CG-OD1	8.83	126.25	118.30
5	e	86	ARG	NE-CZ-NH1	8.82	124.71	120.30
32	M	128	PHE	CB-CG-CD2	-8.82	114.63	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	110	TYR	CB-CG-CD2	8.81	126.29	121.00
29	I	135	PHE	CB-CG-CD1	8.81	126.97	120.80
3	c	213	PHE	CB-CG-CD1	8.81	126.97	120.80
27	O	137	TYR	CB-CG-CD1	8.80	126.28	121.00
27	O	190	TYR	CB-CG-CD2	-8.80	115.72	121.00
21	N	856	PHE	CB-CG-CD2	8.80	126.96	120.80
20	Z	738	TYR	CB-CG-CD1	-8.79	115.72	121.00
5	e	136	ARG	NE-CZ-NH2	-8.78	115.91	120.30
10	j	198	ARG	NE-CZ-NH2	8.78	124.69	120.30
24	Q	294	ARG	N-CA-CB	8.78	126.40	110.60
8	1	183	ARG	NE-CZ-NH1	8.77	124.68	120.30
27	O	106	PHE	CB-CG-CD2	-8.76	114.67	120.80
2	B	97	TYR	CD1-CE1-CZ	-8.76	111.92	119.80
21	N	406	TYR	CB-CG-CD2	-8.75	115.75	121.00
26	U	288	PHE	CB-CG-CD1	-8.75	114.67	120.80
15	W	157	PHE	CB-CG-CD2	-8.75	114.68	120.80
8	h	152	ARG	NE-CZ-NH1	8.74	124.67	120.30
5	e	123	PHE	CB-CG-CD2	8.74	126.92	120.80
23	P	221	TYR	CB-CG-CD1	8.74	126.24	121.00
21	N	549	TYR	CB-CG-CD1	-8.73	115.76	121.00
28	H	87	ASP	CB-CG-OD2	-8.73	110.44	118.30
1	a	71	TYR	CB-CG-CD1	8.73	126.24	121.00
1	A	144	VAL	CA-CB-CG1	-8.73	97.81	110.90
21	N	908	ARG	NE-CZ-NH1	8.73	124.66	120.30
16	V	108	TYR	CB-CG-CD1	-8.72	115.77	121.00
8	h	152	ARG	NE-CZ-NH2	-8.71	115.94	120.30
3	C	50	ARG	NE-CZ-NH1	-8.71	115.94	120.30
13	6	56	ASP	CB-CG-OD2	-8.71	110.46	118.30
16	V	175	SER	N-CA-CB	8.70	123.55	110.50
7	G	78	TYR	CB-CG-CD2	8.70	126.22	121.00
23	P	213	TYR	CB-CG-CD1	8.69	126.21	121.00
4	D	6	ARG	NE-CZ-NH1	8.69	124.64	120.30
13	6	193	ARG	NE-CZ-NH1	8.68	124.64	120.30
10	j	74	TYR	CB-CG-CD2	-8.67	115.80	121.00
11	4	36	ARG	NE-CZ-NH1	8.67	124.63	120.30
1	a	218	PHE	CB-CG-CD1	-8.65	114.74	120.80
25	R	301	TYR	CB-CG-CD1	-8.64	115.81	121.00
4	d	18	PHE	CB-CG-CD1	8.64	126.84	120.80
28	H	283	TYR	CB-CG-CD1	-8.63	115.82	121.00
13	m	99	ARG	NE-CZ-NH1	8.63	124.61	120.30
10	j	183	TRP	CB-CG-CD2	-8.62	115.39	126.60
21	N	148	SER	N-CA-CB	8.62	123.43	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	262	TYR	CB-CG-CD2	-8.62	115.83	121.00
4	d	11	PHE	CB-CG-CD2	-8.62	114.77	120.80
30	K	344	ARG	NE-CZ-NH2	-8.61	115.99	120.30
2	b	148	TYR	CG-CD2-CE2	8.61	128.19	121.30
10	j	183	TRP	CB-CG-CD1	8.60	138.18	127.00
25	R	400	TYR	CB-CG-CD2	-8.60	115.84	121.00
11	k	171	ARG	NE-CZ-NH2	8.60	124.60	120.30
3	C	24	TYR	CB-CG-CD2	8.59	126.16	121.00
4	d	156	TYR	CG-CD1-CE1	-8.58	114.44	121.30
16	V	135	ARG	NE-CZ-NH2	-8.58	116.01	120.30
7	g	112	PHE	CB-CG-CD2	8.56	126.79	120.80
27	O	263	PHE	CB-CG-CD2	-8.56	114.81	120.80
15	W	31	ASP	CB-CG-OD2	-8.55	110.60	118.30
22	S	286	TYR	CB-CG-CD1	8.55	126.13	121.00
29	I	319	ARG	NE-CZ-NH1	8.54	124.57	120.30
11	k	93	ARG	NE-CZ-NH1	8.54	124.57	120.30
1	A	244	ARG	NE-CZ-NH2	-8.54	116.03	120.30
9	i	236	ARG	NE-CZ-NH2	-8.53	116.03	120.30
3	c	137	TYR	CG-CD2-CE2	-8.53	114.47	121.30
30	K	255	ARG	NE-CZ-NH2	-8.53	116.03	120.30
10	3	188	TYR	CB-CG-CD2	-8.53	115.89	121.00
12	5	144	ARG	NE-CZ-NH2	8.52	124.56	120.30
14	7	189	ARG	NE-CZ-NH2	-8.50	116.05	120.30
4	D	29	ARG	NE-CZ-NH2	-8.49	116.06	120.30
32	M	281	ASP	CB-CG-OD2	8.48	125.93	118.30
17	T	244	ASP	CB-CG-OD2	-8.47	110.68	118.30
7	g	56	SER	N-CA-CB	8.46	123.19	110.50
4	D	232	TYR	CB-CG-CD2	-8.45	115.93	121.00
21	N	398	ARG	NE-CZ-NH2	-8.44	116.08	120.30
7	G	190	ARG	NE-CZ-NH1	-8.44	116.08	120.30
21	N	857	TYR	CB-CG-CD1	8.43	126.06	121.00
24	Q	116	PHE	CB-CG-CD2	-8.43	114.90	120.80
23	P	390	TYR	CB-CG-CD1	8.42	126.05	121.00
12	5	212	TYR	CG-CD1-CE1	8.42	128.03	121.30
1	A	105	ARG	NE-CZ-NH1	8.42	124.51	120.30
7	G	157	TYR	CB-CG-CD2	8.42	126.05	121.00
25	R	331	ARG	NE-CZ-NH2	-8.41	116.10	120.30
28	H	454	TYR	CG-CD1-CE1	-8.40	114.58	121.30
10	3	164	PHE	CB-CG-CD1	8.40	126.68	120.80
25	R	63	TYR	CB-CG-CD2	-8.39	115.96	121.00
11	k	107	TYR	CB-CG-CD1	8.39	126.03	121.00
24	Q	434	TYR	CB-CG-CD1	8.38	126.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	129	TYR	CB-CG-CD1	-8.38	115.97	121.00
11	k	187	ASP	CB-CG-OD2	-8.37	110.77	118.30
9	2	117	PHE	CB-CG-CD2	8.36	126.65	120.80
3	c	217	ARG	NE-CZ-NH2	-8.36	116.12	120.30
7	g	72	ARG	NE-CZ-NH2	-8.35	116.12	120.30
14	n	98	ARG	NE-CZ-NH2	-8.35	116.12	120.30
4	d	181	ARG	NE-CZ-NH2	-8.35	116.13	120.30
12	5	245	TYR	CB-CG-CD2	8.35	126.01	121.00
33	J	368	TYR	CB-CG-CD1	-8.34	116.00	121.00
22	S	481	TYR	CB-CG-CD1	-8.33	116.00	121.00
12	l	242	ARG	NE-CZ-NH2	-8.31	116.14	120.30
15	W	37	PHE	CB-CG-CD2	-8.31	114.98	120.80
30	K	49	PHE	CB-CG-CD1	8.30	126.61	120.80
24	Q	153	ASP	CB-CG-OD2	-8.30	110.83	118.30
24	Q	13	ARG	NE-CZ-NH1	8.29	124.45	120.30
24	Q	20	TYR	CB-CG-CD2	-8.29	116.03	121.00
27	O	185	PHE	CB-CG-CD2	8.28	126.60	120.80
5	e	169	ALA	N-CA-CB	8.28	121.69	110.10
11	k	20	ALA	N-CA-CB	8.28	121.69	110.10
29	I	416	PHE	CB-CG-CD1	8.28	126.59	120.80
23	P	10	ASP	CB-CG-OD2	-8.27	110.86	118.30
22	S	475	TYR	CB-CG-CD1	-8.27	116.04	121.00
28	H	409	ARG	NE-CZ-NH2	8.27	124.44	120.30
17	T	157	TYR	CB-CG-CD1	-8.26	116.04	121.00
23	P	193	TYR	CG-CD1-CE1	-8.24	114.71	121.30
19	Y	37	ASP	CB-CG-OD1	8.23	125.71	118.30
20	Z	738	TYR	CE1-CZ-CE2	-8.23	106.63	119.80
5	e	123	PHE	CB-CG-CD1	-8.23	115.04	120.80
21	N	866	TYR	CB-CG-CD1	8.23	125.94	121.00
26	U	52	PHE	CB-CG-CD2	8.23	126.56	120.80
33	J	246	PHE	CB-CG-CD1	-8.23	115.04	120.80
13	m	13	TYR	CB-CG-CD2	8.22	125.94	121.00
11	k	130	TYR	CB-CG-CD1	-8.22	116.07	121.00
13	6	62	ALA	N-CA-CB	8.22	121.61	110.10
7	G	103	TYR	CB-CG-CD2	-8.22	116.07	121.00
10	3	177	ARG	NE-CZ-NH2	8.21	124.41	120.30
22	S	188	TYR	CB-CG-CD1	-8.20	116.08	121.00
28	H	62	ARG	NE-CZ-NH2	-8.20	116.20	120.30
5	E	150	ASP	CB-CG-OD1	-8.20	110.92	118.30
30	K	398	ASN	N-CA-CB	8.19	125.34	110.60
5	e	136	ARG	NE-CZ-NH1	8.18	124.39	120.30
13	m	221	ARG	NE-CZ-NH2	-8.18	116.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	137	PHE	CB-CG-CD1	8.18	126.53	120.80
16	V	230	TYR	CB-CG-CD1	8.18	125.91	121.00
33	J	373	ARG	NE-CZ-NH2	-8.17	116.21	120.30
12	5	148	ARG	NE-CZ-NH2	-8.17	116.22	120.30
31	L	126	ARG	NE-CZ-NH2	-8.16	116.22	120.30
22	S	241	PHE	CB-CG-CD2	-8.16	115.09	120.80
22	S	88	PHE	CB-CG-CD2	8.14	126.50	120.80
10	j	96	TYR	CB-CG-CD2	-8.14	116.12	121.00
29	I	129	TYR	CG-CD1-CE1	-8.13	114.79	121.30
13	6	110	PHE	CB-CG-CD1	8.13	126.49	120.80
30	K	325	ASP	CB-CG-OD1	-8.13	110.98	118.30
23	P	240	TYR	CB-CG-CD2	8.13	125.88	121.00
25	R	357	PHE	CB-CG-CD1	8.13	126.49	120.80
21	N	682	PHE	CB-CG-CD1	8.13	126.49	120.80
1	a	134	MET	CG-SD-CE	-8.13	87.20	100.20
17	T	224	ARG	NE-CZ-NH2	-8.12	116.24	120.30
7	g	157	TYR	CB-CG-CD2	-8.11	116.13	121.00
15	W	41	ARG	NE-CZ-NH1	8.11	124.36	120.30
21	N	322	ASP	CB-CG-OD2	8.11	125.60	118.30
11	4	8	ARG	NE-CZ-NH1	8.11	124.35	120.30
22	S	114	TYR	CB-CG-CD2	8.11	125.86	121.00
29	I	181	TYR	CB-CG-CD2	8.11	125.86	121.00
32	M	255	TYR	CB-CG-CD1	8.11	125.86	121.00
4	d	181	ARG	NE-CZ-NH1	-8.10	116.25	120.30
25	R	238	PHE	CB-CG-CD2	-8.10	115.13	120.80
1	a	234	PHE	CB-CG-CD1	-8.09	115.14	120.80
30	K	290	ARG	NE-CZ-NH2	8.08	124.34	120.30
9	2	98	TYR	CB-CG-CD1	-8.06	116.16	121.00
6	F	18	ARG	NE-CZ-NH1	8.06	124.33	120.30
23	P	397	ALA	N-CA-CB	8.06	121.38	110.10
5	e	153	TYR	CB-CG-CD1	8.05	125.83	121.00
16	V	57	PHE	CB-CG-CD1	-8.05	115.17	120.80
32	M	77	TYR	CD1-CE1-CZ	-8.04	112.56	119.80
22	S	88	PHE	CB-CG-CD1	-8.03	115.18	120.80
30	K	393	ARG	NE-CZ-NH2	-8.03	116.28	120.30
8	1	142	PHE	CB-CG-CD1	-8.03	115.18	120.80
31	L	434	TYR	CB-CG-CD1	-8.03	116.18	121.00
7	G	26	TYR	CG-CD1-CE1	-8.02	114.88	121.30
5	e	8	TYR	CB-CG-CD2	-8.01	116.19	121.00
1	a	113	PRO	N-CA-CB	8.01	112.91	103.30
21	N	884	PHE	CB-CG-CD2	8.01	126.40	120.80
20	Z	970	TYR	CB-CG-CD2	-8.00	116.20	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	727	GLU	CA-CB-CG	7.99	130.98	113.40
12	l	245	TYR	CB-CG-CD2	7.98	125.79	121.00
2	B	101	TYR	CB-CG-CD2	-7.98	116.21	121.00
24	Q	153	ASP	CB-CG-OD1	7.98	125.48	118.30
2	b	104	TYR	CB-CG-CD2	-7.98	116.22	121.00
9	i	152	TYR	CG-CD2-CE2	-7.97	114.92	121.30
31	L	376	PHE	CB-CG-CD2	7.97	126.38	120.80
5	e	151	ASP	CB-CG-OD1	-7.97	111.13	118.30
18	X	116	ALA	N-CA-CB	7.96	121.25	110.10
28	H	190	ARG	NE-CZ-NH2	7.96	124.28	120.30
2	b	178	ARG	NE-CZ-NH2	-7.94	116.33	120.30
21	N	328	PHE	CB-CG-CD2	-7.94	115.24	120.80
1	A	128	TYR	CG-CD2-CE2	-7.93	114.95	121.30
30	K	289	ASP	CB-CG-OD2	-7.93	111.16	118.30
20	Z	634	ASP	C-N-CA	7.92	141.51	121.70
18	X	75	TRP	CG-CD2-CE3	-7.91	126.78	133.90
5	e	103	TYR	CB-CG-CD2	-7.91	116.26	121.00
9	i	186	ASP	CB-CG-OD1	7.91	125.42	118.30
2	B	97	TYR	CG-CD1-CE1	7.90	127.62	121.30
10	j	96	TYR	CB-CG-CD1	7.89	125.74	121.00
32	M	207	PHE	CB-CG-CD2	-7.89	115.28	120.80
10	3	100	PHE	CB-CG-CD2	-7.88	115.29	120.80
21	N	584	ARG	NE-CZ-NH1	7.87	124.23	120.30
25	R	82	ASP	CB-CG-OD1	7.86	125.38	118.30
3	c	39	MET	CG-SD-CE	-7.86	87.62	100.20
17	T	109	TYR	CG-CD1-CE1	-7.86	115.01	121.30
22	S	425	ARG	NE-CZ-NH2	-7.86	116.37	120.30
28	H	303	ALA	N-CA-CB	7.86	121.10	110.10
4	d	6	ARG	NE-CZ-NH2	-7.85	116.38	120.30
25	R	24	TYR	CB-CG-CD1	-7.84	116.30	121.00
21	N	208	ARG	NE-CZ-NH1	7.83	124.22	120.30
11	4	149	ARG	NE-CZ-NH2	-7.82	116.39	120.30
11	k	185	ASP	CB-CG-OD1	7.82	125.34	118.30
9	2	164	MET	CG-SD-CE	-7.82	87.69	100.20
14	7	68	ARG	NE-CZ-NH2	-7.81	116.39	120.30
7	G	86	ARG	NE-CZ-NH2	-7.80	116.40	120.30
26	U	22	TYR	CB-CG-CD1	-7.80	116.32	121.00
25	R	70	TYR	CB-CG-CD1	-7.80	116.32	121.00
5	E	26	TYR	CB-CG-CD2	-7.79	116.33	121.00
9	i	65	ARG	NH1-CZ-NH2	-7.78	110.84	119.40
3	C	237	ASP	CB-CG-OD2	7.78	125.30	118.30
6	F	24	TYR	CB-CG-CD2	-7.77	116.34	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	92	PHE	CB-CG-CD1	7.76	126.23	120.80
27	O	387	ARG	NE-CZ-NH1	7.76	124.18	120.30
24	Q	202	ARG	NE-CZ-NH2	-7.76	116.42	120.30
26	U	288	PHE	CB-CG-CD2	7.76	126.23	120.80
33	J	238	ARG	NE-CZ-NH1	7.76	124.18	120.30
24	Q	51	ARG	NE-CZ-NH1	7.76	124.18	120.30
23	P	395	ARG	NE-CZ-NH2	-7.75	116.42	120.30
14	n	218	TYR	CB-CG-CD2	-7.74	116.35	121.00
7	G	138	PHE	CB-CG-CD2	7.74	126.22	120.80
24	Q	321	TYR	CB-CG-CD1	7.74	125.64	121.00
1	a	77	ARG	NE-CZ-NH1	7.73	124.17	120.30
30	K	350	ARG	NE-CZ-NH2	-7.73	116.43	120.30
24	Q	255	TYR	CB-CG-CD1	-7.73	116.36	121.00
2	B	82	TYR	CB-CG-CD1	-7.72	116.36	121.00
25	R	400	TYR	CB-CG-CD1	7.72	125.64	121.00
16	V	84	ASP	CB-CG-OD2	-7.72	111.35	118.30
10	j	154	TYR	CB-CG-CD1	-7.72	116.37	121.00
17	T	211	PHE	CB-CG-CD1	-7.72	115.40	120.80
21	N	782	PHE	CB-CG-CD1	-7.72	115.40	120.80
13	6	65	PHE	CB-CG-CD1	-7.71	115.40	120.80
14	n	194	ARG	NE-CZ-NH2	-7.70	116.45	120.30
33	J	3	ALA	N-CA-CB	7.70	120.89	110.10
3	c	217	ARG	NE-CZ-NH1	-7.70	116.45	120.30
24	Q	189	ARG	NE-CZ-NH2	7.70	124.15	120.30
16	V	53	MET	CG-SD-CE	-7.69	87.89	100.20
5	e	167	TYR	CG-CD2-CE2	-7.69	115.15	121.30
2	B	99	ARG	NE-CZ-NH2	-7.69	116.46	120.30
14	n	162	TYR	CG-CD2-CE2	7.68	127.45	121.30
24	Q	306	TYR	CB-CG-CD2	-7.68	116.39	121.00
1	A	46	ARG	NE-CZ-NH2	7.68	124.14	120.30
27	O	263	PHE	CB-CG-CD1	7.67	126.17	120.80
12	l	163	TYR	CB-CG-CD2	-7.66	116.40	121.00
22	S	259	TYR	CB-CG-CD1	-7.66	116.40	121.00
10	3	176	ASP	CB-CG-OD2	7.66	125.19	118.30
2	b	5	TYR	CG-CD2-CE2	-7.65	115.18	121.30
13	6	202	ARG	NE-CZ-NH1	7.65	124.12	120.30
21	N	365	PHE	CB-CG-CD1	7.65	126.15	120.80
9	i	187	ALA	N-CA-CB	7.64	120.80	110.10
14	7	63	TYR	CB-CG-CD1	7.64	125.58	121.00
21	N	161	TYR	CB-CG-CD2	-7.64	116.42	121.00
33	J	368	TYR	CB-CG-CD2	7.64	125.58	121.00
8	h	162	ASP	CB-CG-OD1	-7.63	111.43	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	120	ARG	NE-CZ-NH2	-7.62	116.49	120.30
8	1	79	TYR	CB-CG-CD1	7.62	125.57	121.00
22	S	464	ARG	NE-CZ-NH1	7.61	124.11	120.30
21	N	9	LEU	CB-CG-CD1	7.61	123.94	111.00
8	h	202	TYR	CB-CG-CD2	7.61	125.56	121.00
14	7	134	TYR	CB-CG-CD2	-7.61	116.44	121.00
27	O	58	ARG	NE-CZ-NH1	7.61	124.10	120.30
30	K	198	TYR	CG-CD1-CE1	-7.61	115.22	121.30
14	7	252	TRP	CG-CD2-CE3	-7.58	127.08	133.90
16	V	268	THR	CA-CB-CG2	-7.58	101.79	112.40
23	P	327	LEU	N-CA-CB	7.57	125.55	110.40
2	b	204	PHE	CB-CG-CD2	7.57	126.10	120.80
4	D	202	VAL	CA-CB-CG1	-7.57	99.54	110.90
24	Q	67	THR	N-CA-CB	7.57	124.68	110.30
4	D	18	PHE	CB-CG-CD1	7.56	126.09	120.80
8	1	75	TYR	CB-CG-CD1	7.56	125.54	121.00
6	F	174	ARG	NE-CZ-NH2	7.56	124.08	120.30
8	1	151	PHE	CB-CG-CD2	7.55	126.09	120.80
8	1	202	TYR	CB-CG-CD2	-7.55	116.47	121.00
32	M	414	ASP	CB-CG-OD2	-7.55	111.50	118.30
20	Z	248	TYR	CB-CG-CD2	-7.54	116.47	121.00
19	Y	7	ALA	CB-CA-C	-7.54	98.80	110.10
20	Z	918	ASP	CB-CA-C	-7.53	95.34	110.40
27	O	210	ARG	NE-CZ-NH1	-7.53	116.54	120.30
12	l	129	PHE	CB-CG-CD2	-7.52	115.53	120.80
21	N	89	PHE	CB-CG-CD2	-7.51	115.54	120.80
13	m	15	ASP	CB-CG-OD2	7.51	125.06	118.30
11	k	85	ARG	NE-CZ-NH2	-7.51	116.55	120.30
19	Y	73	PHE	CB-CG-CD2	-7.50	115.55	120.80
12	5	191	ASP	CB-CG-OD1	-7.50	111.55	118.30
21	N	338	PHE	CB-CG-CD1	7.50	126.05	120.80
12	l	227	ASP	CB-CG-OD2	-7.49	111.56	118.30
13	m	75	ARG	NE-CZ-NH1	7.49	124.04	120.30
20	Z	727	GLU	CB-CA-C	7.49	125.37	110.40
14	7	219	TYR	CB-CG-CD1	7.48	125.49	121.00
4	D	138	PHE	CB-CG-CD1	-7.47	115.57	120.80
21	N	50	TYR	CB-CG-CD2	-7.47	116.52	121.00
29	I	67	ASP	CB-CG-OD1	-7.46	111.58	118.30
18	X	81	SER	N-CA-CB	7.46	121.69	110.50
12	l	282	PHE	CB-CG-CD2	-7.46	115.58	120.80
13	6	86	ASP	CB-CG-OD1	-7.46	111.59	118.30
3	c	24	TYR	CG-CD1-CE1	7.45	127.26	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	h	45	ARG	NE-CZ-NH2	-7.45	116.58	120.30
29	I	316	PHE	CB-CG-CD1	-7.45	115.59	120.80
25	R	171	MET	CG-SD-CE	-7.44	88.29	100.20
28	H	454	TYR	CB-CG-CD1	7.44	125.47	121.00
3	c	183	ASP	N-CA-CB	7.44	123.99	110.60
4	d	18	PHE	CB-CG-CD2	-7.43	115.60	120.80
4	d	4	TYR	CZ-CE2-CD2	7.42	126.48	119.80
13	6	141	ARG	NE-CZ-NH2	7.42	124.01	120.30
21	N	856	PHE	CB-CG-CD1	-7.42	115.61	120.80
14	n	223	ARG	NH1-CZ-NH2	-7.41	111.25	119.40
1	a	163	TYR	CG-CD1-CE1	-7.41	115.37	121.30
15	W	120	ASP	CB-CG-OD1	-7.41	111.63	118.30
30	K	234	PHE	CB-CG-CD1	7.41	125.99	120.80
31	L	68	ARG	NE-CZ-NH1	7.41	124.00	120.30
32	M	38	ASP	CB-CG-OD1	7.41	124.97	118.30
21	N	502	PHE	CB-CG-CD2	-7.41	115.61	120.80
11	k	89	ALA	N-CA-CB	7.40	120.46	110.10
3	c	144	TYR	CB-CG-CD1	-7.40	116.56	121.00
12	l	139	ARG	NE-CZ-NH1	7.40	124.00	120.30
13	m	125	ASP	CB-CG-OD2	-7.39	111.64	118.30
33	J	229	MET	CG-SD-CE	-7.39	88.37	100.20
27	O	181	PHE	CB-CG-CD2	-7.39	115.63	120.80
7	G	15	PHE	CB-CG-CD1	-7.39	115.63	120.80
26	U	92	TRP	CD1-CG-CD2	-7.38	100.39	106.30
7	G	169	ARG	NE-CZ-NH2	-7.38	116.61	120.30
10	3	68	ARG	NE-CZ-NH1	7.38	123.99	120.30
25	R	62	TYR	CB-CG-CD1	7.37	125.42	121.00
31	L	60	PHE	CB-CG-CD1	7.36	125.95	120.80
4	d	4	TYR	CB-CG-CD2	-7.36	116.58	121.00
14	7	110	ASP	CB-CG-OD1	-7.35	111.69	118.30
2	B	4	ARG	NE-CZ-NH1	7.35	123.97	120.30
21	N	330	THR	CA-CB-CG2	7.35	122.69	112.40
5	e	228	PHE	CB-CG-CD2	7.34	125.94	120.80
9	2	80	ASP	CB-CG-OD2	7.34	124.91	118.30
9	2	119	TYR	CB-CG-CD2	-7.34	116.59	121.00
15	W	31	ASP	CB-CG-OD1	7.34	124.91	118.30
30	K	304	ASP	CB-CG-OD1	-7.34	111.70	118.30
23	P	356	TYR	CB-CG-CD1	7.34	125.40	121.00
19	Y	83	ARG	NE-CZ-NH1	-7.33	116.64	120.30
15	W	179	ARG	NE-CZ-NH2	-7.33	116.64	120.30
5	E	150	ASP	CB-CG-OD2	7.32	124.89	118.30
21	N	866	TYR	CB-CG-CD2	-7.32	116.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	549	TYR	CD1-CE1-CZ	7.31	126.38	119.80
6	f	107	ARG	NE-CZ-NH1	7.31	123.95	120.30
1	a	131	ARG	NE-CZ-NH2	7.31	123.95	120.30
29	I	262	ARG	NE-CZ-NH1	7.30	123.95	120.30
13	m	193	ARG	NE-CZ-NH2	-7.30	116.65	120.30
20	Z	253	VAL	CG1-CB-CG2	-7.30	99.22	110.90
2	B	236	ARG	NE-CZ-NH1	7.30	123.95	120.30
28	H	241	ASP	CB-CG-OD2	-7.30	111.73	118.30
8	1	147	CYS	CB-CA-C	-7.29	95.81	110.40
28	H	271	PHE	CB-CG-CD1	7.29	125.91	120.80
28	H	162	ARG	NE-CZ-NH1	7.29	123.94	120.30
33	J	149	MET	CG-SD-CE	-7.28	88.55	100.20
21	N	250	ASP	CB-CG-OD2	7.28	124.85	118.30
25	R	86	ASP	N-CA-CB	7.27	123.69	110.60
31	L	297	ALA	N-CA-CB	7.27	120.28	110.10
5	e	166	ARG	NE-CZ-NH1	7.27	123.93	120.30
8	1	34	TYR	CB-CG-CD1	7.26	125.36	121.00
32	M	77	TYR	CB-CG-CD2	-7.25	116.65	121.00
3	c	217	ARG	NH1-CZ-NH2	7.25	127.38	119.40
10	3	122	ALA	CB-CA-C	-7.25	99.23	110.10
1	a	155	TYR	CB-CG-CD2	-7.25	116.65	121.00
33	J	193	THR	CA-CB-CG2	-7.25	102.25	112.40
32	M	281	ASP	CB-CG-OD1	-7.25	111.78	118.30
27	O	189	TYR	CG-CD2-CE2	-7.24	115.51	121.30
12	l	79	LEU	CB-CG-CD2	7.24	123.31	111.00
11	k	107	TYR	CB-CG-CD2	-7.24	116.66	121.00
32	M	117	ALA	CB-CA-C	-7.24	99.25	110.10
12	5	94	ARG	NE-CZ-NH1	7.24	123.92	120.30
10	3	154	TYR	CG-CD2-CE2	-7.23	115.51	121.30
2	B	224	TYR	CB-CG-CD2	7.23	125.34	121.00
6	F	39	ARG	NE-CZ-NH2	-7.23	116.69	120.30
27	O	58	ARG	NE-CZ-NH2	-7.22	116.69	120.30
2	B	15	SER	C-N-CA	7.22	137.46	122.30
8	h	194	ARG	NE-CZ-NH1	7.22	123.91	120.30
2	B	32	VAL	CA-CB-CG1	-7.22	100.08	110.90
6	F	24	TYR	CB-CG-CD1	7.21	125.33	121.00
27	O	286	PHE	CB-CG-CD2	-7.21	115.75	120.80
32	M	33	ARG	NE-CZ-NH1	7.21	123.91	120.30
5	e	228	PHE	CB-CG-CD1	-7.21	115.75	120.80
2	b	23	TYR	CB-CG-CD2	7.20	125.32	121.00
13	6	229	ARG	NE-CZ-NH1	7.20	123.90	120.30
30	K	56	LYS	N-CA-CB	7.20	123.56	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	174	PHE	CD1-CE1-CZ	-7.19	111.47	120.10
8	1	152	ARG	NE-CZ-NH1	7.19	123.90	120.30
28	H	196	THR	CA-CB-CG2	-7.19	102.33	112.40
23	P	220	TYR	CB-CG-CD2	-7.19	116.69	121.00
21	N	906	ARG	NE-CZ-NH2	-7.19	116.71	120.30
18	X	99	PHE	CB-CG-CD2	-7.18	115.77	120.80
5	e	138	PHE	CB-CG-CD2	-7.18	115.77	120.80
11	4	130	TYR	CB-CG-CD2	-7.18	116.69	121.00
13	m	65	PHE	CB-CG-CD1	7.18	125.82	120.80
7	G	103	TYR	CG-CD2-CE2	-7.17	115.56	121.30
16	V	275	ASP	CB-CG-OD2	-7.17	111.85	118.30
22	S	51	ARG	NE-CZ-NH1	7.17	123.88	120.30
6	f	123	TYR	CB-CG-CD2	-7.17	116.70	121.00
1	A	70	SER	N-CA-CB	7.16	121.24	110.50
2	b	101	TYR	CG-CD1-CE1	-7.16	115.57	121.30
11	k	135	TYR	CB-CG-CD1	7.16	125.30	121.00
30	K	88	ARG	NE-CZ-NH2	7.16	123.88	120.30
18	X	131	ASN	O-C-N	7.16	134.15	122.70
4	d	119	ARG	NE-CZ-NH2	-7.15	116.72	120.30
31	L	244	ILE	N-CA-C	-7.15	91.69	111.00
29	I	412	THR	CA-CB-CG2	-7.15	102.39	112.40
23	P	208	PHE	CB-CG-CD2	-7.14	115.80	120.80
4	d	83	ARG	NE-CZ-NH1	7.14	123.87	120.30
25	R	214	TYR	CB-CG-CD1	-7.14	116.72	121.00
13	6	76	PHE	CB-CG-CD1	7.13	125.79	120.80
11	k	148	TYR	CB-CG-CD1	7.12	125.28	121.00
1	a	182	LEU	CB-CG-CD2	7.12	123.11	111.00
21	N	139	ARG	NE-CZ-NH2	-7.12	116.74	120.30
6	f	137	TYR	CB-CG-CD2	7.12	125.27	121.00
8	1	13	MET	CG-SD-CE	7.12	111.59	100.20
28	H	178	ARG	NE-CZ-NH1	7.12	123.86	120.30
3	C	112	VAL	CA-CB-CG2	-7.12	100.23	110.90
31	L	400	PHE	CB-CG-CD1	-7.12	115.82	120.80
9	2	71	TRP	CE3-CZ3-CH2	-7.11	113.38	121.20
15	W	25	ARG	NE-CZ-NH1	7.11	123.86	120.30
2	b	148	TYR	CZ-CE2-CD2	-7.11	113.40	119.80
8	1	133	TYR	CG-CD2-CE2	7.10	126.98	121.30
4	D	18	PHE	CB-CG-CD2	-7.10	115.83	120.80
14	7	261	TYR	CG-CD2-CE2	-7.10	115.62	121.30
20	Z	358	TYR	CB-CG-CD2	-7.09	116.74	121.00
28	H	267	THR	CA-CB-CG2	-7.09	102.47	112.40
2	b	99	ARG	NE-CZ-NH2	-7.09	116.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	W	120	ASP	CB-CG-OD2	7.09	124.68	118.30
4	D	110	THR	CA-CB-CG2	7.08	122.32	112.40
8	1	79	TYR	CB-CG-CD2	-7.08	116.75	121.00
13	6	225	TYR	CB-CG-CD2	7.08	125.25	121.00
27	O	51	ASP	CB-CG-OD1	-7.08	111.93	118.30
32	M	109	ASP	CB-CG-OD2	7.08	124.67	118.30
31	L	72	ASP	CB-CG-OD1	-7.08	111.93	118.30
4	D	90	ARG	NE-CZ-NH1	7.07	123.84	120.30
25	R	321	TYR	CZ-CE2-CD2	7.07	126.16	119.80
7	g	142	ASP	N-CA-CB	7.06	123.31	110.60
21	N	123	PHE	CB-CG-CD2	-7.06	115.86	120.80
21	N	570	ARG	NE-CZ-NH1	-7.06	116.77	120.30
6	f	13	PHE	O-C-N	-7.05	111.42	122.70
28	H	289	ARG	NE-CZ-NH2	-7.04	116.78	120.30
4	d	197	ARG	NE-CZ-NH1	7.04	123.82	120.30
7	G	78	TYR	CD1-CE1-CZ	7.03	126.13	119.80
16	V	183	ALA	N-CA-CB	7.03	119.94	110.10
6	F	59	TYR	CB-CG-CD2	7.03	125.22	121.00
25	R	345	TYR	CB-CG-CD2	7.03	125.22	121.00
1	A	73	PHE	CD1-CE1-CZ	-7.03	111.67	120.10
3	C	210	ARG	NE-CZ-NH1	-7.03	116.79	120.30
9	2	219	TYR	CD1-CE1-CZ	-7.03	113.48	119.80
16	V	104	VAL	CA-CB-CG2	-7.03	100.36	110.90
25	R	186	TYR	CB-CG-CD1	-7.03	116.78	121.00
18	X	92	SER	N-CA-CB	7.02	121.03	110.50
9	2	186	ASP	CB-CG-OD2	7.02	124.62	118.30
26	U	189	ARG	NE-CZ-NH2	-7.01	116.79	120.30
4	d	108	TYR	CB-CG-CD1	-7.01	116.79	121.00
28	H	462	ARG	NE-CZ-NH1	7.01	123.81	120.30
11	4	39	SER	N-CA-CB	7.00	121.01	110.50
24	Q	236	PHE	CB-CG-CD1	7.00	125.70	120.80
5	e	158	ALA	CB-CA-C	-7.00	99.60	110.10
21	N	781	ALA	N-CA-CB	7.00	119.90	110.10
5	e	122	ARG	NE-CZ-NH1	6.99	123.79	120.30
13	m	110	PHE	CB-CG-CD2	-6.99	115.91	120.80
7	G	181	ASP	CB-CG-OD2	-6.99	112.01	118.30
21	N	322	ASP	CB-CG-OD1	-6.99	112.01	118.30
13	6	75	ARG	NE-CZ-NH2	-6.98	116.81	120.30
32	M	77	TYR	N-CA-CB	6.98	123.16	110.60
9	i	48	ARG	NE-CZ-NH1	-6.97	116.81	120.30
33	J	382	PHE	CB-CG-CD2	-6.97	115.92	120.80
14	n	220	ARG	NE-CZ-NH1	6.96	123.78	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	390	ARG	NH1-CZ-NH2	-6.96	111.74	119.40
7	g	180	VAL	CA-CB-CG1	6.96	121.34	110.90
3	C	146	TYR	CB-CG-CD1	6.96	125.18	121.00
8	1	144	TYR	CZ-CE2-CD2	-6.96	113.54	119.80
11	4	96	ARG	NE-CZ-NH2	-6.96	116.82	120.30
6	F	171	TYR	CG-CD1-CE1	-6.96	115.73	121.30
12	5	219	TYR	CB-CG-CD1	-6.96	116.83	121.00
6	f	59	TYR	CB-CG-CD1	-6.95	116.83	121.00
5	E	102	TYR	CB-CG-CD1	6.95	125.17	121.00
23	P	329	PHE	CB-CG-CD2	-6.95	115.94	120.80
4	d	181	ARG	NH1-CZ-NH2	6.95	127.04	119.40
13	m	109	ARG	NE-CZ-NH2	-6.94	116.83	120.30
2	b	3	ASP	CB-CG-OD2	6.94	124.55	118.30
26	U	113	TYR	CB-CG-CD1	6.93	125.16	121.00
21	N	766	GLN	N-CA-CB	6.92	123.06	110.60
1	a	166	TYR	CB-CG-CD1	-6.92	116.85	121.00
21	N	735	MET	CG-SD-CE	-6.92	89.12	100.20
30	K	304	ASP	CB-CG-OD2	6.92	124.53	118.30
14	7	44	VAL	CA-CB-CG2	6.92	121.28	110.90
11	k	17	SER	N-CA-CB	6.92	120.88	110.50
29	I	385	ASP	CB-CG-OD2	-6.92	112.08	118.30
31	L	315	PHE	CB-CG-CD2	-6.91	115.96	120.80
33	J	120	TYR	CB-CG-CD2	-6.91	116.85	121.00
4	d	4	TYR	CB-CG-CD1	6.91	125.14	121.00
1	A	155	TYR	CB-CG-CD2	-6.91	116.86	121.00
6	F	128	TYR	CB-CG-CD1	-6.91	116.86	121.00
9	2	234	PHE	CB-CG-CD1	-6.91	115.97	120.80
4	D	58	ARG	NE-CZ-NH1	-6.90	116.85	120.30
21	N	418	ASP	CB-CG-OD2	6.90	124.51	118.30
8	1	133	TYR	CB-CG-CD1	-6.90	116.86	121.00
7	G	160	TYR	CB-CG-CD1	-6.89	116.86	121.00
3	C	144	TYR	CB-CG-CD2	-6.89	116.87	121.00
32	M	255	TYR	CB-CG-CD2	-6.89	116.87	121.00
25	R	241	ILE	N-CA-C	-6.88	92.42	111.00
27	O	252	PHE	CB-CG-CD1	6.88	125.61	120.80
1	a	96	ARG	NE-CZ-NH2	-6.88	116.86	120.30
33	J	84	VAL	CA-CB-CG1	-6.87	100.59	110.90
9	2	119	TYR	CB-CG-CD1	6.87	125.12	121.00
14	7	128	TYR	CG-CD1-CE1	-6.87	115.81	121.30
9	2	203	ASP	CB-CG-OD1	6.87	124.48	118.30
27	O	33	TYR	CB-CG-CD1	6.86	125.12	121.00
27	O	181	PHE	CB-CG-CD1	6.86	125.60	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	45	ARG	NE-CZ-NH2	-6.85	116.87	120.30
26	U	100	ARG	NE-CZ-NH1	6.85	123.72	120.30
32	M	124	ARG	NE-CZ-NH1	6.85	123.73	120.30
22	S	76	PHE	CB-CG-CD1	-6.85	116.01	120.80
22	S	475	TYR	CB-CG-CD2	6.85	125.11	121.00
24	Q	340	ASP	CB-CG-OD2	-6.85	112.14	118.30
24	Q	384	LYS	N-CA-CB	6.85	122.93	110.60
9	i	46	ASP	CB-CG-OD2	-6.85	112.14	118.30
2	B	128	ARG	NE-CZ-NH2	-6.85	116.88	120.30
5	e	84	ASP	CB-CG-OD1	-6.84	112.14	118.30
11	4	32	ASP	CB-CG-OD2	6.84	124.46	118.30
27	O	252	PHE	CB-CG-CD2	-6.84	116.01	120.80
14	7	202	THR	CA-CB-CG2	-6.83	102.83	112.40
14	n	49	TYR	CB-CG-CD2	6.83	125.10	121.00
26	U	53	ALA	N-CA-CB	6.83	119.67	110.10
2	B	12	PHE	CB-CG-CD1	-6.83	116.02	120.80
14	7	99	LEU	CB-CG-CD2	6.83	122.61	111.00
31	L	69	ARG	NE-CZ-NH2	-6.83	116.89	120.30
7	G	181	ASP	CB-CG-OD1	6.83	124.44	118.30
2	B	161	ALA	N-CA-CB	6.83	119.66	110.10
11	k	11	ASP	CB-CG-OD2	6.82	124.44	118.30
12	5	235	SER	N-CA-CB	6.82	120.73	110.50
3	c	47	ALA	CB-CA-C	-6.82	99.87	110.10
13	m	86	ASP	CB-CG-OD1	6.82	124.44	118.30
2	b	95	THR	CA-CB-CG2	-6.81	102.87	112.40
12	l	245	TYR	CG-CD2-CE2	6.81	126.75	121.30
18	X	22	ARG	NE-CZ-NH1	6.81	123.70	120.30
13	m	48	GLU	N-CA-C	-6.81	92.62	111.00
1	a	120	ARG	NE-CZ-NH1	6.80	123.70	120.30
12	l	234	ARG	NE-CZ-NH2	-6.80	116.90	120.30
16	V	274	GLN	N-CA-CB	6.80	122.84	110.60
2	B	104	TYR	CB-CG-CD1	-6.80	116.92	121.00
11	k	148	TYR	CZ-CE2-CD2	-6.80	113.68	119.80
12	5	82	ARG	NH1-CZ-NH2	-6.80	111.92	119.40
24	Q	113	ASP	CB-CG-OD2	-6.79	112.19	118.30
24	Q	185	TYR	CB-CG-CD1	-6.79	116.93	121.00
24	Q	291	TYR	CB-CG-CD2	-6.79	116.93	121.00
1	A	71	TYR	CB-CG-CD2	-6.79	116.93	121.00
25	R	321	TYR	CB-CG-CD2	6.79	125.07	121.00
14	7	109	TYR	CB-CG-CD1	-6.78	116.93	121.00
15	W	113	PHE	CB-CG-CD1	6.78	125.55	120.80
13	m	145	ARG	NE-CZ-NH1	-6.78	116.91	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	h	53	CYS	CA-CB-SG	6.78	126.20	114.00
7	G	126	TYR	CB-CG-CD1	-6.78	116.94	121.00
21	N	282	TYR	CB-CG-CD2	-6.77	116.94	121.00
26	U	233	PHE	CB-CG-CD1	6.77	125.54	120.80
10	j	203	ARG	NE-CZ-NH2	-6.77	116.92	120.30
11	k	88	LEU	CB-CA-C	-6.77	97.34	110.20
4	d	174	PHE	CB-CG-CD1	-6.76	116.06	120.80
24	Q	189	ARG	NE-CZ-NH1	-6.76	116.92	120.30
3	c	4	ARG	NE-CZ-NH2	-6.76	116.92	120.30
17	T	149	ASP	CB-CG-OD2	6.75	124.38	118.30
3	c	135	PHE	CB-CA-C	-6.75	96.89	110.40
9	i	163	ALA	N-CA-CB	6.75	119.55	110.10
3	c	20	TYR	CG-CD2-CE2	-6.75	115.90	121.30
13	m	131	TYR	CD1-CE1-CZ	-6.75	113.73	119.80
14	n	80	ASP	CB-CG-OD1	-6.75	112.23	118.30
3	c	131	PHE	CB-CG-CD1	-6.75	116.08	120.80
21	N	50	TYR	CB-CG-CD1	6.75	125.05	121.00
33	J	306	ARG	NE-CZ-NH2	6.75	123.67	120.30
3	c	63	THR	CA-CB-CG2	-6.75	102.96	112.40
31	L	420	ARG	NE-CZ-NH2	-6.74	116.93	120.30
6	F	137	TYR	CG-CD2-CE2	6.74	126.69	121.30
10	j	40	PHE	CB-CG-CD2	-6.74	116.08	120.80
23	P	225	VAL	CG1-CB-CG2	-6.73	100.12	110.90
12	l	121	ALA	N-CA-CB	6.73	119.52	110.10
9	2	101	ARG	NE-CZ-NH2	-6.73	116.94	120.30
5	E	33	LEU	CB-CG-CD1	-6.73	99.56	111.00
6	F	14	SER	N-CA-CB	6.72	120.58	110.50
23	P	213	TYR	CG-CD2-CE2	-6.72	115.93	121.30
6	f	169	LYS	CB-CA-C	-6.72	96.97	110.40
27	O	255	LEU	CB-CA-C	-6.71	97.44	110.20
6	f	87	TYR	CB-CG-CD1	-6.71	116.98	121.00
4	d	127	ARG	NE-CZ-NH2	6.70	123.65	120.30
28	H	462	ARG	NE-CZ-NH2	-6.70	116.95	120.30
2	b	246	ARG	NE-CZ-NH1	6.70	123.65	120.30
30	K	198	TYR	CD1-CG-CD2	6.70	125.27	117.90
23	P	364	ARG	NE-CZ-NH1	6.70	123.65	120.30
1	A	26	TYR	CG-CD2-CE2	-6.70	115.94	121.30
17	T	88	TYR	CB-CG-CD1	6.70	125.02	121.00
22	S	263	ASP	CB-CG-OD1	-6.70	112.27	118.30
10	3	198	ARG	NE-CZ-NH2	6.70	123.65	120.30
22	S	384	ARG	NE-CZ-NH1	6.70	123.65	120.30
3	c	113	ARG	NE-CZ-NH2	6.69	123.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	188	TYR	CB-CG-CD2	-6.69	116.99	121.00
22	S	288	THR	CA-CB-CG2	-6.69	103.04	112.40
7	g	9	ASP	CB-CG-OD2	6.68	124.31	118.30
3	C	183	ASP	CB-CG-OD1	6.68	124.32	118.30
20	Z	746	ILE	CB-CA-C	6.68	124.97	111.60
21	N	365	PHE	CB-CG-CD2	-6.68	116.12	120.80
24	Q	20	TYR	CD1-CE1-CZ	6.68	125.81	119.80
3	c	230	PHE	CG-CD2-CE2	-6.68	113.45	120.80
30	K	128	ARG	NE-CZ-NH2	6.68	123.64	120.30
8	h	45	ARG	NE-CZ-NH1	6.67	123.64	120.30
24	Q	130	ARG	NE-CZ-NH2	-6.67	116.96	120.30
6	F	225	TYR	CB-CG-CD2	-6.67	117.00	121.00
3	C	18	ARG	NE-CZ-NH1	6.67	123.64	120.30
12	5	153	ALA	O-C-N	-6.67	112.03	122.70
25	R	252	TYR	CB-CG-CD2	-6.67	117.00	121.00
12	l	227	ASP	CB-CG-OD1	6.67	124.30	118.30
21	N	782	PHE	CB-CG-CD2	6.67	125.47	120.80
10	3	74	TYR	CB-CG-CD2	6.66	125.00	121.00
6	F	137	TYR	CB-CG-CD1	6.66	125.00	121.00
1	A	140	ILE	O-C-N	6.66	133.36	122.70
30	K	171	TYR	CB-CG-CD2	-6.66	117.00	121.00
16	V	221	TRP	CH2-CZ2-CE2	6.66	124.06	117.40
21	N	139	ARG	CD-NE-CZ	-6.66	114.28	123.60
27	O	185	PHE	CB-CG-CD1	-6.66	116.14	120.80
2	b	234	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	b	178	ARG	NE-CZ-NH1	6.65	123.63	120.30
6	f	164	ARG	NE-CZ-NH1	6.64	123.62	120.30
26	U	60	GLU	OE1-CD-OE2	-6.64	115.33	123.30
9	2	152	TYR	CB-CG-CD1	-6.63	117.02	121.00
3	C	9	ARG	NE-CZ-NH1	-6.63	116.98	120.30
9	i	251	ASP	CB-CG-OD1	-6.63	112.34	118.30
31	L	144	VAL	CA-CB-CG2	-6.63	100.96	110.90
16	V	194	ARG	NE-CZ-NH1	6.62	123.61	120.30
21	N	702	ALA	CB-CA-C	-6.62	100.17	110.10
2	b	86	VAL	CA-CB-CG1	6.62	120.83	110.90
14	n	157	ASP	CB-CG-OD1	-6.62	112.34	118.30
16	V	202	ASP	CB-CG-OD1	6.62	124.25	118.30
21	N	884	PHE	CB-CG-CD1	-6.62	116.17	120.80
2	b	234	ARG	CD-NE-CZ	6.61	132.86	123.60
20	Z	748	LEU	O-C-N	-6.61	111.96	123.20
1	a	110	TYR	CB-CG-CD2	-6.61	117.03	121.00
17	T	46	ILE	N-CA-C	-6.61	93.15	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	181	ARG	NE-CZ-NH2	-6.61	117.00	120.30
8	1	70	TYR	N-CA-CB	-6.61	98.71	110.60
24	Q	431	SER	N-CA-CB	6.60	120.40	110.50
11	k	23	ARG	NE-CZ-NH1	6.59	123.60	120.30
25	R	132	GLN	O-C-N	-6.59	112.16	122.70
15	W	157	PHE	CB-CG-CD1	6.59	125.41	120.80
14	n	134	TYR	CB-CG-CD2	-6.59	117.05	121.00
21	N	88	ARG	N-CA-CB	6.59	122.46	110.60
17	T	109	TYR	CB-CG-CD1	-6.58	117.05	121.00
23	P	51	ASP	CB-CG-OD1	-6.58	112.38	118.30
17	T	148	LEU	CB-CG-CD1	6.58	122.18	111.00
7	g	119	TYR	CB-CG-CD2	-6.57	117.06	121.00
12	l	242	ARG	NE-CZ-NH1	6.57	123.59	120.30
8	1	38	ARG	NE-CZ-NH1	6.57	123.59	120.30
13	6	46	ARG	NE-CZ-NH1	-6.57	117.02	120.30
11	k	195	PHE	CB-CG-CD2	-6.56	116.21	120.80
5	E	138	PHE	CB-CG-CD1	6.56	125.39	120.80
14	7	110	ASP	CB-CG-OD2	6.56	124.20	118.30
31	L	180	PHE	CB-CG-CD1	6.55	125.39	120.80
32	M	158	THR	CA-CB-CG2	-6.55	103.23	112.40
17	T	266	TYR	CG-CD1-CE1	-6.55	116.06	121.30
33	J	222	TYR	CB-CG-CD1	-6.55	117.07	121.00
24	Q	47	ASP	CB-CG-OD2	-6.55	112.41	118.30
1	A	17	THR	CA-CB-CG2	-6.55	103.23	112.40
6	F	172	LEU	CB-CG-CD2	6.54	122.12	111.00
27	O	38	TRP	CB-CG-CD2	-6.54	118.09	126.60
6	F	94	TYR	CB-CG-CD1	-6.54	117.08	121.00
10	3	67	PHE	CB-CG-CD2	6.54	125.38	120.80
1	A	96	ARG	NE-CZ-NH2	-6.54	117.03	120.30
13	6	10	PHE	CB-CG-CD2	6.54	125.38	120.80
3	c	24	TYR	CB-CG-CD1	6.53	124.92	121.00
9	i	35	VAL	CG1-CB-CG2	-6.53	100.45	110.90
7	g	130	ARG	NE-CZ-NH1	6.53	123.56	120.30
5	E	231	TYR	CB-CG-CD1	-6.53	117.08	121.00
10	j	50	PHE	CB-CG-CD2	6.52	125.37	120.80
33	J	325	ALA	CB-CA-C	-6.52	100.31	110.10
18	X	17	TYR	CB-CG-CD2	6.52	124.91	121.00
25	R	233	ASP	CB-CG-OD2	-6.52	112.43	118.30
26	U	103	ASP	CB-CG-OD1	-6.51	112.44	118.30
30	K	185	ARG	NE-CZ-NH1	6.51	123.55	120.30
4	d	172	ARG	NE-CZ-NH2	-6.50	117.05	120.30
28	H	297	MET	CG-SD-CE	-6.50	89.80	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	230	PHE	CB-CG-CD1	-6.50	116.25	120.80
6	f	179	PHE	CB-CG-CD1	6.50	125.35	120.80
21	N	124	TYR	CB-CG-CD1	6.50	124.90	121.00
32	M	433	TYR	CB-CG-CD2	-6.50	117.10	121.00
5	e	26	TYR	CG-CD2-CE2	6.50	126.50	121.30
22	S	259	TYR	CG-CD1-CE1	-6.50	116.10	121.30
29	I	436	TYR	CD1-CG-CD2	6.49	125.04	117.90
3	c	122	TYR	CB-CG-CD1	-6.49	117.11	121.00
9	i	65	ARG	NE-CZ-NH1	6.49	123.54	120.30
30	K	196	ASP	CB-CG-OD1	6.48	124.13	118.30
31	L	173	PHE	CB-CG-CD2	-6.48	116.27	120.80
2	b	130	PHE	CB-CG-CD2	6.47	125.33	120.80
22	S	464	ARG	CG-CD-NE	-6.47	98.20	111.80
1	A	24	ARG	NE-CZ-NH1	-6.47	117.06	120.30
11	k	21	VAL	CA-CB-CG2	-6.47	101.19	110.90
32	M	73	ARG	NE-CZ-NH1	6.47	123.53	120.30
10	3	122	ALA	N-CA-CB	6.47	119.15	110.10
21	N	599	TYR	CG-CD1-CE1	-6.46	116.13	121.30
21	N	748	PHE	CB-CG-CD1	-6.46	116.27	120.80
9	2	104	ARG	NH1-CZ-NH2	6.46	126.51	119.40
8	1	34	TYR	CG-CD1-CE1	-6.46	116.13	121.30
11	4	121	TYR	CB-CG-CD2	-6.45	117.13	121.00
13	6	109	ARG	NE-CZ-NH1	6.45	123.53	120.30
26	U	154	PHE	CB-CG-CD2	-6.45	116.28	120.80
16	V	95	LEU	CB-CA-C	-6.45	97.95	110.20
7	g	157	TYR	CZ-CE2-CD2	-6.45	114.00	119.80
2	b	5	TYR	CG-CD1-CE1	-6.45	116.14	121.30
30	K	111	SER	N-CA-CB	6.45	120.17	110.50
12	5	115	PHE	CB-CG-CD1	-6.44	116.29	120.80
1	a	246	VAL	CA-CB-CG1	6.44	120.56	110.90
1	A	124	LEU	CB-CG-CD1	-6.44	100.05	111.00
14	7	179	PHE	CZ-CE2-CD2	-6.44	112.37	120.10
5	E	54	ALA	N-CA-CB	6.44	119.12	110.10
14	7	115	ASP	CB-CG-OD2	-6.44	112.50	118.30
22	S	211	ARG	NE-CZ-NH1	6.44	123.52	120.30
20	Z	780	MET	CG-SD-CE	-6.44	89.90	100.20
11	k	44	MET	CG-SD-CE	-6.44	89.90	100.20
8	1	102	LEU	CB-CG-CD2	6.43	121.94	111.00
29	I	424	MET	CG-SD-CE	-6.43	89.91	100.20
22	S	461	PHE	CD1-CE1-CZ	6.43	127.82	120.10
13	m	56	ASP	CB-CG-OD2	-6.43	112.51	118.30
6	F	80	ASP	CB-CG-OD1	6.43	124.09	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	340	ASP	CB-CG-OD1	6.43	124.09	118.30
1	A	108	TYR	CD1-CE1-CZ	6.43	125.58	119.80
12	l	186	THR	CA-CB-CG2	-6.43	103.40	112.40
21	N	328	PHE	CB-CG-CD1	6.42	125.30	120.80
9	i	105	VAL	CA-CB-CG1	6.42	120.53	110.90
32	M	88	MET	CG-SD-CE	-6.42	89.93	100.20
2	B	195	THR	N-CA-CB	6.42	122.50	110.30
29	I	200	LEU	CA-C-N	6.42	135.07	117.10
30	K	313	LYS	N-CA-CB	6.42	122.15	110.60
21	N	162	ARG	NE-CZ-NH2	-6.42	117.09	120.30
26	U	160	THR	CA-CB-CG2	-6.42	103.42	112.40
25	R	382	ASP	CB-CG-OD1	6.41	124.07	118.30
31	L	245	PHE	CB-CG-CD1	6.41	125.29	120.80
32	M	376	TRP	CE2-CD2-CG	-6.41	102.17	107.30
25	R	214	TYR	CB-CG-CD2	6.41	124.84	121.00
8	h	146	TYR	CB-CG-CD1	-6.41	117.16	121.00
10	j	71	THR	N-CA-CB	6.41	122.47	110.30
18	X	47	ASP	CB-CG-OD2	-6.41	112.53	118.30
31	L	70	TYR	CB-CG-CD1	-6.40	117.16	121.00
5	E	223	THR	CA-CB-CG2	-6.40	103.44	112.40
27	O	143	LEU	CB-CG-CD2	6.40	121.88	111.00
4	D	180	ASP	CB-CG-OD1	-6.39	112.55	118.30
17	T	17	ASN	CB-CA-C	-6.39	97.61	110.40
4	d	20	VAL	CA-CB-CG2	-6.39	101.32	110.90
5	E	16	SER	N-CA-CB	6.39	120.08	110.50
22	S	92	LEU	CB-CG-CD2	6.39	121.86	111.00
6	F	101	ARG	NE-CZ-NH1	6.39	123.49	120.30
25	R	232	VAL	CA-CB-CG1	6.39	120.48	110.90
32	M	433	TYR	CB-CG-CD1	6.39	124.83	121.00
5	E	208	MET	CG-SD-CE	6.38	110.42	100.20
13	m	109	ARG	NE-CZ-NH1	6.38	123.49	120.30
15	W	80	GLN	N-CA-C	-6.38	93.77	111.00
25	R	312	TYR	CB-CG-CD1	-6.38	117.17	121.00
26	U	113	TYR	CB-CG-CD2	-6.38	117.17	121.00
16	V	84	ASP	CB-CG-OD1	6.38	124.04	118.30
17	T	109	TYR	CD1-CE1-CZ	6.38	125.54	119.80
31	L	245	PHE	N-CA-CB	6.38	122.08	110.60
2	B	183	LEU	CB-CG-CD1	6.38	121.84	111.00
4	d	166	ARG	NE-CZ-NH2	-6.38	117.11	120.30
3	C	141	ASP	N-CA-CB	6.38	122.08	110.60
11	4	31	SER	N-CA-CB	6.38	120.06	110.50
3	c	20	TYR	CB-CG-CD1	-6.37	117.18	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	329	ARG	NE-CZ-NH1	-6.37	117.11	120.30
12	l	116	LEU	CB-CG-CD2	6.37	121.83	111.00
23	P	364	ARG	NE-CZ-NH2	-6.37	117.11	120.30
12	5	234	ARG	NE-CZ-NH1	-6.37	117.12	120.30
28	H	194	SER	CB-CA-C	-6.37	98.00	110.10
14	n	161	ARG	NE-CZ-NH1	6.37	123.48	120.30
14	n	74	ARG	NE-CZ-NH1	6.36	123.48	120.30
29	I	422	ARG	NE-CZ-NH2	-6.36	117.12	120.30
3	c	179	ASP	CB-CG-OD1	-6.36	112.58	118.30
4	d	91	VAL	CA-CB-CG2	-6.36	101.36	110.90
2	B	111	VAL	CA-CB-CG2	-6.36	101.36	110.90
6	F	24	TYR	CD1-CE1-CZ	-6.36	114.08	119.80
10	3	136	PHE	CB-CG-CD1	-6.36	116.35	120.80
16	V	108	TYR	CG-CD2-CE2	-6.36	116.21	121.30
9	i	152	TYR	CD1-CG-CD2	6.36	124.89	117.90
2	B	130	PHE	CB-CG-CD2	6.36	125.25	120.80
26	U	156	HIS	N-CA-CB	6.35	122.03	110.60
13	m	145	ARG	NE-CZ-NH2	6.35	123.47	120.30
25	R	134	TRP	CZ3-CH2-CZ2	-6.35	113.98	121.60
27	O	310	PHE	CG-CD1-CE1	-6.35	113.82	120.80
1	A	143	PHE	CB-CG-CD1	-6.34	116.36	120.80
11	4	20	ALA	N-CA-CB	6.34	118.98	110.10
21	N	232	LEU	O-C-N	-6.34	112.55	122.70
8	h	194	ARG	NH1-CZ-NH2	-6.34	112.42	119.40
11	k	126	VAL	CA-CB-CG1	-6.34	101.39	110.90
14	n	162	TYR	CD1-CG-CD2	-6.34	110.92	117.90
2	b	187	ASP	CB-CG-OD1	6.34	124.01	118.30
12	l	204	VAL	CA-CB-CG2	-6.34	101.39	110.90
33	J	174	PHE	CG-CD1-CE1	6.34	127.77	120.80
2	B	64	VAL	CA-CB-CG1	-6.34	101.39	110.90
7	g	26	TYR	CB-CG-CD2	-6.34	117.20	121.00
27	O	189	TYR	CB-CG-CD1	-6.34	117.20	121.00
3	C	146	TYR	CB-CG-CD2	-6.33	117.20	121.00
29	I	386	ASP	CB-CG-OD1	6.33	124.00	118.30
12	5	273	TRP	CH2-CZ2-CE2	6.33	123.73	117.40
21	N	674	GLN	N-CA-CB	6.33	121.99	110.60
28	H	355	THR	CA-CB-CG2	-6.32	103.55	112.40
31	L	65	LEU	CB-CG-CD2	6.32	121.75	111.00
5	e	167	TYR	CB-CG-CD2	-6.32	117.21	121.00
33	J	212	ARG	NE-CZ-NH2	-6.31	117.14	120.30
25	R	321	TYR	CB-CG-CD1	-6.31	117.21	121.00
3	C	137	TYR	CB-CG-CD2	-6.31	117.22	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	241	PHE	CB-CG-CD1	6.31	125.22	120.80
11	k	73	TYR	CB-CG-CD1	6.31	124.78	121.00
12	l	144	ARG	CD-NE-CZ	-6.31	114.77	123.60
13	m	152	SER	N-CA-CB	-6.30	101.04	110.50
13	6	168	TYR	CG-CD1-CE1	-6.30	116.26	121.30
21	N	415	PHE	CB-CG-CD1	6.30	125.21	120.80
11	k	85	ARG	NE-CZ-NH1	6.30	123.45	120.30
3	C	92	ARG	NE-CZ-NH2	-6.30	117.15	120.30
6	F	225	TYR	CB-CG-CD1	6.30	124.78	121.00
33	J	64	LEU	CB-CG-CD2	6.30	121.71	111.00
4	d	156	TYR	CB-CG-CD2	-6.30	117.22	121.00
32	M	109	ASP	CB-CG-OD1	-6.30	112.63	118.30
13	m	202	ARG	NE-CZ-NH1	6.29	123.45	120.30
21	N	578	ASP	N-CA-CB	6.29	121.93	110.60
7	G	103	TYR	CZ-CE2-CD2	6.29	125.46	119.80
21	N	380	LEU	CB-CG-CD2	6.29	121.70	111.00
21	N	88	ARG	NE-CZ-NH2	-6.29	117.16	120.30
10	3	96	TYR	CZ-CE2-CD2	6.29	125.46	119.80
20	Z	358	TYR	CB-CG-CD1	6.29	124.77	121.00
3	c	213	PHE	CB-CG-CD2	-6.29	116.40	120.80
24	Q	48	ASP	CB-CG-OD1	-6.28	112.64	118.30
18	X	65	SER	N-CA-CB	6.28	119.92	110.50
28	H	55	ASP	CB-CG-OD1	-6.28	112.65	118.30
7	g	8	TYR	CA-CB-CG	-6.28	101.48	113.40
14	n	219	TYR	CB-CG-CD2	-6.28	117.23	121.00
4	D	83	ARG	NE-CZ-NH2	-6.28	117.16	120.30
28	H	432	ARG	NE-CZ-NH2	6.28	123.44	120.30
3	C	137	TYR	CD1-CE1-CZ	-6.27	114.15	119.80
4	d	91	VAL	CA-CB-CG1	-6.27	101.49	110.90
23	P	234	TYR	CZ-CE2-CD2	-6.27	114.16	119.80
10	j	188	TYR	CB-CG-CD1	-6.27	117.24	121.00
2	B	90	ARG	NE-CZ-NH2	-6.27	117.16	120.30
28	H	135	ASP	CB-CG-OD2	6.26	123.94	118.30
30	K	77	ARG	NE-CZ-NH2	-6.26	117.17	120.30
17	T	175	ASP	CB-CG-OD2	-6.26	112.66	118.30
21	N	188	TYR	CD1-CE1-CZ	6.26	125.44	119.80
31	L	145	ARG	NE-CZ-NH1	6.26	123.43	120.30
12	l	268	VAL	CA-CB-CG1	6.26	120.29	110.90
16	V	22	ASP	CB-CG-OD2	6.26	123.93	118.30
30	K	317	ALA	N-CA-CB	6.26	118.86	110.10
33	J	270	ARG	NE-CZ-NH2	-6.26	117.17	120.30
28	H	69	VAL	CG1-CB-CG2	-6.25	100.89	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	221	ASP	CB-CG-OD2	-6.25	112.67	118.30
22	S	422	MET	CB-CA-C	-6.25	97.90	110.40
29	I	376	ASN	N-CA-CB	6.25	121.85	110.60
11	4	148	TYR	CB-CG-CD2	-6.24	117.25	121.00
16	V	87	PHE	CB-CG-CD2	-6.24	116.43	120.80
21	N	477	SER	N-CA-CB	6.24	119.87	110.50
28	H	272	ILE	N-CA-C	-6.24	94.15	111.00
24	Q	48	ASP	CB-CG-OD2	6.24	123.92	118.30
29	I	304	ARG	NE-CZ-NH1	6.24	123.42	120.30
6	F	126	ARG	NH1-CZ-NH2	-6.24	112.54	119.40
29	I	126	PRO	N-CD-CG	6.24	112.55	103.20
26	U	225	ILE	CA-CB-CG1	-6.23	99.16	111.00
30	K	289	ASP	CB-CG-OD1	6.23	123.91	118.30
18	X	122	TYR	CG-CD2-CE2	-6.23	116.31	121.30
21	N	788	TYR	N-CA-CB	6.23	121.81	110.60
11	4	21	VAL	CG1-CB-CG2	6.22	120.86	110.90
15	W	62	LEU	CB-CG-CD2	6.22	121.58	111.00
26	U	99	LEU	CB-CG-CD1	6.22	121.58	111.00
33	J	279	LEU	CB-CG-CD1	-6.22	100.42	111.00
26	U	67	PHE	CB-CG-CD1	6.22	125.16	120.80
21	N	387	ALA	N-CA-CB	6.22	118.81	110.10
12	l	219	TYR	CB-CG-CD2	-6.22	117.27	121.00
13	6	144	CYS	N-CA-CB	6.22	121.79	110.60
29	I	377	LEU	CB-CG-CD2	6.22	121.57	111.00
30	K	340	PHE	CB-CG-CD1	-6.22	116.45	120.80
12	l	147	GLU	N-CA-C	-6.21	94.23	111.00
7	G	115	ARG	NE-CZ-NH2	-6.21	117.20	120.30
31	L	168	TYR	CD1-CE1-CZ	6.21	125.39	119.80
21	N	334	VAL	CA-CB-CG2	-6.21	101.59	110.90
22	S	442	PHE	CD1-CE1-CZ	-6.21	112.65	120.10
33	J	214	SER	CB-CA-C	-6.21	98.31	110.10
7	G	212	PHE	CB-CG-CD1	-6.20	116.46	120.80
29	I	316	PHE	CB-CG-CD2	6.20	125.14	120.80
11	4	46	PHE	CB-CG-CD2	-6.20	116.46	120.80
24	Q	146	TYR	CB-CG-CD2	-6.19	117.28	121.00
9	2	101	ARG	NE-CZ-NH1	-6.19	117.20	120.30
32	M	384	ASP	CB-CG-OD2	6.19	123.87	118.30
33	J	207	ASP	N-CA-CB	6.19	121.74	110.60
11	4	138	PHE	CB-CG-CD1	6.19	125.13	120.80
29	I	256	TYR	CB-CG-CD2	-6.19	117.29	121.00
17	T	186	ARG	NE-CZ-NH1	6.18	123.39	120.30
4	d	85	LEU	CB-CA-C	-6.18	98.45	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	210	LEU	CB-CG-CD2	-6.18	100.49	111.00
28	H	222	ARG	NE-CZ-NH2	-6.18	117.21	120.30
6	F	67	ASP	CB-CG-OD1	-6.18	112.74	118.30
15	W	35	PHE	CG-CD1-CE1	6.18	127.60	120.80
3	C	6	TYR	CB-CG-CD2	-6.17	117.30	121.00
9	2	162	ALA	N-CA-CB	6.17	118.75	110.10
23	P	202	LYS	CB-CA-C	-6.17	98.05	110.40
24	Q	50	ARG	NE-CZ-NH1	6.17	123.39	120.30
25	R	62	TYR	CB-CG-CD2	-6.17	117.30	121.00
5	e	5	ARG	NE-CZ-NH1	6.17	123.38	120.30
29	I	128	TYR	CZ-CE2-CD2	6.17	125.35	119.80
21	N	873	ARG	NE-CZ-NH2	-6.17	117.22	120.30
25	R	350	LEU	O-C-N	6.17	132.56	122.70
6	F	13	PHE	C-N-CA	6.16	137.10	121.70
27	O	178	TYR	CZ-CE2-CD2	-6.16	114.26	119.80
26	U	233	PHE	CG-CD2-CE2	6.16	127.57	120.80
7	g	48	PHE	CB-CG-CD1	6.15	125.11	120.80
30	K	113	THR	CA-CB-CG2	-6.15	103.79	112.40
21	N	161	TYR	CB-CG-CD1	6.15	124.69	121.00
15	W	101	ARG	NE-CZ-NH1	-6.15	117.23	120.30
27	O	248	TYR	CB-CG-CD1	6.15	124.69	121.00
2	b	5	TYR	CD1-CG-CD2	6.14	124.66	117.90
5	e	62	ASP	CB-CG-OD1	-6.14	112.77	118.30
24	Q	20	TYR	CG-CD1-CE1	-6.14	116.39	121.30
20	Z	748	LEU	CB-CA-C	6.14	121.86	110.20
21	N	804	LEU	CB-CG-CD1	6.14	121.44	111.00
30	K	281	ARG	NE-CZ-NH1	6.14	123.37	120.30
22	S	481	TYR	CB-CG-CD2	6.13	124.68	121.00
3	c	117	ASP	CB-CG-OD1	6.13	123.82	118.30
1	A	19	PHE	CB-CG-CD1	-6.13	116.51	120.80
27	O	149	LEU	CB-CG-CD1	6.13	121.42	111.00
30	K	88	ARG	NE-CZ-NH1	-6.13	117.24	120.30
7	g	21	ASN	N-CA-CB	6.13	121.63	110.60
2	B	212	ALA	N-CA-CB	6.13	118.68	110.10
22	S	55	ARG	NE-CZ-NH2	-6.13	117.24	120.30
8	h	162	ASP	CB-CG-OD2	6.12	123.81	118.30
17	T	20	TYR	CB-CG-CD1	-6.12	117.33	121.00
22	S	352	VAL	CA-CB-CG1	6.12	120.09	110.90
27	O	166	ARG	NE-CZ-NH2	-6.12	117.24	120.30
11	k	70	ARG	NE-CZ-NH2	-6.12	117.24	120.30
12	l	80	ALA	N-CA-CB	6.12	118.67	110.10
23	P	1	MET	CG-SD-CE	-6.12	90.40	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	173	PHE	CB-CG-CD1	6.12	125.08	120.80
18	X	17	TYR	CB-CG-CD1	-6.12	117.33	121.00
29	I	416	PHE	CB-CG-CD2	-6.12	116.52	120.80
2	B	101	TYR	CB-CG-CD1	6.11	124.67	121.00
11	4	171	ARG	NE-CZ-NH1	6.11	123.36	120.30
25	R	371	PHE	CB-CG-CD2	-6.11	116.52	120.80
21	N	888	ASP	CB-CG-OD1	6.11	123.80	118.30
24	Q	231	ASP	CB-CG-OD1	-6.11	112.80	118.30
23	P	43	GLU	CB-CA-C	-6.10	98.19	110.40
17	T	96	LEU	N-CA-CB	6.10	122.60	110.40
30	K	393	ARG	CD-NE-CZ	6.10	132.14	123.60
21	N	503	THR	CA-CB-CG2	-6.10	103.86	112.40
27	O	70	TYR	CG-CD2-CE2	-6.10	116.42	121.30
5	E	112	LEU	CB-CG-CD2	6.10	121.37	111.00
28	H	373	ARG	NE-CZ-NH1	6.10	123.35	120.30
23	P	253	ASP	N-CA-CB	6.10	121.58	110.60
12	5	97	ALA	N-CA-CB	6.09	118.63	110.10
29	I	246	ARG	NE-CZ-NH1	6.09	123.35	120.30
32	M	325	ALA	N-CA-CB	6.09	118.63	110.10
4	d	90	ARG	NE-CZ-NH2	6.09	123.34	120.30
20	Z	255	LEU	CA-CB-CG	6.09	129.30	115.30
10	j	66	MET	CG-SD-CE	-6.08	90.47	100.20
30	K	411	TYR	CG-CD1-CE1	6.08	126.17	121.30
28	H	432	ARG	NE-CZ-NH1	-6.08	117.26	120.30
10	j	40	PHE	N-CA-C	-6.08	94.60	111.00
13	m	83	TYR	CB-CG-CD2	-6.08	117.36	121.00
28	H	299	ARG	NE-CZ-NH2	-6.08	117.26	120.30
6	f	137	TYR	CB-CG-CD1	-6.07	117.36	121.00
16	V	156	PHE	CB-CG-CD2	-6.07	116.55	120.80
24	Q	434	TYR	CG-CD2-CE2	-6.07	116.44	121.30
8	1	118	GLU	N-CA-CB	6.07	121.53	110.60
32	M	234	ALA	CB-CA-C	-6.07	101.00	110.10
30	K	336	ARG	NE-CZ-NH2	6.06	123.33	120.30
1	a	12	TYR	CZ-CE2-CD2	6.06	125.25	119.80
14	7	183	MET	CG-SD-CE	-6.06	90.50	100.20
20	Z	550	PHE	CB-CG-CD1	6.06	125.04	120.80
10	3	131	ASP	N-CA-C	-6.06	94.64	111.00
12	l	239	ALA	N-CA-CB	6.05	118.57	110.10
1	a	26	TYR	CG-CD2-CE2	-6.05	116.46	121.30
12	5	165	TYR	CG-CD1-CE1	-6.05	116.46	121.30
7	g	179	LEU	CB-CG-CD1	6.04	121.28	111.00
21	N	857	TYR	CB-CG-CD2	-6.04	117.37	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	15	PHE	C-N-CA	6.04	136.80	121.70
18	X	81	SER	CB-CA-C	-6.04	98.62	110.10
30	K	290	ARG	CD-NE-CZ	-6.04	115.14	123.60
18	X	51	ARG	N-CA-CB	6.04	121.47	110.60
31	L	344	ASP	CB-CG-OD2	6.04	123.73	118.30
8	h	44	THR	CA-CB-CG2	-6.03	103.95	112.40
3	C	4	ARG	NE-CZ-NH1	6.03	123.32	120.30
16	V	270	TYR	CB-CG-CD1	-6.03	117.38	121.00
30	K	406	ASP	CB-CA-C	-6.03	98.34	110.40
20	Z	727	GLU	CA-C-N	6.03	130.46	117.20
23	P	31	ASP	CB-CG-OD2	6.03	123.72	118.30
7	G	60	VAL	CB-CA-C	-6.03	99.95	111.40
13	m	229	ARG	NE-CZ-NH2	-6.02	117.29	120.30
33	J	339	ARG	NE-CZ-NH1	6.02	123.31	120.30
14	7	215	ARG	CD-NE-CZ	6.02	132.03	123.60
5	E	167	TYR	CB-CG-CD1	6.02	124.61	121.00
11	k	13	VAL	CA-CB-CG1	-6.02	101.87	110.90
28	H	390	ARG	NE-CZ-NH2	6.01	123.31	120.30
1	A	162	TYR	CB-CG-CD1	-6.01	117.39	121.00
5	e	106	ASP	CB-CG-OD1	-6.01	112.89	118.30
16	V	20	ARG	NE-CZ-NH2	-6.01	117.29	120.30
13	m	150	ALA	N-CA-CB	-6.01	101.69	110.10
3	C	122	TYR	CD1-CE1-CZ	6.01	125.21	119.80
14	7	128	TYR	CB-CG-CD1	-6.01	117.40	121.00
32	M	243	PHE	CB-CG-CD2	6.01	125.00	120.80
21	N	235	ALA	N-CA-CB	6.00	118.51	110.10
21	N	819	LYS	CB-CA-C	-6.00	98.39	110.40
1	A	166	TYR	CB-CG-CD1	-6.00	117.40	121.00
22	S	467	PHE	CB-CG-CD1	-6.00	116.60	120.80
23	P	439	MET	CG-SD-CE	6.00	109.80	100.20
29	I	267	ILE	CB-CA-C	-6.00	99.60	111.60
9	i	57	ASP	CB-CG-OD2	6.00	123.70	118.30
27	O	26	PHE	CB-CG-CD2	6.00	125.00	120.80
21	N	20	VAL	CA-CB-CG2	-6.00	101.91	110.90
10	3	142	ALA	N-CA-CB	5.99	118.49	110.10
24	Q	382	LEU	CB-CG-CD2	5.99	121.19	111.00
30	K	427	TYR	CB-CG-CD1	-5.99	117.41	121.00
6	F	159	THR	CA-CB-CG2	5.99	120.78	112.40
9	2	65	ARG	NE-CZ-NH2	-5.99	117.31	120.30
22	S	333	PHE	CG-CD1-CE1	-5.99	114.21	120.80
5	e	103	TYR	CZ-CE2-CD2	-5.98	114.41	119.80
23	P	394	ASN	CB-CG-OD1	5.98	133.57	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	239	PHE	CB-CG-CD2	-5.98	116.61	120.80
8	1	192	VAL	CA-CB-CG2	5.98	119.87	110.90
9	2	215	TYR	CB-CG-CD1	5.98	124.59	121.00
25	R	213	TYR	CB-CG-CD2	-5.98	117.41	121.00
11	4	50	ALA	CB-CA-C	-5.97	101.14	110.10
20	Z	748	LEU	CA-CB-CG	5.97	129.04	115.30
13	6	85	PHE	CB-CG-CD2	-5.97	116.62	120.80
26	U	210	TYR	CG-CD1-CE1	-5.97	116.52	121.30
9	2	87	LEU	CB-CG-CD1	5.97	121.15	111.00
27	O	60	ARG	NE-CZ-NH1	-5.97	117.31	120.30
31	L	91	THR	CA-CB-CG2	-5.97	104.04	112.40
2	b	3	ASP	CB-CG-OD1	-5.97	112.93	118.30
11	k	139	TYR	CB-CA-C	-5.97	98.46	110.40
25	R	48	GLU	N-CA-CB	-5.97	99.86	110.60
21	N	604	ARG	NE-CZ-NH2	-5.97	117.32	120.30
29	I	181	TYR	CB-CG-CD1	-5.97	117.42	121.00
20	Z	251	ALA	CB-CA-C	-5.96	101.16	110.10
8	h	183	ARG	NE-CZ-NH1	5.96	123.28	120.30
11	4	172	MET	CG-SD-CE	-5.96	90.66	100.20
23	P	379	TYR	CZ-CE2-CD2	5.96	125.16	119.80
20	Z	247	GLN	CA-CB-CG	5.96	126.50	113.40
23	P	221	TYR	CB-CG-CD2	-5.96	117.43	121.00
4	D	74	SER	CB-CA-C	5.96	121.42	110.10
15	W	5	ALA	N-CA-CB	5.96	118.44	110.10
1	A	186	PHE	CB-CG-CD2	-5.95	116.63	120.80
31	L	392	ARG	NE-CZ-NH1	5.95	123.28	120.30
30	K	340	PHE	CB-CG-CD2	5.95	124.97	120.80
4	D	22	TYR	CB-CG-CD2	-5.95	117.43	121.00
4	D	112	TYR	CB-CG-CD1	5.95	124.57	121.00
28	H	169	GLU	N-CA-CB	5.95	121.31	110.60
2	b	43	VAL	N-CA-C	-5.95	94.94	111.00
7	g	16	SER	CB-CA-C	-5.94	98.81	110.10
9	2	215	TYR	CB-CG-CD2	-5.94	117.43	121.00
12	5	163	TYR	CB-CG-CD2	-5.94	117.44	121.00
28	H	442	ASP	CB-CG-OD2	-5.94	112.95	118.30
30	K	267	SER	N-CA-CB	5.94	119.41	110.50
5	E	53	ARG	NE-CZ-NH1	5.94	123.27	120.30
1	a	234	PHE	CB-CG-CD2	5.93	124.95	120.80
21	N	208	ARG	NE-CZ-NH2	-5.93	117.33	120.30
33	J	257	ARG	NE-CZ-NH1	5.93	123.27	120.30
23	P	3	ARG	N-CA-CB	5.93	121.27	110.60
21	N	784	TYR	CB-CG-CD1	-5.93	117.44	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	43	LYS	N-CA-CB	5.93	121.27	110.60
24	Q	243	PHE	CB-CG-CD2	-5.93	116.65	120.80
14	7	170	TYR	CB-CG-CD2	5.92	124.56	121.00
23	P	304	THR	CA-CB-CG2	-5.92	104.11	112.40
7	g	48	PHE	CB-CG-CD2	-5.92	116.66	120.80
8	1	11	SER	N-CA-CB	5.91	119.36	110.50
23	P	328	ALA	O-C-N	-5.91	113.24	122.70
30	K	169	VAL	CA-CB-CG1	5.91	119.77	110.90
21	N	13	LEU	CB-CG-CD2	5.91	121.04	111.00
21	N	311	ILE	CA-CB-CG1	5.91	122.23	111.00
11	k	98	TYR	CB-CG-CD1	5.91	124.54	121.00
10	3	74	TYR	CG-CD1-CE1	5.91	126.03	121.30
23	P	170	SER	C-N-CA	5.91	136.47	121.70
31	L	264	ARG	NE-CZ-NH2	-5.90	117.35	120.30
5	e	86	ARG	NE-CZ-NH2	-5.90	117.35	120.30
2	B	208	THR	CA-CB-CG2	-5.90	104.14	112.40
17	T	129	LEU	CB-CA-C	-5.90	98.99	110.20
4	D	105	THR	CA-CB-CG2	-5.90	104.14	112.40
8	1	194	ARG	CD-NE-CZ	5.90	131.86	123.60
22	S	431	VAL	CA-CB-CG1	5.90	119.75	110.90
9	i	50	THR	CA-CB-CG2	-5.90	104.14	112.40
14	n	144	TRP	CB-CG-CD2	-5.89	118.94	126.60
4	D	120	TYR	CZ-CE2-CD2	5.89	125.11	119.80
10	3	154	TYR	CB-CG-CD2	5.89	124.54	121.00
21	N	762	ARG	NE-CZ-NH2	-5.89	117.35	120.30
28	H	216	ASP	CB-CG-OD1	-5.89	113.00	118.30
7	G	132	PHE	CB-CG-CD1	5.89	124.92	120.80
1	A	110	TYR	CB-CG-CD1	-5.89	117.47	121.00
19	Y	82	ASP	CB-CG-OD2	-5.89	113.00	118.30
33	J	113	VAL	CA-CB-CG1	-5.89	102.07	110.90
6	F	99	PHE	CB-CG-CD1	-5.89	116.68	120.80
9	2	234	PHE	CB-CG-CD2	5.89	124.92	120.80
24	Q	192	ALA	N-CA-CB	5.89	118.34	110.10
3	C	6	TYR	CG-CD1-CE1	-5.88	116.59	121.30
11	4	148	TYR	CB-CG-CD1	5.88	124.53	121.00
16	V	69	PHE	N-CA-CB	5.88	121.19	110.60
21	N	230	VAL	CA-CB-CG2	-5.88	102.08	110.90
27	O	210	ARG	NH1-CZ-NH2	5.88	125.87	119.40
22	S	428	ARG	NE-CZ-NH2	5.88	123.24	120.30
12	l	172	MET	CA-CB-CG	5.88	123.30	113.30
12	l	266	HIS	CB-CA-C	-5.88	98.64	110.40
3	C	9	ARG	CD-NE-CZ	5.88	131.83	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	117	TRP	CE2-CD2-CG	-5.88	102.60	107.30
18	X	98	PHE	N-CA-C	-5.88	95.13	111.00
22	S	453	ASP	CB-CG-OD1	-5.88	113.01	118.30
27	O	71	ASP	CB-CG-OD2	-5.88	113.01	118.30
31	L	434	TYR	CB-CG-CD2	5.88	124.53	121.00
12	5	262	TYR	CB-CG-CD1	5.88	124.53	121.00
21	N	721	ASP	CB-CG-OD2	5.88	123.59	118.30
23	P	261	LEU	CB-CG-CD1	5.87	120.98	111.00
16	V	56	GLU	OE1-CD-OE2	5.87	130.34	123.30
7	G	72	ARG	NE-CZ-NH2	-5.87	117.37	120.30
3	c	84	ALA	CB-CA-C	-5.86	101.31	110.10
6	f	14	SER	N-CA-CB	5.86	119.29	110.50
14	n	157	ASP	CB-CG-OD2	5.86	123.58	118.30
27	O	349	THR	N-CA-C	-5.86	95.18	111.00
3	C	98	TYR	CB-CG-CD2	5.86	124.52	121.00
11	4	83	PHE	CB-CG-CD1	-5.86	116.70	120.80
12	5	253	TYR	CB-CG-CD1	5.86	124.52	121.00
14	7	84	VAL	CA-CB-CG1	-5.86	102.11	110.90
13	m	139	TYR	CG-CD2-CE2	-5.86	116.62	121.30
3	c	113	ARG	NE-CZ-NH1	-5.85	117.37	120.30
22	S	467	PHE	CB-CG-CD2	5.85	124.90	120.80
20	Z	248	TYR	N-CA-CB	5.85	121.13	110.60
30	K	246	TYR	N-CA-CB	5.85	121.12	110.60
30	K	322	ASP	N-CA-CB	5.85	121.12	110.60
4	D	111	ARG	CD-NE-CZ	5.84	131.78	123.60
11	4	139	TYR	CB-CG-CD2	-5.84	117.49	121.00
22	S	330	LEU	CB-CG-CD2	5.84	120.93	111.00
11	4	8	ARG	NH1-CZ-NH2	-5.84	112.97	119.40
27	O	280	LEU	CB-CG-CD1	5.84	120.93	111.00
28	H	385	ARG	NE-CZ-NH1	5.84	123.22	120.30
31	L	126	ARG	NE-CZ-NH1	5.84	123.22	120.30
12	5	130	TRP	CG-CD2-CE3	-5.84	128.65	133.90
3	C	222	ASP	N-CA-CB	5.84	121.11	110.60
29	I	187	LEU	N-CA-CB	5.84	122.08	110.40
10	j	24	ALA	N-CA-CB	5.84	118.27	110.10
33	J	187	LEU	CB-CG-CD1	5.84	120.92	111.00
26	U	45	THR	CA-CB-CG2	-5.83	104.23	112.40
14	7	137	ARG	NE-CZ-NH1	5.83	123.22	120.30
26	U	243	ASP	CB-CG-OD1	-5.83	113.05	118.30
13	6	109	ARG	NE-CZ-NH2	-5.83	117.38	120.30
25	R	99	TYR	CA-CB-CG	5.83	124.48	113.40
29	I	256	TYR	CB-CG-CD1	5.83	124.50	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	106	PRO	N-CD-CG	5.83	111.94	103.20
12	l	127	CYS	CA-CB-SG	-5.83	103.51	114.00
1	A	91	ARG	NE-CZ-NH2	-5.83	117.39	120.30
32	M	416	VAL	N-CA-CB	-5.83	98.68	111.50
3	C	209	ASP	CB-CG-OD2	-5.83	113.06	118.30
6	F	92	CYS	CA-CB-SG	-5.83	103.51	114.00
9	i	117	PHE	CB-CG-CD2	-5.82	116.72	120.80
33	J	120	TYR	N-CA-CB	5.82	121.08	110.60
28	H	308	PHE	O-C-N	5.82	132.01	122.70
3	c	66	LEU	N-CA-CB	5.82	122.04	110.40
21	N	123	PHE	CB-CG-CD1	5.82	124.88	120.80
26	U	113	TYR	CD1-CE1-CZ	-5.82	114.56	119.80
6	f	122	SER	N-CA-CB	5.82	119.23	110.50
4	D	232	TYR	CG-CD1-CE1	-5.82	116.65	121.30
24	Q	77	PHE	CZ-CE2-CD2	-5.82	113.12	120.10
9	2	43	ILE	N-CA-C	-5.81	95.30	111.00
33	J	281	GLY	O-C-N	5.81	132.00	122.70
9	2	148	THR	CA-CB-CG2	-5.81	104.27	112.40
28	H	112	SER	N-CA-CB	5.81	119.22	110.50
1	A	106	TYR	CB-CG-CD2	-5.80	117.52	121.00
9	2	101	ARG	NH1-CZ-NH2	5.80	125.78	119.40
1	a	14	ARG	NE-CZ-NH2	-5.80	117.40	120.30
12	5	124	ALA	N-CA-CB	5.80	118.22	110.10
21	N	297	ASP	CB-CG-OD1	5.80	123.52	118.30
27	O	179	PHE	CZ-CE2-CD2	-5.80	113.14	120.10
15	W	15	TYR	CB-CG-CD1	-5.80	117.52	121.00
26	U	290	ASP	CB-CG-OD1	-5.80	113.08	118.30
27	O	202	SER	N-CA-CB	5.80	119.20	110.50
31	L	207	PHE	CB-CG-CD1	-5.80	116.74	120.80
2	b	148	TYR	CB-CG-CD1	5.80	124.48	121.00
5	E	82	THR	CA-CB-CG2	-5.80	104.28	112.40
11	4	120	ASP	CB-CG-OD2	5.80	123.52	118.30
20	Z	767	TYR	CB-CG-CD1	5.80	124.48	121.00
17	T	244	ASP	N-CA-CB	5.79	121.03	110.60
14	n	102	ASP	CB-CG-OD2	-5.79	113.09	118.30
31	L	262	ILE	O-C-N	5.79	131.97	122.70
7	G	149	TYR	CD1-CE1-CZ	-5.79	114.59	119.80
2	b	133	SER	N-CA-CB	5.79	119.18	110.50
14	n	220	ARG	NE-CZ-NH2	-5.79	117.41	120.30
1	a	246	VAL	CA-CB-CG2	-5.79	102.22	110.90
25	R	140	TYR	CZ-CE2-CD2	-5.79	114.59	119.80
13	m	111	PHE	CB-CG-CD1	-5.79	116.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	353	PHE	CG-CD1-CE1	5.79	127.17	120.80
6	f	146	GLU	N-CA-C	-5.78	95.38	111.00
2	B	250	LEU	CB-CG-CD2	5.78	120.83	111.00
2	b	83	ARG	NE-CZ-NH1	5.78	123.19	120.30
18	X	83	SER	N-CA-CB	5.77	119.16	110.50
30	K	375	ASN	CB-CG-OD1	5.77	133.15	121.60
11	4	103	LEU	CB-CG-CD2	5.77	120.81	111.00
12	5	253	TYR	CG-CD2-CE2	-5.77	116.68	121.30
1	A	71	TYR	CG-CD1-CE1	-5.77	116.68	121.30
32	M	236	ALA	CB-CA-C	-5.77	101.44	110.10
13	6	157	PHE	CB-CG-CD1	-5.77	116.76	120.80
24	Q	15	VAL	CB-CA-C	-5.77	100.44	111.40
25	R	63	TYR	CB-CG-CD1	5.77	124.46	121.00
8	1	23	LEU	CB-CG-CD1	5.77	120.80	111.00
32	M	404	ARG	NE-CZ-NH2	-5.76	117.42	120.30
3	c	144	TYR	CB-CG-CD2	5.76	124.46	121.00
7	g	172	ALA	N-CA-CB	5.76	118.17	110.10
10	3	40	PHE	CB-CG-CD2	5.76	124.83	120.80
10	3	183	TRP	CG-CD2-CE3	-5.76	128.72	133.90
11	4	149	ARG	NE-CZ-NH1	5.76	123.18	120.30
20	Z	287	ARG	CG-CD-NE	-5.76	99.71	111.80
32	M	18	LEU	N-CA-CB	5.76	121.92	110.40
6	F	222	PHE	CB-CG-CD2	5.75	124.83	120.80
21	N	741	TYR	CB-CG-CD2	-5.75	117.55	121.00
19	Y	64	TRP	CE2-CD2-CG	5.75	111.90	107.30
4	d	129	PHE	CD1-CE1-CZ	-5.75	113.20	120.10
12	l	105	THR	N-CA-CB	5.75	121.22	110.30
30	K	58	TYR	CB-CG-CD2	5.75	124.45	121.00
31	L	364	HIS	N-CA-CB	5.75	120.94	110.60
27	O	120	LYS	N-CA-CB	5.74	120.94	110.60
27	O	250	TRP	CG-CD2-CE3	-5.74	128.73	133.90
9	i	209	ILE	C-N-CA	5.74	134.36	122.30
24	Q	27	TYR	CB-CG-CD2	-5.74	117.56	121.00
6	f	44	ALA	N-CA-CB	5.74	118.14	110.10
12	5	210	PHE	CB-CG-CD2	5.74	124.82	120.80
14	n	252	TRP	CB-CG-CD2	-5.74	119.14	126.60
26	U	291	LEU	CB-CG-CD2	5.74	120.75	111.00
12	5	210	PHE	CB-CG-CD1	-5.74	116.78	120.80
10	3	154	TYR	CZ-CE2-CD2	5.73	124.96	119.80
20	Z	513	ALA	N-CA-CB	5.73	118.12	110.10
24	Q	77	PHE	CB-CG-CD1	5.73	124.81	120.80
8	1	202	TYR	CG-CD1-CE1	-5.73	116.72	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	193	ASP	CB-CG-OD1	5.73	123.45	118.30
21	N	861	TYR	CG-CD2-CE2	-5.73	116.72	121.30
21	N	889	ARG	NE-CZ-NH2	-5.73	117.44	120.30
24	Q	98	LYS	O-C-N	-5.73	113.53	122.70
29	I	246	ARG	NE-CZ-NH2	-5.73	117.44	120.30
7	G	97	ALA	O-C-N	-5.72	113.54	122.70
33	J	385	ALA	N-CA-CB	5.72	118.11	110.10
7	G	138	PHE	CB-CG-CD1	-5.72	116.80	120.80
23	P	436	GLU	N-CA-CB	5.72	120.90	110.60
31	L	261	ARG	NE-CZ-NH2	-5.72	117.44	120.30
21	N	515	ARG	NE-CZ-NH1	5.72	123.16	120.30
24	Q	360	SER	N-CA-CB	5.72	119.08	110.50
26	U	43	SER	CB-CA-C	5.72	120.96	110.10
2	b	177	LYS	CB-CA-C	-5.72	98.97	110.40
23	P	398	LYS	CA-CB-CG	5.72	125.97	113.40
27	O	36	LYS	N-CA-CB	5.72	120.89	110.60
14	7	132	VAL	CG1-CB-CG2	-5.71	101.76	110.90
14	n	133	MET	CG-SD-CE	-5.71	91.06	100.20
33	J	106	ASP	CB-CG-OD1	5.71	123.44	118.30
33	J	257	ARG	CD-NE-CZ	-5.71	115.61	123.60
24	Q	51	ARG	NE-CZ-NH2	-5.71	117.45	120.30
10	j	136	PHE	CB-CG-CD1	5.71	124.80	120.80
12	5	260	TRP	CG-CD2-CE3	-5.70	128.77	133.90
24	Q	335	PHE	CB-CG-CD1	-5.70	116.81	120.80
30	K	121	ARG	NE-CZ-NH2	-5.70	117.45	120.30
33	J	329	ARG	NE-CZ-NH1	5.70	123.15	120.30
28	H	295	PHE	CB-CG-CD1	5.70	124.79	120.80
8	h	79	TYR	CB-CG-CD2	-5.70	117.58	121.00
32	M	332	VAL	CA-CB-CG1	-5.70	102.35	110.90
12	5	209	THR	CA-CB-CG2	-5.70	104.42	112.40
21	N	851	GLU	N-CA-CB	5.70	120.86	110.60
9	2	125	ALA	CB-CA-C	-5.70	101.56	110.10
13	6	76	PHE	CB-CG-CD2	-5.70	116.81	120.80
33	J	381	ASP	CB-CG-OD1	5.69	123.42	118.30
4	D	141	ARG	N-CA-CB	5.69	120.84	110.60
14	7	138	SER	N-CA-CB	5.69	119.03	110.50
21	N	711	ARG	NE-CZ-NH2	-5.69	117.45	120.30
13	m	123	ASP	CB-CG-OD2	-5.69	113.18	118.30
16	V	94	MET	CA-CB-CG	5.69	122.97	113.30
24	Q	150	GLN	O-C-N	-5.69	113.60	122.70
23	P	318	TYR	CG-CD1-CE1	-5.68	116.75	121.30
27	O	213	LEU	CB-CG-CD2	-5.68	101.33	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	57	GLU	O-C-N	-5.68	113.61	122.70
8	1	99	LYS	N-CA-CB	5.68	120.83	110.60
27	O	188	PHE	CB-CG-CD1	-5.68	116.82	120.80
29	I	422	ARG	NE-CZ-NH1	5.68	123.14	120.30
21	N	896	PHE	CB-CG-CD1	-5.68	116.82	120.80
31	L	344	ASP	CB-CG-OD1	-5.68	113.19	118.30
20	Z	745	LEU	O-C-N	5.68	131.78	122.70
12	l	115	PHE	CB-CG-CD1	-5.67	116.83	120.80
3	C	122	TYR	CG-CD1-CE1	-5.67	116.76	121.30
27	O	193	LEU	N-CA-CB	5.67	121.75	110.40
32	M	151	ASP	CB-CG-OD1	5.67	123.41	118.30
22	S	110	LEU	CB-CG-CD1	5.67	120.64	111.00
25	R	359	VAL	C-N-CA	5.67	135.87	121.70
32	M	117	ALA	O-C-N	5.67	131.77	122.70
32	M	184	GLY	N-CA-C	-5.67	98.92	113.10
13	m	86	ASP	CB-CG-OD2	-5.67	113.20	118.30
1	a	59	VAL	N-CA-C	-5.67	95.70	111.00
10	j	198	ARG	NH1-CZ-NH2	-5.66	113.17	119.40
13	m	168	TYR	CB-CG-CD2	-5.66	117.60	121.00
7	G	160	TYR	CG-CD1-CE1	-5.66	116.77	121.30
28	H	463	TYR	CZ-CE2-CD2	5.66	124.89	119.80
32	M	264	ARG	NE-CZ-NH1	5.66	123.13	120.30
14	n	166	LEU	CB-CG-CD2	5.66	120.62	111.00
14	7	108	ALA	CB-CA-C	-5.66	101.61	110.10
2	b	82	TYR	CB-CG-CD1	-5.66	117.61	121.00
3	C	187	ASP	CB-CG-OD2	5.66	123.39	118.30
5	E	106	ASP	CB-CG-OD2	5.66	123.39	118.30
16	V	221	TRP	N-CA-CB	5.66	120.78	110.60
28	H	403	ARG	NE-CZ-NH1	5.66	123.13	120.30
32	M	77	TYR	CG-CD2-CE2	-5.65	116.78	121.30
4	d	57	THR	CA-CB-CG2	-5.65	104.49	112.40
4	d	156	TYR	CD1-CG-CD2	5.65	124.12	117.90
5	E	2	PHE	CG-CD1-CE1	-5.65	114.58	120.80
11	4	44	MET	CA-CB-CG	5.65	122.91	113.30
17	T	234	TYR	CB-CG-CD1	-5.65	117.61	121.00
21	N	884	PHE	N-CA-CB	5.65	120.78	110.60
22	S	285	ASP	CB-CG-OD2	5.65	123.39	118.30
14	n	63	TYR	CB-CG-CD1	-5.65	117.61	121.00
17	T	245	TYR	O-C-N	-5.65	113.66	122.70
26	U	134	THR	CA-CB-CG2	-5.65	104.49	112.40
31	L	137	ARG	NE-CZ-NH1	5.65	123.12	120.30
1	A	244	ARG	N-CA-CB	5.65	120.77	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	228	PHE	CG-CD1-CE1	-5.65	114.59	120.80
21	N	54	THR	CA-CB-CG2	-5.65	104.50	112.40
32	M	126	THR	N-CA-CB	5.65	121.03	110.30
32	M	207	PHE	CG-CD2-CE2	-5.65	114.59	120.80
2	B	181	ASP	CB-CG-OD2	-5.65	113.22	118.30
7	G	93	ARG	CD-NE-CZ	5.65	131.50	123.60
21	N	365	PHE	CD1-CE1-CZ	5.65	126.88	120.10
30	K	171	TYR	CD1-CE1-CZ	-5.65	114.72	119.80
10	j	50	PHE	CB-CG-CD1	-5.64	116.85	120.80
12	l	273	TRP	CD2-CE3-CZ3	5.64	126.14	118.80
14	7	233	ILE	N-CA-C	-5.64	95.76	111.00
23	P	207	THR	CA-CB-CG2	-5.64	104.50	112.40
29	I	227	THR	N-CA-CB	5.64	121.02	110.30
3	c	208	TYR	CG-CD2-CE2	-5.64	116.79	121.30
13	m	187	GLU	OE1-CD-OE2	5.64	130.07	123.30
17	T	43	ASP	N-CA-CB	5.64	120.76	110.60
19	Y	57	THR	CA-CB-CG2	-5.64	104.50	112.40
20	Z	287	ARG	NE-CZ-NH2	-5.64	117.48	120.30
32	M	85	VAL	N-CA-C	-5.64	95.77	111.00
3	C	210	ARG	NH1-CZ-NH2	5.64	125.60	119.40
14	7	44	VAL	N-CA-C	-5.64	95.78	111.00
30	K	353	PHE	N-CA-CB	5.63	120.74	110.60
33	J	351	ASN	CA-CB-CG	-5.63	101.00	113.40
30	K	187	ALA	CB-CA-C	-5.63	101.65	110.10
29	I	168	VAL	CG1-CB-CG2	5.63	119.91	110.90
8	h	19	ASP	O-C-N	-5.63	113.63	123.20
30	K	142	HIS	O-C-N	-5.63	113.69	122.70
19	Y	43	TRP	CB-CG-CD1	5.63	134.31	127.00
27	O	130	ASP	CB-CG-OD2	5.63	123.36	118.30
11	k	128	LEU	CB-CA-C	-5.62	99.51	110.20
21	N	682	PHE	CB-CG-CD2	-5.62	116.86	120.80
22	S	196	ARG	NE-CZ-NH1	5.62	123.11	120.30
10	3	103	TYR	CB-CG-CD1	5.62	124.37	121.00
18	X	57	VAL	O-C-N	-5.62	113.65	123.20
30	K	185	ARG	NE-CZ-NH2	-5.62	117.49	120.30
33	J	329	ARG	NE-CZ-NH2	-5.62	117.49	120.30
8	h	155	MET	CG-SD-CE	-5.61	91.22	100.20
21	N	862	SER	N-CA-CB	5.61	118.92	110.50
13	m	134	ASP	CB-CG-OD1	5.61	123.35	118.30
1	A	10	ALA	N-CA-CB	5.61	117.95	110.10
2	B	171	ALA	CB-CA-C	-5.61	101.68	110.10
4	D	197	ARG	NE-CZ-NH2	-5.61	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	103	TYR	CG-CD1-CE1	-5.61	116.81	121.30
24	Q	291	TYR	CB-CG-CD1	5.61	124.37	121.00
10	3	50	PHE	N-CA-CB	5.61	120.70	110.60
21	N	385	VAL	CG1-CB-CG2	5.61	119.87	110.90
7	g	79	SER	N-CA-CB	5.61	118.91	110.50
7	G	148	LEU	CA-CB-CG	5.61	128.20	115.30
20	Z	767	TYR	CB-CG-CD2	-5.61	117.64	121.00
28	H	125	SER	N-CA-CB	5.61	118.91	110.50
22	S	186	TYR	CB-CG-CD2	-5.60	117.64	121.00
25	R	150	ALA	CB-CA-C	5.60	118.50	110.10
26	U	103	ASP	CB-CG-OD2	5.60	123.34	118.30
26	U	167	GLU	OE1-CD-OE2	5.60	130.02	123.30
12	l	80	ALA	CB-CA-C	-5.60	101.70	110.10
22	S	423	VAL	CA-CB-CG2	-5.60	102.50	110.90
8	h	87	ALA	CB-CA-C	-5.60	101.70	110.10
8	h	174	TRP	CB-CG-CD2	-5.60	119.32	126.60
15	W	103	ASN	N-CA-CB	5.60	120.67	110.60
2	b	156	TYR	N-CA-C	-5.59	95.90	111.00
3	c	214	ALA	N-CA-CB	5.59	117.93	110.10
4	D	179	TYR	CB-CG-CD2	-5.59	117.64	121.00
26	U	67	PHE	CB-CG-CD2	-5.59	116.88	120.80
30	K	337	LYS	N-CA-CB	-5.59	100.53	110.60
4	D	218	ASP	N-CA-CB	5.59	120.67	110.60
21	N	907	ASP	CB-CG-OD1	5.59	123.33	118.30
26	U	69	ASP	CB-CG-OD1	-5.59	113.27	118.30
6	f	101	ARG	NE-CZ-NH2	-5.59	117.51	120.30
27	O	187	SER	N-CA-CB	5.59	118.88	110.50
30	K	393	ARG	NH1-CZ-NH2	5.59	125.55	119.40
31	L	226	THR	C-N-CA	5.59	134.03	122.30
3	C	50	ARG	NE-CZ-NH2	5.58	123.09	120.30
6	F	101	ARG	NE-CZ-NH2	-5.58	117.51	120.30
7	G	162	GLY	N-CA-C	-5.58	99.14	113.10
13	6	155	MET	CG-SD-CE	-5.58	91.26	100.20
31	L	168	TYR	N-CA-CB	5.58	120.65	110.60
4	d	97	ARG	NE-CZ-NH1	5.58	123.09	120.30
4	d	111	ARG	NE-CZ-NH2	5.58	123.09	120.30
12	l	82	ARG	NE-CZ-NH1	-5.58	117.51	120.30
24	Q	51	ARG	N-CA-C	5.58	126.07	111.00
27	O	150	LEU	N-CA-CB	5.58	121.57	110.40
16	V	269	ARG	NE-CZ-NH1	5.58	123.09	120.30
20	Z	245	VAL	N-CA-C	5.58	126.07	111.00
21	N	179	THR	CA-CB-CG2	-5.58	104.59	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	67	ILE	N-CA-CB	5.58	123.63	110.80
17	T	230	ASN	CB-CA-C	5.58	121.56	110.40
8	1	79	TYR	N-CA-CB	5.58	120.64	110.60
14	7	184	ALA	N-CA-CB	5.58	117.91	110.10
2	b	93	ALA	O-C-N	5.58	131.62	122.70
13	m	39	THR	N-CA-C	-5.58	95.94	111.00
11	4	2	ASP	CB-CG-OD1	-5.58	113.28	118.30
30	K	48	TYR	CB-CG-CD1	-5.57	117.66	121.00
30	K	411	TYR	CD1-CE1-CZ	-5.57	114.78	119.80
25	R	338	TYR	CB-CA-C	-5.57	99.26	110.40
1	a	237	SER	N-CA-CB	5.57	118.86	110.50
9	i	171	TRP	CE2-CD2-CE3	5.57	125.38	118.70
12	5	196	ARG	NE-CZ-NH1	5.57	123.08	120.30
22	S	95	PHE	CB-CG-CD1	-5.57	116.90	120.80
27	O	139	LEU	CB-CA-C	-5.57	99.61	110.20
27	O	77	SER	N-CA-CB	5.57	118.85	110.50
12	l	189	TYR	CB-CA-C	5.57	121.54	110.40
11	4	131	GLY	N-CA-C	-5.57	99.18	113.10
12	5	272	PHE	CB-CG-CD2	5.57	124.70	120.80
33	J	324	ARG	NE-CZ-NH2	5.57	123.08	120.30
11	4	60	ILE	CB-CA-C	5.57	122.73	111.60
8	h	111	TYR	CB-CG-CD1	5.56	124.34	121.00
13	6	168	TYR	CB-CG-CD2	-5.56	117.66	121.00
12	l	144	ARG	NE-CZ-NH1	-5.56	117.52	120.30
27	O	254	LEU	CB-CG-CD1	5.56	120.46	111.00
23	P	266	TYR	CG-CD1-CE1	-5.56	116.85	121.30
22	S	239	ARG	NE-CZ-NH2	-5.56	117.52	120.30
20	Z	728	LYS	CD-CE-NZ	5.56	124.48	111.70
4	d	138	PHE	CB-CG-CD1	5.55	124.69	120.80
25	R	31	PHE	CB-CG-CD1	-5.55	116.91	120.80
3	c	180	TYR	CG-CD2-CE2	5.55	125.74	121.30
1	a	164	VAL	CA-CB-CG2	-5.55	102.58	110.90
3	c	94	HIS	N-CA-CB	5.55	120.59	110.60
7	G	20	ARG	NH1-CZ-NH2	-5.55	113.30	119.40
14	7	163	VAL	CB-CA-C	5.55	121.94	111.40
22	S	176	LEU	CB-CG-CD2	-5.55	101.56	111.00
23	P	193	TYR	CB-CG-CD1	-5.55	117.67	121.00
10	j	168	SER	N-CA-CB	5.55	118.82	110.50
9	2	195	ASP	CB-CG-OD2	5.55	123.29	118.30
14	7	214	MET	CG-SD-CE	-5.55	91.33	100.20
1	A	105	ARG	NE-CZ-NH2	-5.54	117.53	120.30
31	L	342	ARG	NE-CZ-NH2	-5.54	117.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	12	VAL	CA-CB-CG1	5.54	119.22	110.90
14	7	221	ASP	CB-CG-OD1	5.54	123.29	118.30
25	R	304	TYR	CB-CG-CD2	5.54	124.33	121.00
21	N	365	PHE	CG-CD1-CE1	-5.54	114.70	120.80
5	E	93	ARG	NE-CZ-NH1	5.54	123.07	120.30
22	S	232	MET	CG-SD-CE	-5.54	91.34	100.20
31	L	245	PHE	CB-CG-CD2	-5.54	116.92	120.80
3	c	66	LEU	CB-CG-CD2	5.54	120.41	111.00
14	n	49	TYR	CB-CG-CD1	-5.54	117.68	121.00
6	f	108	ALA	N-CA-CB	5.54	117.85	110.10
5	E	13	SER	N-CA-CB	5.54	118.80	110.50
13	m	65	PHE	CB-CG-CD2	-5.53	116.93	120.80
14	n	110	ASP	CB-CG-OD2	5.53	123.28	118.30
8	1	111	TYR	O-C-N	5.53	131.55	122.70
21	N	146	LYS	CB-CA-C	-5.53	99.34	110.40
29	I	61	ARG	NE-CZ-NH2	5.53	123.07	120.30
2	b	170	ALA	N-CA-CB	5.53	117.84	110.10
1	A	135	ARG	NH1-CZ-NH2	-5.53	113.32	119.40
7	G	93	ARG	N-CA-CB	5.53	120.55	110.60
20	Z	550	PHE	CB-CG-CD2	-5.53	116.93	120.80
3	C	129	ARG	NE-CZ-NH1	5.53	123.06	120.30
8	1	79	TYR	CG-CD1-CE1	-5.53	116.88	121.30
25	R	124	ASP	CB-CG-OD2	5.53	123.27	118.30
25	R	164	THR	CA-CB-CG2	-5.52	104.67	112.40
6	F	16	THR	CA-CB-CG2	-5.52	104.67	112.40
10	3	35	GLY	N-CA-C	-5.52	99.29	113.10
2	b	43	VAL	N-CA-CB	5.52	123.65	111.50
1	A	190	LYS	N-CA-CB	5.52	120.54	110.60
17	T	213	ASN	N-CA-CB	5.52	120.53	110.60
2	B	249	ALA	CB-CA-C	-5.52	101.82	110.10
1	A	111	ASP	CB-CG-OD2	5.52	123.26	118.30
30	K	259	ARG	NE-CZ-NH2	-5.52	117.54	120.30
31	L	149	ASP	N-CA-CB	5.52	120.53	110.60
8	h	98	ASN	CB-CG-OD1	-5.51	110.57	121.60
21	N	98	VAL	CA-CB-CG2	-5.51	102.63	110.90
8	h	183	ARG	NE-CZ-NH2	-5.51	117.54	120.30
27	O	392	TRP	CB-CG-CD1	5.51	134.16	127.00
8	h	10	THR	N-CA-C	-5.51	96.12	111.00
16	V	117	TRP	CE3-CZ3-CH2	-5.51	115.14	121.20
25	R	50	VAL	CA-CB-CG2	-5.51	102.64	110.90
25	R	82	ASP	CB-CG-OD2	-5.50	113.35	118.30
29	I	423	VAL	CA-CB-CG2	-5.50	102.64	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	831	GLU	CA-CB-CG	5.50	125.50	113.40
22	S	188	TYR	CD1-CE1-CZ	-5.50	114.85	119.80
27	O	228	TYR	CB-CG-CD2	5.50	124.30	121.00
1	a	39	ASN	N-CA-CB	5.50	120.50	110.60
10	3	96	TYR	CG-CD2-CE2	-5.50	116.90	121.30
22	S	82	TYR	CB-CG-CD2	5.50	124.30	121.00
5	e	82	THR	CA-CB-OG1	5.50	120.54	109.00
2	B	101	TYR	CA-CB-CG	-5.50	102.96	113.40
12	5	242	ARG	CB-CA-C	-5.50	99.41	110.40
4	D	34	VAL	CA-CB-CG2	-5.49	102.66	110.90
20	Z	264	PHE	CB-CG-CD1	5.49	124.65	120.80
7	G	171	SER	N-CA-CB	5.49	118.74	110.50
16	V	71	MET	CA-CB-CG	-5.49	103.96	113.30
21	N	674	GLN	C-N-CA	5.49	135.43	121.70
3	c	4	ARG	N-CA-CB	5.49	120.48	110.60
6	f	51	ARG	N-CA-CB	5.49	120.48	110.60
1	A	19	PHE	CG-CD2-CE2	5.49	126.84	120.80
8	1	79	TYR	CD1-CE1-CZ	5.49	124.74	119.80
15	W	179	ARG	NE-CZ-NH1	5.49	123.05	120.30
18	X	39	GLU	OE1-CD-OE2	5.49	129.89	123.30
24	Q	286	TYR	CB-CG-CD1	5.49	124.30	121.00
32	M	111	THR	N-CA-CB	5.49	120.73	110.30
16	V	122	ASP	CB-CG-OD2	-5.49	113.36	118.30
22	S	272	TYR	CB-CG-CD1	5.49	124.29	121.00
28	H	312	ASP	O-C-N	-5.49	113.92	122.70
1	a	186	PHE	CB-CG-CD2	-5.49	116.96	120.80
9	i	83	ALA	N-CA-CB	5.49	117.78	110.10
21	N	314	LEU	CB-CG-CD1	5.49	120.33	111.00
24	Q	396	TRP	CB-CG-CD1	5.49	134.13	127.00
14	n	144	TRP	CB-CG-CD1	5.48	134.13	127.00
25	R	362	ALA	N-CA-CB	-5.48	102.42	110.10
10	j	59	ASP	CB-CG-OD1	5.48	123.23	118.30
2	B	76	SER	N-CA-CB	5.48	118.72	110.50
12	5	126	ASP	CB-CG-OD1	-5.48	113.37	118.30
21	N	543	ASP	CB-CG-OD2	-5.48	113.37	118.30
24	Q	34	ASP	CB-CG-OD2	-5.48	113.37	118.30
4	d	112	TYR	CD1-CE1-CZ	5.48	124.73	119.80
23	P	99	LYS	N-CA-CB	5.48	120.46	110.60
24	Q	32	ASP	CB-CG-OD1	-5.48	113.37	118.30
29	I	436	TYR	CG-CD1-CE1	-5.48	116.92	121.30
3	c	35	ALA	N-CA-CB	5.47	117.76	110.10
3	C	48	ALA	N-CA-CB	5.47	117.76	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	782	PHE	N-CA-CB	5.47	120.45	110.60
24	Q	34	ASP	CB-CG-OD1	5.47	123.23	118.30
30	K	265	ALA	CB-CA-C	-5.47	101.89	110.10
17	T	267	ALA	N-CA-CB	5.47	117.76	110.10
12	5	260	TRP	CB-CG-CD2	-5.47	119.49	126.60
2	b	134	LEU	CB-CG-CD2	5.47	120.30	111.00
12	l	83	PHE	CB-CG-CD1	5.47	124.63	120.80
12	l	119	THR	N-CA-CB	5.47	120.69	110.30
29	I	268	PHE	CB-CG-CD2	-5.47	116.97	120.80
23	P	269	VAL	CA-CB-CG1	5.46	119.10	110.90
26	U	9	THR	N-CA-CB	5.46	120.68	110.30
2	b	151	ASP	CB-CG-OD1	5.46	123.22	118.30
5	e	223	THR	CA-CB-CG2	-5.46	104.75	112.40
7	g	111	ALA	CB-CA-C	-5.46	101.91	110.10
23	P	123	ARG	NE-CZ-NH2	-5.46	117.57	120.30
27	O	262	ASP	CB-CG-OD2	-5.46	113.39	118.30
33	J	296	ARG	NE-CZ-NH1	5.46	123.03	120.30
12	l	200	ASP	CB-CG-OD2	-5.46	113.39	118.30
5	E	167	TYR	CG-CD2-CE2	-5.46	116.93	121.30
8	h	120	TYR	CA-CB-CG	-5.46	103.03	113.40
11	4	53	THR	CA-CB-OG1	5.46	120.46	109.00
8	h	159	GLU	CB-CA-C	-5.45	99.49	110.40
5	E	143	LEU	CB-CG-CD1	5.45	120.27	111.00
2	b	224	TYR	CB-CG-CD2	-5.45	117.73	121.00
5	e	165	TYR	CB-CG-CD2	5.45	124.27	121.00
7	g	160	TYR	CB-CG-CD2	5.45	124.27	121.00
13	m	46	ARG	NE-CZ-NH1	5.45	123.03	120.30
10	3	120	PHE	CB-CG-CD2	-5.45	116.98	120.80
17	T	239	SER	N-CA-CB	5.45	118.68	110.50
30	K	89	ILE	CA-CB-CG1	5.45	121.36	111.00
3	C	226	TYR	N-CA-C	-5.45	96.29	111.00
33	J	361	VAL	CG1-CB-CG2	-5.45	102.18	110.90
27	O	210	ARG	NE-CZ-NH2	-5.45	117.58	120.30
1	A	13	ASP	CB-CG-OD2	5.45	123.20	118.30
7	G	201	TYR	CZ-CE2-CD2	-5.45	114.90	119.80
8	1	74	LEU	CB-CG-CD1	5.45	120.26	111.00
15	W	39	ALA	CB-CA-C	-5.45	101.93	110.10
22	S	367	TYR	CG-CD1-CE1	5.45	125.66	121.30
29	I	192	GLN	N-CA-CB	5.45	120.40	110.60
31	L	354	GLU	OE1-CD-OE2	5.45	129.83	123.30
2	b	90	ARG	NE-CZ-NH2	-5.44	117.58	120.30
4	d	156	TYR	CG-CD2-CE2	-5.44	116.94	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	234	ARG	NE-CZ-NH2	-5.44	117.58	120.30
31	L	232	ALA	CB-CA-C	-5.44	101.93	110.10
8	1	28	ARG	NE-CZ-NH2	-5.44	117.58	120.30
10	3	155	GLU	N-CA-C	-5.44	96.30	111.00
16	V	223	SER	O-C-N	-5.44	113.95	123.20
24	Q	332	ARG	NE-CZ-NH1	-5.44	117.58	120.30
12	l	144	ARG	NE-CZ-NH2	5.44	123.02	120.30
22	S	487	THR	CA-CB-CG2	-5.44	104.78	112.40
21	N	353	LEU	CA-C-N	5.44	132.32	117.10
27	O	179	PHE	CD1-CE1-CZ	-5.44	113.58	120.10
29	I	346	ARG	N-CA-CB	5.44	120.38	110.60
32	M	117	ALA	N-CA-CB	5.44	117.71	110.10
29	I	437	LEU	CB-CA-C	-5.43	99.87	110.20
31	L	373	GLU	OE1-CD-OE2	5.43	129.82	123.30
21	N	367	ALA	CB-CA-C	-5.43	101.95	110.10
25	R	404	VAL	N-CA-CB	5.43	123.45	111.50
1	A	168	ALA	N-CA-CB	5.43	117.70	110.10
18	X	122	TYR	CZ-CE2-CD2	5.43	124.69	119.80
21	N	870	ASN	C-N-CA	5.43	135.28	121.70
26	U	72	TYR	CB-CG-CD2	-5.43	117.74	121.00
33	J	32	LEU	CB-CG-CD1	5.43	120.23	111.00
5	e	84	ASP	CB-CG-OD2	5.42	123.18	118.30
7	G	48	PHE	CB-CG-CD1	5.42	124.60	120.80
8	1	198	TYR	CB-CG-CD1	-5.42	117.75	121.00
21	N	778	LYS	C-N-CA	5.42	135.26	121.70
29	I	208	TYR	CB-CG-CD1	-5.42	117.75	121.00
3	c	92	ARG	C-N-CA	5.42	135.26	121.70
13	m	39	THR	N-CA-CB	5.42	120.60	110.30
17	T	229	VAL	C-N-CA	5.42	135.25	121.70
28	H	331	ARG	NE-CZ-NH2	5.42	123.01	120.30
10	j	138	VAL	CB-CA-C	-5.42	101.10	111.40
11	4	159	ASP	CB-CG-OD1	-5.42	113.42	118.30
8	h	70	TYR	CD1-CE1-CZ	5.42	124.67	119.80
13	m	83	TYR	CB-CG-CD1	5.42	124.25	121.00
1	A	110	TYR	CG-CD1-CE1	5.42	125.63	121.30
4	D	162	GLN	CA-CB-CG	5.42	125.31	113.40
14	7	239	LEU	CB-CG-CD1	5.42	120.20	111.00
2	B	236	ARG	NE-CZ-NH2	-5.41	117.59	120.30
16	V	141	VAL	CA-CB-CG1	-5.41	102.78	110.90
21	N	137	PHE	CG-CD1-CE1	5.41	126.75	120.80
12	5	237	LEU	CB-CG-CD1	5.41	120.20	111.00
13	6	39	THR	N-CA-CB	5.41	120.58	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	383	THR	CA-CB-CG2	-5.41	104.82	112.40
7	g	72	ARG	CB-CA-C	-5.41	99.58	110.40
8	1	132	PRO	N-CD-CG	5.41	111.31	103.20
15	W	78	ASP	CB-CG-OD1	-5.41	113.43	118.30
2	b	96	SER	O-C-N	-5.41	114.05	122.70
10	j	67	PHE	CB-CG-CD1	-5.41	117.02	120.80
30	K	399	ARG	NE-CZ-NH1	5.41	123.00	120.30
13	6	82	TRP	CG-CD2-CE3	-5.41	129.03	133.90
3	c	24	TYR	CD1-CE1-CZ	-5.40	114.94	119.80
7	G	38	ILE	CB-CA-C	-5.40	100.80	111.60
21	N	697	PHE	CG-CD2-CE2	5.40	126.74	120.80
31	L	230	LEU	CB-CG-CD1	5.40	120.18	111.00
1	A	19	PHE	CD1-CG-CD2	-5.40	111.28	118.30
24	Q	112	ASP	N-CA-CB	5.40	120.32	110.60
32	M	29	GLU	N-CA-CB	5.40	120.32	110.60
5	e	130	GLU	CA-CB-CG	5.40	125.28	113.40
22	S	339	GLN	N-CA-CB	5.40	120.32	110.60
9	i	48	ARG	N-CA-CB	5.40	120.31	110.60
16	V	225	LEU	CB-CG-CD2	5.40	120.18	111.00
10	3	83	GLU	OE1-CD-OE2	-5.40	116.83	123.30
6	F	213	ILE	N-CA-C	-5.39	96.44	111.00
18	X	99	PHE	CG-CD1-CE1	-5.39	114.87	120.80
27	O	352	TRP	CD1-CG-CD2	-5.39	101.98	106.30
1	A	66	PRO	O-C-N	5.39	131.33	122.70
21	N	188	TYR	N-CA-CB	5.39	120.31	110.60
25	R	357	PHE	CB-CG-CD2	-5.39	117.03	120.80
26	U	113	TYR	CG-CD1-CE1	5.39	125.61	121.30
30	K	236	ARG	NE-CZ-NH2	-5.39	117.60	120.30
33	J	229	MET	N-CA-CB	5.39	120.31	110.60
4	d	75	PHE	CB-CG-CD1	-5.39	117.03	120.80
27	O	135	ARG	NE-CZ-NH2	-5.39	117.60	120.30
6	f	194	VAL	CG1-CB-CG2	-5.39	102.28	110.90
9	i	60	CYS	N-CA-C	-5.39	96.45	111.00
14	n	198	ILE	CA-CB-CG2	5.39	121.68	110.90
5	E	157	HIS	N-CA-CB	5.39	120.30	110.60
11	4	72	ASP	CB-CG-OD2	5.39	123.15	118.30
22	S	408	CYS	CA-CB-SG	-5.39	104.30	114.00
29	I	76	VAL	CA-CB-CG2	-5.39	102.81	110.90
30	K	382	VAL	O-C-N	-5.39	114.08	122.70
33	J	4	ALA	CB-CA-C	-5.39	102.02	110.10
9	2	141	SER	N-CA-CB	5.39	118.58	110.50
15	W	178	PRO	O-C-N	5.39	131.32	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	440	ASP	CB-CG-OD2	5.39	123.15	118.30
3	c	187	ASP	CB-CG-OD1	5.38	123.15	118.30
10	j	86	THR	N-CA-CB	5.38	120.53	110.30
4	d	160	SER	N-CA-CB	5.38	118.57	110.50
4	D	112	TYR	CG-CD2-CE2	5.38	125.61	121.30
7	G	190	ARG	NE-CZ-NH2	5.38	122.99	120.30
33	J	35	ARG	NE-CZ-NH2	-5.38	117.61	120.30
3	C	210	ARG	NE-CZ-NH2	-5.38	117.61	120.30
13	6	36	ARG	CA-CB-CG	5.38	125.24	113.40
25	R	49	PHE	CB-CA-C	-5.38	99.64	110.40
29	I	300	ARG	CD-NE-CZ	5.38	131.13	123.60
30	K	294	ARG	NE-CZ-NH2	-5.38	117.61	120.30
19	Y	54	VAL	C-N-CA	5.38	135.15	121.70
22	S	276	LEU	CB-CA-C	-5.38	99.98	110.20
32	M	50	ARG	NE-CZ-NH2	-5.38	117.61	120.30
5	e	169	ALA	CB-CA-C	-5.38	102.03	110.10
14	7	146	ALA	N-CA-C	-5.38	96.49	111.00
29	I	75	PHE	CB-CG-CD2	-5.38	117.04	120.80
8	1	175	ASP	CB-CG-OD2	5.38	123.14	118.30
13	6	97	ALA	CB-CA-C	-5.38	102.04	110.10
16	V	223	SER	CA-C-N	5.37	126.95	116.20
31	L	241	ALA	N-CA-CB	5.37	117.62	110.10
1	a	113	PRO	CA-N-CD	-5.37	103.98	111.50
5	e	2	PHE	CB-CG-CD1	-5.37	117.04	120.80
14	n	168	VAL	CG1-CB-CG2	-5.37	102.30	110.90
12	l	286	ILE	CA-CB-CG1	5.37	121.20	111.00
15	W	115	CYS	CB-CA-C	-5.37	99.66	110.40
9	i	171	TRP	CA-C-N	-5.37	105.39	117.20
13	m	168	TYR	CG-CD1-CE1	-5.36	117.01	121.30
2	B	204	PHE	CB-CG-CD1	5.36	124.55	120.80
12	5	275	VAL	CA-CB-CG2	-5.36	102.85	110.90
30	K	401	VAL	CA-CB-CG1	-5.36	102.85	110.90
8	h	55	SER	N-CA-CB	5.36	118.54	110.50
22	S	462	ASP	CB-CG-OD1	-5.36	113.47	118.30
31	L	299	ARG	CB-CA-C	-5.36	99.68	110.40
31	L	308	LEU	CB-CA-C	-5.36	100.02	110.20
33	J	320	SER	N-CA-CB	5.36	118.54	110.50
23	P	143	LEU	CB-CG-CD2	-5.36	101.89	111.00
3	c	42	ASP	CB-CG-OD1	5.35	123.12	118.30
2	b	174	PHE	CB-CG-CD2	-5.35	117.06	120.80
3	c	165	VAL	CA-CB-CG2	5.35	118.92	110.90
6	f	13	PHE	C-N-CA	5.35	135.07	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	328	PHE	CB-CG-CD1	-5.35	117.06	120.80
1	a	199	TRP	CH2-CZ2-CE2	5.35	122.75	117.40
9	i	154	LEU	CB-CG-CD1	5.35	120.09	111.00
3	c	131	PHE	CZ-CE2-CD2	5.34	126.51	120.10
7	G	124	THR	CA-CB-OG1	5.34	120.22	109.00
12	5	249	SER	N-CA-CB	5.34	118.52	110.50
13	6	47	TYR	CD1-CE1-CZ	5.34	124.61	119.80
24	Q	265	MET	CG-SD-CE	5.34	108.75	100.20
33	J	125	VAL	CA-CB-CG1	-5.34	102.88	110.90
6	f	201	LEU	CB-CG-CD2	5.34	120.08	111.00
11	k	93	ARG	NH1-CZ-NH2	5.34	125.28	119.40
1	A	43	LEU	CB-CG-CD2	5.34	120.08	111.00
5	e	156	PHE	CB-CG-CD1	-5.34	117.06	120.80
1	a	108	TYR	CB-CG-CD2	-5.34	117.80	121.00
4	d	99	THR	CA-CB-CG2	-5.34	104.93	112.40
1	A	91	ARG	CG-CD-NE	-5.34	100.59	111.80
14	7	120	LEU	N-CA-CB	5.33	121.07	110.40
23	P	218	LEU	CB-CG-CD2	5.33	120.07	111.00
10	j	136	PHE	CB-CG-CD2	-5.33	117.07	120.80
12	5	230	TYR	CZ-CE2-CD2	5.33	124.60	119.80
21	N	250	ASP	CB-CG-OD1	-5.33	113.50	118.30
31	L	89	ASP	CB-CG-OD2	-5.33	113.50	118.30
4	D	196	VAL	CA-CB-CG2	-5.33	102.90	110.90
31	L	267	PHE	CB-CG-CD1	-5.33	117.07	120.80
2	B	238	LEU	N-CA-CB	5.33	121.06	110.40
14	7	46	SER	N-CA-CB	5.33	118.49	110.50
26	U	136	ALA	N-CA-CB	5.33	117.56	110.10
8	h	14	ALA	N-CA-CB	5.33	117.56	110.10
9	i	149	ASP	N-CA-CB	5.33	120.19	110.60
13	6	144	CYS	CB-CA-C	-5.33	99.75	110.40
21	N	70	TYR	CB-CG-CD2	-5.33	117.81	121.00
30	K	349	ARG	NE-CZ-NH2	-5.33	117.64	120.30
33	J	222	TYR	CG-CD2-CE2	-5.33	117.04	121.30
11	k	190	ARG	NE-CZ-NH2	5.32	122.96	120.30
21	N	548	ARG	NH1-CZ-NH2	5.32	125.26	119.40
28	H	447	VAL	CA-CB-CG2	-5.32	102.91	110.90
27	O	188	PHE	CB-CG-CD2	5.32	124.52	120.80
17	T	177	PHE	CB-CG-CD2	-5.32	117.08	120.80
9	2	153	TYR	CB-CG-CD1	-5.32	117.81	121.00
30	K	246	TYR	CB-CG-CD2	5.32	124.19	121.00
10	j	69	TYR	CB-CG-CD2	-5.32	117.81	121.00
9	2	236	ARG	NE-CZ-NH2	-5.32	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	92	TRP	CG-CD1-NE1	5.32	115.42	110.10
32	M	74	GLN	C-N-CA	5.32	134.99	121.70
21	N	713	VAL	CA-CB-CG1	-5.31	102.93	110.90
6	F	36	VAL	CG1-CB-CG2	-5.31	102.40	110.90
8	1	201	GLU	OE1-CD-OE2	5.31	129.67	123.30
28	H	307	PHE	CB-CG-CD2	-5.31	117.08	120.80
6	f	108	ALA	CB-CA-C	-5.31	102.14	110.10
2	B	52	SER	CB-CA-C	-5.31	100.01	110.10
27	O	133	ILE	CB-CA-C	-5.31	100.98	111.60
1	a	180	THR	CA-CB-CG2	-5.31	104.97	112.40
7	g	138	PHE	CB-CG-CD1	5.31	124.52	120.80
8	h	31	THR	N-CA-CB	5.31	120.38	110.30
12	l	191	ASP	CB-CG-OD2	5.31	123.08	118.30
11	4	70	ARG	NE-CZ-NH2	-5.31	117.65	120.30
20	Z	918	ASP	N-CA-CB	5.31	120.15	110.60
29	I	54	ARG	NE-CZ-NH1	5.31	122.95	120.30
8	1	108	VAL	O-C-N	-5.30	114.22	122.70
8	1	160	THR	CA-CB-CG2	-5.30	104.98	112.40
14	7	63	TYR	N-CA-C	-5.30	96.69	111.00
18	X	124	LYS	N-CA-CB	5.30	120.14	110.60
30	K	330	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
2	B	247	LEU	CB-CG-CD1	-5.30	101.99	111.00
1	A	199	TRP	CG-CD2-CE3	-5.30	129.13	133.90
2	B	52	SER	N-CA-CB	5.30	118.44	110.50
19	Y	55	THR	CA-CB-CG2	-5.30	104.99	112.40
24	Q	255	TYR	CZ-CE2-CD2	-5.30	115.03	119.80
33	J	10	ILE	C-N-CA	5.30	134.94	121.70
7	g	93	ARG	CD-NE-CZ	5.29	131.01	123.60
10	j	144	ASP	CB-CG-OD1	5.29	123.06	118.30
15	W	136	ASN	N-CA-CB	5.29	120.13	110.60
24	Q	156	ALA	N-CA-CB	5.29	117.51	110.10
4	d	42	VAL	O-C-N	-5.29	114.23	122.70
12	l	260	TRP	CB-CG-CD1	5.29	133.88	127.00
23	P	173	MET	CG-SD-CE	-5.29	91.73	100.20
25	R	86	ASP	CB-CG-OD2	-5.29	113.54	118.30
25	R	220	ALA	CB-CA-C	-5.29	102.16	110.10
28	H	156	VAL	CA-CB-CG1	-5.29	102.96	110.90
22	S	459	GLN	N-CA-CB	5.29	120.12	110.60
12	l	124	ALA	CB-CA-C	-5.29	102.17	110.10
13	m	99	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
3	C	162	ALA	N-CA-CB	5.29	117.51	110.10
25	R	363	PHE	CB-CG-CD1	5.29	124.50	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	222	ASN	N-CA-CB	5.29	120.12	110.60
2	b	113	GLU	N-CA-CB	5.29	120.12	110.60
2	b	12	PHE	CB-CG-CD2	-5.29	117.10	120.80
13	m	167	GLN	N-CA-CB	5.29	120.11	110.60
21	N	260	ASP	CB-CG-OD2	5.29	123.06	118.30
5	e	153	TYR	CA-CB-CG	-5.28	103.36	113.40
12	l	165	TYR	CG-CD1-CE1	-5.28	117.07	121.30
6	F	125	GLY	O-C-N	-5.28	114.25	122.70
6	f	123	TYR	CB-CG-CD1	5.28	124.17	121.00
32	M	323	VAL	CG1-CB-CG2	5.28	119.35	110.90
21	N	332	VAL	CG1-CB-CG2	-5.28	102.45	110.90
24	Q	32	ASP	CB-CG-OD2	5.28	123.05	118.30
13	6	182	TYR	CB-CG-CD2	-5.28	117.83	121.00
16	V	230	TYR	CG-CD1-CE1	5.28	125.52	121.30
25	R	197	MET	CB-CA-C	-5.28	99.85	110.40
21	N	7	ALA	CA-C-O	-5.27	109.03	120.10
24	Q	146	TYR	CB-CG-CD1	5.27	124.17	121.00
24	Q	278	VAL	CA-CB-CG1	5.27	118.81	110.90
1	a	46	ARG	NE-CZ-NH2	5.27	122.94	120.30
7	g	62	GLN	N-CA-CB	5.27	120.09	110.60
13	6	30	VAL	N-CA-C	-5.27	96.76	111.00
15	W	48	THR	CA-CB-OG1	5.27	120.07	109.00
20	Z	258	PRO	N-CA-C	5.27	125.81	112.10
23	P	234	TYR	CB-CG-CD1	-5.27	117.84	121.00
4	d	127	ARG	CD-NE-CZ	-5.27	116.22	123.60
7	G	171	SER	CB-CA-C	-5.27	100.09	110.10
28	H	338	THR	CA-CB-CG2	-5.27	105.02	112.40
30	K	107	THR	N-CA-CB	5.27	120.31	110.30
5	e	207	VAL	CA-CB-CG1	-5.27	103.00	110.90
13	m	30	VAL	N-CA-CB	5.27	123.09	111.50
22	S	148	ASP	CB-CG-OD1	-5.27	113.56	118.30
28	H	450	VAL	CG1-CB-CG2	5.27	119.33	110.90
4	d	138	PHE	CB-CG-CD2	-5.27	117.11	120.80
13	6	99	ARG	NE-CZ-NH1	5.27	122.93	120.30
21	N	345	ASP	CB-CA-C	-5.27	99.87	110.40
11	k	73	TYR	CG-CD1-CE1	5.26	125.51	121.30
6	F	182	ILE	N-CA-C	-5.26	96.78	111.00
31	L	401	PHE	CB-CG-CD1	5.26	124.48	120.80
32	M	216	LYS	CB-CA-C	5.26	120.93	110.40
23	P	351	ARG	NE-CZ-NH1	5.26	122.93	120.30
3	C	115	LEU	CB-CG-CD2	5.26	119.95	111.00
5	E	249	ALA	CB-CA-C	-5.26	102.21	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	234	ARG	NH1-CZ-NH2	5.26	125.19	119.40
4	D	50	SER	N-CA-CB	5.26	118.39	110.50
13	6	208	ASP	CB-CG-OD1	5.26	123.03	118.30
21	N	749	LEU	CB-CG-CD1	5.26	119.94	111.00
27	O	234	LEU	CB-CG-CD2	5.26	119.94	111.00
23	P	318	TYR	CB-CG-CD2	-5.26	117.84	121.00
25	R	345	TYR	CZ-CE2-CD2	5.26	124.53	119.80
29	I	242	ALA	N-CA-C	-5.26	96.81	111.00
6	f	164	ARG	NE-CZ-NH2	-5.25	117.67	120.30
32	M	131	MET	CG-SD-CE	-5.25	91.79	100.20
7	g	156	SER	N-CA-CB	5.25	118.38	110.50
12	l	82	ARG	NE-CZ-NH2	-5.25	117.67	120.30
15	W	113	PHE	CG-CD2-CE2	5.25	126.58	120.80
2	B	36	GLY	N-CA-C	-5.25	99.97	113.10
11	4	57	ALA	N-CA-CB	5.25	117.45	110.10
17	T	13	ILE	O-C-N	-5.25	114.30	122.70
21	N	848	GLU	N-CA-CB	5.25	120.05	110.60
23	P	96	MET	N-CA-CB	-5.25	101.15	110.60
30	K	406	ASP	CB-CG-OD2	-5.25	113.58	118.30
8	1	123	PRO	N-CD-CG	5.25	111.07	103.20
30	K	104	ASP	N-CA-CB	5.25	120.04	110.60
32	M	291	PHE	N-CA-CB	5.25	120.05	110.60
25	R	297	TYR	CB-CG-CD1	-5.25	117.85	121.00
10	3	110	ALA	N-CA-CB	5.24	117.44	110.10
32	M	290	ARG	NE-CZ-NH1	5.24	122.92	120.30
21	N	464	GLU	OE1-CD-OE2	5.24	129.59	123.30
25	R	95	ASP	N-CA-CB	5.24	120.04	110.60
10	j	17	GLY	N-CA-C	-5.24	100.00	113.10
21	N	127	ASP	CB-CG-OD1	-5.24	113.58	118.30
3	c	147	GLN	CB-CA-C	-5.24	99.92	110.40
10	j	98	ARG	NE-CZ-NH1	-5.24	117.68	120.30
10	j	124	PHE	CB-CG-CD1	-5.24	117.13	120.80
12	l	215	LEU	CB-CG-CD2	-5.24	102.09	111.00
16	V	85	ASP	CB-CG-OD1	-5.24	113.59	118.30
25	R	124	ASP	CB-CG-OD1	-5.24	113.59	118.30
14	n	54	ILE	CB-CA-C	-5.24	101.13	111.60
24	Q	88	PHE	CB-CG-CD1	-5.24	117.14	120.80
6	F	47	VAL	CG1-CB-CG2	-5.23	102.53	110.90
12	5	165	TYR	CB-CG-CD2	-5.23	117.86	121.00
32	M	25	LEU	CB-CG-CD1	5.23	119.90	111.00
33	J	150	VAL	CG1-CB-CG2	-5.23	102.53	110.90
8	h	118	GLU	N-CA-CB	5.23	120.02	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	134	TYR	CD1-CG-CD2	5.23	123.65	117.90
15	W	2	VAL	N-CA-C	-5.23	96.88	111.00
20	Z	726	GLU	C-N-CA	5.23	134.77	121.70
32	M	303	ARG	NE-CZ-NH2	5.23	122.92	120.30
15	W	131	THR	N-CA-CB	5.23	120.23	110.30
7	g	107	ILE	CG1-CB-CG2	5.23	122.90	111.40
15	W	108	GLN	N-CA-CB	5.23	120.01	110.60
15	W	123	ASP	CA-CB-CG	-5.23	101.90	113.40
23	P	13	TYR	CG-CD2-CE2	-5.23	117.12	121.30
24	Q	132	PHE	CB-CG-CD1	-5.22	117.14	120.80
31	L	307	GLU	N-CA-CB	-5.22	101.19	110.60
9	2	34	GLY	N-CA-C	-5.22	100.04	113.10
14	7	137	ARG	CA-CB-CG	5.22	124.89	113.40
30	K	104	ASP	CB-CG-OD2	-5.22	113.60	118.30
10	3	100	PHE	CG-CD1-CE1	-5.22	115.06	120.80
6	f	59	TYR	CB-CG-CD2	5.22	124.13	121.00
7	g	114	ASP	CB-CG-OD1	-5.22	113.60	118.30
16	V	160	ASP	CB-CG-OD1	-5.22	113.61	118.30
24	Q	170	ASP	CB-CG-OD2	-5.22	113.60	118.30
29	I	320	GLY	CA-C-O	5.22	129.99	120.60
3	C	131	PHE	CB-CG-CD1	-5.21	117.15	120.80
14	7	170	TYR	CB-CG-CD1	-5.21	117.87	121.00
25	R	311	THR	CA-CB-CG2	-5.21	105.10	112.40
12	5	212	TYR	CD1-CE1-CZ	-5.21	115.11	119.80
22	S	222	SER	N-CA-CB	5.21	118.32	110.50
28	H	94	GLU	N-CA-CB	5.21	119.98	110.60
26	U	51	SER	N-CA-CB	5.21	118.31	110.50
26	U	283	ARG	NE-CZ-NH2	5.21	122.91	120.30
4	d	232	TYR	CG-CD1-CE1	5.21	125.47	121.30
2	B	221	LEU	CB-CG-CD2	5.21	119.85	111.00
13	6	153	LEU	CB-CG-CD1	-5.21	102.15	111.00
30	K	294	ARG	NE-CZ-NH1	5.21	122.91	120.30
6	f	126	ARG	N-CA-CB	5.21	119.97	110.60
9	i	254	GLU	OE1-CD-OE2	5.21	129.55	123.30
6	F	171	TYR	CB-CG-CD2	-5.21	117.88	121.00
20	Z	743	ILE	CA-CB-CG1	-5.21	101.11	111.00
33	J	339	ARG	O-C-N	-5.21	114.35	123.20
9	2	126	TYR	CD1-CE1-CZ	-5.20	115.12	119.80
25	R	268	SER	N-CA-CB	5.20	118.30	110.50
3	C	47	ALA	N-CA-CB	5.20	117.38	110.10
4	D	138	PHE	CB-CG-CD2	5.20	124.44	120.80
7	G	65	VAL	CA-CB-CG1	-5.20	103.10	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	X	20	ASP	CA-CB-CG	-5.20	101.96	113.40
24	Q	12	ARG	CB-CA-C	5.20	120.80	110.40
2	B	7	PHE	N-CA-CB	5.20	119.95	110.60
24	Q	343	LEU	CB-CG-CD2	5.20	119.83	111.00
7	G	192	ALA	CB-CA-C	-5.19	102.31	110.10
6	f	26	LEU	CB-CA-C	5.19	120.07	110.20
8	h	195	LEU	N-CA-CB	5.19	120.79	110.40
10	3	116	SER	CB-CA-C	-5.19	100.23	110.10
11	4	36	ARG	CB-CA-C	-5.19	100.01	110.40
31	L	435	GLN	N-CA-CB	-5.19	101.25	110.60
14	n	144	TRP	CG-CD2-CE3	-5.19	129.23	133.90
17	T	222	LEU	CB-CA-C	-5.19	100.34	110.20
9	2	104	ARG	NE-CZ-NH2	-5.19	117.70	120.30
27	O	138	LEU	O-C-N	-5.19	114.40	122.70
13	6	145	ARG	CD-NE-CZ	5.19	130.86	123.60
30	K	250	GLY	CA-C-O	-5.19	111.26	120.60
11	k	8	ARG	NH1-CZ-NH2	5.19	125.11	119.40
27	O	110	ASP	CB-CG-OD2	-5.19	113.63	118.30
29	I	104	LEU	N-CA-C	-5.19	97.00	111.00
3	C	216	ILE	O-C-N	-5.18	114.41	122.70
11	4	59	TYR	CZ-CE2-CD2	-5.18	115.13	119.80
13	6	125	ASP	CB-CG-OD2	-5.18	113.63	118.30
14	n	202	THR	CA-CB-CG2	-5.18	105.14	112.40
3	C	16	GLU	CG-CD-OE1	5.18	128.67	118.30
7	G	22	PHE	CB-CG-CD2	-5.18	117.17	120.80
14	7	185	ASN	CB-CA-C	5.18	120.76	110.40
16	V	114	PHE	CB-CG-CD2	-5.18	117.17	120.80
5	E	231	TYR	CG-CD2-CE2	-5.18	117.16	121.30
30	K	61	LEU	CB-CG-CD1	-5.18	102.19	111.00
2	b	93	ALA	CB-CA-C	-5.18	102.33	110.10
23	P	103	TYR	CB-CG-CD2	5.18	124.11	121.00
7	g	44	ASP	CB-CG-OD2	5.18	122.96	118.30
1	A	147	ASP	CB-CG-OD2	-5.18	113.64	118.30
22	S	171	TYR	CZ-CE2-CD2	-5.18	115.14	119.80
11	4	144	LEU	CB-CG-CD1	5.17	119.79	111.00
12	5	91	VAL	CB-CA-C	-5.17	101.57	111.40
23	P	76	ASN	N-CA-CB	5.17	119.91	110.60
8	h	18	LYS	O-C-N	-5.17	114.43	122.70
11	k	59	TYR	CD1-CE1-CZ	5.17	124.45	119.80
13	m	141	ARG	CA-CB-CG	5.17	124.77	113.40
6	f	181	LYS	N-CA-CB	-5.17	101.30	110.60
11	4	93	ARG	NE-CZ-NH1	5.17	122.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	134	ALA	CB-CA-C	-5.17	102.35	110.10
32	M	77	TYR	CG-CD1-CE1	5.17	125.44	121.30
33	J	288	ILE	N-CA-CB	5.17	122.69	110.80
10	j	129	CYS	CA-CB-SG	5.17	123.30	114.00
15	W	183	GLU	OE1-CD-OE2	5.17	129.50	123.30
18	X	101	LEU	CB-CG-CD1	5.17	119.78	111.00
21	N	355	TRP	CH2-CZ2-CE2	5.17	122.57	117.40
23	P	411	LEU	CB-CG-CD2	5.17	119.78	111.00
29	I	112	ILE	CA-CB-CG2	-5.17	100.57	110.90
33	J	335	MET	CG-SD-CE	5.17	108.47	100.20
4	d	206	GLY	O-C-N	-5.17	114.44	122.70
8	h	26	ASP	CB-CG-OD1	5.17	122.95	118.30
21	N	813	ARG	NE-CZ-NH2	-5.17	117.72	120.30
30	K	278	ALA	N-CA-CB	5.17	117.33	110.10
27	O	178	TYR	CG-CD2-CE2	5.16	125.43	121.30
2	b	88	LYS	CB-CA-C	-5.16	100.08	110.40
7	g	156	SER	CB-CA-C	-5.16	100.30	110.10
7	G	50	VAL	CA-CB-CG2	-5.16	103.16	110.90
16	V	251	TYR	CB-CG-CD1	-5.16	117.90	121.00
33	J	374	ARG	NE-CZ-NH1	5.16	122.88	120.30
9	i	133	ASP	CB-CG-OD1	-5.16	113.66	118.30
28	H	193	PRO	N-CA-CB	5.16	109.49	103.30
31	L	77	ARG	O-C-N	-5.16	114.44	122.70
10	j	200	LEU	CB-CG-CD2	5.16	119.77	111.00
2	B	177	LYS	CB-CA-C	-5.16	100.09	110.40
11	4	118	GLN	N-CA-CB	5.16	119.88	110.60
12	5	221	TRP	CH2-CZ2-CE2	5.16	122.56	117.40
26	U	29	GLU	CB-CA-C	5.16	120.71	110.40
33	J	301	ASP	CB-CG-OD2	-5.16	113.66	118.30
32	M	143	ASN	N-CA-CB	5.15	119.88	110.60
29	I	244	PHE	CB-CG-CD2	5.15	124.41	120.80
33	J	324	ARG	NE-CZ-NH1	-5.15	117.72	120.30
17	T	234	TYR	C-N-CA	5.15	134.58	121.70
21	N	17	GLN	N-CA-C	-5.15	97.09	111.00
27	O	110	ASP	CB-CG-OD1	5.15	122.94	118.30
33	J	55	VAL	CG1-CB-CG2	-5.15	102.66	110.90
1	a	137	LEU	CB-CG-CD2	5.15	119.75	111.00
20	Z	268	ALA	CB-CA-C	-5.15	102.38	110.10
21	N	310	ASP	CB-CG-OD2	5.15	122.93	118.30
18	X	18	ASN	CB-CA-C	-5.15	100.11	110.40
22	S	73	THR	CA-CB-CG2	-5.15	105.20	112.40
2	B	9	LEU	CB-CG-CD1	-5.14	102.25	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	112	VAL	CG1-CB-CG2	5.14	119.13	110.90
21	N	801	THR	CA-CB-CG2	-5.14	105.20	112.40
28	H	464	MET	C-N-CA	5.14	134.55	121.70
29	I	121	THR	CA-CB-CG2	-5.14	105.20	112.40
13	6	168	TYR	CD1-CG-CD2	5.14	123.56	117.90
22	S	160	ARG	NE-CZ-NH2	-5.14	117.73	120.30
4	D	155	ILE	N-CA-C	-5.14	97.12	111.00
4	D	186	ALA	N-CA-CB	5.14	117.30	110.10
19	Y	31	GLU	N-CA-CB	5.14	119.85	110.60
21	N	299	TYR	CD1-CE1-CZ	-5.14	115.17	119.80
23	P	83	SER	N-CA-CB	5.14	118.21	110.50
24	Q	208	ILE	CA-CB-CG2	-5.14	100.62	110.90
11	k	187	ASP	CB-CG-OD1	5.14	122.92	118.30
27	O	71	ASP	CB-CA-C	-5.14	100.13	110.40
8	h	79	TYR	CB-CG-CD1	5.13	124.08	121.00
3	C	178	MET	CB-CA-C	-5.13	100.13	110.40
11	4	115	GLU	OE1-CD-OE2	-5.13	117.14	123.30
7	g	206	ASP	CB-CG-OD1	-5.13	113.68	118.30
13	6	190	LYS	CG-CD-CE	5.13	127.30	111.90
6	f	116	ALA	O-C-N	5.13	130.91	122.70
13	m	182	TYR	CG-CD1-CE1	-5.13	117.20	121.30
4	D	190	GLU	N-CA-CB	-5.13	101.37	110.60
33	J	382	PHE	CB-CA-C	-5.13	100.14	110.40
5	e	243	LEU	CB-CG-CD2	5.13	119.72	111.00
9	i	173	GLN	C-N-CA	5.13	134.52	121.70
5	E	188	HIS	N-CA-CB	5.13	119.83	110.60
21	N	578	ASP	CB-CG-OD1	5.13	122.91	118.30
21	N	788	TYR	CB-CA-C	-5.13	100.15	110.40
4	d	58	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	c	63	THR	N-CA-C	-5.12	97.17	111.00
6	f	225	TYR	CB-CG-CD2	-5.12	117.92	121.00
3	C	75	VAL	CG1-CB-CG2	5.12	119.10	110.90
1	a	141	LEU	N-CA-CB	5.12	120.64	110.40
7	g	149	TYR	CB-CG-CD2	5.12	124.07	121.00
6	F	198	SER	N-CA-CB	5.12	118.18	110.50
10	3	100	PHE	N-CA-C	-5.12	97.18	111.00
21	N	434	SER	N-CA-CB	5.12	118.18	110.50
29	I	404	LEU	CB-CA-C	-5.12	100.48	110.20
21	N	834	GLU	OE1-CD-OE2	-5.11	117.17	123.30
27	O	249	ASP	N-CA-CB	5.11	119.80	110.60
29	I	415	ASP	N-CA-CB	5.11	119.80	110.60
32	M	220	MET	CG-SD-CE	-5.11	92.02	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	44	LEU	N-CA-CB	5.11	120.62	110.40
19	Y	89	GLN	N-CA-CB	5.11	119.80	110.60
22	S	452	TYR	CA-CB-CG	-5.11	103.69	113.40
13	m	208	ASP	N-CA-CB	5.11	119.79	110.60
2	B	151	ASP	CB-CG-OD2	5.11	122.90	118.30
29	I	178	THR	CA-CB-CG2	-5.11	105.25	112.40
11	k	87	GLU	OE1-CD-OE2	-5.11	117.17	123.30
13	6	68	ASP	CB-CG-OD2	-5.11	113.70	118.30
12	l	225	VAL	CG1-CB-CG2	-5.10	102.73	110.90
33	J	168	VAL	N-CA-CB	5.10	122.73	111.50
1	a	44	ALA	CB-CA-C	-5.10	102.45	110.10
2	b	244	ASN	O-C-N	-5.10	114.53	122.70
4	d	135	ILE	CA-CB-CG2	-5.10	100.70	110.90
6	f	85	SER	N-CA-CB	5.10	118.15	110.50
21	N	469	VAL	CG1-CB-CG2	-5.10	102.73	110.90
26	U	32	ARG	NE-CZ-NH2	-5.10	117.75	120.30
27	O	44	SER	N-CA-CB	5.10	118.15	110.50
29	I	343	ARG	NE-CZ-NH2	5.10	122.85	120.30
9	2	48	ARG	N-CA-CB	5.10	119.78	110.60
5	e	50	VAL	N-CA-C	-5.10	97.23	111.00
3	C	54	SER	N-CA-C	-5.10	97.23	111.00
22	S	49	ASP	CB-CG-OD1	-5.10	113.71	118.30
27	O	174	THR	N-CA-CB	5.10	119.99	110.30
8	1	177	SER	N-CA-CB	5.10	118.15	110.50
13	6	131	TYR	CG-CD1-CE1	-5.10	117.22	121.30
21	N	648	PRO	CA-CB-CG	-5.10	94.31	104.00
25	R	309	LEU	CB-CG-CD1	-5.10	102.34	111.00
27	O	255	LEU	N-CA-CB	5.10	120.60	110.40
3	c	5	ARG	NE-CZ-NH2	-5.09	117.75	120.30
3	c	16	GLU	OE1-CD-OE2	-5.09	117.19	123.30
16	V	21	ASP	CA-CB-CG	-5.09	102.19	113.40
20	Z	857	LEU	CB-CG-CD1	5.09	119.66	111.00
30	K	116	MET	N-CA-C	-5.09	97.25	111.00
17	T	265	ASP	CB-CG-OD2	5.09	122.88	118.30
22	S	477	VAL	CA-CB-CG2	-5.09	103.26	110.90
30	K	268	ILE	N-CA-C	-5.09	97.25	111.00
8	h	137	GLY	N-CA-C	-5.09	100.37	113.10
13	m	36	ARG	NH1-CZ-NH2	5.09	125.00	119.40
4	D	22	TYR	CB-CG-CD1	5.09	124.06	121.00
30	K	246	TYR	CB-CG-CD1	-5.09	117.94	121.00
20	Z	246	CYS	C-N-CA	5.09	134.42	121.70
8	1	182	ILE	N-CA-C	-5.09	97.26	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	64	GLY	N-CA-C	-5.09	100.38	113.10
2	b	68	THR	CA-CB-CG2	-5.08	105.28	112.40
11	k	70	ARG	NE-CZ-NH1	5.08	122.84	120.30
29	I	358	LYS	CB-CA-C	-5.08	100.23	110.40
14	n	80	ASP	CB-CG-OD2	5.08	122.88	118.30
13	6	93	SER	N-CA-CB	-5.08	102.87	110.50
24	Q	129	LYS	N-CA-CB	5.08	119.75	110.60
29	I	60	LEU	CB-CG-CD1	5.08	119.64	111.00
29	I	277	SER	N-CA-CB	5.08	118.13	110.50
6	F	161	ILE	CA-CB-CG2	-5.08	100.73	110.90
25	R	328	PHE	N-CA-CB	-5.08	101.46	110.60
4	d	218	ASP	CB-CG-OD2	5.08	122.87	118.30
10	j	74	TYR	CB-CG-CD1	5.08	124.05	121.00
16	V	196	TYR	N-CA-CB	5.08	119.74	110.60
24	Q	170	ASP	CB-CG-OD1	5.08	122.87	118.30
17	T	264	MET	CG-SD-CE	-5.08	92.08	100.20
22	S	173	LEU	CB-CG-CD2	5.08	119.63	111.00
32	M	404	ARG	NE-CZ-NH1	-5.08	117.76	120.30
1	A	34	ALA	N-CA-CB	5.07	117.20	110.10
12	5	273	TRP	CZ3-CH2-CZ2	-5.07	115.51	121.60
27	O	137	TYR	CB-CA-C	-5.07	100.25	110.40
8	h	197	PHE	CB-CG-CD2	-5.07	117.25	120.80
3	C	207	THR	CA-CB-CG2	-5.07	105.30	112.40
11	k	107	TYR	CD1-CE1-CZ	-5.07	115.24	119.80
7	G	244	GLN	CA-CB-CG	5.07	124.56	113.40
8	1	147	CYS	CA-CB-SG	-5.07	104.87	114.00
13	6	82	TRP	CB-CG-CD1	5.07	133.59	127.00
17	T	213	ASN	N-CA-C	-5.07	97.31	111.00
21	N	582	ASP	N-CA-CB	5.07	119.73	110.60
1	a	71	TYR	CG-CD2-CE2	-5.07	117.25	121.30
1	A	147	ASP	CB-CA-C	-5.07	100.27	110.40
1	A	209	HIS	N-CA-CB	-5.07	101.48	110.60
6	F	94	TYR	CG-CD2-CE2	-5.07	117.25	121.30
2	b	127	VAL	O-C-N	5.07	130.80	122.70
31	L	413	ASP	CB-CA-C	-5.07	100.27	110.40
8	h	26	ASP	CB-CG-OD2	-5.06	113.74	118.30
21	N	585	ARG	NE-CZ-NH1	5.06	122.83	120.30
9	i	79	ALA	N-CA-CB	-5.06	103.01	110.10
10	j	80	ARG	N-CA-CB	5.06	119.71	110.60
9	2	206	VAL	CB-CA-C	-5.06	101.78	111.40
12	5	212	TYR	CD1-CG-CD2	-5.06	112.33	117.90
19	Y	38	PHE	CB-CG-CD1	5.06	124.34	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	264	PHE	CB-CG-CD2	-5.06	117.26	120.80
26	U	277	TYR	CB-CG-CD1	-5.06	117.96	121.00
7	g	201	TYR	CD1-CG-CD2	5.06	123.47	117.90
1	A	104	PHE	CB-CG-CD1	5.06	124.34	120.80
14	7	228	PHE	CB-CG-CD1	5.06	124.34	120.80
14	n	134	TYR	CB-CG-CD1	5.06	124.03	121.00
2	B	130	PHE	CB-CG-CD1	-5.06	117.26	120.80
21	N	210	SER	N-CA-CB	5.06	118.08	110.50
33	J	309	ARG	NE-CZ-NH2	5.06	122.83	120.30
2	b	90	ARG	N-CA-CB	5.05	119.70	110.60
22	S	256	LYS	C-N-CA	5.05	134.34	121.70
4	d	247	ASP	CB-CG-OD2	5.05	122.85	118.30
26	U	93	TYR	CB-CG-CD1	5.05	124.03	121.00
11	4	130	TYR	CG-CD2-CE2	-5.05	117.26	121.30
15	W	155	ASP	CB-CG-OD2	-5.05	113.75	118.30
32	M	255	TYR	CZ-CE2-CD2	-5.05	115.25	119.80
15	W	35	PHE	CB-CG-CD1	5.05	124.33	120.80
22	S	473	ASP	CB-CG-OD1	5.05	122.84	118.30
21	N	147	ALA	O-C-N	5.05	130.78	122.70
22	S	450	ASN	N-CA-CB	5.05	119.69	110.60
3	c	180	TYR	CB-CG-CD2	5.05	124.03	121.00
8	1	84	THR	CA-CB-CG2	5.05	119.47	112.40
17	T	247	ASP	CB-CG-OD1	-5.05	113.76	118.30
33	J	331	HIS	N-CA-CB	-5.05	101.52	110.60
31	L	400	PHE	CB-CG-CD2	5.04	124.33	120.80
14	n	40	THR	CA-CB-OG1	5.04	119.59	109.00
6	F	176	LEU	CB-CA-C	-5.04	100.62	110.20
17	T	225	ASN	N-CA-CB	5.04	119.68	110.60
20	Z	825	ALA	N-CA-CB	5.04	117.16	110.10
29	I	231	LEU	N-CA-CB	5.04	120.49	110.40
31	L	258	GLU	OE1-CD-OE2	5.04	129.35	123.30
4	D	81	ASP	CB-CG-OD1	-5.04	113.76	118.30
21	N	599	TYR	CB-CG-CD1	-5.04	117.97	121.00
30	K	377	SER	N-CA-CB	5.04	118.06	110.50
17	T	165	GLN	CG-CD-OE1	-5.04	111.52	121.60
31	L	106	GLY	O-C-N	5.04	130.76	122.70
2	B	224	TYR	N-CA-C	-5.04	97.39	111.00
8	1	31	THR	N-CA-CB	5.04	119.87	110.30
20	Z	748	LEU	CA-C-N	5.04	126.28	116.20
31	L	354	GLU	CG-CD-OE1	-5.04	108.22	118.30
3	c	137	TYR	CZ-CE2-CD2	5.04	124.33	119.80
7	G	40	ILE	N-CA-C	-5.04	97.41	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	55	THR	CA-CB-CG2	-5.04	105.35	112.40
17	T	261	GLU	N-CA-CB	5.03	119.66	110.60
20	Z	747	ALA	N-CA-CB	5.03	117.15	110.10
27	O	373	TRP	CB-CG-CD1	5.03	133.54	127.00
2	b	64	VAL	C-N-CA	5.03	134.28	121.70
5	e	167	TYR	CB-CA-C	-5.03	100.34	110.40
4	D	159	TRP	CE3-CZ3-CH2	-5.03	115.67	121.20
22	S	442	PHE	CZ-CE2-CD2	-5.03	114.06	120.10
32	M	26	SER	N-CA-CB	5.03	118.05	110.50
2	B	156	TYR	CB-CG-CD1	-5.03	117.98	121.00
12	5	273	TRP	CD2-CE2-CZ2	-5.03	116.27	122.30
33	J	125	VAL	CG1-CB-CG2	5.03	118.95	110.90
3	c	64	GLU	OE1-CD-OE2	5.03	129.33	123.30
8	1	38	ARG	NE-CZ-NH2	-5.03	117.79	120.30
26	U	93	TYR	CD1-CE1-CZ	-5.03	115.28	119.80
7	g	80	GLY	N-CA-C	-5.03	100.53	113.10
21	N	36	TRP	CD1-CG-CD2	5.03	110.32	106.30
12	5	144	ARG	CB-CA-C	-5.02	100.35	110.40
5	e	39	GLY	N-CA-C	-5.02	100.55	113.10
11	k	122	LEU	O-C-N	-5.02	114.66	123.20
1	A	94	ALA	N-CA-CB	5.02	117.13	110.10
22	S	158	PHE	CB-CG-CD2	-5.02	117.28	120.80
24	Q	400	TYR	N-CA-CB	5.02	119.64	110.60
31	L	189	GLN	N-CA-CB	5.02	119.64	110.60
22	S	31	VAL	CG1-CB-CG2	-5.02	102.87	110.90
29	I	167	MET	CA-CB-CG	-5.02	104.77	113.30
33	J	214	SER	N-CA-CB	5.02	118.03	110.50
6	f	143	HIS	N-CA-C	-5.02	97.45	111.00
6	F	147	PHE	CB-CG-CD2	-5.02	117.29	120.80
11	4	125	LYS	N-CA-CB	5.02	119.63	110.60
13	6	65	PHE	CZ-CE2-CD2	-5.02	114.08	120.10
17	T	157	TYR	CB-CG-CD2	5.02	124.01	121.00
24	Q	334	HIS	CA-CB-CG	-5.02	105.07	113.60
28	H	44	PRO	N-CA-CB	5.02	109.32	103.30
7	g	196	ALA	CB-CA-C	-5.02	102.58	110.10
6	F	55	GLU	OE1-CD-OE2	5.02	129.32	123.30
7	G	32	GLU	O-C-N	-5.02	114.67	122.70
33	J	138	MET	CA-CB-CG	5.02	121.83	113.30
3	c	157	TYR	CB-CG-CD1	-5.01	117.99	121.00
11	k	124	THR	CA-CB-CG2	-5.01	105.38	112.40
12	l	260	TRP	CB-CG-CD2	-5.01	120.08	126.60
10	3	46	TYR	CB-CG-CD2	5.01	124.01	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	85	SER	CB-CA-C	-5.01	100.57	110.10
8	h	146	TYR	CB-CG-CD2	5.01	124.01	121.00
32	M	17	GLU	N-CA-CB	5.01	119.62	110.60
14	7	136	ARG	NE-CZ-NH2	-5.01	117.79	120.30
20	Z	385	PHE	CB-CG-CD1	5.01	124.31	120.80
30	K	219	LYS	CB-CA-C	-5.01	100.38	110.40
1	a	216	THR	C-N-CA	5.01	134.22	121.70
11	4	181	VAL	CA-CB-CG1	-5.01	103.39	110.90
16	V	108	TYR	CD1-CG-CD2	5.01	123.41	117.90
16	V	124	ASN	N-CA-CB	5.01	119.62	110.60
20	Z	244	ARG	C-N-CA	5.01	134.22	121.70
23	P	214	GLU	N-CA-CB	5.01	119.62	110.60
24	Q	41	ALA	N-CA-CB	5.01	117.11	110.10
26	U	149	SER	C-N-CA	5.01	134.22	121.70
29	I	174	ASP	CB-CG-OD1	5.01	122.81	118.30
4	d	48	ARG	NE-CZ-NH2	-5.01	117.80	120.30
4	d	126	VAL	N-CA-C	-5.01	97.48	111.00
12	5	129	PHE	CB-CG-CD1	-5.01	117.30	120.80
27	O	93	ASP	CB-CG-OD2	-5.01	113.80	118.30
29	I	125	MET	N-CA-CB	5.01	119.61	110.60
32	M	252	VAL	CA-CB-CG1	-5.01	103.39	110.90
32	M	425	ARG	N-CA-CB	5.01	119.61	110.60
15	W	143	ASN	CB-CA-C	-5.00	100.39	110.40
27	O	250	TRP	CA-CB-CG	5.00	123.21	113.70
12	l	89	VAL	N-CA-C	-5.00	97.50	111.00
14	n	57	ALA	N-CA-C	-5.00	97.49	111.00
10	3	11	ILE	CB-CA-C	-5.00	101.59	111.60
19	Y	7	ALA	N-CA-CB	5.00	117.10	110.10
21	N	888	ASP	CB-CG-OD2	-5.00	113.80	118.30
31	L	168	TYR	CB-CG-CD1	5.00	124.00	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
20	Z	748	LEU	CA

All (350) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	133	TYR	Sidechain
8	1	144	TYR	Sidechain
8	1	146	TYR	Sidechain

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Mol	Chain	Res	Type	Group
8	1	75	TYR	Sidechain
9	2	119	TYR	Sidechain
9	2	140	PHE	Sidechain
9	2	219	TYR	Sidechain
9	2	232	TYR	Sidechain
9	2	98	TYR	Sidechain
10	3	136	PHE	Sidechain
10	3	154	TYR	Sidechain
10	3	199	TYR	Sidechain
10	3	203	ARG	Sidechain
10	3	69	TYR	Sidechain
10	3	96	TYR	Sidechain
11	4	121	TYR	Sidechain
11	4	176	PHE	Sidechain
11	4	59	TYR	Sidechain
12	5	148	ARG	Sidechain
12	5	176	ILE	Mainchain
12	5	179	TYR	Sidechain
12	5	188	TYR	Sidechain
12	5	219	TYR	Sidechain
13	6	114	TYR	Sidechain
13	6	203	HIS	Sidechain
13	6	229	ARG	Peptide
13	6	47	TYR	Sidechain
13	6	75	ARG	Sidechain
13	6	83	TYR	Sidechain
13	6	99	ARG	Sidechain
14	7	124	TYR	Sidechain
14	7	162	TYR	Sidechain
14	7	170	TYR	Sidechain
14	7	179	PHE	Sidechain
14	7	223	ARG	Sidechain
14	7	49	TYR	Sidechain
14	7	63	TYR	Sidechain
1	A	110	TYR	Sidechain
1	A	131	ARG	Sidechain
1	A	244	ARG	Sidechain
1	A	71	TYR	Sidechain
1	A	91	ARG	Sidechain
2	B	104	TYR	Sidechain
2	B	178	ARG	Sidechain
2	B	23	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	235	PHE	Sidechain
2	B	236	ARG	Sidechain
2	B	5	TYR	Sidechain
2	B	90	ARG	Sidechain
2	B	97	TYR	Sidechain
3	C	131	PHE	Sidechain
3	C	140	TYR	Sidechain
3	C	157	TYR	Sidechain
3	C	180	TYR	Sidechain
3	C	226	TYR	Sidechain
3	C	4	ARG	Sidechain
4	D	112	TYR	Sidechain
4	D	172	ARG	Sidechain
4	D	179	TYR	Sidechain
4	D	41	CYS	Peptide
4	D	49	ARG	Sidechain
4	D	83	ARG	Sidechain
4	D	96	HIS	Sidechain
4	D	97	ARG	Sidechain
5	E	10	ARG	Sidechain
5	E	102	TYR	Sidechain
5	E	103	TYR	Sidechain
5	E	132	ARG	Sidechain
5	E	136	ARG	Sidechain
5	E	138	PHE	Sidechain
5	E	15	PHE	Sidechain
5	E	20	ARG	Sidechain
5	E	228	PHE	Sidechain
5	E	231	TYR	Sidechain
6	F	101	ARG	Sidechain
6	F	137	TYR	Sidechain
6	F	157	TYR	Sidechain
6	F	174	ARG	Sidechain
6	F	179	PHE	Sidechain
6	F	18	ARG	Peptide
6	F	233	TYR	Sidechain
6	F	51	ARG	Sidechain
6	F	89	ARG	Sidechain
6	F	94	TYR	Sidechain
7	G	149	TYR	Sidechain
7	G	16	SER	Peptide
7	G	190	ARG	Sidechain

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Mol	Chain	Res	Type	Group
7	G	201	TYR	Sidechain
7	G	21	ASN	Peptide
7	G	78	TYR	Sidechain
7	G	93	ARG	Sidechain
28	H	190	ARG	Sidechain
28	H	249	TYR	Sidechain
28	H	318	ARG	Sidechain
28	H	385	ARG	Sidechain
28	H	429	PHE	Sidechain
28	H	434	ARG	Sidechain
28	H	463	TYR	Sidechain
28	H	73	ASP	Peptide
29	I	181	TYR	Sidechain
29	I	208	TYR	Sidechain
29	I	340	ARG	Sidechain
29	I	408	ARG	Sidechain
29	I	422	ARG	Sidechain
29	I	429	GLU	Peptide
29	I	54	ARG	Sidechain
29	I	68	HIS	Sidechain
33	J	124	LYS	Peptide
33	J	147	TYR	Sidechain
33	J	22	TYR	Sidechain
33	J	222	TYR	Sidechain
33	J	270	ARG	Sidechain
33	J	286	LYS	Peptide
33	J	309	ARG	Sidechain
33	J	312	ARG	Sidechain
33	J	35	ARG	Sidechain
33	J	94	TYR	Sidechain
30	K	118	TYR	Sidechain
30	K	141	ARG	Sidechain
30	K	185	ARG	Sidechain
30	K	198	TYR	Sidechain
30	K	236	ARG	Mainchain,Sidechain
30	K	246	TYR	Sidechain
30	K	262	ARG	Sidechain
30	K	67	TYR	Sidechain
30	K	88	ARG	Sidechain
31	L	131	VAL	Peptide
31	L	168	TYR	Sidechain
31	L	209	ARG	Sidechain

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Mol	Chain	Res	Type	Group
31	L	243	PHE	Mainchain,Peptide
31	L	244	ILE	Mainchain,Peptide
31	L	255	TYR	Sidechain
31	L	261	ARG	Sidechain
31	L	264	ARG	Sidechain
31	L	303	ARG	Sidechain
31	L	315	PHE	Peptide
31	L	318	LEU	Peptide
31	L	342	ARG	Peptide
31	L	345	ARG	Sidechain
31	L	374	PHE	Sidechain
31	L	376	PHE	Peptide
31	L	407	ARG	Sidechain
31	L	409	HIS	Sidechain
31	L	434	TYR	Sidechain
31	L	62	ARG	Sidechain
31	L	70	TYR	Sidechain
31	L	77	ARG	Sidechain
32	M	124	ARG	Sidechain
32	M	153	TYR	Sidechain
32	M	213	ARG	Sidechain
32	M	291	PHE	Sidechain
32	M	314	GLY	Peptide
32	M	320	ARG	Sidechain
32	M	329	ARG	Sidechain
32	M	349	PHE	Sidechain
32	M	423	GLN	Peptide
21	N	109	TYR	Sidechain
21	N	139	ARG	Sidechain
21	N	161	TYR	Sidechain
21	N	202	PHE	Sidechain
21	N	282	TYR	Sidechain
21	N	329	HIS	Sidechain
21	N	348	PHE	Sidechain
21	N	389	TYR	Sidechain
21	N	412	TYR	Sidechain
21	N	415	PHE	Sidechain
21	N	471	TYR	Sidechain
21	N	549	TYR	Sidechain
21	N	599	TYR	Sidechain
21	N	653	ARG	Sidechain
21	N	69	TYR	Sidechain

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Mol	Chain	Res	Type	Group
21	N	762	ARG	Sidechain
21	N	771	PHE	Sidechain
21	N	782	PHE	Sidechain
21	N	784	TYR	Sidechain
21	N	788	TYR	Sidechain
21	N	81	TYR	Sidechain
21	N	884	PHE	Sidechain
21	N	889	ARG	Sidechain
21	N	894	ARG	Sidechain
27	O	15	ARG	Sidechain
27	O	172	TYR	Sidechain
27	O	195	TYR	Sidechain
27	O	32	PHE	Sidechain
27	O	58	ARG	Sidechain
23	P	138	ARG	Sidechain
23	P	21	PHE	Sidechain
23	P	213	TYR	Sidechain
23	P	220	TYR	Sidechain
23	P	310	ARG	Sidechain
23	P	351	ARG	Sidechain
23	P	356	TYR	Sidechain
23	P	47	ARG	Sidechain
24	Q	161	LEU	Peptide
24	Q	209	TYR	Sidechain
24	Q	232	TYR	Sidechain
24	Q	243	PHE	Sidechain
24	Q	246	TYR	Sidechain
24	Q	255	TYR	Sidechain
24	Q	264	TYR	Sidechain
24	Q	306	TYR	Sidechain
24	Q	321	TYR	Sidechain
24	Q	332	ARG	Sidechain
24	Q	400	TYR	Sidechain
24	Q	50	ARG	Sidechain
24	Q	67	THR	Peptide
24	Q	84	TYR	Sidechain
25	R	140	TYR	Sidechain
25	R	141	TYR	Sidechain
25	R	176	ARG	Sidechain
25	R	181	TYR	Sidechain
25	R	20	ARG	Sidechain
25	R	209	ARG	Sidechain

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Mol	Chain	Res	Type	Group
25	R	210	TYR	Sidechain
25	R	224	PHE	Sidechain
25	R	24	TYR	Sidechain
25	R	307	TYR	Sidechain
25	R	312	TYR	Sidechain
25	R	325	HIS	Sidechain
25	R	345	TYR	Sidechain
25	R	62	TYR	Sidechain
25	R	65	TYR	Sidechain
25	R	70	TYR	Peptide
25	R	99	TYR	Sidechain
22	S	185	PHE	Sidechain
22	S	186	TYR	Sidechain
22	S	197	SER	Peptide
22	S	211	ARG	Sidechain
22	S	259	TYR	Sidechain
22	S	272	TYR	Sidechain
22	S	345	TYR	Sidechain
22	S	442	PHE	Sidechain
22	S	481	TYR	Sidechain
22	S	64	ARG	Sidechain
22	S	76	PHE	Sidechain
22	S	82	TYR	Sidechain
17	T	144	TYR	Sidechain
17	T	251	HIS	Peptide
17	T	266	TYR	Sidechain
17	T	88	TYR	Sidechain
17	T	91	SER	Peptide
26	U	22	TYR	Sidechain
26	U	283	ARG	Sidechain
26	U	47	ARG	Sidechain
26	U	94	HIS	Sidechain
16	V	135	ARG	Sidechain
16	V	230	TYR	Sidechain
16	V	269	ARG	Sidechain
16	V	28	TYR	Sidechain
16	V	40	HIS	Sidechain
16	V	87	PHE	Sidechain
15	W	122	ARG	Sidechain
15	W	17	ARG	Sidechain
15	W	179	ARG	Sidechain
15	W	41	ARG	Sidechain

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Mol	Chain	Res	Type	Group
18	X	17	TYR	Sidechain
18	X	97	TYR	Sidechain
18	X	98	PHE	Sidechain
20	Z	248	TYR	Sidechain
20	Z	269	TYR	Sidechain
20	Z	287	ARG	Sidechain
20	Z	623	ARG	Sidechain
20	Z	738	TYR	Sidechain
1	a	108	TYR	Sidechain
1	a	110	TYR	Sidechain
1	a	209	HIS	Sidechain
1	a	26	TYR	Sidechain
1	a	71	TYR	Sidechain
1	a	77	ARG	Sidechain
2	b	178	ARG	Sidechain
2	b	90	ARG	Sidechain
2	b	97	TYR	Sidechain
3	c	140	TYR	Sidechain
3	c	143	ARG	Sidechain
3	c	157	TYR	Sidechain
3	c	18	ARG	Sidechain
3	c	210	ARG	Sidechain
3	c	217	ARG	Sidechain
3	c	5	ARG	Sidechain
3	c	6	TYR	Sidechain
4	d	108	TYR	Sidechain
4	d	11	PHE	Sidechain
4	d	22	TYR	Sidechain
4	d	49	ARG	Sidechain
4	d	83	ARG	Sidechain
5	e	10	ARG	Sidechain
5	e	136	ARG	Sidechain
5	e	138	PHE	Sidechain
5	e	164	PHE	Sidechain
5	e	165	TYR	Sidechain
5	e	86	ARG	Sidechain
5	e	91	HIS	Sidechain
6	f	12	THR	Peptide
6	f	137	TYR	Sidechain
6	f	147	PHE	Sidechain
6	f	18	ARG	Peptide
6	f	225	TYR	Sidechain

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Mol	Chain	Res	Type	Group
6	f	233	TYR	Sidechain
6	f	24	TYR	Sidechain
6	f	43	HIS	Sidechain
7	g	130	ARG	Sidechain
7	g	169	ARG	Sidechain
7	g	190	ARG	Sidechain
7	g	20	ARG	Sidechain
7	g	21	ASN	Peptide
7	g	72	ARG	Sidechain
7	g	8	TYR	Sidechain
8	h	111	TYR	Sidechain
8	h	133	TYR	Sidechain
8	h	142	PHE	Sidechain
8	h	144	TYR	Sidechain
8	h	34	TYR	Sidechain
8	h	45	ARG	Sidechain
8	h	96	TYR	Sidechain
9	i	145	HIS	Sidechain
9	i	215	TYR	Sidechain
9	i	219	TYR	Sidechain
10	j	103	TYR	Sidechain
10	j	177	ARG	Sidechain
10	j	188	TYR	Sidechain
10	j	44	PHE	Sidechain
10	j	46	TYR	Sidechain
10	j	69	TYR	Sidechain
10	j	74	TYR	Sidechain
11	k	139	TYR	Sidechain
11	k	56	PHE	Sidechain
11	k	67	TYR	Sidechain
11	k	8	ARG	Sidechain
12	l	144	ARG	Sidechain
12	l	179	TYR	Sidechain
12	l	210	PHE	Sidechain
12	l	253	TYR	Sidechain
12	l	81	PHE	Sidechain
13	m	106	TYR	Sidechain
13	m	113	TYR	Sidechain
13	m	114	TYR	Sidechain
13	m	13	TYR	Sidechain
13	m	182	TYR	Sidechain
13	m	225	TYR	Sidechain

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Mol	Chain	Res	Type	Group
13	m	41	TYR	Sidechain
13	m	83	TYR	Sidechain
14	n	136	ARG	Sidechain
14	n	162	TYR	Sidechain
14	n	189	ARG	Sidechain
14	n	226	ARG	Sidechain
14	n	49	TYR	Sidechain
14	n	63	TYR	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%)	221 (92%)	18 (8%)	1 (0%)	34 72
1	a	240/242 (99%)	224 (93%)	15 (6%)	1 (0%)	34 72
2	B	247/249 (99%)	230 (93%)	16 (6%)	1 (0%)	34 72
2	b	247/249 (99%)	230 (93%)	13 (5%)	4 (2%)	9 45
3	C	242/244 (99%)	230 (95%)	11 (4%)	1 (0%)	34 72
3	c	242/244 (99%)	233 (96%)	8 (3%)	1 (0%)	34 72
4	D	235/251 (94%)	215 (92%)	17 (7%)	3 (1%)	12 48
4	d	249/251 (99%)	235 (94%)	9 (4%)	5 (2%)	7 40
5	E	247/249 (99%)	231 (94%)	10 (4%)	6 (2%)	6 36
5	e	247/249 (99%)	229 (93%)	13 (5%)	5 (2%)	7 40
6	F	229/231 (99%)	211 (92%)	16 (7%)	2 (1%)	17 56
6	f	229/231 (99%)	208 (91%)	16 (7%)	5 (2%)	6 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
7	G	240/242 (99%)	227 (95%)	13 (5%)	0	100	100
7	g	240/242 (99%)	231 (96%)	9 (4%)	0	100	100
8	1	194/196 (99%)	187 (96%)	6 (3%)	1 (0%)	29	68
8	h	194/196 (99%)	175 (90%)	16 (8%)	3 (2%)	10	46
9	2	224/226 (99%)	212 (95%)	12 (5%)	0	100	100
9	i	224/226 (99%)	203 (91%)	18 (8%)	3 (1%)	12	48
10	3	202/204 (99%)	183 (91%)	19 (9%)	0	100	100
10	j	202/204 (99%)	182 (90%)	15 (7%)	5 (2%)	5	35
11	4	193/195 (99%)	176 (91%)	13 (7%)	4 (2%)	7	39
11	k	193/195 (99%)	179 (93%)	13 (7%)	1 (0%)	29	68
12	5	210/212 (99%)	198 (94%)	11 (5%)	1 (0%)	29	68
12	l	210/212 (99%)	192 (91%)	14 (7%)	4 (2%)	8	41
13	6	220/222 (99%)	201 (91%)	16 (7%)	3 (1%)	11	47
13	m	220/222 (99%)	207 (94%)	10 (4%)	3 (1%)	11	47
14	7	227/232 (98%)	204 (90%)	20 (9%)	3 (1%)	12	48
14	n	230/232 (99%)	207 (90%)	21 (9%)	2 (1%)	17	56
15	W	195/197 (99%)	174 (89%)	18 (9%)	3 (2%)	10	46
16	V	287/289 (99%)	265 (92%)	17 (6%)	5 (2%)	9	43
17	T	264/266 (99%)	246 (93%)	11 (4%)	7 (3%)	5	34
18	X	125/127 (98%)	106 (85%)	15 (12%)	4 (3%)	4	30
19	Y	87/89 (98%)	72 (83%)	11 (13%)	4 (5%)	2	24
20	Z	902/970 (93%)	823 (91%)	56 (6%)	23 (2%)	5	35
21	N	920/922 (100%)	857 (93%)	47 (5%)	16 (2%)	9	43
22	S	473/475 (100%)	428 (90%)	33 (7%)	12 (2%)	5	35
23	P	438/440 (100%)	408 (93%)	24 (6%)	6 (1%)	11	47
24	Q	432/434 (100%)	393 (91%)	24 (6%)	15 (4%)	3	29
25	R	403/405 (100%)	380 (94%)	19 (5%)	4 (1%)	15	54
26	U	302/304 (99%)	292 (97%)	8 (3%)	2 (1%)	22	62
27	O	386/388 (100%)	367 (95%)	13 (3%)	6 (2%)	9	45
28	H	424/426 (100%)	376 (89%)	36 (8%)	12 (3%)	5	33
29	I	382/384 (100%)	335 (88%)	35 (9%)	12 (3%)	4	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
30	K	392/394 (100%)	361 (92%)	22 (6%)	9 (2%)	6 37
31	L	386/388 (100%)	355 (92%)	25 (6%)	6 (2%)	9 45
32	M	419/421 (100%)	375 (90%)	30 (7%)	14 (3%)	4 30
33	J	403/405 (100%)	342 (85%)	49 (12%)	12 (3%)	4 31
All	All	13937/14114 (99%)	12816 (92%)	881 (6%)	240 (2%)	13 43

All (240) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	101	GLU
5	e	16	SER
6	f	11	VAL
5	E	9	ASP
6	F	14	SER
12	5	172	MET
13	6	89	ASP
13	6	138	SER
16	V	73	GLN
17	T	92	ASN
17	T	96	LEU
17	T	173	GLU
20	Z	24	THR
20	Z	85	VAL
20	Z	728	LYS
20	Z	870	ALA
20	Z	923	ILE
21	N	175	ASP
21	N	708	ALA
21	N	779	GLU
23	P	397	ALA
24	Q	68	MET
24	Q	384	LYS
25	R	280	ILE
27	O	120	LYS
28	H	124	ASN
28	H	162	ARG
28	H	458	SER
28	H	465	GLN
29	I	125	MET
29	I	142	GLU
29	I	213	ILE

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Mol	Chain	Res	Type
30	K	314	VAL
31	L	245	PHE
31	L	246	SER
31	L	343	LEU
32	M	97	SER
32	M	316	SER
32	M	424	ALA
33	J	282	PHE
3	c	168	ASN
5	e	9	ASP
5	e	122	ARG
5	e	169	ALA
6	f	9	ASP
8	h	101	ASN
10	j	7	ILE
11	k	4	ILE
5	E	122	ARG
5	E	169	ALA
11	4	150	PRO
14	7	260	GLY
16	V	61	TYR
16	V	117	TRP
16	V	200	ASN
17	T	225	ASN
18	X	116	ALA
19	Y	44	ALA
19	Y	55	THR
20	Z	612	GLY
20	Z	926	ASN
21	N	17	GLN
21	N	120	ASP
21	N	148	SER
21	N	178	SER
21	N	395	ALA
21	N	725	LEU
21	N	856	PHE
21	N	871	MET
22	S	44	THR
22	S	47	THR
22	S	128	ILE
22	S	132	ALA
23	P	130	ILE

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Mol	Chain	Res	Type
24	Q	46	VAL
24	Q	253	ASN
24	Q	309	ARG
25	R	263	ARG
26	U	150	THR
27	O	225	ASP
27	O	243	VAL
29	I	86	GLU
29	I	187	LEU
31	L	179	THR
32	M	92	GLU
32	M	124	ARG
32	M	240	ASN
32	M	408	SER
32	M	433	TYR
33	J	2	THR
33	J	3	ALA
33	J	284	THR
2	b	4	ARG
2	b	17	LYS
6	f	14	SER
6	f	164	ARG
9	i	146	GLY
9	i	174	ASP
10	j	40	PHE
13	m	27	ASP
1	A	13	ASP
2	B	106	PRO
5	E	16	SER
5	E	128	SER
5	E	216	ASN
8	1	123	PRO
11	4	2	ASP
13	6	27	ASP
14	7	244	ASN
15	W	169	SER
16	V	184	ASN
17	T	138	ASP
18	X	77	PRO
20	Z	82	MET
20	Z	205	LEU
20	Z	825	ALA

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Mol	Chain	Res	Type
20	Z	887	GLY
20	Z	940	GLY
20	Z	947	GLY
20	Z	951	GLN
21	N	739	PHE
21	N	851	GLU
22	S	100	HIS
22	S	107	SER
22	S	111	ARG
22	S	225	HIS
22	S	329	GLU
23	P	111	ASP
24	Q	48	ASP
24	Q	75	ARG
24	Q	149	LYS
24	Q	170	ASP
25	R	125	GLU
26	U	30	ASN
27	O	52	ALA
28	H	194	SER
29	I	143	PRO
29	I	291	ARG
30	K	41	SER
30	K	155	ASP
30	K	162	GLY
30	K	399	ARG
32	M	87	ASP
32	M	108	LEU
32	M	179	THR
32	M	427	SER
33	J	252	SER
5	e	53	ARG
10	j	116	SER
10	j	194	GLU
12	l	147	GLU
12	l	281	SER
13	m	208	ASP
14	n	252	TRP
3	C	222	ASP
4	D	219	SER
11	4	11	ASP
15	W	179	ARG

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Mol	Chain	Res	Type
18	X	38	ASN
19	Y	31	GLU
20	Z	142	ASP
20	Z	233	LEU
20	Z	578	GLY
21	N	832	HIS
23	P	129	LYS
24	Q	47	ASP
24	Q	67	THR
25	R	245	SER
27	O	70	TYR
28	H	135	ASP
28	H	323	ALA
28	H	457	PHE
29	I	216	PRO
31	L	289	ARG
33	J	4	ALA
33	J	82	LYS
33	J	283	GLU
33	J	353	CYS
1	a	49	ASP
4	d	5	ASP
4	d	40	ASN
4	d	70	HIS
6	f	69	HIS
8	h	123	PRO
8	h	154	ASN
13	m	138	SER
14	n	249	ASN
4	D	101	GLU
4	D	208	LYS
6	F	41	ASN
11	4	176	PHE
14	7	114	ALA
17	T	95	LYS
17	T	257	THR
18	X	112	ASN
19	Y	52	ASN
20	Z	25	PRO
20	Z	65	GLU
20	Z	557	GLU
21	N	32	VAL

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Mol	Chain	Res	Type
21	N	86	LYS
22	S	83	PRO
22	S	97	THR
22	S	153	GLU
23	P	89	LEU
23	P	108	LYS
24	Q	40	ALA
24	Q	89	ALA
24	Q	283	ASN
28	H	94	GLU
29	I	198	VAL
29	I	283	GLU
29	I	292	TYR
30	K	167	PRO
30	K	398	ASN
30	K	426	PHE
31	L	244	ILE
32	M	106	VAL
32	M	282	GLU
33	J	118	ASP
33	J	141	LYS
2	b	97	TYR
2	b	161	ALA
4	d	102	ASP
10	j	193	ASP
20	Z	463	HIS
24	Q	18	LYS
28	H	143	ALA
29	I	329	ASN
33	J	261	SER
12	l	106	VAL
12	l	173	GLY
20	Z	920	GLY
20	Z	886	VAL
28	H	191	ILE
28	H	314	VAL
30	K	175	GLY
9	i	222	PRO
27	O	201	PRO
15	W	164	PRO

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	206/206 (100%)	200 (97%)	6 (3%)	42	64
1	a	206/206 (100%)	200 (97%)	6 (3%)	42	64
2	B	208/208 (100%)	205 (99%)	3 (1%)	67	81
2	b	208/208 (100%)	204 (98%)	4 (2%)	57	75
3	C	203/203 (100%)	200 (98%)	3 (2%)	65	80
3	c	203/203 (100%)	199 (98%)	4 (2%)	55	73
4	D	210/224 (94%)	204 (97%)	6 (3%)	42	64
4	d	224/224 (100%)	219 (98%)	5 (2%)	52	71
5	E	205/205 (100%)	200 (98%)	5 (2%)	49	69
5	e	205/205 (100%)	197 (96%)	8 (4%)	32	57
6	F	190/190 (100%)	183 (96%)	7 (4%)	34	59
6	f	190/190 (100%)	185 (97%)	5 (3%)	46	67
7	G	200/200 (100%)	194 (97%)	6 (3%)	41	63
7	g	200/200 (100%)	191 (96%)	9 (4%)	27	54
8	1	162/162 (100%)	158 (98%)	4 (2%)	47	68
8	h	162/162 (100%)	159 (98%)	3 (2%)	57	75
9	2	185/185 (100%)	183 (99%)	2 (1%)	73	85
9	i	185/185 (100%)	185 (100%)	0	100	100
10	3	172/172 (100%)	165 (96%)	7 (4%)	30	56
10	j	172/172 (100%)	170 (99%)	2 (1%)	71	84
11	4	173/173 (100%)	170 (98%)	3 (2%)	60	78
11	k	173/173 (100%)	169 (98%)	4 (2%)	50	70
12	5	169/169 (100%)	160 (95%)	9 (5%)	22	49
12	l	169/169 (100%)	161 (95%)	8 (5%)	26	52
13	6	185/185 (100%)	182 (98%)	3 (2%)	62	79
13	m	185/185 (100%)	181 (98%)	4 (2%)	52	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	7	195/198 (98%)	192 (98%)	3 (2%)	65	80
14	n	198/198 (100%)	191 (96%)	7 (4%)	36	60
15	W	171/171 (100%)	164 (96%)	7 (4%)	30	56
16	V	253/253 (100%)	244 (96%)	9 (4%)	35	60
17	T	249/249 (100%)	244 (98%)	5 (2%)	55	73
18	X	116/116 (100%)	111 (96%)	5 (4%)	29	55
19	Y	81/81 (100%)	81 (100%)	0	100	100
20	Z	773/828 (93%)	750 (97%)	23 (3%)	41	63
21	N	776/776 (100%)	765 (99%)	11 (1%)	67	81
22	S	447/447 (100%)	439 (98%)	8 (2%)	59	77
23	P	412/412 (100%)	407 (99%)	5 (1%)	71	84
24	Q	391/391 (100%)	378 (97%)	13 (3%)	38	61
25	R	356/356 (100%)	345 (97%)	11 (3%)	40	63
26	U	277/277 (100%)	272 (98%)	5 (2%)	59	77
27	O	363/363 (100%)	358 (99%)	5 (1%)	67	81
28	H	361/361 (100%)	351 (97%)	10 (3%)	43	65
29	I	341/341 (100%)	330 (97%)	11 (3%)	39	62
30	K	346/346 (100%)	336 (97%)	10 (3%)	42	64
31	L	332/332 (100%)	323 (97%)	9 (3%)	44	66
32	M	364/364 (100%)	350 (96%)	14 (4%)	33	58
33	J	352/352 (100%)	334 (95%)	18 (5%)	24	50
All	All	12104/12176 (99%)	11789 (97%)	315 (3%)	49	67

All (315) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	14	ARG
1	a	134	MET
1	a	158	ASP
1	a	175	GLN
1	a	210	MET
1	a	237	SER
2	b	35	LEU
2	b	70	ASP
2	b	76	SER

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Mol	Chain	Res	Type
2	b	128	ARG
3	c	14	SER
3	c	66	LEU
3	c	153	PRO
3	c	232	PRO
4	d	4	TYR
4	d	70	HIS
4	d	126	VAL
4	d	149	GLN
4	d	241	GLN
5	e	2	PHE
5	e	36	THR
5	e	53	ARG
5	e	68	VAL
5	e	121	LEU
5	e	136	ARG
5	e	213	ASP
5	e	214	GLU
6	f	74	LEU
6	f	117	GLN
6	f	120	THR
6	f	154	THR
6	f	207	THR
7	g	35	THR
7	g	41	LYS
7	g	71	ASP
7	g	74	ILE
7	g	134	VAL
7	g	187	LEU
7	g	208	LYS
7	g	218	TRP
7	g	220	SER
8	h	44	THR
8	h	101	ASN
8	h	135	ILE
10	j	84	PRO
10	j	183	TRP
11	k	85	ARG
11	k	126	VAL
11	k	130	TYR
11	k	141	PHE
12	l	79	LEU

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Mol	Chain	Res	Type
12	l	105	THR
12	l	109	VAL
12	l	179	TYR
12	l	181	ARG
12	l	201	ILE
12	l	212	TYR
12	l	276	LYS
13	m	49	PRO
13	m	115	VAL
13	m	136	VAL
13	m	196	PHE
14	n	36	GLN
14	n	137	ARG
14	n	162	TYR
14	n	186	PRO
14	n	195	GLU
14	n	220	ARG
14	n	258	ILE
1	A	43	LEU
1	A	110	TYR
1	A	131	ARG
1	A	134	MET
1	A	175	GLN
1	A	192	ASP
2	B	14	PRO
2	B	45	ILE
2	B	128	ARG
3	C	120	GLN
3	C	129	ARG
3	C	152	ASN
4	D	70	HIS
4	D	120	TYR
4	D	156	TYR
4	D	158	SER
4	D	202	VAL
4	D	240	LYS
5	E	20	ARG
5	E	36	THR
5	E	53	ARG
5	E	104	ASP
5	E	136	ARG
6	F	23	GLU

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Mol	Chain	Res	Type
6	F	74	LEU
6	F	80	ASP
6	F	117	GLN
6	F	145	LEU
6	F	153	VAL
6	F	161	ILE
7	G	15	PHE
7	G	73	HIS
7	G	185	GLU
7	G	208	LYS
7	G	218	TRP
7	G	220	SER
8	1	30	THR
8	1	44	THR
8	1	61	THR
8	1	135	ILE
9	2	167	LEU
9	2	233	LYS
10	3	33	SER
10	3	48	HIS
10	3	51	LEU
10	3	69	TYR
10	3	80	ARG
10	3	147	PHE
10	3	192	LYS
11	4	2	ASP
11	4	3	ILE
11	4	119	ILE
12	5	79	LEU
12	5	109	VAL
12	5	117	LEU
12	5	159	SER
12	5	179	TYR
12	5	181	ARG
12	5	190	VAL
12	5	212	TYR
12	5	268	VAL
13	6	20	ILE
13	6	39	THR
13	6	125	ASP
14	7	39	VAL
14	7	185	ASN

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Mol	Chain	Res	Type
14	7	241	PHE
15	W	58	ASN
15	W	59	PRO
15	W	76	LEU
15	W	79	THR
15	W	120	ASP
15	W	155	ASP
15	W	182	TYR
16	V	67	ASP
16	V	91	MET
16	V	117	TRP
16	V	130	GLU
16	V	160	ASP
16	V	196	TYR
16	V	199	LEU
16	V	229	ASP
16	V	274	GLN
17	T	27	LEU
17	T	53	ASN
17	T	193	THR
17	T	197	TYR
17	T	236	ASN
18	X	14	VAL
18	X	28	PRO
18	X	57	VAL
18	X	62	ASP
18	X	115	SER
20	Z	27	LYS
20	Z	64	TYR
20	Z	171	LYS
20	Z	206	ASP
20	Z	213	LYS
20	Z	222	ASP
20	Z	236	PHE
20	Z	402	ASP
20	Z	411	LYS
20	Z	548	ASP
20	Z	557	GLU
20	Z	563	VAL
20	Z	566	LEU
20	Z	728	LYS
20	Z	734	ASP

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Mol	Chain	Res	Type
20	Z	748	LEU
20	Z	756	MET
20	Z	767	TYR
20	Z	809	MET
20	Z	842	GLN
20	Z	850	LEU
20	Z	874	ASN
20	Z	942	PRO
21	N	83	LEU
21	N	261	LEU
21	N	282	TYR
21	N	324	LYS
21	N	398	ARG
21	N	530	GLU
21	N	669	GLU
21	N	680	LYS
21	N	739	PHE
21	N	876	PRO
21	N	888	ASP
22	S	54	TRP
22	S	128	ILE
22	S	165	PRO
22	S	170	TYR
22	S	332	PHE
22	S	369	GLN
22	S	452	TYR
22	S	486	LYS
23	P	34	SER
23	P	69	ARG
23	P	145	GLU
23	P	394	ASN
23	P	403	GLU
24	Q	61	LEU
24	Q	73	LYS
24	Q	77	PHE
24	Q	79	PRO
24	Q	88	PHE
24	Q	95	LYS
24	Q	96	VAL
24	Q	198	LEU
24	Q	250	THR
24	Q	285	LYS

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Mol	Chain	Res	Type
24	Q	294	ARG
24	Q	338	LEU
24	Q	406	ASP
25	R	68	GLU
25	R	71	LEU
25	R	95	ASP
25	R	124	ASP
25	R	137	LEU
25	R	141	TYR
25	R	146	ASP
25	R	176	ARG
25	R	306	PRO
25	R	348	LEU
25	R	373	PRO
26	U	70	HIS
26	U	79	MET
26	U	115	GLN
26	U	134	THR
26	U	176	ARG
27	O	58	ARG
27	O	115	ARG
27	O	243	VAL
27	O	343	GLN
27	O	348	VAL
28	H	82	TRP
28	H	95	HIS
28	H	162	ARG
28	H	194	SER
28	H	221	LEU
28	H	271	PHE
28	H	281	GLN
28	H	307	PHE
28	H	450	VAL
28	H	464	MET
29	I	86	GLU
29	I	102	ASN
29	I	127	ASP
29	I	147	VAL
29	I	177	PRO
29	I	246	ARG
29	I	300	ARG
29	I	328	THR

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Mol	Chain	Res	Type
29	I	347	LYS
29	I	410	GLN
29	I	432	LEU
30	K	37	ASN
30	K	160	VAL
30	K	236	ARG
30	K	237	VAL
30	K	252	ARG
30	K	275	ASP
30	K	335	ASP
30	K	360	MET
30	K	387	MET
30	K	405	SER
31	L	147	THR
31	L	174	GLU
31	L	177	GLU
31	L	199	LEU
31	L	244	ILE
31	L	246	SER
31	L	354	GLU
31	L	361	PHE
31	L	416	MET
32	M	15	ASP
32	M	36	LEU
32	M	73	ARG
32	M	77	TYR
32	M	109	ASP
32	M	127	VAL
32	M	143	ASN
32	M	173	ASP
32	M	291	PHE
32	M	335	PRO
32	M	344	ASP
32	M	352	PRO
32	M	375	ASN
32	M	433	TYR
33	J	12	LEU
33	J	37	LYS
33	J	63	ARG
33	J	125	VAL
33	J	149	MET
33	J	179	ILE

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Mol	Chain	Res	Type
33	J	207	ASP
33	J	222	TYR
33	J	261	SER
33	J	274	GLU
33	J	279	LEU
33	J	282	PHE
33	J	287	ASN
33	J	309	ARG
33	J	311	ASP
33	J	320	SER
33	J	358	VAL
33	J	359	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (129) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	27	GLN
1	a	39	ASN
2	b	94	HIS
2	b	244	ASN
4	d	149	GLN
4	d	231	GLN
6	f	5	ASN
6	f	152	ASN
7	g	12	ASN
7	g	144	ASN
7	g	182	HIS
7	g	204	HIS
8	h	47	HIS
10	j	204	GLN
11	k	63	ASN
12	l	128	GLN
12	l	284	ASN
13	m	44	ASN
13	m	57	ASN
13	m	63	ASN
13	m	116	HIS
14	n	51	ASN
14	n	107	ASN
14	n	227	ASN
14	n	246	GLN
14	n	249	ASN

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Mol	Chain	Res	Type
1	A	27	GLN
1	A	181	ASN
1	A	185	HIS
3	C	152	ASN
4	D	118	GLN
4	D	122	GLN
5	E	73	HIS
5	E	100	ASN
5	E	157	HIS
6	F	93	ASN
7	G	64	ASN
7	G	182	HIS
7	G	204	HIS
8	1	150	ASN
9	2	120	GLN
10	3	89	GLN
10	3	204	GLN
11	4	37	GLN
11	4	55	GLN
11	4	86	GLN
11	4	99	GLN
12	5	84	GLN
12	5	128	GLN
12	5	160	ASN
12	5	241	HIS
13	6	44	ASN
13	6	163	ASN
14	7	36	GLN
15	W	108	GLN
15	W	150	ASN
15	W	184	ASN
16	V	176	ASN
16	V	200	ASN
17	T	47	GLN
17	T	123	HIS
17	T	236	ASN
20	Z	15	GLN
20	Z	214	HIS
20	Z	235	GLN
20	Z	247	GLN
20	Z	622	HIS
20	Z	771	HIS

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Mol	Chain	Res	Type
20	Z	823	ASN
20	Z	829	GLN
20	Z	951	GLN
21	N	16	ASN
21	N	111	GLN
21	N	336	ASN
21	N	525	ASN
21	N	859	ASN
21	N	870	ASN
22	S	65	ASN
22	S	191	HIS
22	S	469	ASN
22	S	472	HIS
23	P	88	GLN
23	P	98	GLN
23	P	230	HIS
23	P	263	HIS
23	P	285	GLN
23	P	296	GLN
23	P	306	ASN
23	P	334	ASN
23	P	425	HIS
23	P	431	HIS
24	Q	87	GLN
24	Q	145	HIS
24	Q	334	HIS
25	R	73	ASN
26	U	5	HIS
26	U	94	HIS
26	U	116	ASN
26	U	156	HIS
26	U	230	GLN
26	U	251	ASN
26	U	252	HIS
27	O	183	ASN
27	O	235	HIS
27	O	236	HIS
27	O	282	GLN
28	H	128	ASN
28	H	151	GLN
28	H	392	HIS
28	H	413	ASN

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Mol	Chain	Res	Type
29	I	161	GLN
29	I	274	ASN
29	I	431	ASN
30	K	37	ASN
30	K	142	HIS
30	K	244	HIS
30	K	293	GLN
31	L	67	HIS
31	L	302	GLN
31	L	393	ASN
32	M	65	ASN
32	M	107	ASN
32	M	125	GLN
32	M	143	ASN
32	M	364	HIS
32	M	375	ASN
32	M	423	GLN
33	J	240	HIS
33	J	376	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 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	$\#\|Z\| > 2$
34	ATP	M	501	35	26,33,33	1.96	7 (26%)	31,52,52	1.58	5 (16%)
34	ATP	K	501	35	26,33,33	1.01	1 (3%)	31,52,52	1.63	6 (19%)
34	ATP	H	501	35	26,33,33	1.38	3 (11%)	31,52,52	2.09	6 (19%)
34	ATP	I	501	35	26,33,33	1.37	4 (15%)	31,52,52	1.86	8 (25%)
36	ADP	J	501	35	24,29,29	1.22	2 (8%)	29,45,45	1.87	6 (20%)
34	ATP	L	501	35	26,33,33	1.71	6 (23%)	31,52,52	2.16	6 (19%)

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
34	ATP	M	501	35	-	6/18/38/38	0/3/3/3
34	ATP	K	501	35	-	4/18/38/38	0/3/3/3
34	ATP	H	501	35	-	3/18/38/38	0/3/3/3
34	ATP	I	501	35	-	5/18/38/38	0/3/3/3
36	ADP	J	501	35	-	7/12/32/32	0/3/3/3
34	ATP	L	501	35	-	3/18/38/38	0/3/3/3

All (23) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	M	501	ATP	C2'-C1'	-6.73	1.43	1.53
34	L	501	ATP	C2-N3	4.43	1.39	1.32
36	J	501	ADP	C8-N7	-3.93	1.27	1.34
34	H	501	ATP	C8-N7	-3.68	1.28	1.34
34	I	501	ATP	C2-N3	3.64	1.38	1.32
34	L	501	ATP	C5'-C4'	3.62	1.62	1.51
34	L	501	ATP	O4'-C1'	3.01	1.45	1.41
34	K	501	ATP	C8-N7	-2.80	1.29	1.34
34	M	501	ATP	C4-N3	-2.71	1.31	1.35
34	L	501	ATP	C8-N7	-2.46	1.30	1.34
34	M	501	ATP	PA-O2A	-2.40	1.44	1.55
34	I	501	ATP	O4'-C4'	2.35	1.50	1.45
34	M	501	ATP	O2'-C2'	-2.35	1.37	1.43
34	M	501	ATP	O4'-C1'	-2.34	1.37	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	I	501	ATP	O2'-C2'	-2.33	1.37	1.43
34	L	501	ATP	O3'-C3'	-2.32	1.37	1.43
34	H	501	ATP	PA-O2A	-2.28	1.44	1.55
34	M	501	ATP	C8-N7	-2.24	1.30	1.34
34	M	501	ATP	C3'-C4'	-2.21	1.47	1.53
34	L	501	ATP	PA-O2A	-2.12	1.45	1.55
34	H	501	ATP	C5'-C4'	2.10	1.58	1.51
34	I	501	ATP	C4-N3	-2.05	1.32	1.35
36	J	501	ADP	C5'-C4'	2.02	1.57	1.51

All (37) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	H	501	ATP	PA-O3A-PB	8.29	161.26	132.83
34	L	501	ATP	PA-O3A-PB	7.71	159.28	132.83
34	I	501	ATP	PA-O3A-PB	6.18	154.04	132.83
36	J	501	ADP	PA-O3A-PB	5.89	153.04	132.83
34	L	501	ATP	N6-C6-N1	4.58	128.08	118.57
34	K	501	ATP	PA-O3A-PB	4.52	148.33	132.83
34	M	501	ATP	PA-O3A-PB	4.45	148.08	132.83
34	H	501	ATP	N6-C6-N1	4.03	126.94	118.57
36	J	501	ADP	C5-C6-N1	-3.94	111.42	120.35
34	K	501	ATP	C5-C6-N1	-3.67	112.02	120.35
34	M	501	ATP	C5-C6-N1	-3.53	112.36	120.35
34	I	501	ATP	N6-C6-N1	3.51	125.87	118.57
34	K	501	ATP	N3-C2-N1	3.42	134.02	128.68
34	L	501	ATP	C4-C5-N7	-3.34	105.92	109.40
34	M	501	ATP	C5-C6-N6	3.12	125.09	120.35
34	H	501	ATP	N3-C2-N1	2.73	132.94	128.68
36	J	501	ADP	N6-C6-N1	2.69	124.17	118.57
34	K	501	ATP	N6-C6-N1	2.67	124.11	118.57
34	L	501	ATP	O4'-C1'-C2'	2.61	110.74	106.93
36	J	501	ADP	C5-C6-N6	2.60	124.31	120.35
34	I	501	ATP	C5-C6-N1	-2.59	114.48	120.35
34	H	501	ATP	C5-C6-N1	-2.54	114.61	120.35
34	L	501	ATP	C5-C6-N1	-2.43	114.84	120.35
34	K	501	ATP	O3G-PG-O1G	2.38	120.00	110.68
34	K	501	ATP	O4'-C4'-C5'	2.37	117.18	109.37
34	I	501	ATP	O4'-C1'-C2'	-2.36	103.48	106.93
34	H	501	ATP	C1'-N9-C4	2.35	130.77	126.64
36	J	501	ADP	O4'-C1'-C2'	-2.34	103.50	106.93
34	I	501	ATP	C4-C5-N7	-2.31	106.99	109.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	M	501	ATP	O3G-PG-O3B	-2.25	97.08	104.64
34	L	501	ATP	C5-C6-N6	-2.16	117.08	120.35
34	M	501	ATP	PB-O3B-PG	2.15	140.20	132.83
34	I	501	ATP	C3'-C2'-C1'	2.08	104.11	100.98
34	I	501	ATP	C2'-C3'-C4'	-2.08	98.60	102.64
34	I	501	ATP	O3G-PG-O3B	2.07	111.57	104.64
34	H	501	ATP	C5'-C4'-C3'	-2.04	107.54	115.18
36	J	501	ADP	O3B-PB-O3A	2.02	111.42	104.64

There are no chirality outliers.

All (28) torsion outliers are listed below:

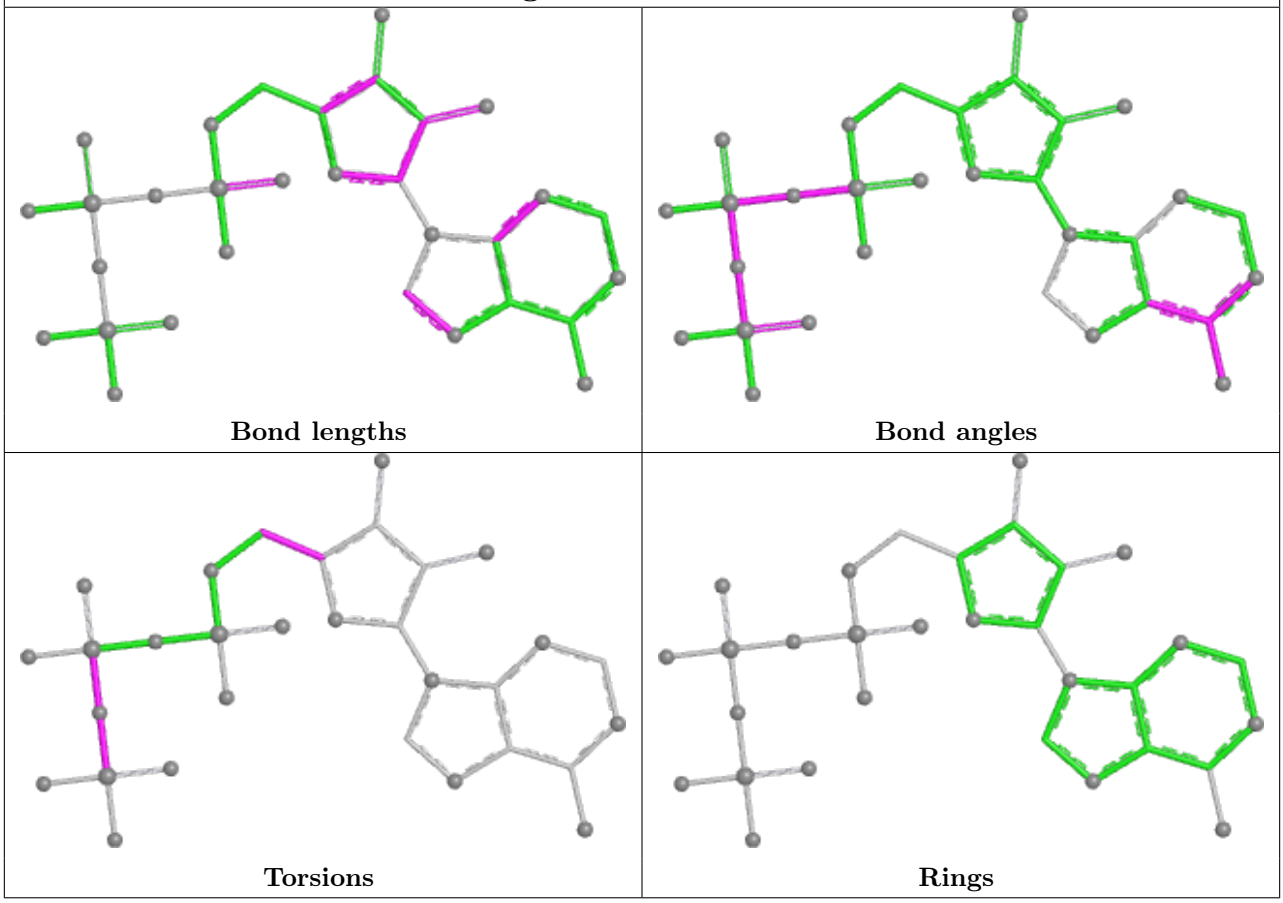
Mol	Chain	Res	Type	Atoms
34	H	501	ATP	C5'-O5'-PA-O3A
34	I	501	ATP	C5'-O5'-PA-O1A
34	I	501	ATP	C5'-O5'-PA-O2A
34	L	501	ATP	C5'-O5'-PA-O3A
34	M	501	ATP	PB-O3B-PG-O3G
36	J	501	ADP	PA-O3A-PB-O3B
36	J	501	ADP	C5'-O5'-PA-O1A
36	J	501	ADP	C5'-O5'-PA-O2A
34	M	501	ATP	O4'-C4'-C5'-O5'
34	I	501	ATP	PA-O3A-PB-O1B
34	M	501	ATP	PG-O3B-PB-O1B
34	K	501	ATP	PB-O3B-PG-O1G
36	J	501	ADP	PA-O3A-PB-O2B
36	J	501	ADP	C5'-O5'-PA-O3A
34	K	501	ATP	PG-O3B-PB-O1B
34	H	501	ATP	C5'-O5'-PA-O2A
34	L	501	ATP	C5'-O5'-PA-O2A
34	M	501	ATP	C3'-C4'-C5'-O5'
34	H	501	ATP	O4'-C4'-C5'-O5'
34	L	501	ATP	O4'-C4'-C5'-O5'
36	J	501	ADP	C4'-C5'-O5'-PA
34	M	501	ATP	PG-O3B-PB-O2B
34	M	501	ATP	PB-O3B-PG-O1G
34	I	501	ATP	PB-O3B-PG-O3G
34	K	501	ATP	PB-O3B-PG-O2G
34	K	501	ATP	PB-O3B-PG-O3G
34	I	501	ATP	C5'-O5'-PA-O3A
36	J	501	ADP	PA-O3A-PB-O1B

There are no ring outliers.

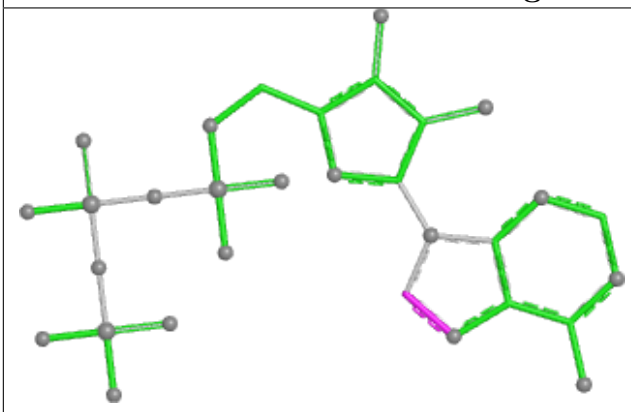
No monomer is involved in short contacts.

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.

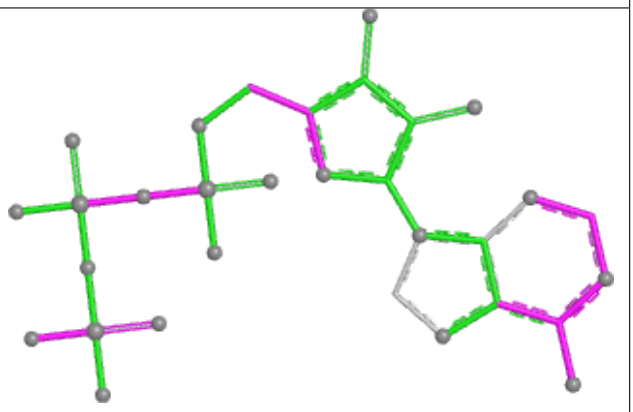
Ligand ATP M 501



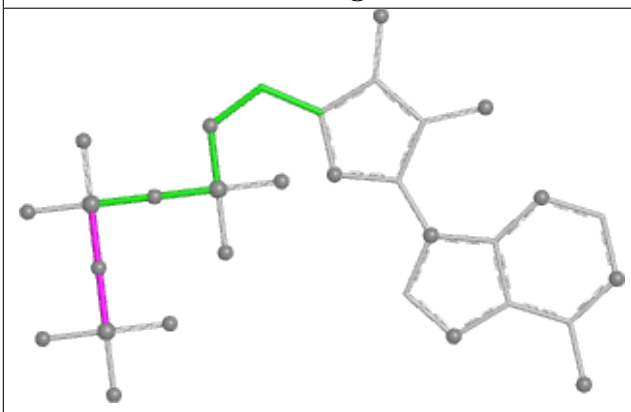
Ligand ATP K 501



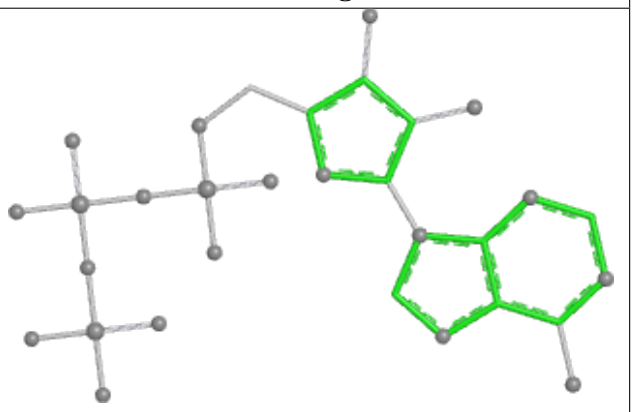
Bond lengths



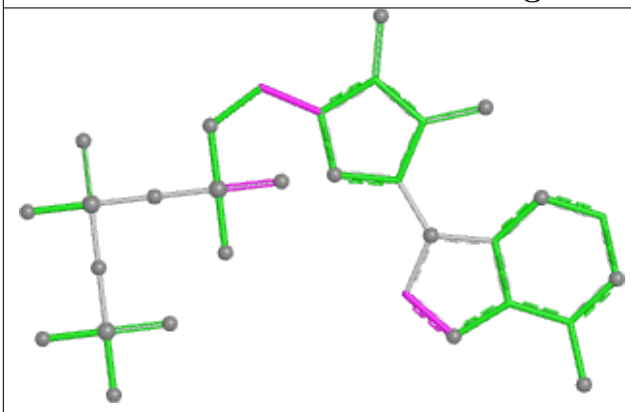
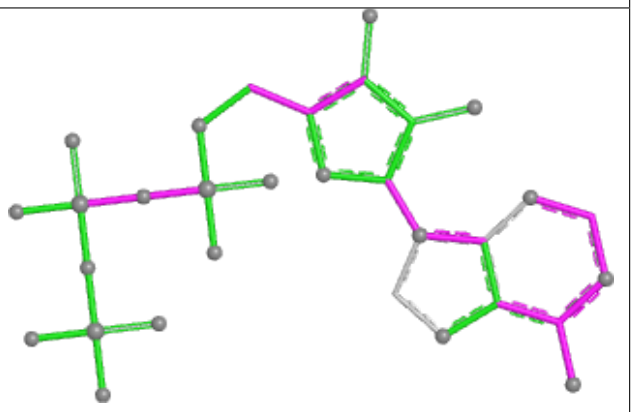
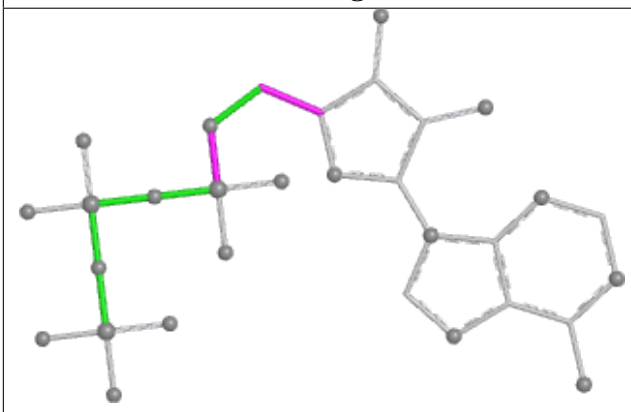
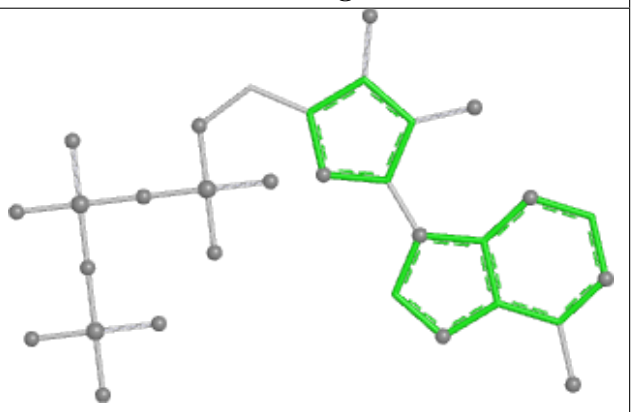
Bond angles

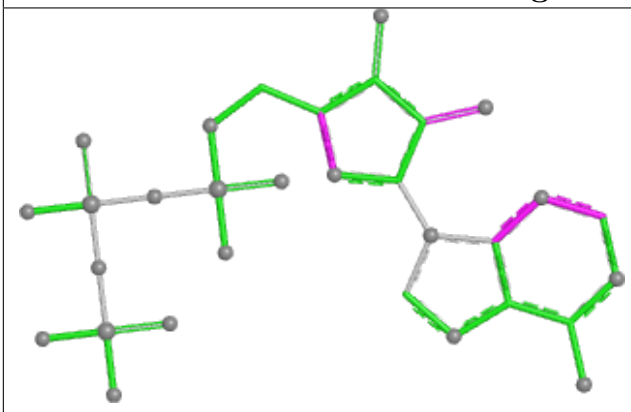
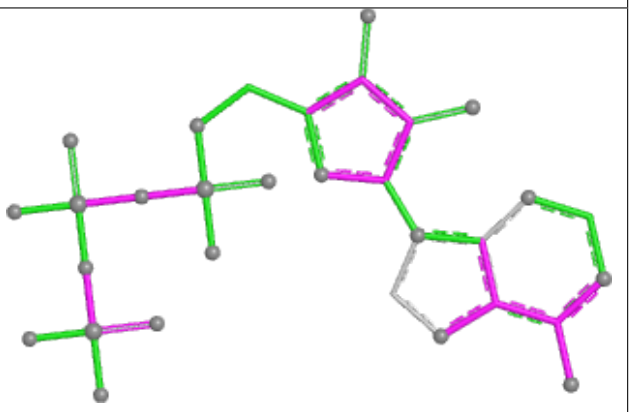
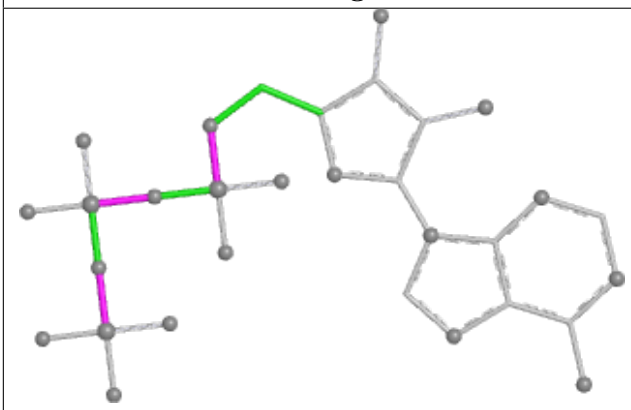
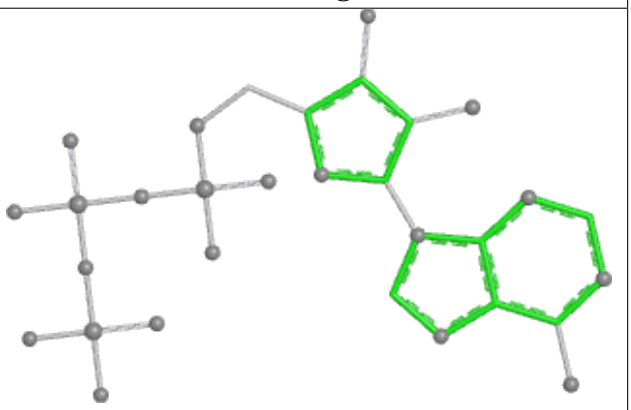


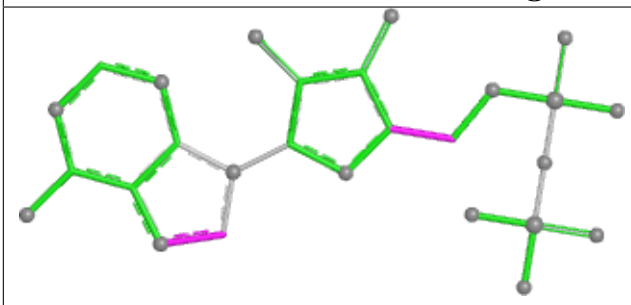
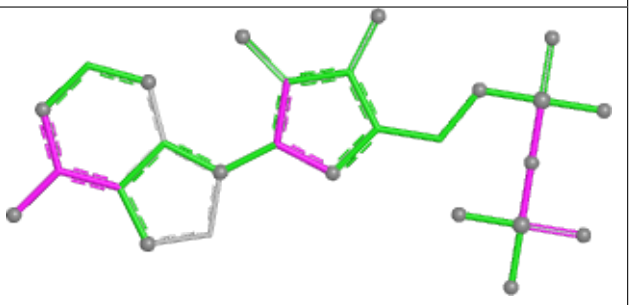
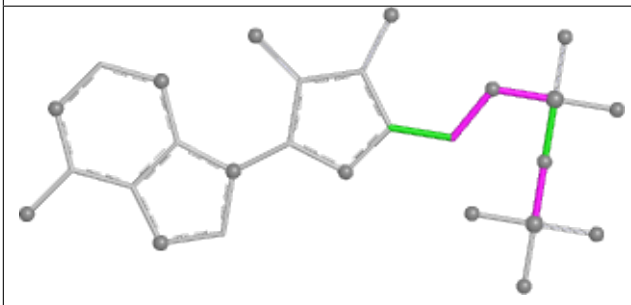
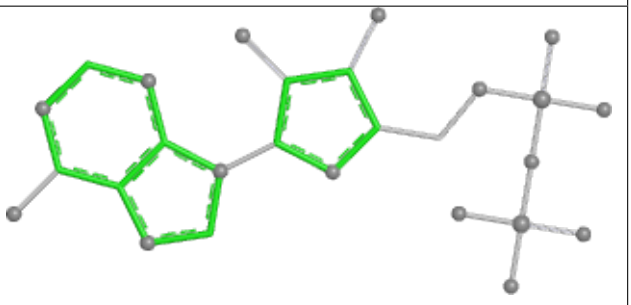
Torsions



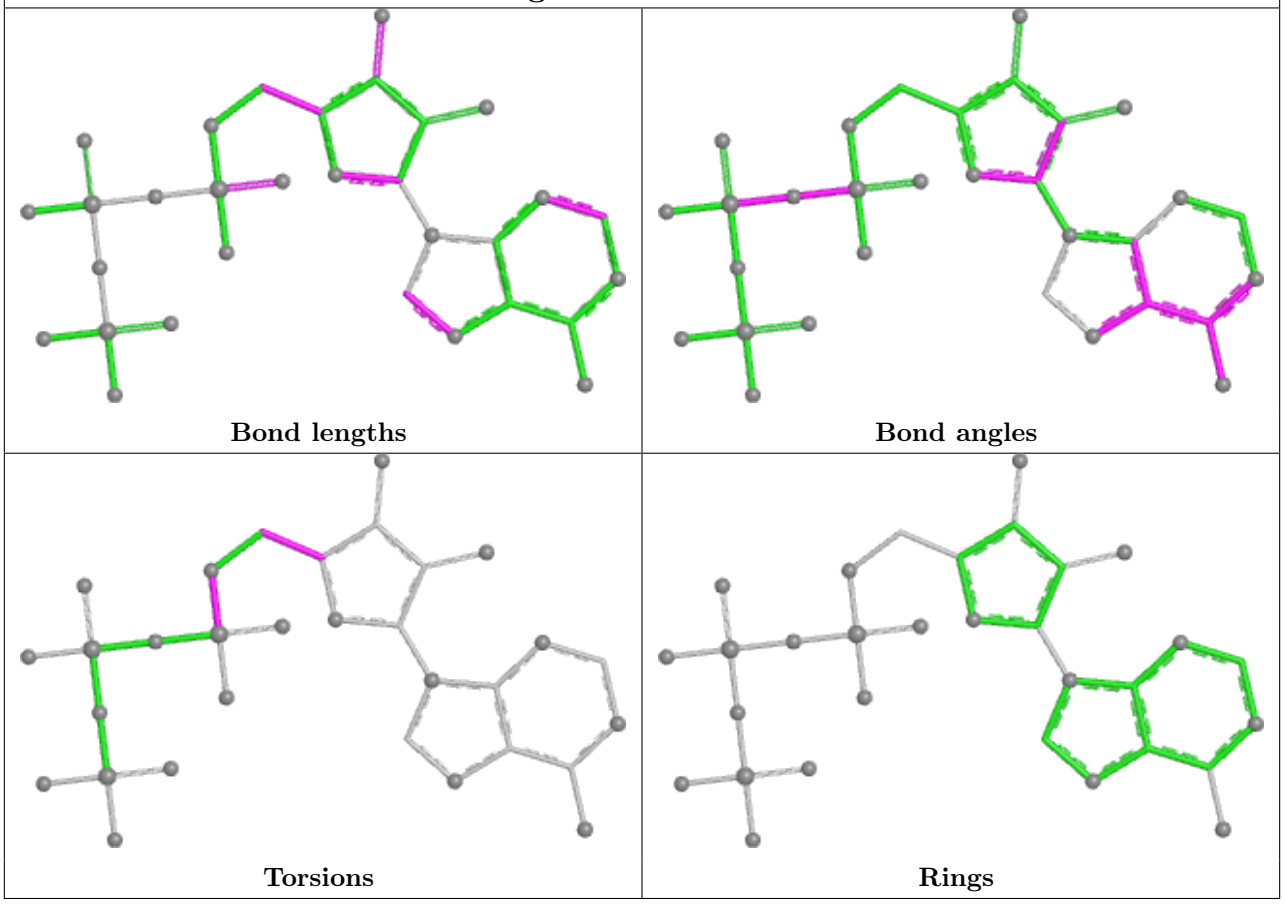
Rings

Ligand ATP H 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP I 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP J 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP L 501



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
28	H	2
29	I	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	H	307:PHE	C	308:PHE	N	1.91
1	I	322:VAL	C	323:LYS	N	1.82
1	H	308:PHE	C	309:ASP	N	1.81

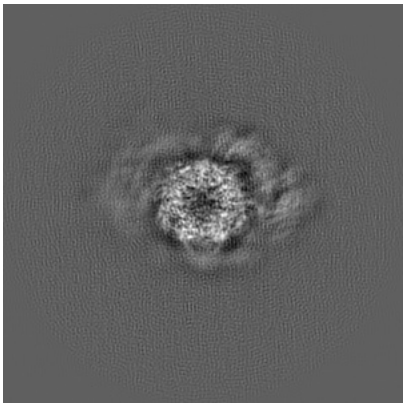
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3535. These allow visual inspection of the internal detail of the map and identification of artifacts.

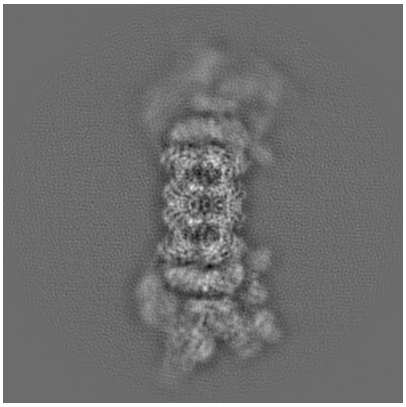
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

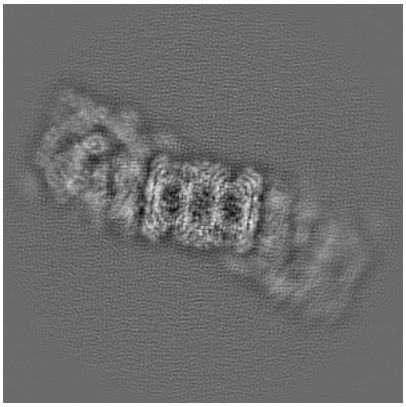
6.1.1 Primary map



X



Y

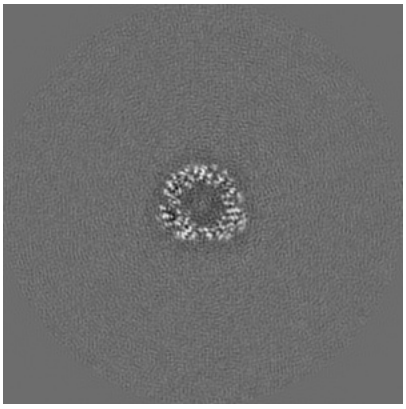


Z

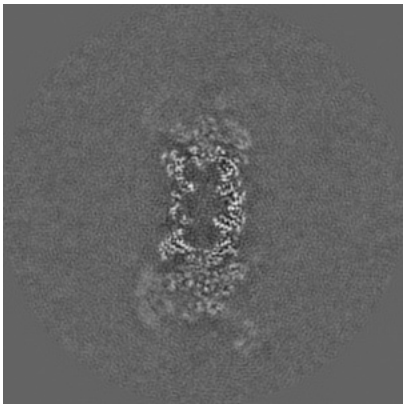
The images above show the map projected in three orthogonal directions.

6.2 Central slices

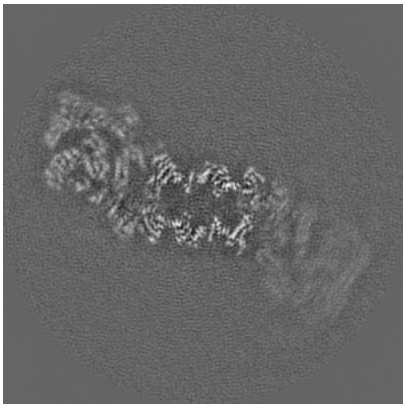
6.2.1 Primary map



X Index: 192



Y Index: 192

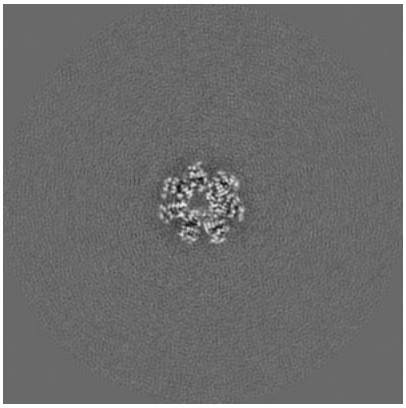


Z Index: 192

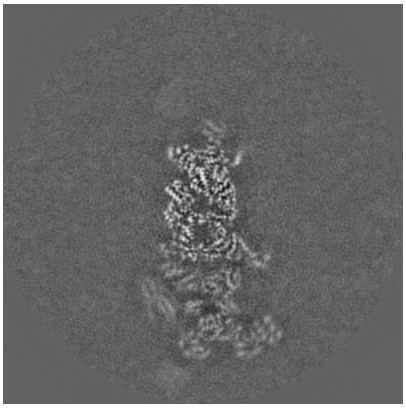
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

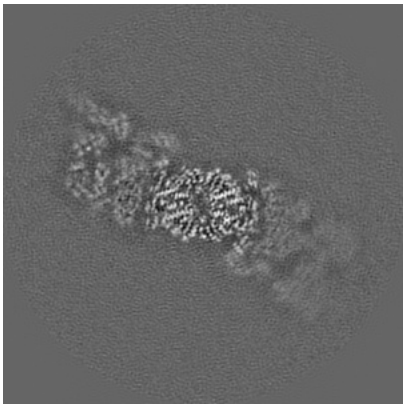
6.3.1 Primary map



X Index: 206



Y Index: 210



Z Index: 210

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 0.017. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

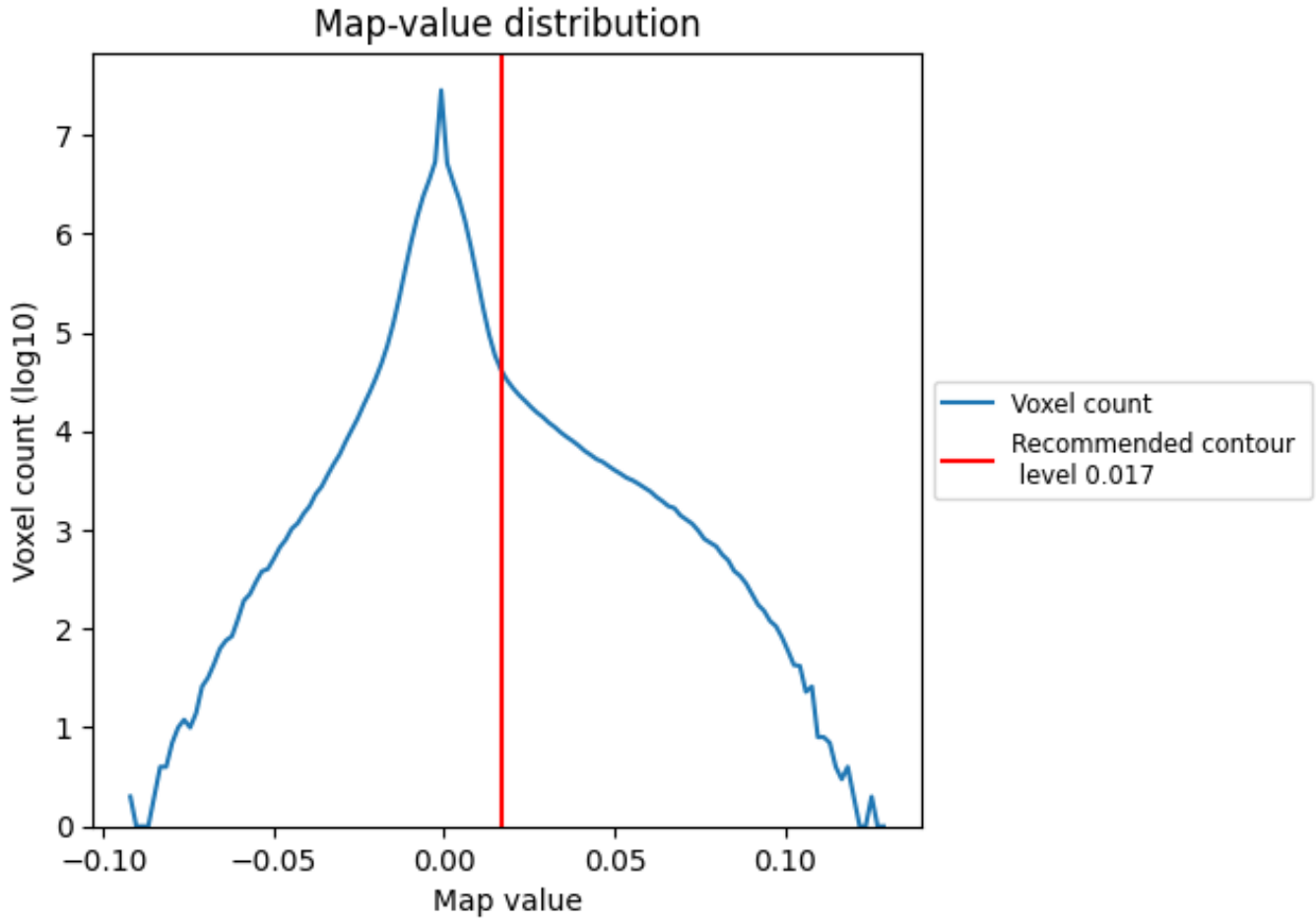
6.5 Mask visualisation (i)

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

7 Map analysis

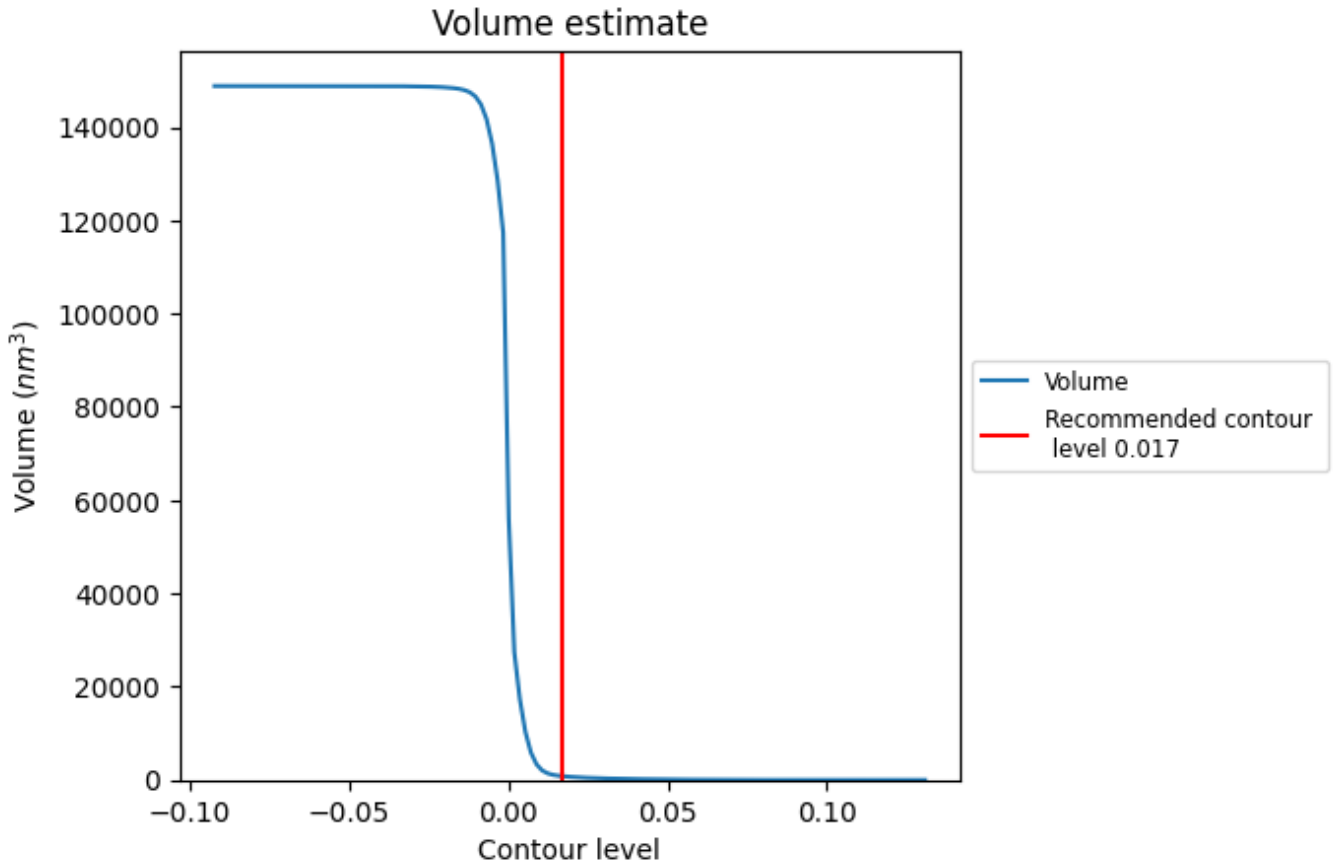
This section contains the results of statistical analysis of the map.

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.

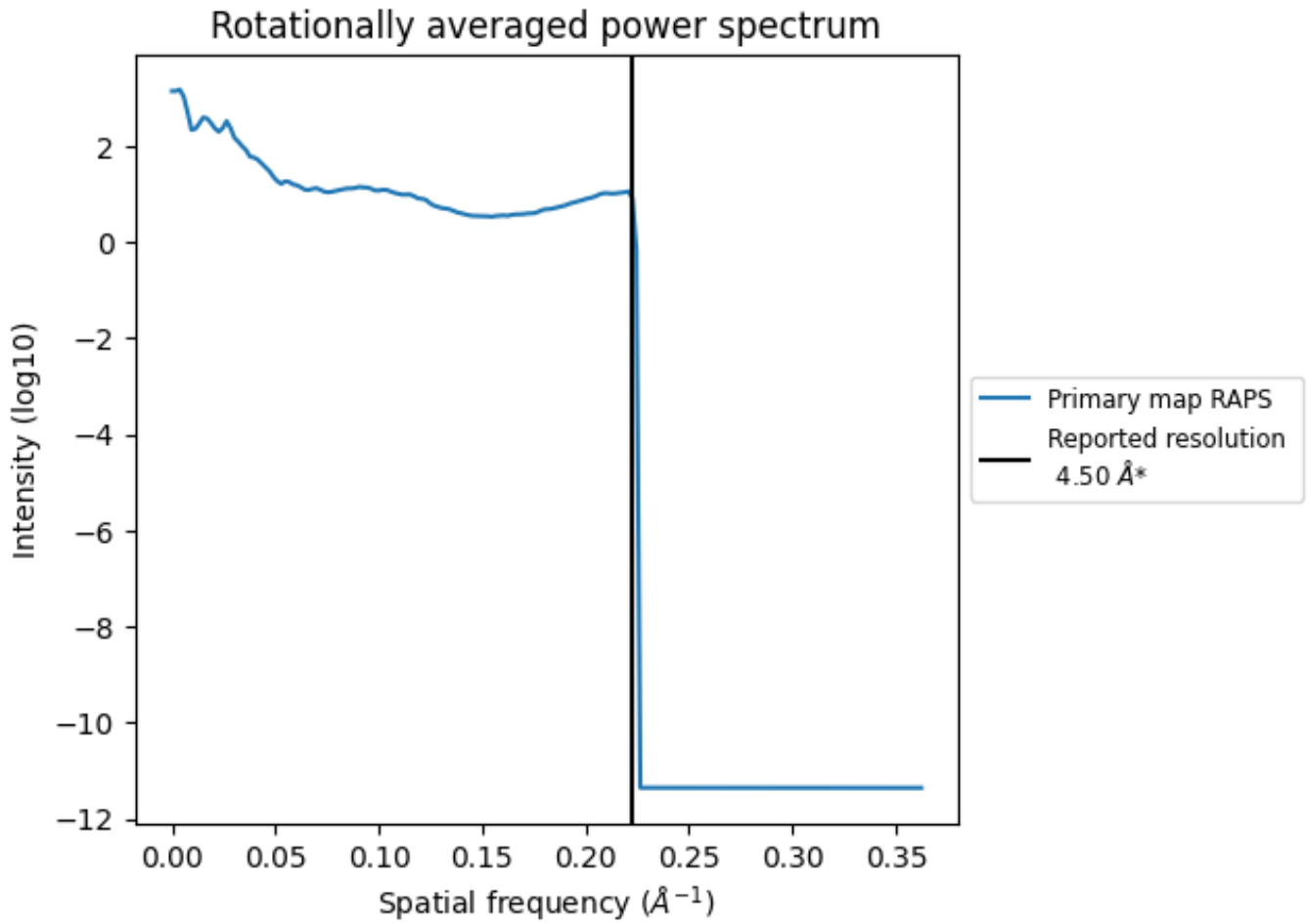
7.2 Volume estimate



The volume at the recommended contour level is 813 nm^3; this corresponds to an approximate mass of 734 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 0.222 Å^{-1}

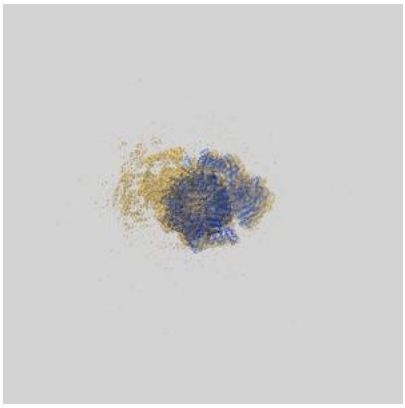
8 Fourier-Shell correlation

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

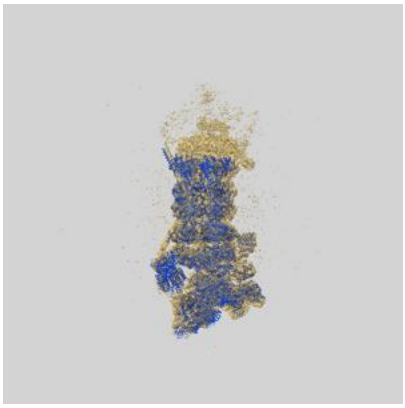
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3535 and PDB model 6FVU. Per-residue inclusion information can be found in section 3 on page 13.

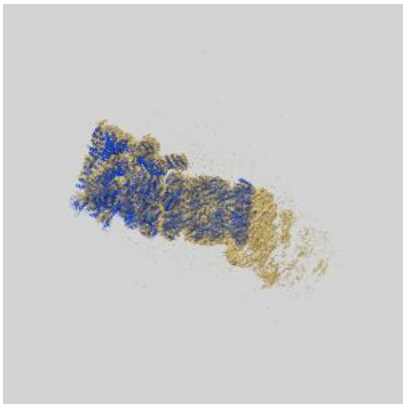
9.1 Map-model overlay



X



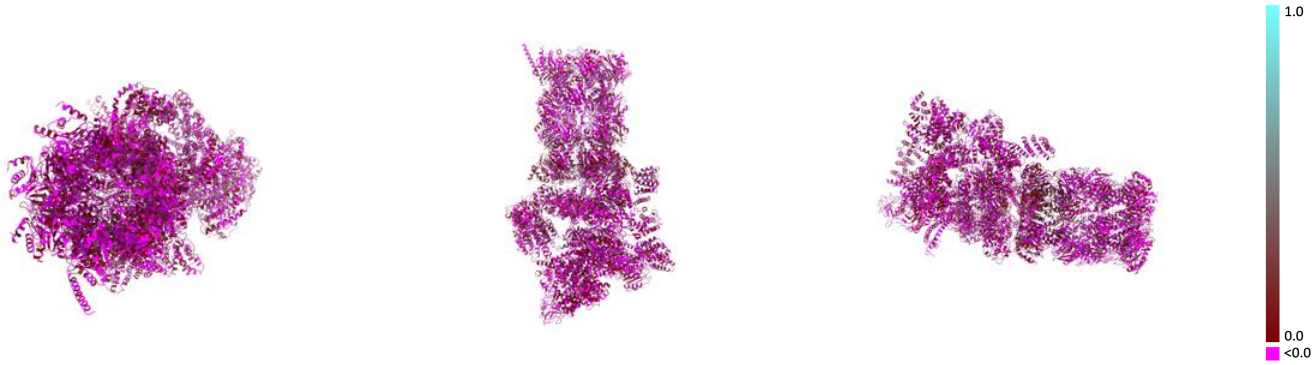
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.017 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.

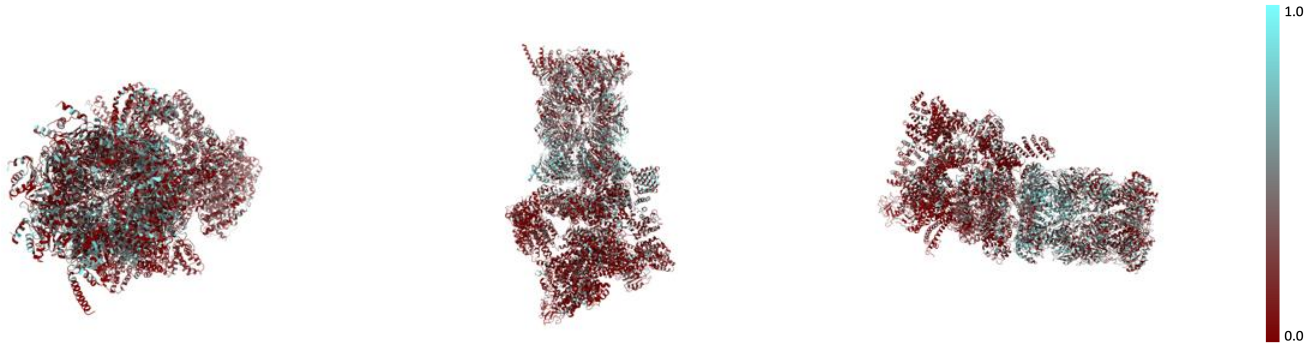
9.2 Q-score mapped to coordinate model



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.

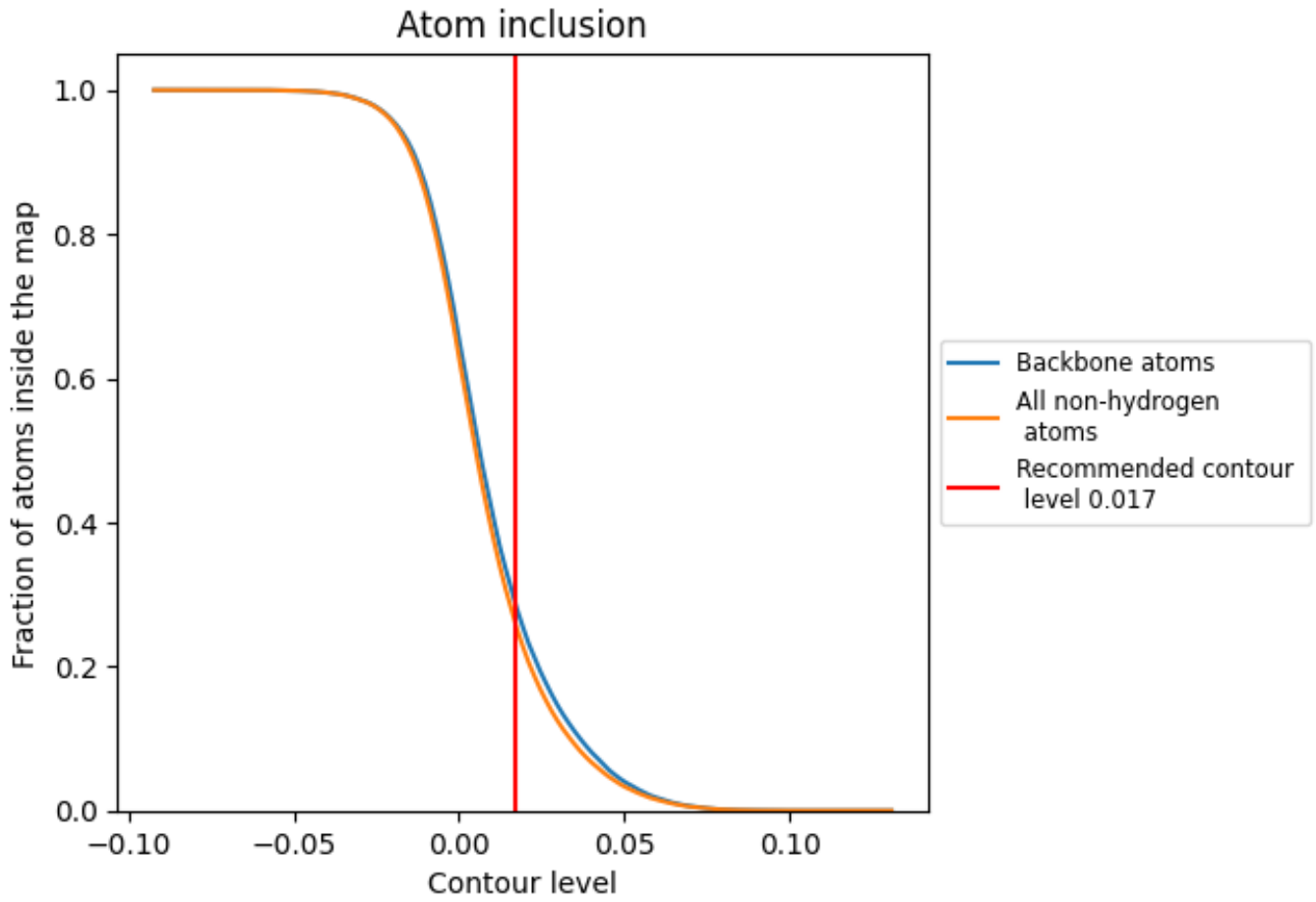
9.3 Atom inclusion mapped to coordinate model



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 (0.017).

9.4 Atom inclusion (i)



At the recommended contour level, 29% of all backbone atoms, 26% 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 (0.017) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.2603	0.0040
1	0.5101	0.0490
2	0.3853	-0.0120
3	0.3541	-0.0510
4	0.4598	0.0150
5	0.4506	0.0080
6	0.3897	-0.0200
7	0.3793	-0.0460
A	0.5482	0.1340
B	0.4571	0.0990
C	0.4362	0.0400
D	0.5718	0.1650
E	0.5240	0.1260
F	0.4123	0.0270
G	0.4262	0.0230
H	0.2041	0.0000
I	0.1898	-0.0150
J	0.1929	0.0020
K	0.2450	0.0040
L	0.2003	-0.0180
M	0.1934	0.0090
N	0.1601	0.0000
O	0.1771	0.0090
P	0.2649	0.0170
Q	0.2027	-0.0040
R	0.1734	-0.0050
S	0.1350	-0.0030
T	0.1005	0.0060
U	0.1758	-0.0150
V	0.1432	-0.0180
W	0.1362	0.0160
X	0.0059	0.0150
Y	0.2116	0.0080
Z	0.0565	0.0060
a	0.2952	-0.0420

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	0.2802	-0.0060
c	0.3262	0.0140
d	0.2582	-0.0230
e	0.2512	-0.0090
f	0.2777	-0.0350
g	0.3173	-0.0010
h	0.3005	-0.0610
i	0.3192	-0.0170
j	0.3246	-0.0420
k	0.3061	-0.0220
l	0.3288	-0.0330
m	0.3200	-0.0410
n	0.3401	-0.0260