Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 02:06 pm GMT

PDB ID	:	5MPC
EMDB ID	:	EMD-3537
Title	:	26S proteasome in presence of BeFx (s4)
Authors	:	Wehmer, M.; Rudack, T.; Beck, F.; Aufderheide, A.; Pfeifer, G.; Plitzko, J.M.; Foerster, F.; Schulten, K.; Baumeister, W.; Sakata, E.
Deposited on	:	2016-12-16
Resolution	:	7.70 Å(reported)

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

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

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

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

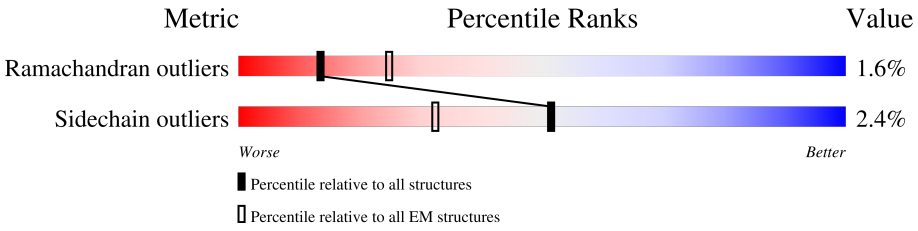
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.70 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	252	15% 73% 21%
1	a	252	21% 72% 21%
2	B	250	20% 81% 17%
2	b	250	30% 78% 19%
3	C	258	22% 72% 19% 5%
3	c	258	24% 69% 20% 5% 5%
4	D	254	19% 70% 21% 6%
4	d	254	18% 70% 20% 6%
5	E	260	19% 73% 17% 7%

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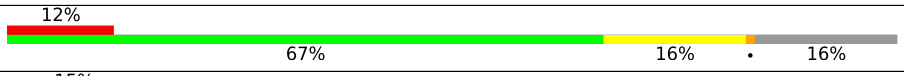
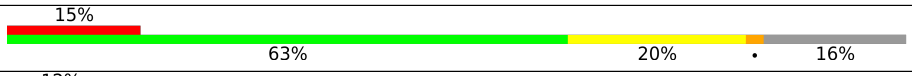
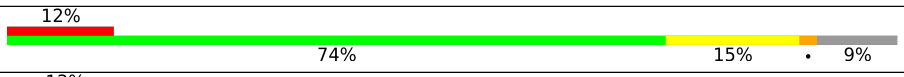
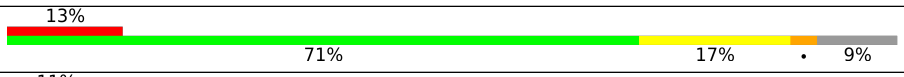
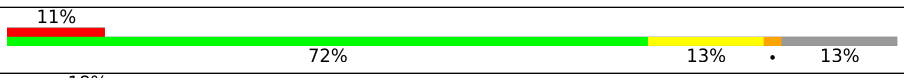
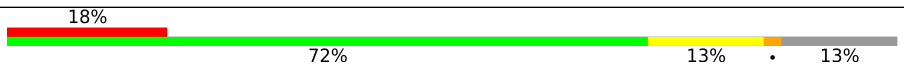
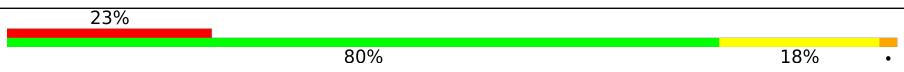
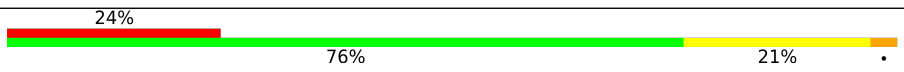
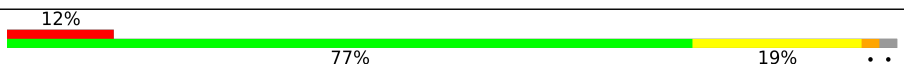
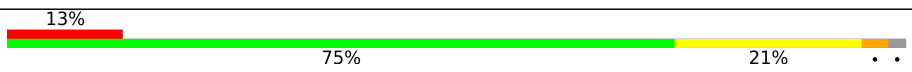
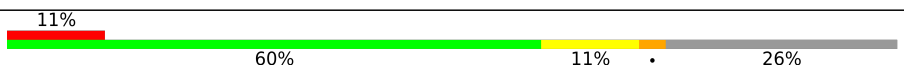
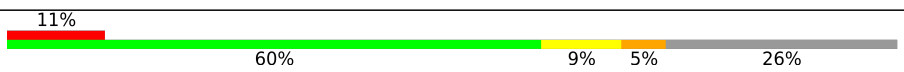
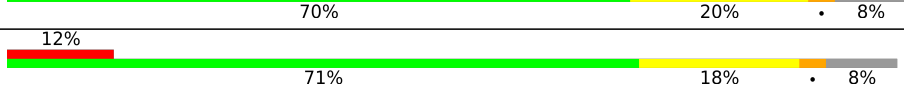
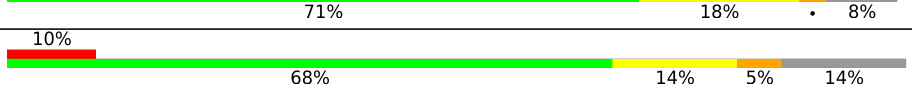
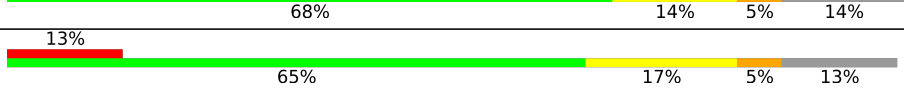
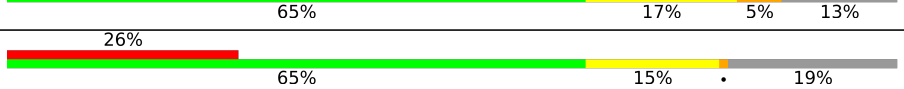
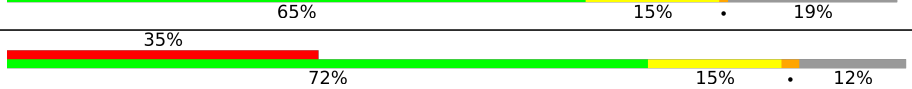
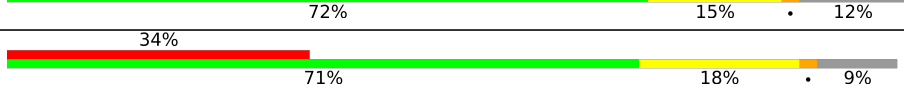
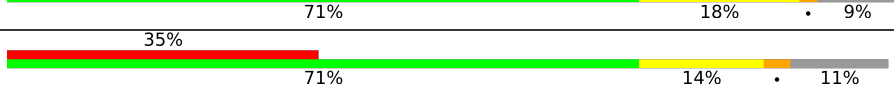
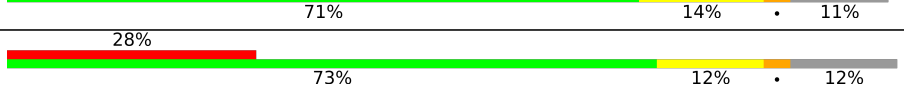
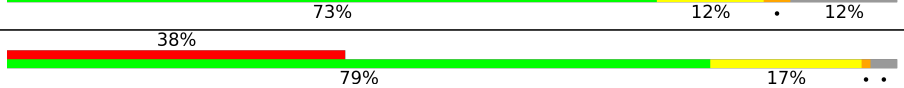
Mol	Chain	Length	Quality of chain
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	1	215	
8	h	215	
9	2	261	
9	i	261	
10	3	205	
10	j	205	
11	4	198	
11	k	198	
12	5	287	
12	l	287	
13	6	241	
13	m	241	
14	7	266	
14	n	266	
15	H	467	
16	I	437	
17	K	428	
18	L	437	
19	M	434	
20	J	405	

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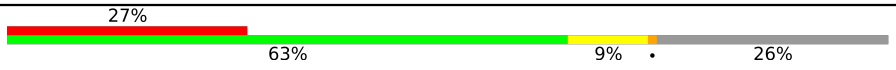
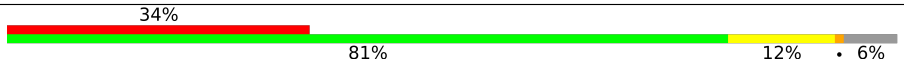
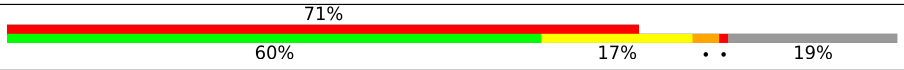
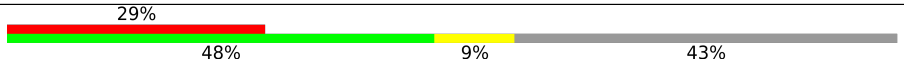
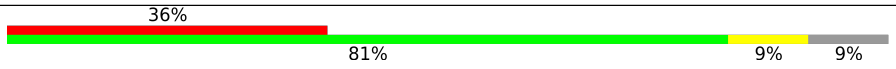
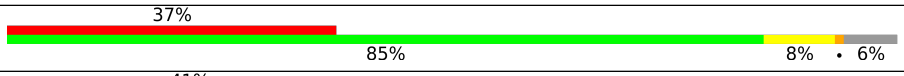
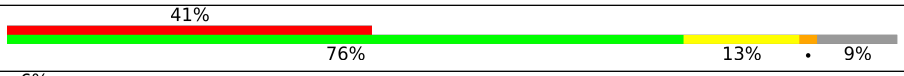
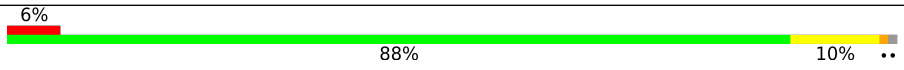
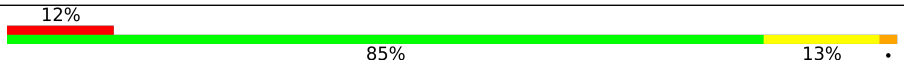
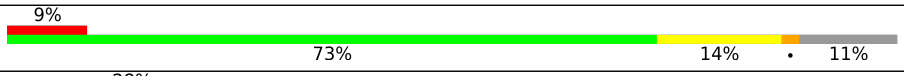
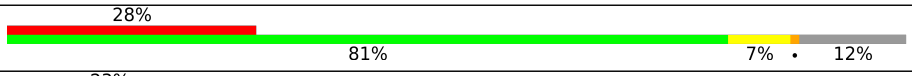
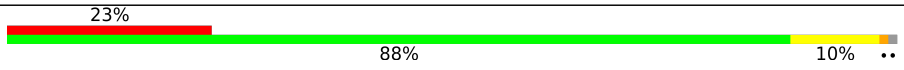
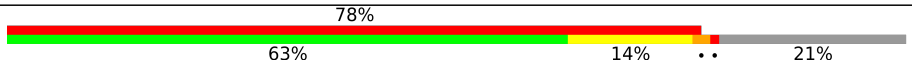
Mol	Chain	Length	Quality of chain
21	W	268	
22	V	306	
23	T	274	
24	X	156	
25	Y	89	
26	Z	993	
27	N	945	
28	S	523	
29	P	445	
30	Q	434	
31	R	429	
32	U	338	
33	O	393	
34	8	499	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 112042 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	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
1	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		
2	B	250	Total	C	N	O	S	0	0
			1915	1219	315	377	4		

- 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
			1904	1201	321	379	3		
3	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		
4	D	240	Total	C	N	O	S	0	0
			1881	1176	329	372	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	242	Total	C	N	O	S	0	0
			1861	1162	314	378	7		
5	E	242	Total	C	N	O	S	0	0
			1861	1162	314	378	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	233	Total	C	N	O	S	0	0
			1795	1129	312	350	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	243	Total	C	N	O	S	0	0
			1892	1203	329	356	4		
7	G	243	Total	C	N	O	S	0	0
			1892	1203	329	356	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
			1719	1082	298	332	7		
9	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	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
			1561	992	264	299	6		
11	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	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
			1815	1148	311	349	7		
14	7	229	Total	C	N	O	S	0	0
			1790	1133	306	344	7		

- Molecule 15 is a protein called 26S protease regulatory subunit 7 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	H	380	Total	C	N	O	S	0	0
			2967	1869	531	551	16		

- Molecule 16 is a protein called 26S protease regulatory subunit 4 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	I	385	Total	C	N	O	S	0	0
			3022	1899	508	598	17		

- Molecule 17 is a protein called 26S protease regulatory subunit 6B homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	K	389	Total	C	N	O	S	0	0
			3078	1933	540	595	10		

- Molecule 18 is a protein called 26S protease subunit RPT4.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	L	388	Total	C	N	O	S	0	0
			3082	1942	548	580	12		

- Molecule 19 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	M	381	Total	C	N	O	S	0	0
			2986	1870	524	580	12		

- Molecule 20 is a protein called 26S protease regulatory subunit 8 homolog.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	J	393	Total	C	N	O	S	0	0
			3089	1944	552	576	17		

- Molecule 21 is a protein called 26S proteasome regulatory subunit RPN10.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	197	Total	C	N	O	S	0	0
			1534	962	269	300	3		

- Molecule 22 is a protein called Ubiquitin carboxyl-terminal hydrolase RPN11.

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

- Molecule 23 is a protein called 26S proteasome regulatory subunit RPN12.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	T	266	Total	C	N	O	S	0	0
			2192	1405	349	432	6		

- Molecule 24 is a protein called 26S proteasome regulatory subunit RPN13.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	X	127	Total	C	N	O	S	0	0
			1032	664	169	195	4		

- Molecule 25 is a protein called 26S proteasome complex subunit SEM1.

Mol	Chain	Residues	Atoms				AltConf	Trace
25	Y	51	Total	C	N	O	0	0
			435	264	69	102		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	Z	906	Total	C	N	O	S	0	0
			7005	4416	1150	1409	30		

- Molecule 27 is a protein called 26S proteasome regulatory subunit RPN2.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	N	890	Total	C	N	O	S	0	0
			6882	4373	1156	1325	28		

- Molecule 28 is a protein called 26S proteasome regulatory subunit RPN3.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	S	475	Total	C	N	O	S	0	0
			3894	2488	653	738	15		

- Molecule 29 is a protein called 26S proteasome regulatory subunit RPN5.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	P	440	Total	C	N	O	S	0	0
			3608	2297	604	697	10		

- Molecule 30 is a protein called 26S proteasome regulatory subunit RPN6.

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

- Molecule 31 is a protein called 26S proteasome regulatory subunit RPN7.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	R	381	Total	C	N	O	S	0	0
			3060	1955	502	593	10		

- Molecule 32 is a protein called 26S proteasome regulatory subunit RPN8.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	U	298	Total	C	N	O	S	0	0
			2373	1496	404	466	7		

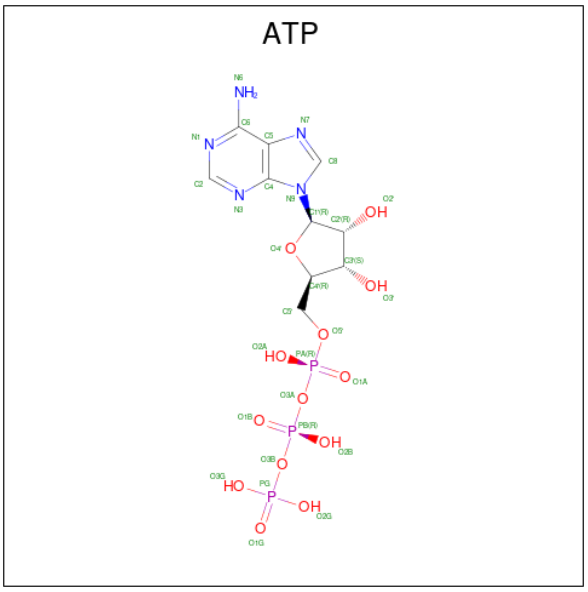
- Molecule 33 is a protein called 26S proteasome regulatory subunit RPN9.

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

- Molecule 34 is a protein called Ubiquitin carboxyl-terminal hydrolase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	395	Total	C	N	O	S	0	0
			3219	2029	554	623	13		

- Molecule 35 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

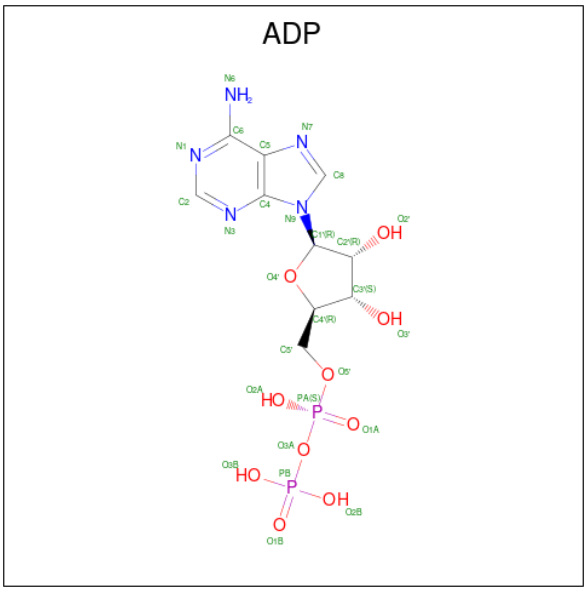


Mol	Chain	Residues	Atoms					AltConf
35	H	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	M	1	Total	C	N	O	P	0
			31	10	5	13	3	
35	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

- Molecule 36 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

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

- Molecule 37 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



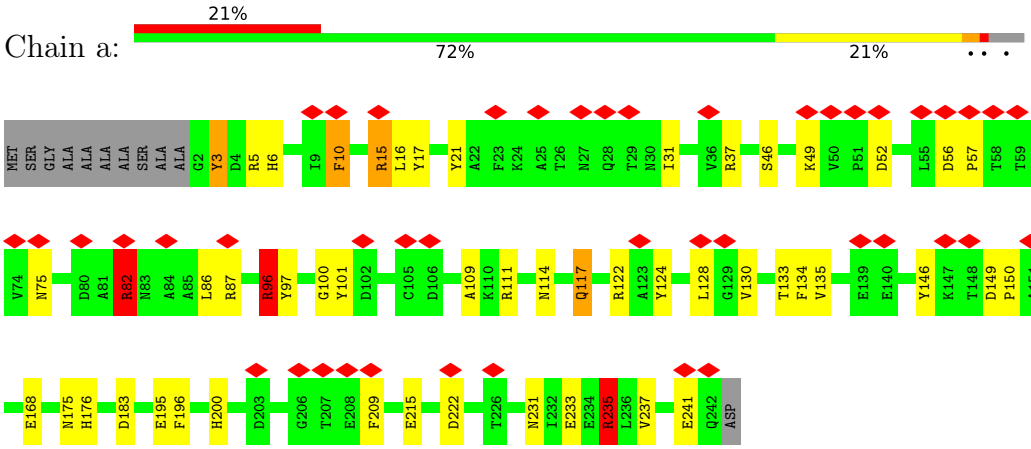
Mol	Chain	Residues	Atoms					AltConf
37	K	1	Total	C	N	O	P	0
			27	10	5	10	2	
37	L	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots

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

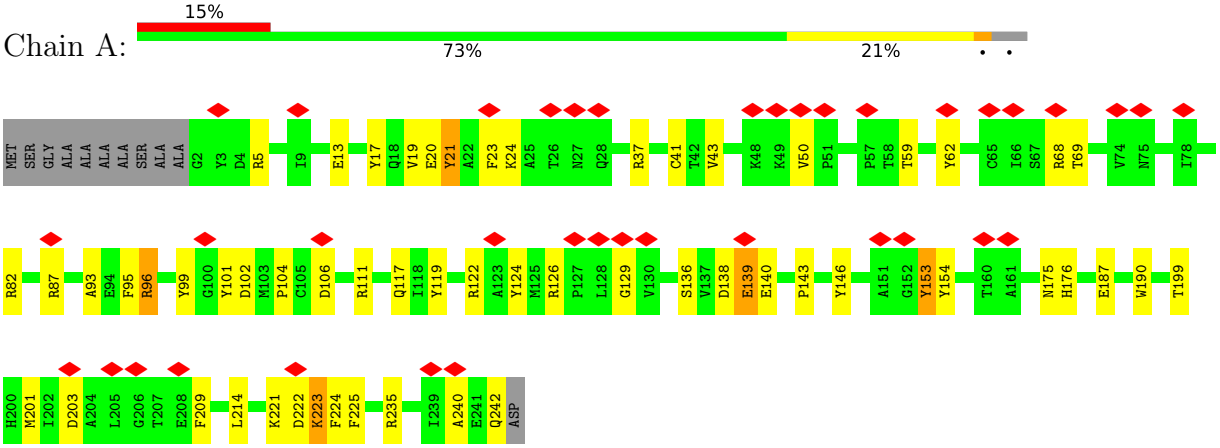
• Molecule 1: Proteasome subunit alpha type-1

Chain a:



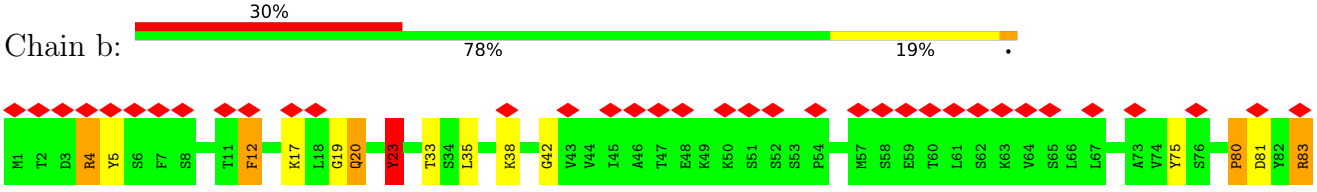
• Molecule 1: Proteasome subunit alpha type-1

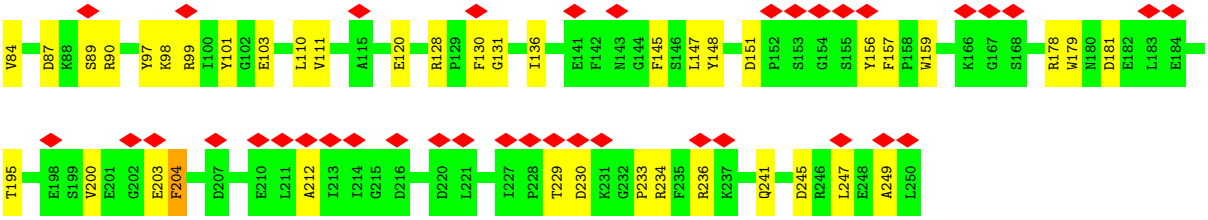
Chain A:



• Molecule 2: Proteasome subunit alpha type-2

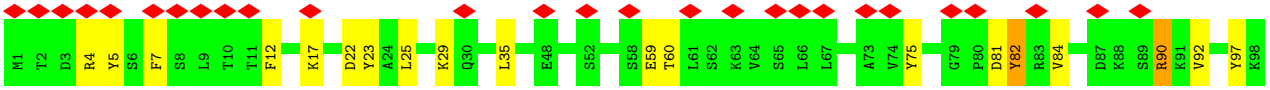
Chain b:





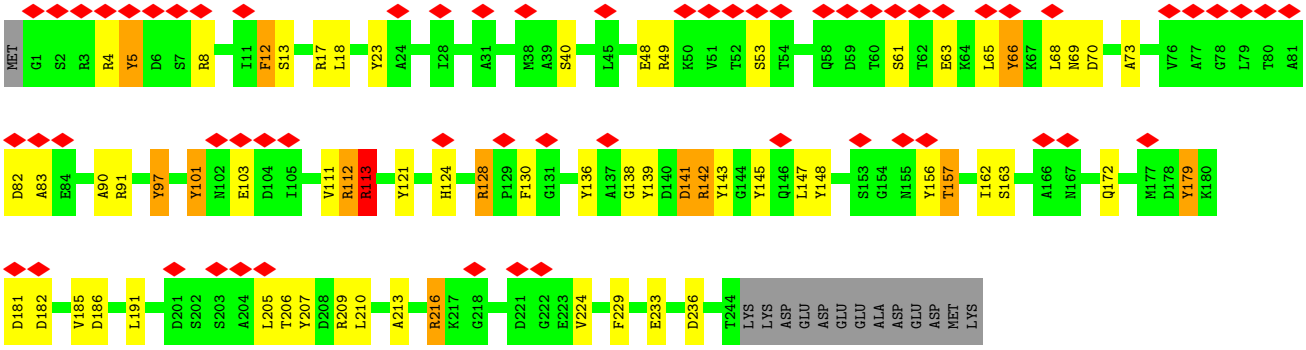
• Molecule 2: Proteasome subunit alpha type-2

Chain B:



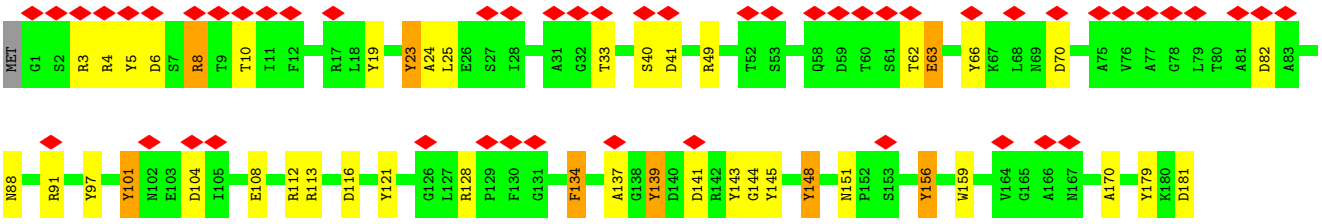
• Molecule 3: Proteasome subunit alpha type-3

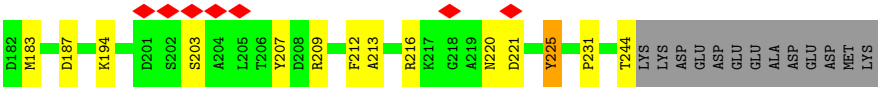
Chain c:



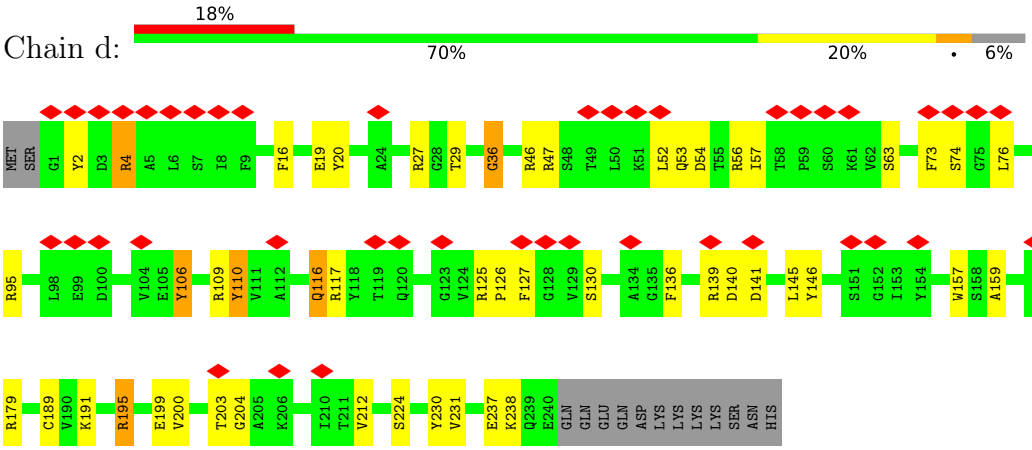
• Molecule 3: Proteasome subunit alpha type-3

Chain C:

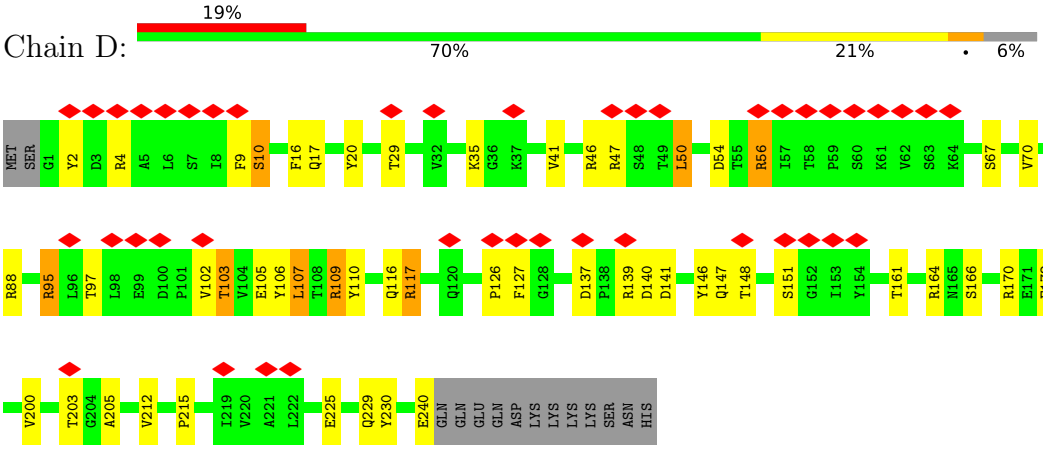




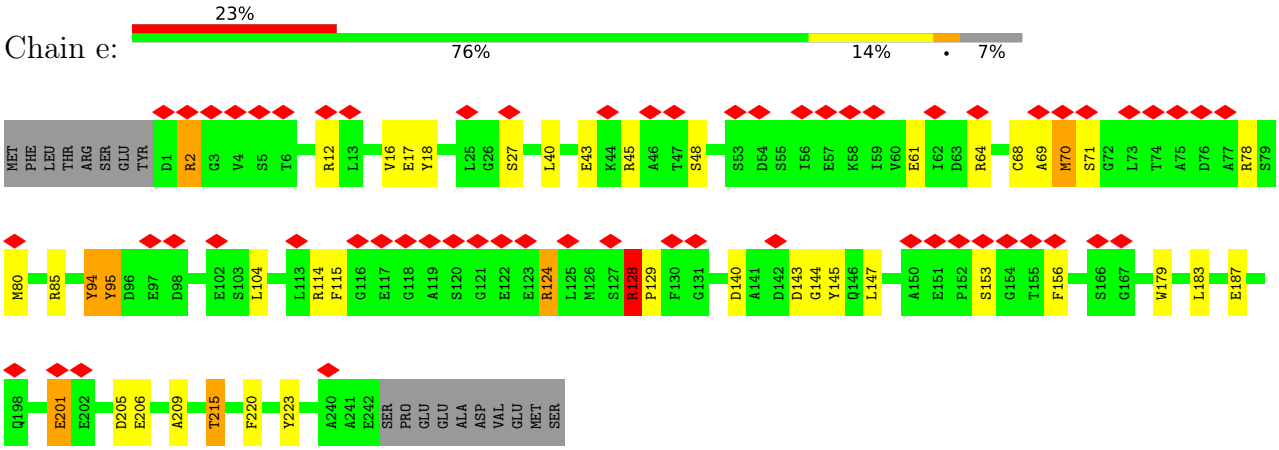
• Molecule 4: Proteasome subunit alpha type-4



• Molecule 4: Proteasome subunit alpha type-4

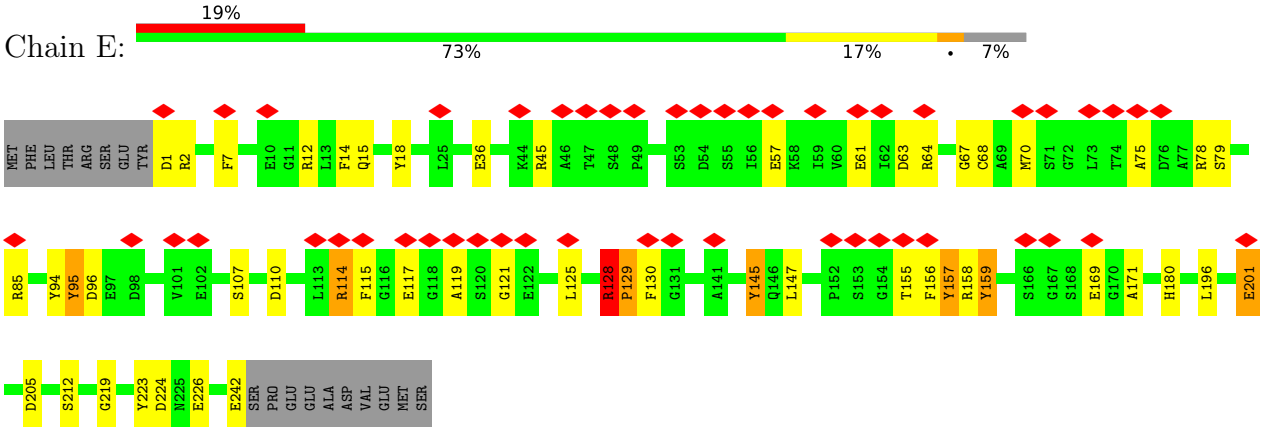


• Molecule 5: Proteasome subunit alpha type-5



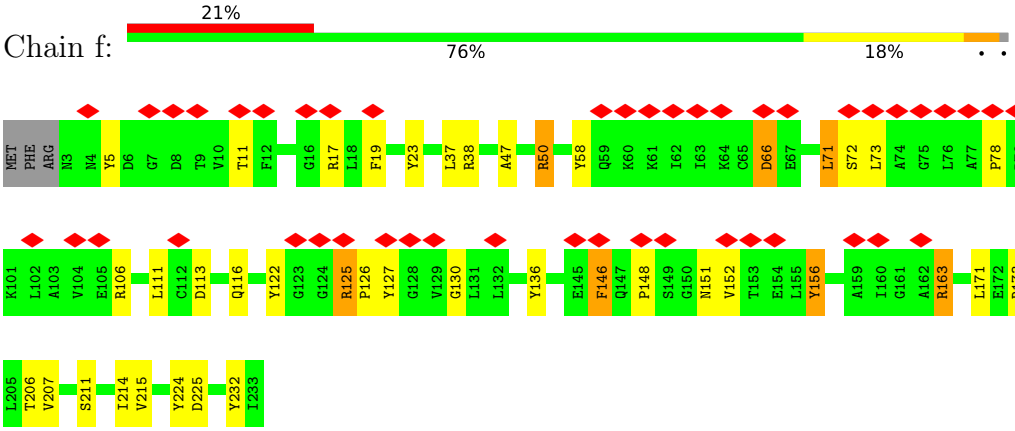
• Molecule 5: Proteasome subunit alpha type-5

Chain E:



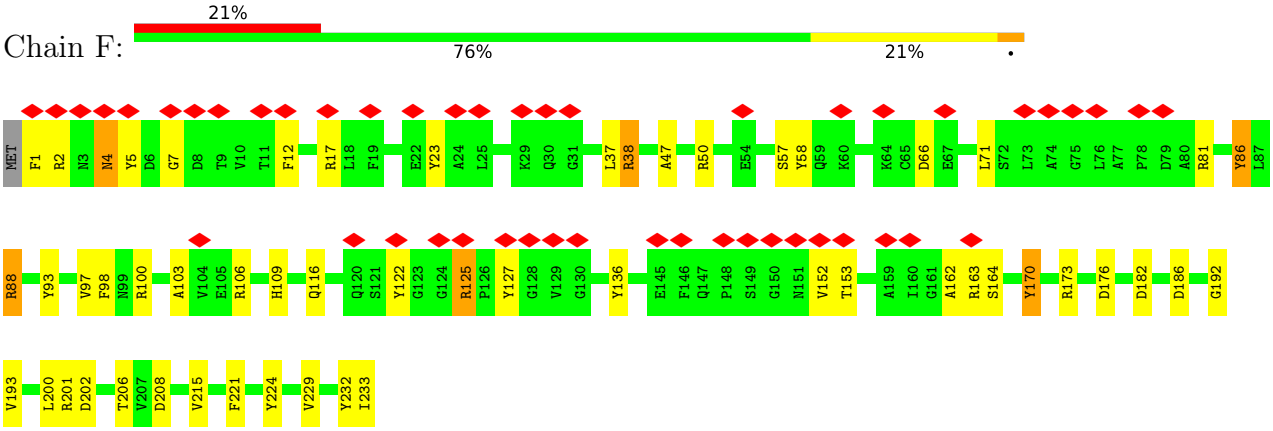
• Molecule 6: Proteasome subunit alpha type-6

Chain f:



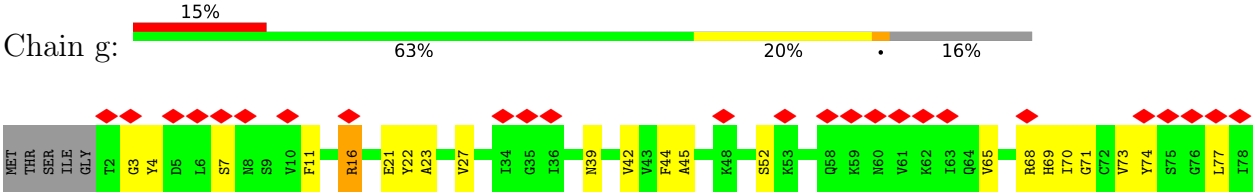
• Molecule 6: Proteasome subunit alpha type-6

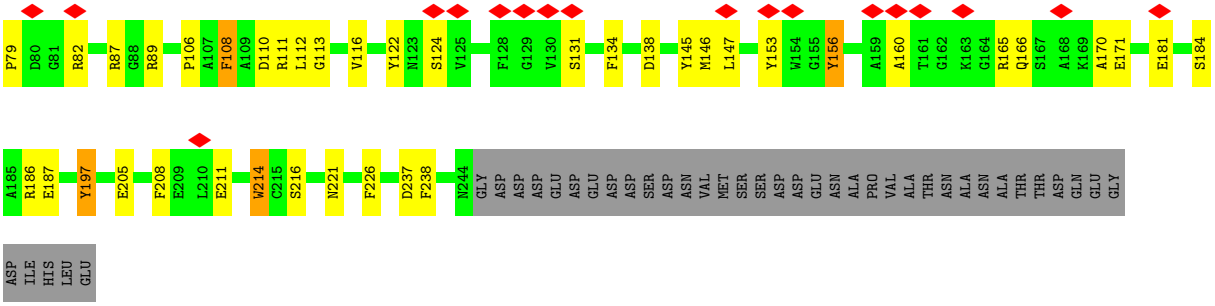
Chain F:



• Molecule 7: Probable proteasome subunit alpha type-7

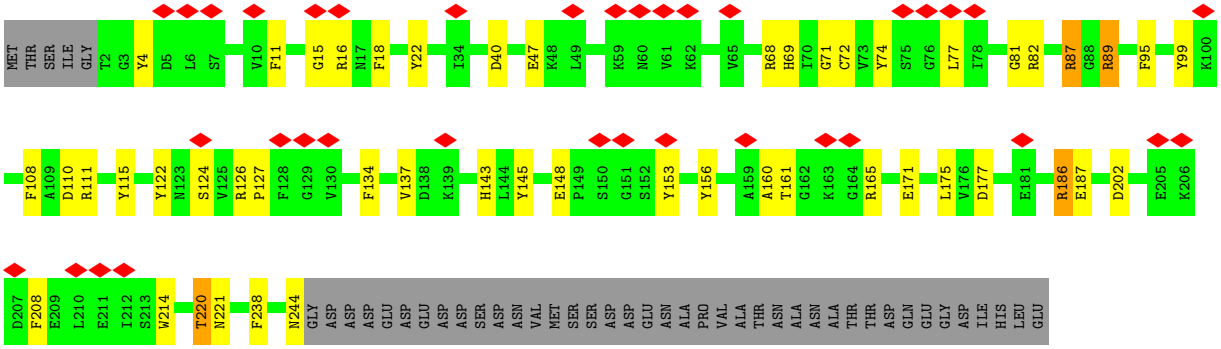
Chain g:





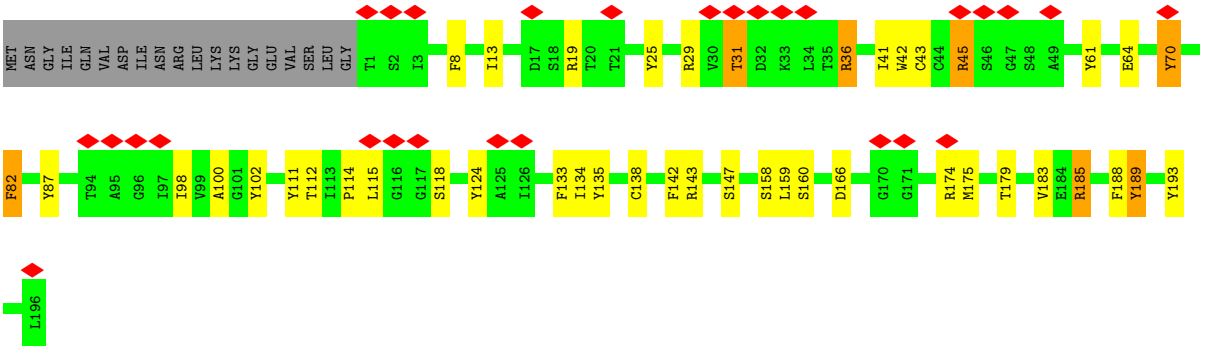
• Molecule 7: Probable proteasome subunit alpha type-7

Chain G:



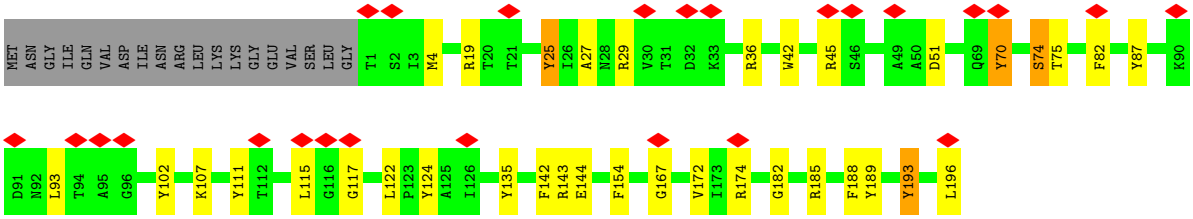
• Molecule 8: Proteasome subunit beta type-1

Chain h:



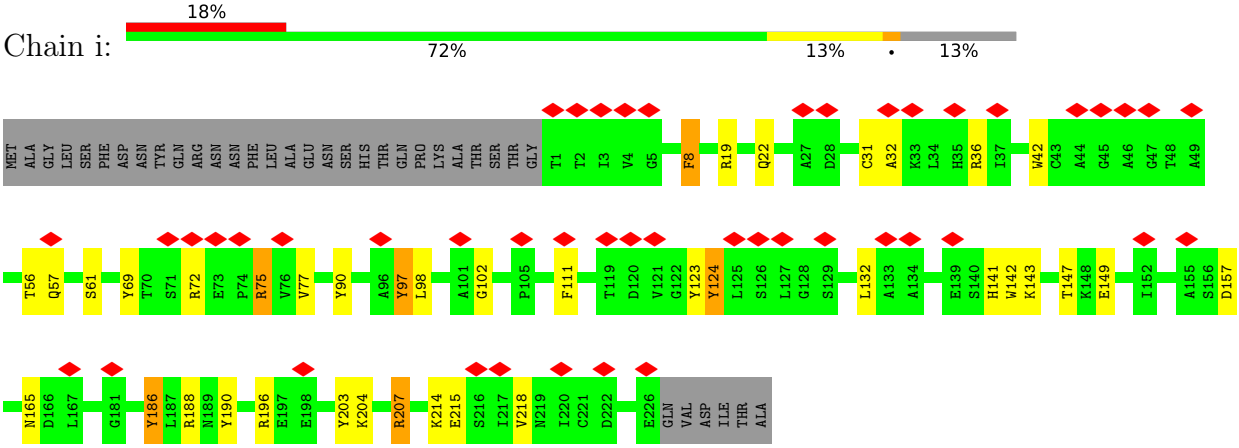
• Molecule 8: Proteasome subunit beta type-1

Chain 1:



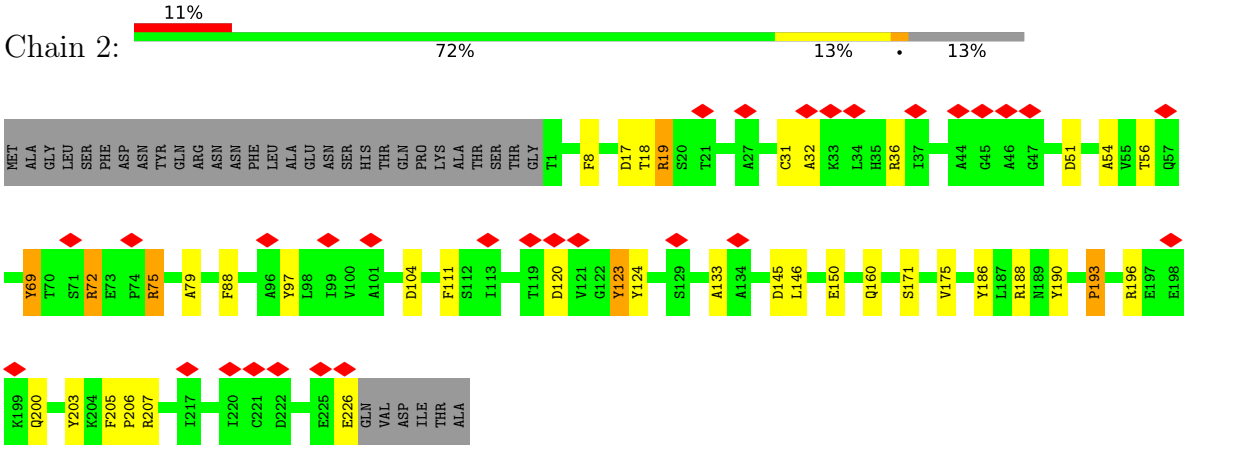
• Molecule 9: Proteasome subunit beta type-2

Chain i:



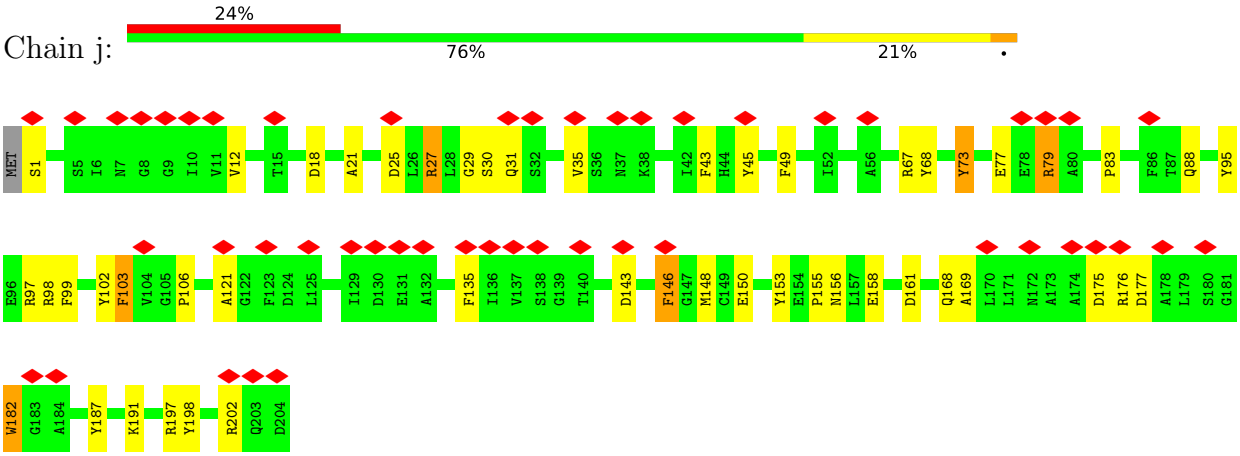
• Molecule 9: Proteasome subunit beta type-2

Chain 2:



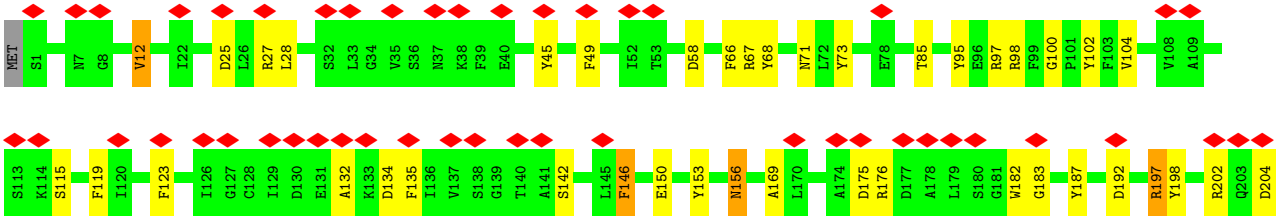
• Molecule 10: Proteasome subunit beta type-3

Chain j:

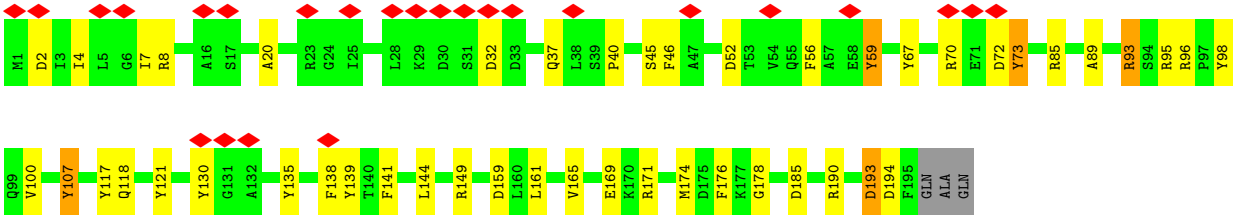


• Molecule 10: Proteasome subunit beta type-3

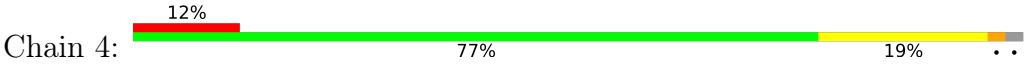
Chain 3:

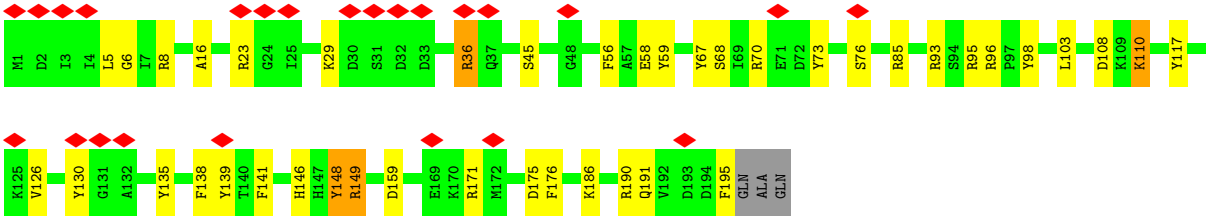


• Molecule 11: Proteasome subunit beta type-4

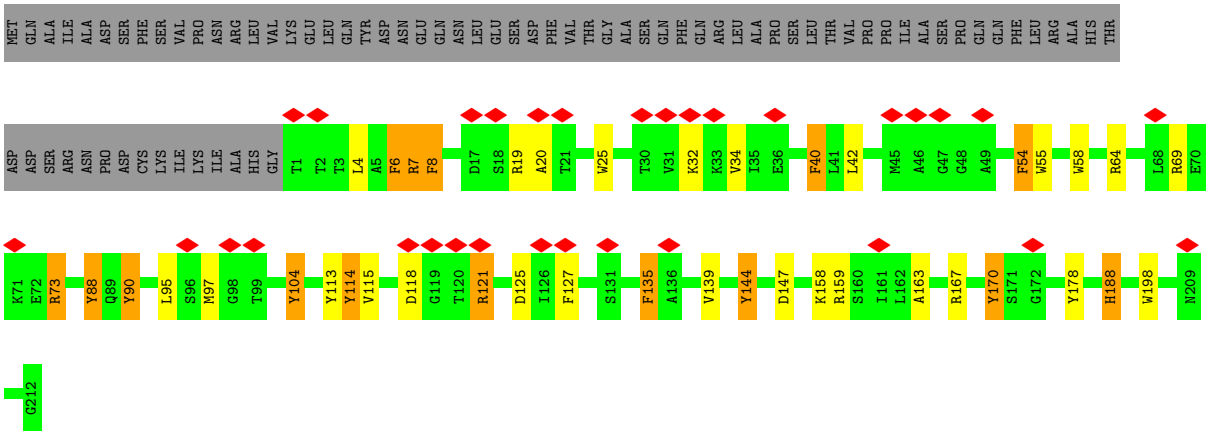


• Molecule 11: Proteasome subunit beta type-4

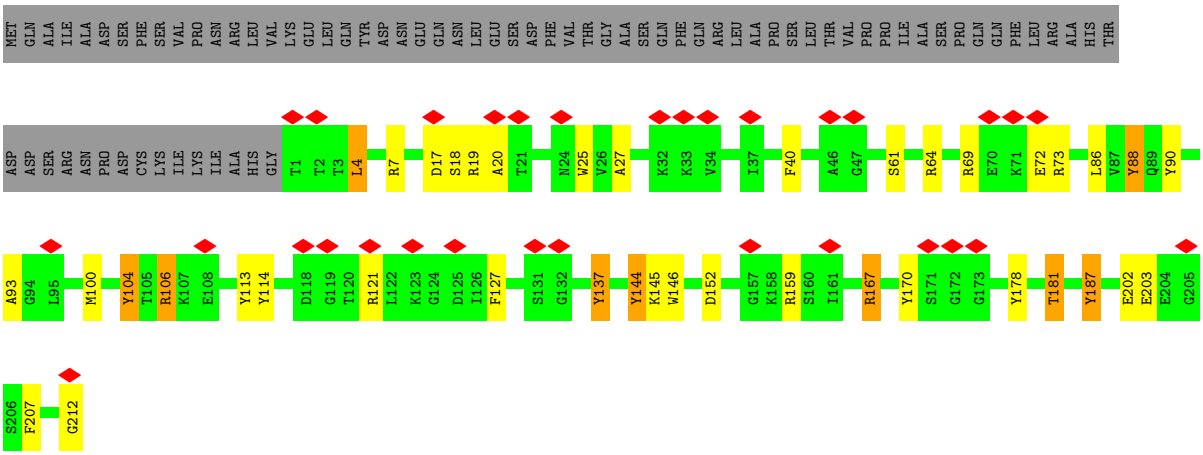




• Molecule 12: Proteasome subunit beta type-5

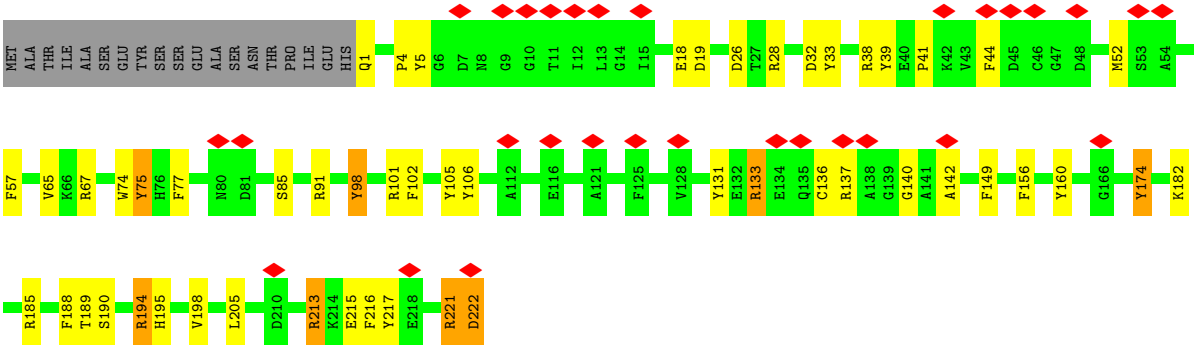


• Molecule 12: Proteasome subunit beta type-5



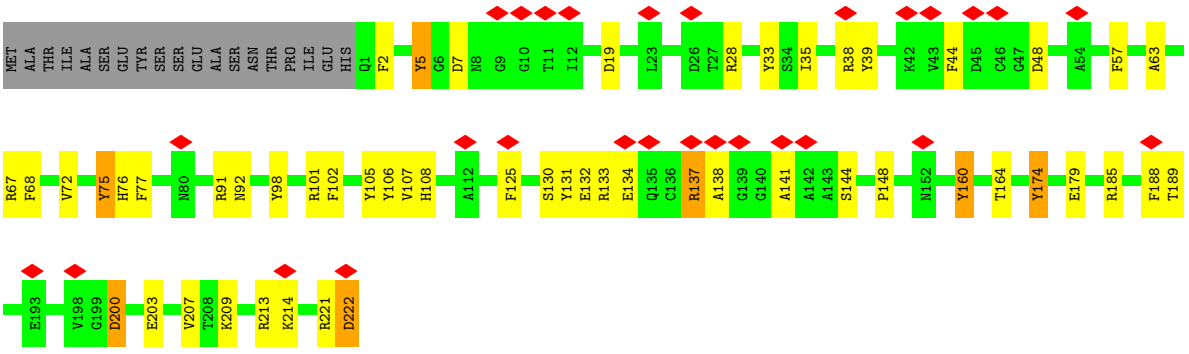
• Molecule 13: Proteasome subunit beta type-6

Chain m:



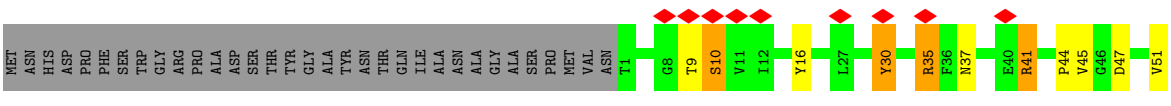
• Molecule 13: Proteasome subunit beta type-6

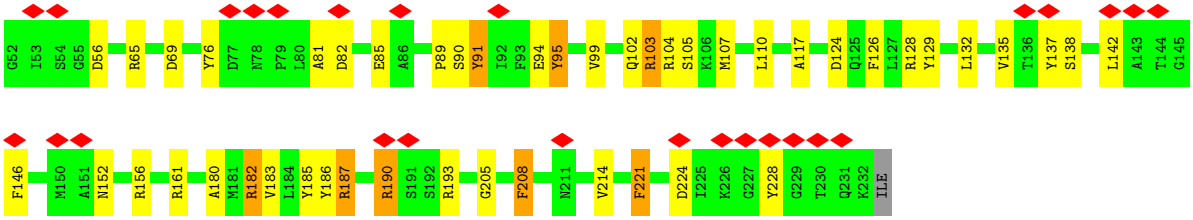
Chain 6:



• Molecule 14: Proteasome subunit beta type-7

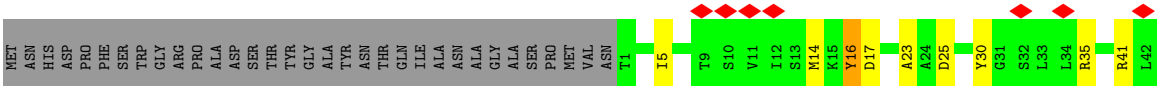
Chain n:

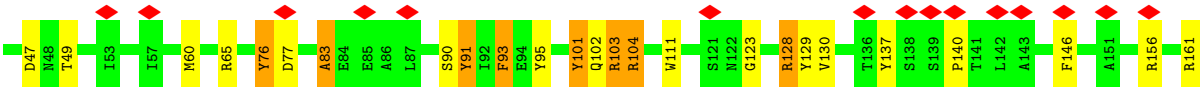


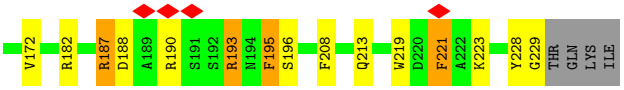


• Molecule 14: Proteasome subunit beta type-7

Chain 7:

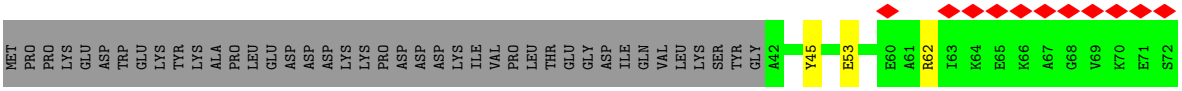


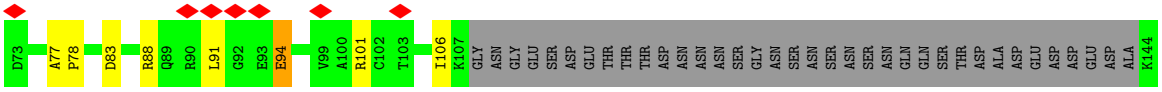


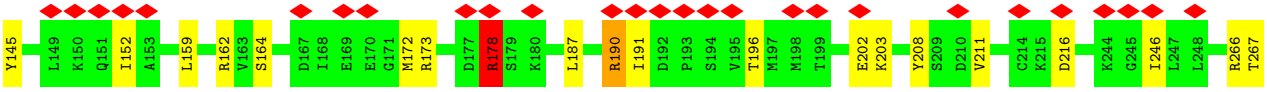


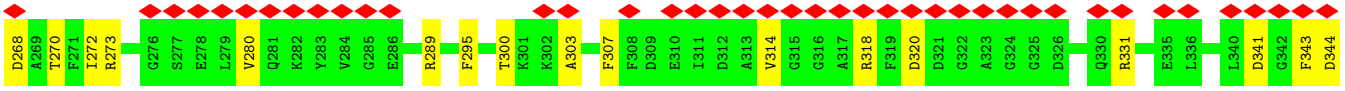
• Molecule 15: 26S protease regulatory subunit 7 homolog

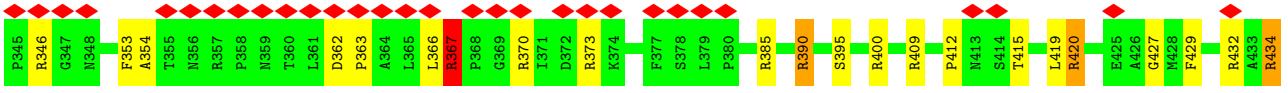
Chain H:

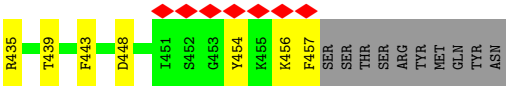






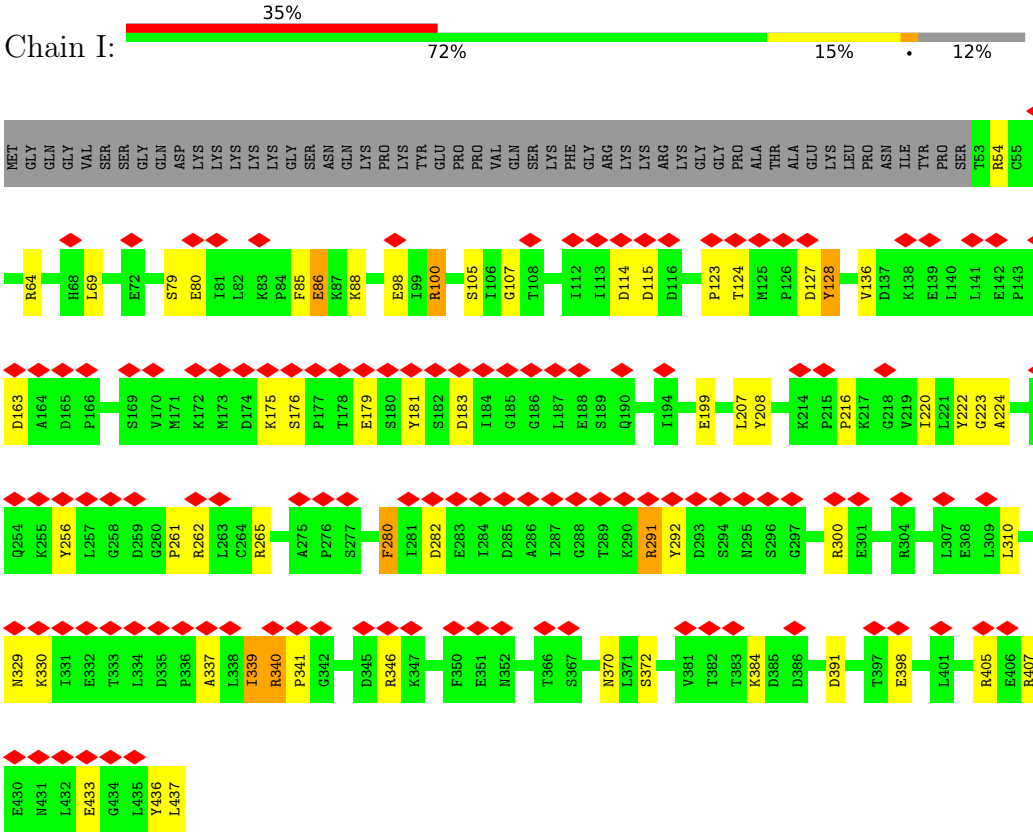






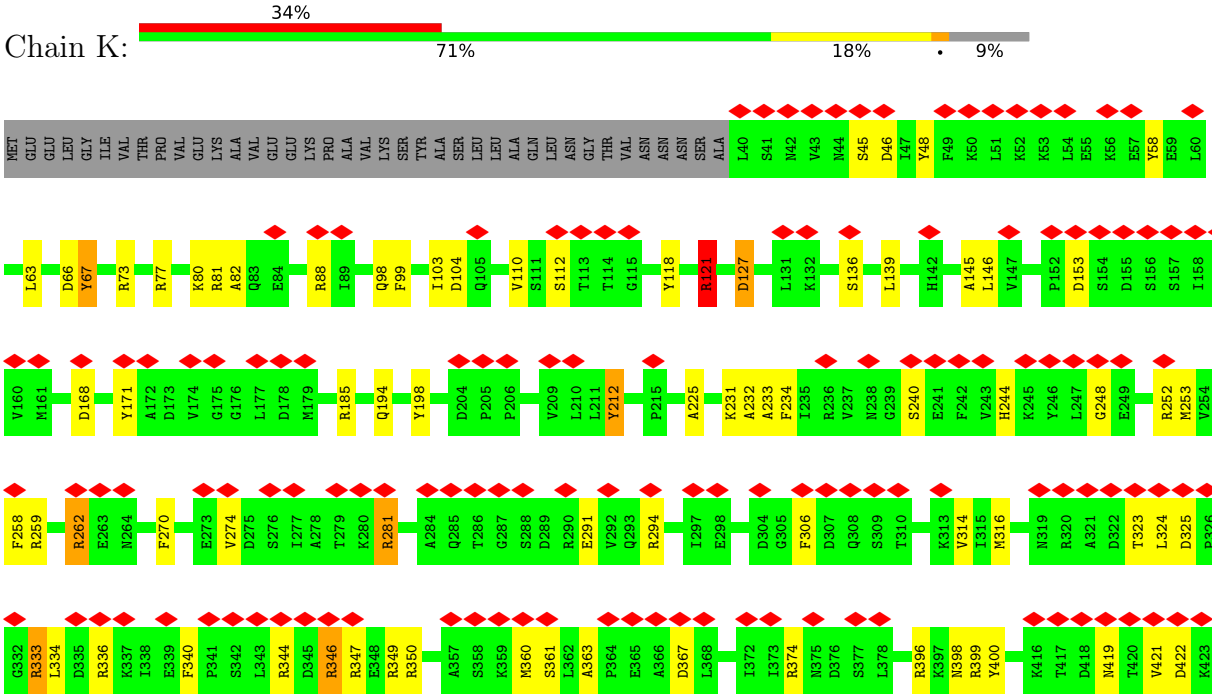
• Molecule 16: 26S protease regulatory subunit 4 homolog

Chain I:



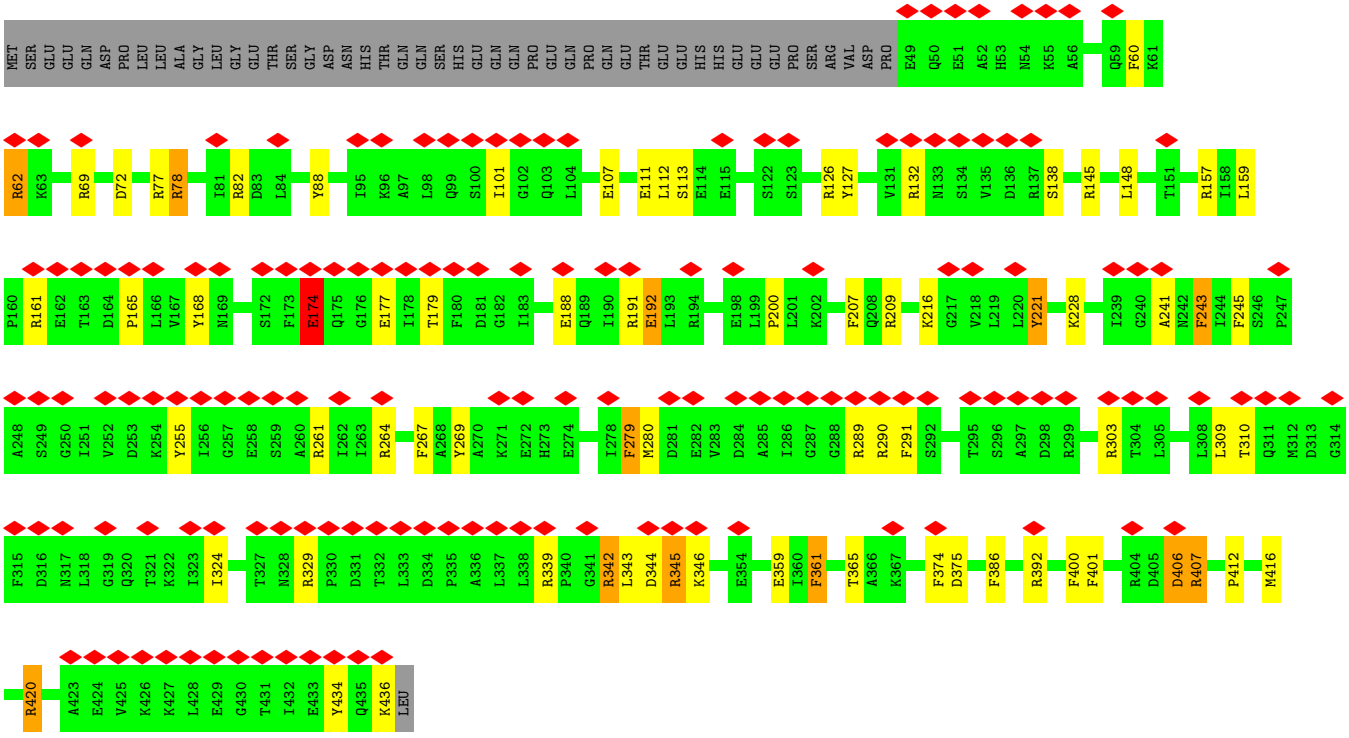
• Molecule 17: 26S protease regulatory subunit 6B homolog

Chain K:



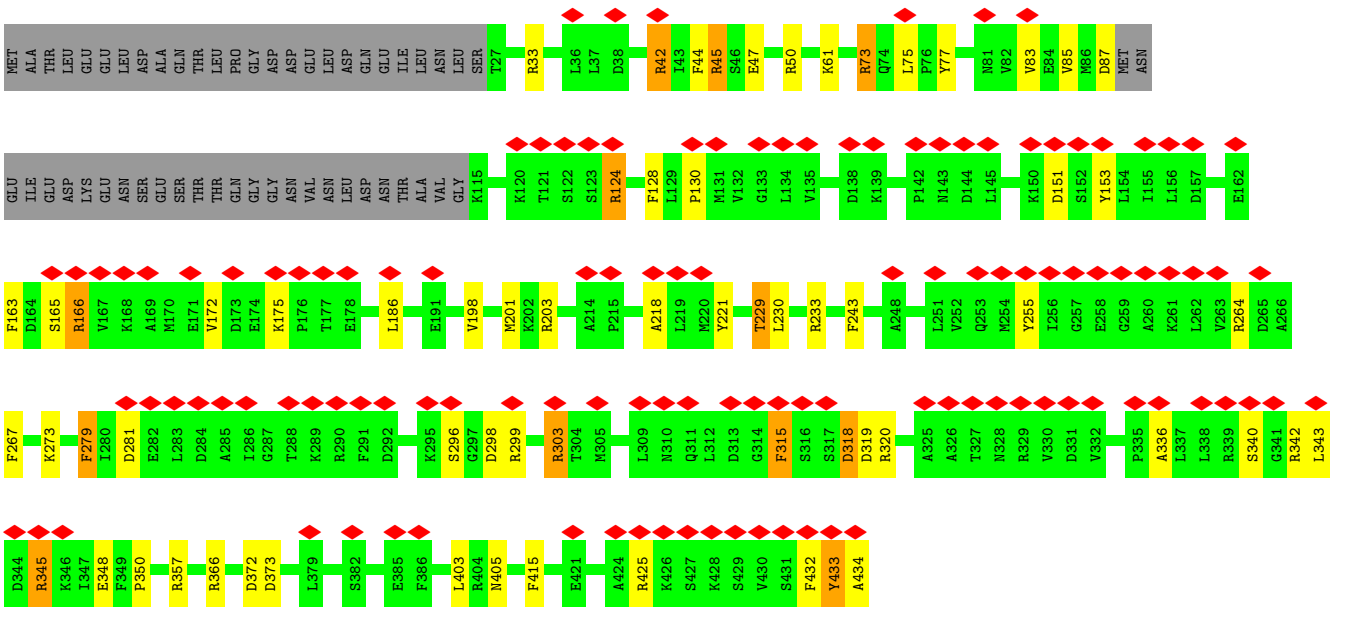
• Molecule 18: 26S protease subunit RPT4

Chain L:



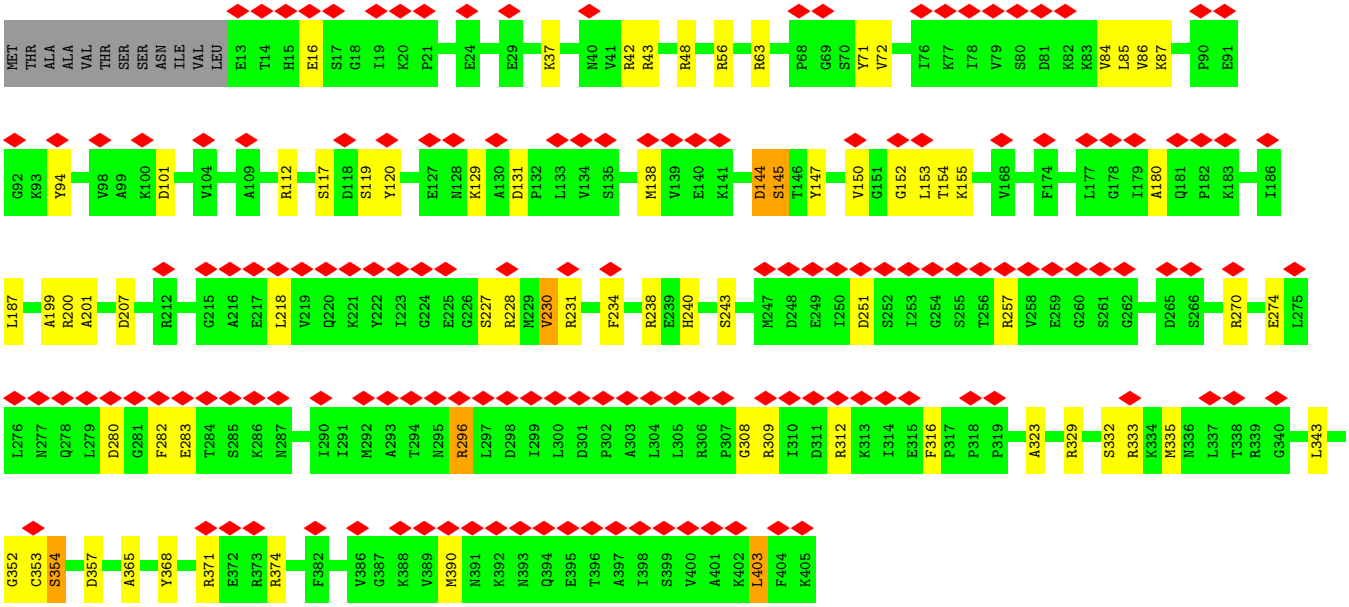
• Molecule 19: 26S protease regulatory subunit 6A

Chain M:



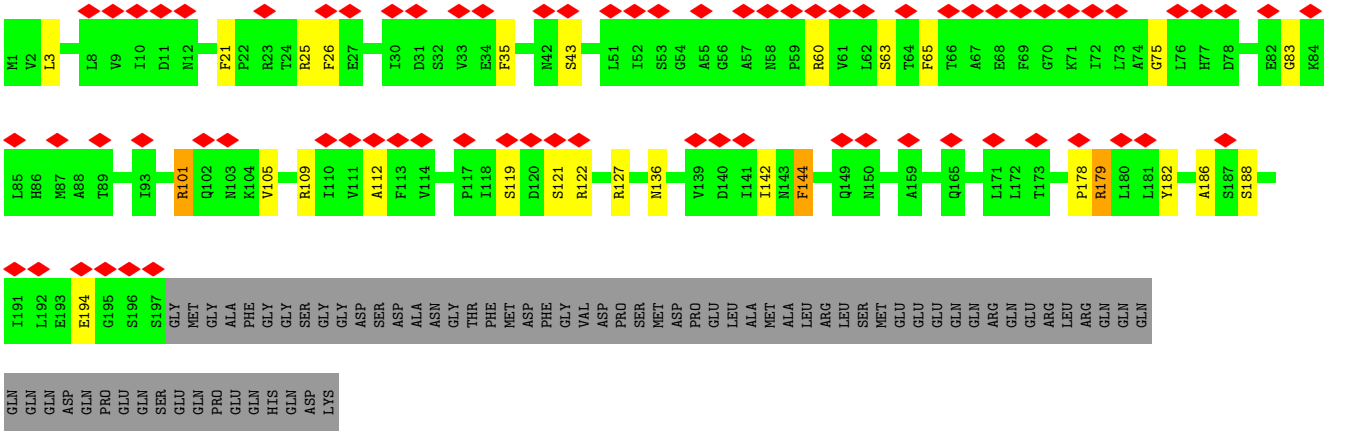
• Molecule 20: 26S protease regulatory subunit 8 homolog

Chain J:



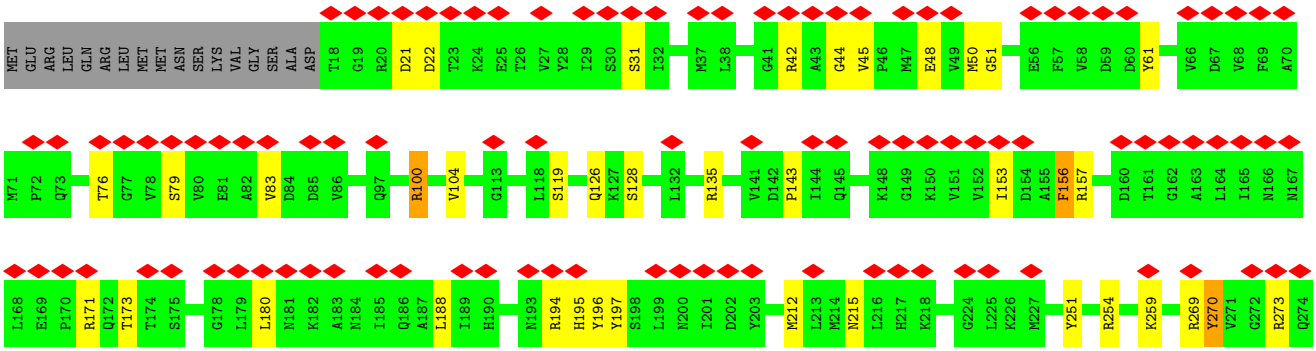
• Molecule 21: 26S proteasome regulatory subunit RPN10

Chain W:



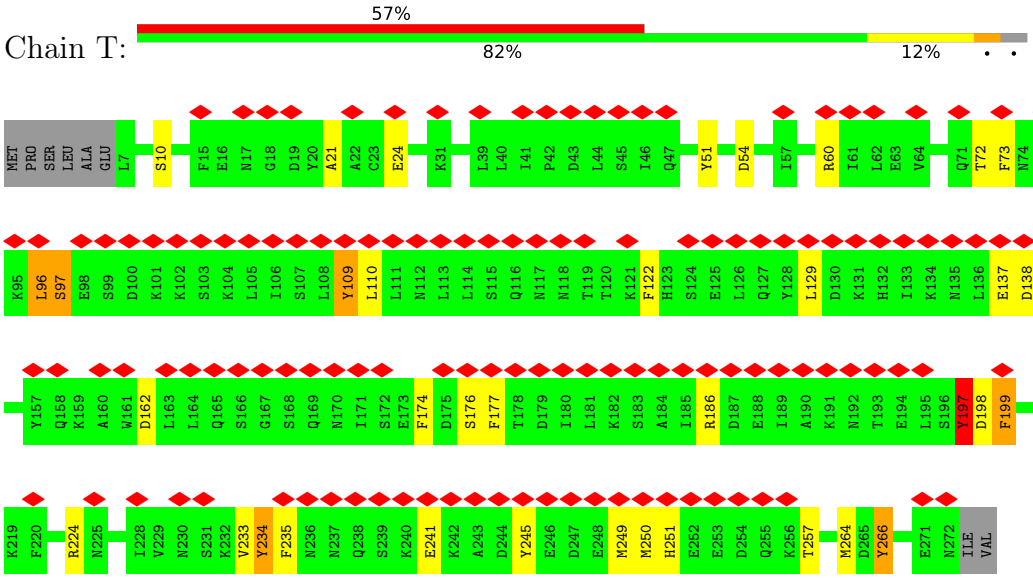
• Molecule 22: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:



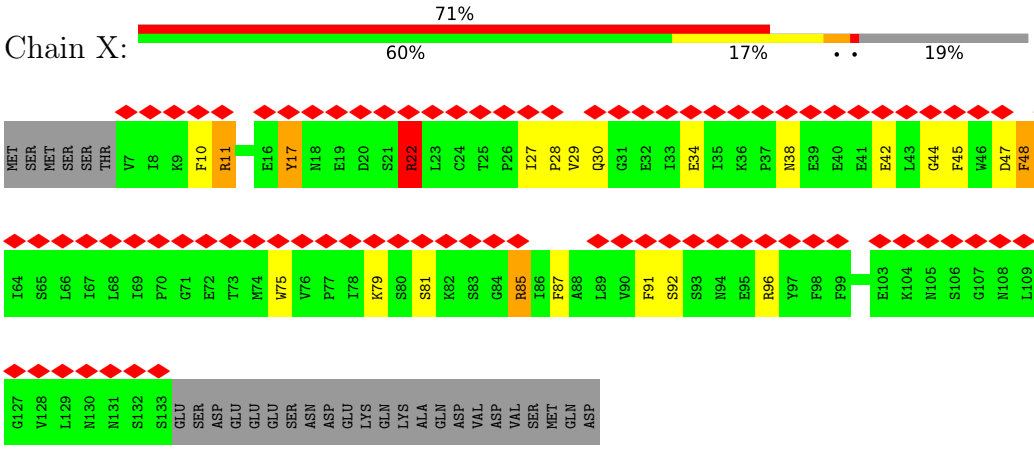
• Molecule 23: 26S proteasome regulatory subunit RPN12

Chain T:



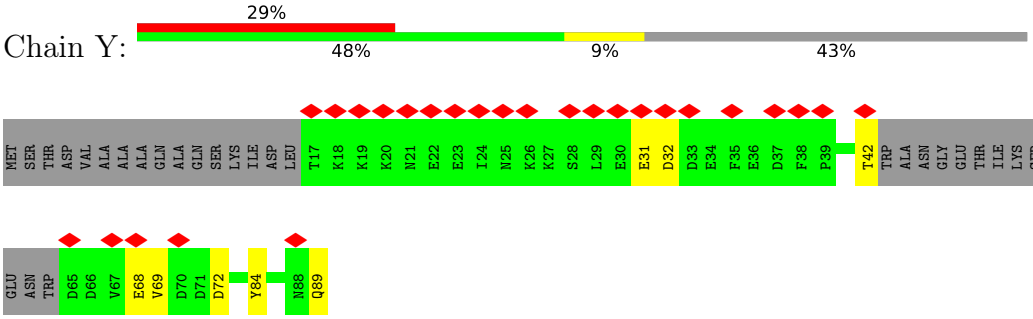
• Molecule 24: 26S proteasome regulatory subunit RPN13

Chain X:



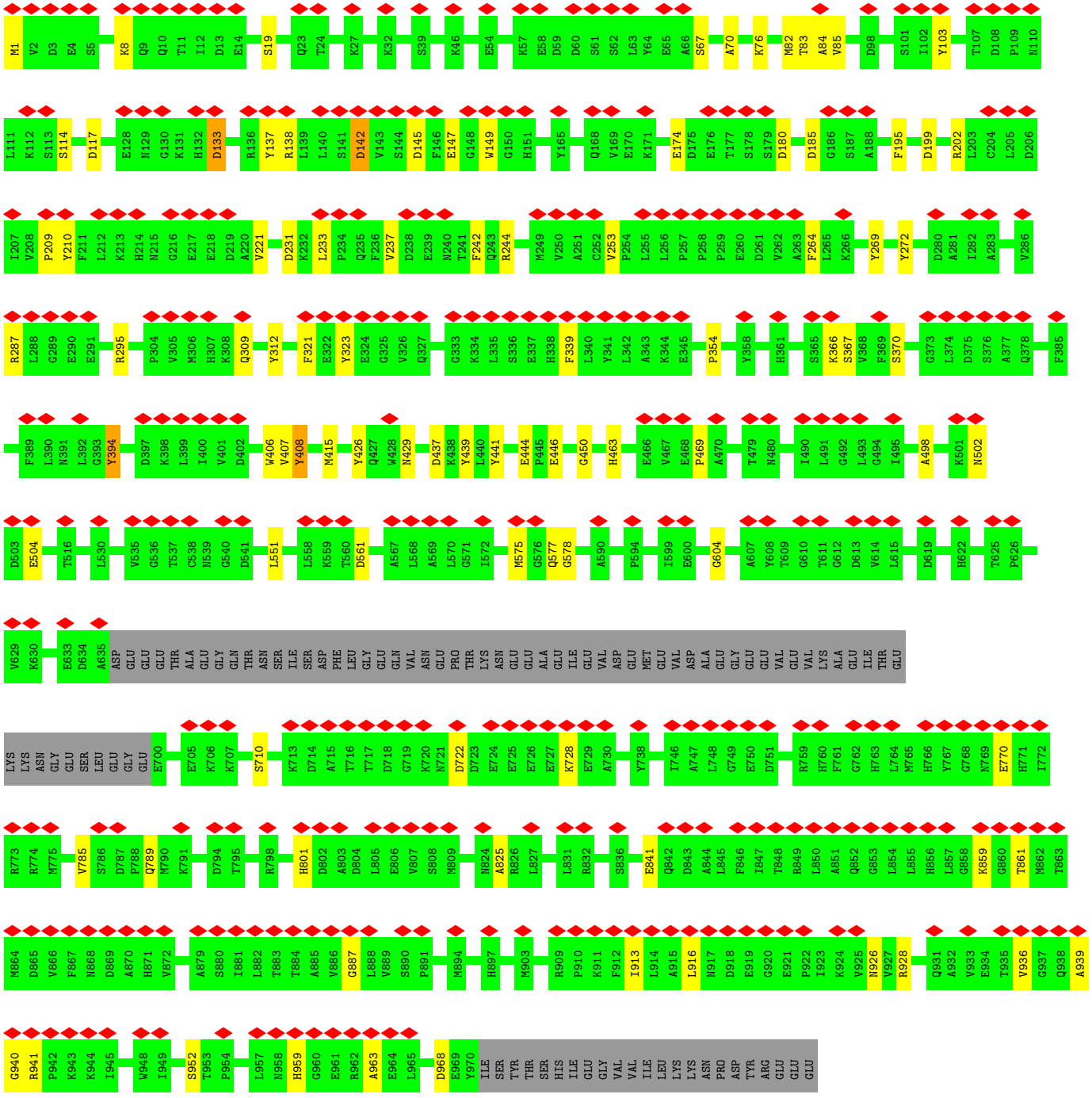
• Molecule 25: 26S proteasome complex subunit SEM1

Chain Y:



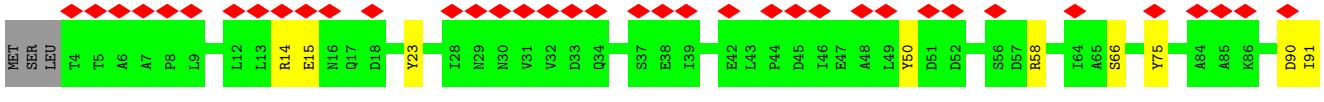
• Molecule 26: 26S proteasome regulatory subunit RPN1

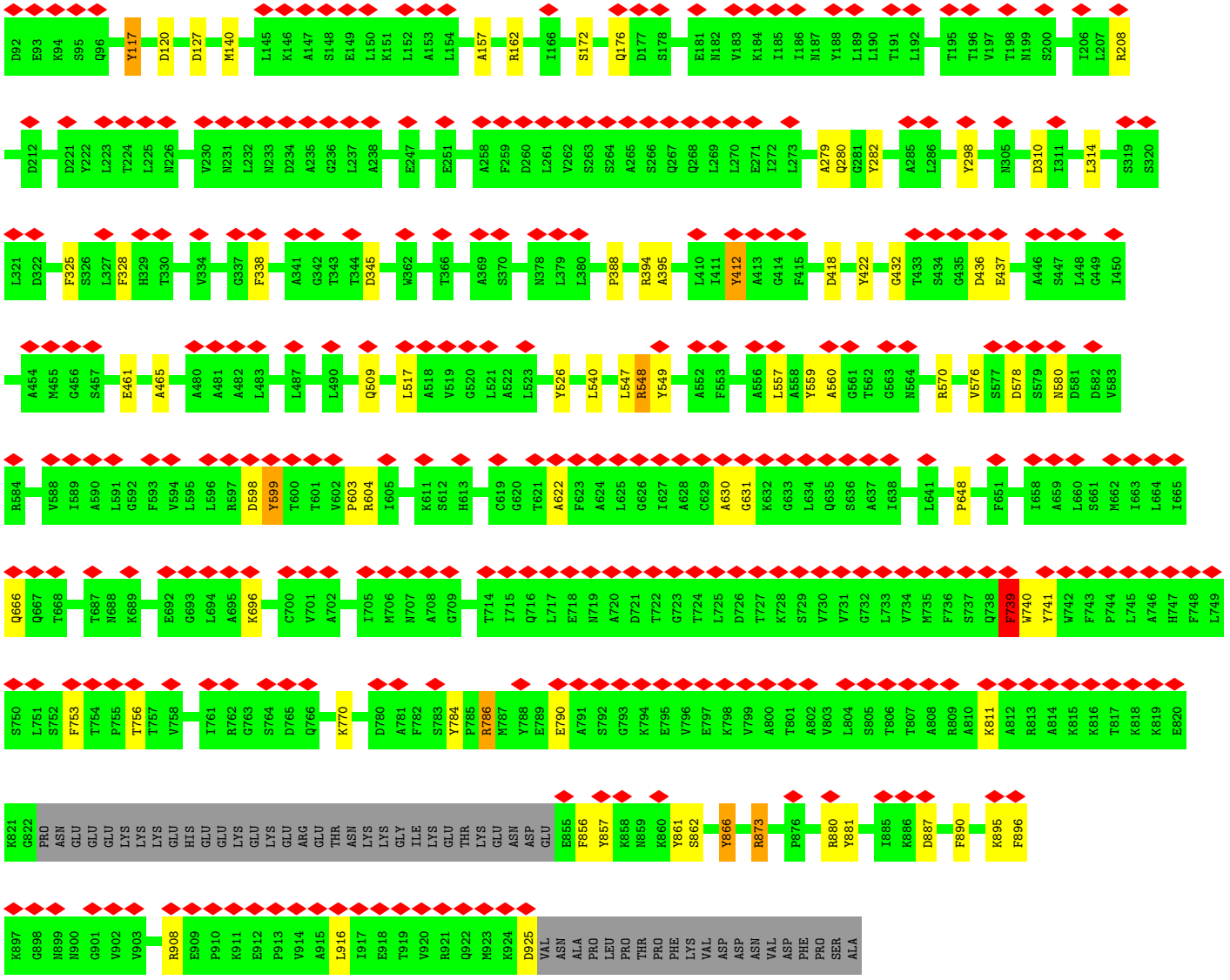
Chain Z:



• Molecule 27: 26S proteasome regulatory subunit RPN2

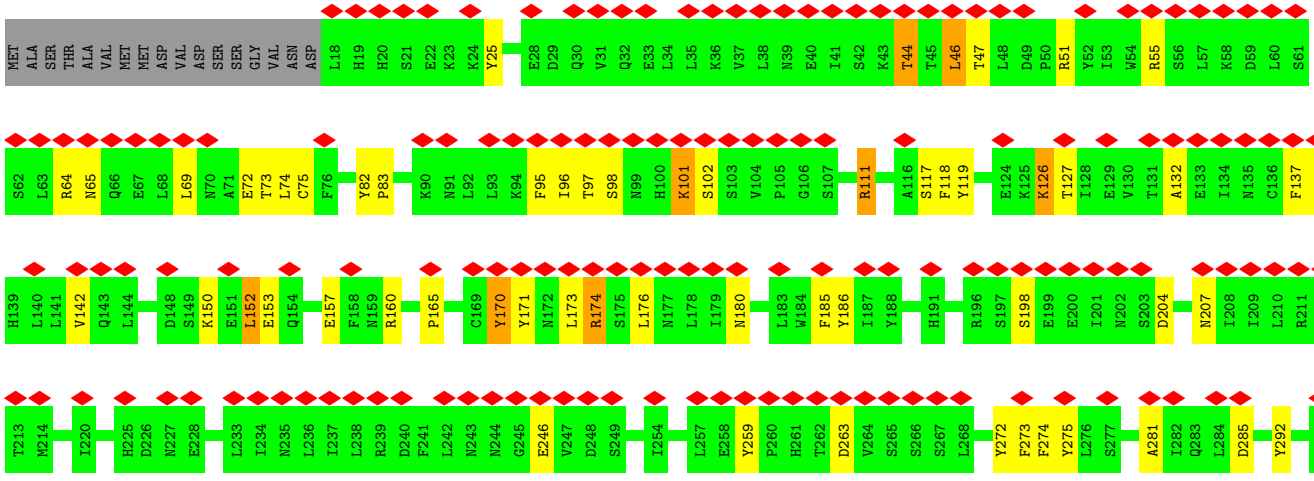
Chain N:

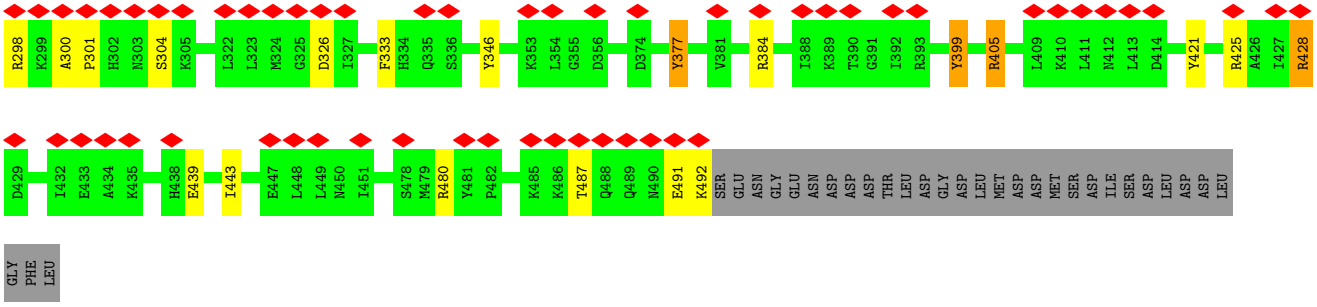




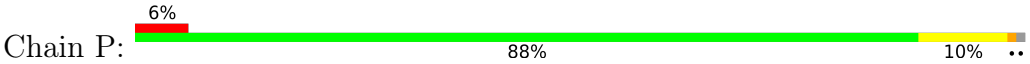
• Molecule 28: 26S proteasome regulatory subunit RPN3

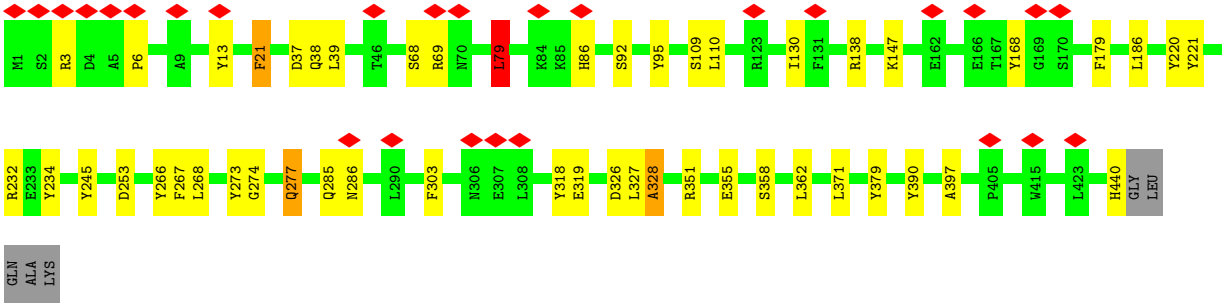
Chain S:



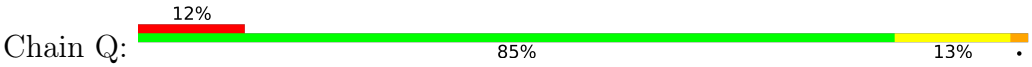


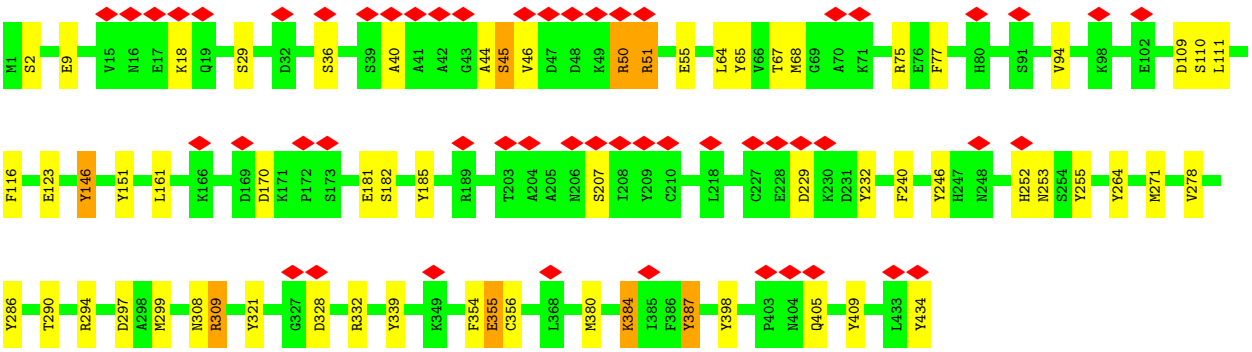
• Molecule 29: 26S proteasome regulatory subunit RPN5



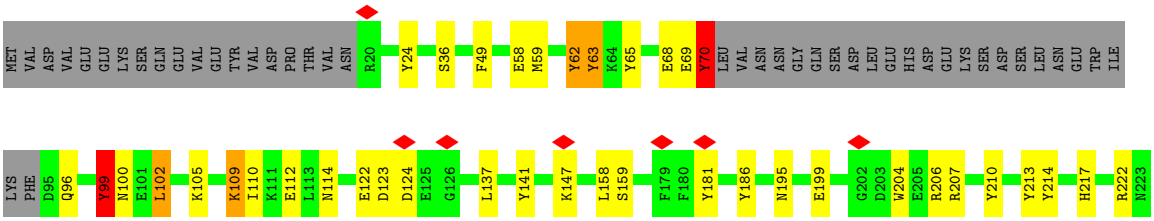


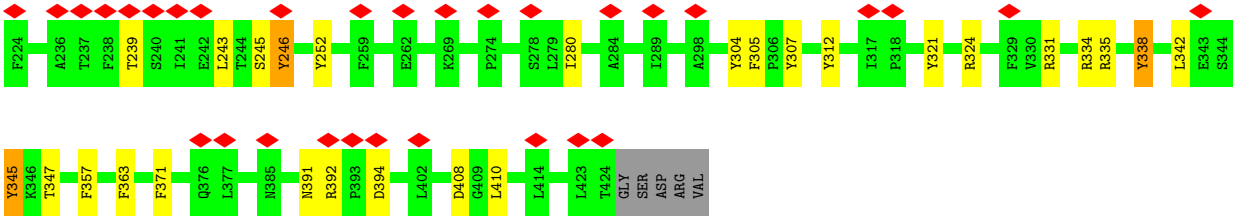
• Molecule 30: 26S proteasome regulatory subunit RPN6



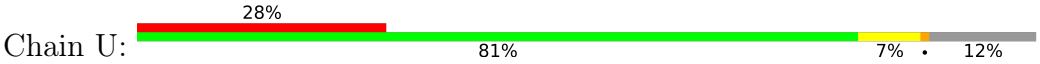


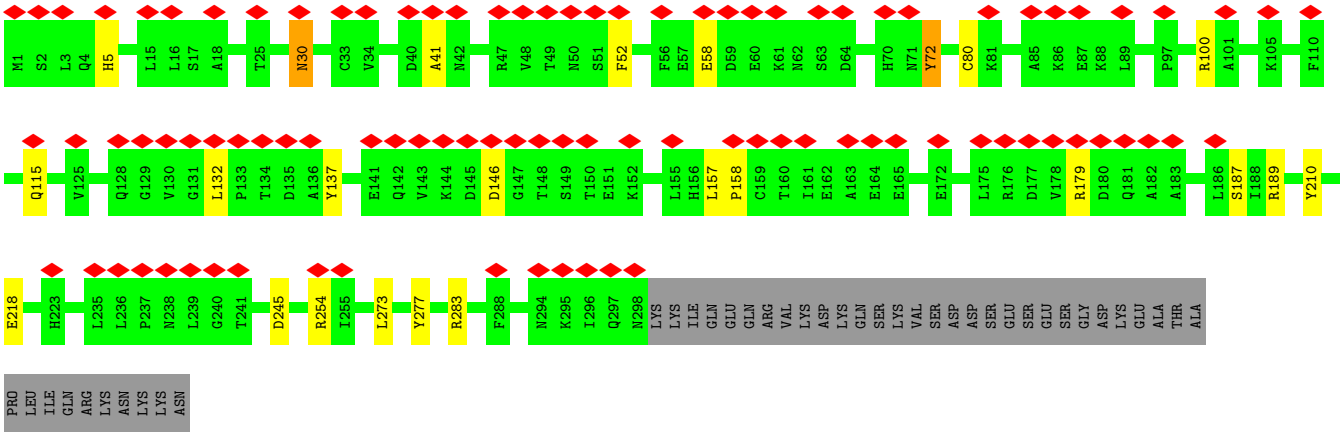
• Molecule 31: 26S proteasome regulatory subunit RPN7



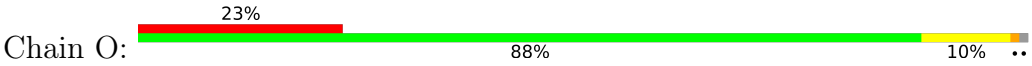


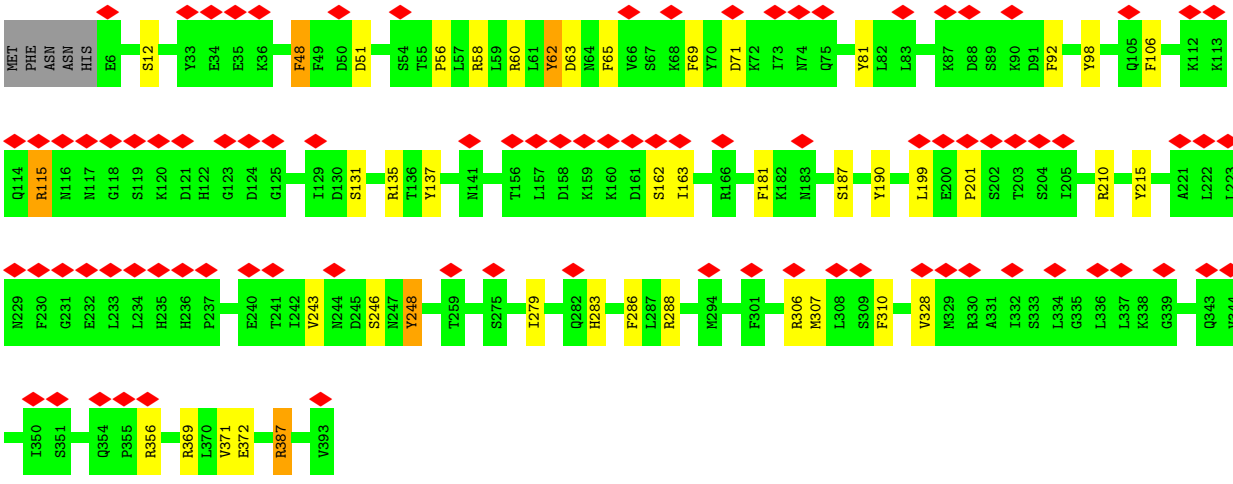
• Molecule 32: 26S proteasome regulatory subunit RPN8



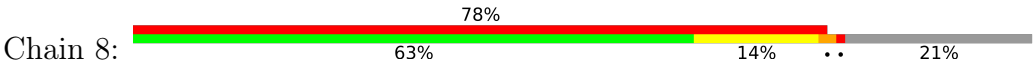


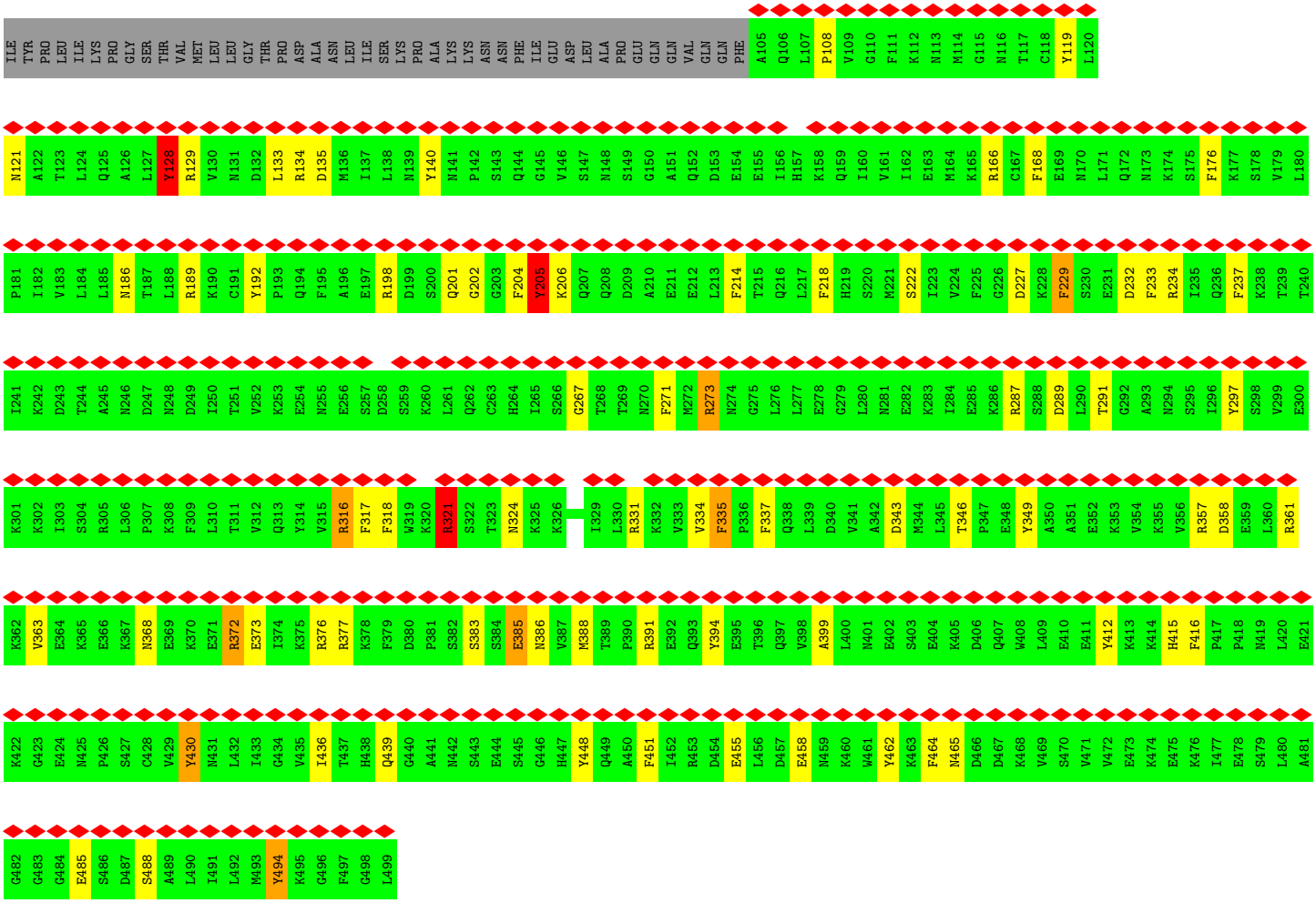
• Molecule 33: 26S proteasome regulatory subunit RPN9





• Molecule 34: Ubiquitin carboxyl-terminal hydrolase 6




ILE TYR PRO LEU ILE LYS PRO GLY SER THR VAL MET LEU LEU GLY THR PRO ASP ALA ASN LEU ILE SER LYS PRO ALA LYS LYS ASN ASN PHE ILE GLU ASP LEU ALA PRO GLU GLN GLN VAL GLN GLN PHE A105 Q106 L107 P108 V109 G110 F111 K112 N113 M114 G115 N116 T117 C118 Y119 L120
N121 A122 T123 L124 Q125 A126 L127 Y128 R129 V130 N131 D132 L133 R134 D135 M136 I137 L138 N139 Y140 N141 P142 S143 Q144 G145 V146 S147 N148 S149 G150 A151 Q152 D153 E154 E155 I156 H157 K158 Q159 I160 V161 I162 E163 M164 K165 R166 C167 F168 E169 N170 L171 Q172 N173 K174 S175 F176 K177 S178 V179 L180
P181 I182 V183 L184 L185 N186 T187 L188 R189 K190 C191 Y192 P193 Q194 F195 A196 E197 R198 D199 S200 Q201 G202 G203 F204 Y205 K206 Q207 Q208 D209 A210 E211 E212 L213 F214 T215 Q216 L217 F218 H219 S220 M221 S222 I223 V224 F225 G226 D227 K228 F229 S230 E231 D232 F233 R234 I235 Q236 F237 K238 T239 T240
I241 K242 D243 T244 A245 N246 D247 N248 D249 I250 T251 V252 K253 E254 N255 E256 S257 D258 S259 K260 L261 Q262 C263 H264 I265 S266 G267 T268 T269 N270 F271 M272 R273 N274 G275 L276 L277 E278 G279 L280 N281 E282 K283 I284 E285 K286 R287 S288 D289 L290 T291 G292 A293 N294 S295 I296 Y297 S298 V299 E300
K301 K302 I303 S304 R305 L306 P307 K308 F309 L310 T311 V312 Q313 Y314 V315 R316 F317 F318 W319 K320 R321 S322 T323 N324 K325 K326 I329 L330 R331 K332 V333 V334 F335 P336 F337 Q338 L339 D340 V341 A342 D343 M344 L345 T346 P347 E348 Y349 A350 A351 E352 K353 V354 K355 V356 R357 D358 E359 L360 R361
K362 V363 E364 K365 E366 K367 N368 E369 K370 E371 R372 E373 I374 K375 R376 R377 K378 F379 D380 P381 S382 S383 S384 E385 N386 V387 M388 T389 P390 R391 E392 Q393 Y394 E395 T396 Q397 V398 A399 L400 N401 E402 S403 E404 K405 D406 Q407 W408 L409 E410 E411 Y412 K413 K414 H415 F416 P417 P418 N419 L420 E421
K422 G423 E424 N425 P426 S427 C428 V429 Y430 N431 L432 I433 G434 V435 I436 T437 H438 Q439 G440 A441 N442 S443 E444 S445 G446 H447 Y448 Q449 A450 F451 I452 R453 D454 E455 L456 D457 E458 N459 K460 W461 Y462 K463 F464 N465 D466 D467 K468 V469 S470 V471 V472 E473 K474 E475 K476 I477 E478 S479 L480 A481
G482 G483 G484 E485 S486 D487 S488 A489 L490 I491 L492 M493 Y494 K495 G496 F497 G498 L499

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	27600	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)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.117	Depositor
Minimum map value	-0.080	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.023	Depositor
Map size (Å)	1.0, 1.0, 1.0	wwPDB
Map dimensions	416, 416, 416	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.3500001, 1.3500001, 1.3500001	Depositor

5 Model quality

5.1 Standard geometry

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	27/1945 (1.4%)	1.95	52/2634 (2.0%)
1	a	1.78	25/1945 (1.3%)	1.93	47/2634 (1.8%)
2	B	1.74	21/1952 (1.1%)	1.87	40/2642 (1.5%)
2	b	1.73	19/1952 (1.0%)	1.92	46/2642 (1.7%)
3	C	1.73	18/1934 (0.9%)	1.96	58/2618 (2.2%)
3	c	1.73	20/1934 (1.0%)	2.04	69/2618 (2.6%)
4	D	1.82	29/1910 (1.5%)	1.88	50/2586 (1.9%)
4	d	1.76	23/1910 (1.2%)	1.94	55/2586 (2.1%)
5	E	1.77	16/1886 (0.8%)	1.87	43/2541 (1.7%)
5	e	1.72	11/1886 (0.6%)	1.95	45/2541 (1.8%)
6	F	1.75	21/1823 (1.2%)	1.95	48/2463 (1.9%)
6	f	1.77	21/1800 (1.2%)	1.95	48/2433 (2.0%)
7	G	1.73	16/1932 (0.8%)	1.91	42/2609 (1.6%)
7	g	1.76	21/1932 (1.1%)	1.93	61/2609 (2.3%)
8	1	1.77	20/1541 (1.3%)	1.97	41/2087 (2.0%)
8	h	1.73	12/1541 (0.8%)	1.93	47/2087 (2.3%)
9	2	1.65	12/1750 (0.7%)	1.84	40/2373 (1.7%)
9	i	1.72	24/1750 (1.4%)	1.86	31/2373 (1.3%)
10	3	1.80	15/1611 (0.9%)	1.92	41/2174 (1.9%)
10	j	1.78	14/1611 (0.9%)	1.98	43/2174 (2.0%)
11	4	1.80	25/1589 (1.6%)	1.96	39/2142 (1.8%)
11	k	1.73	14/1589 (0.9%)	2.03	43/2142 (2.0%)
12	5	1.80	18/1681 (1.1%)	1.89	37/2274 (1.6%)
12	l	1.79	12/1681 (0.7%)	2.03	49/2274 (2.2%)
13	6	1.82	22/1795 (1.2%)	1.88	45/2420 (1.9%)
13	m	1.76	26/1795 (1.4%)	2.00	52/2420 (2.1%)
14	7	1.75	20/1821 (1.1%)	2.01	46/2470 (1.9%)
14	n	1.82	31/1846 (1.7%)	1.98	48/2503 (1.9%)
15	H	1.64	24/3014 (0.8%)	1.75	47/4058 (1.2%)
16	I	1.60	26/3061 (0.8%)	1.73	41/4121 (1.0%)
17	K	1.63	28/3121 (0.9%)	1.79	70/4213 (1.7%)
18	L	1.63	25/3128 (0.8%)	1.79	70/4204 (1.7%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	M	1.59	24/3023 (0.8%)	1.76	47/4070 (1.2%)
20	J	1.56	16/3130 (0.5%)	1.72	50/4203 (1.2%)
21	W	1.48	11/1557 (0.7%)	1.63	19/2111 (0.9%)
22	V	1.45	14/2309 (0.6%)	1.59	28/3115 (0.9%)
23	T	1.46	8/2235 (0.4%)	1.67	36/3017 (1.2%)
24	X	1.66	9/1058 (0.9%)	1.78	22/1432 (1.5%)
25	Y	1.66	2/438 (0.5%)	1.61	5/583 (0.9%)
26	Z	1.46	21/7122 (0.3%)	1.51	62/9645 (0.6%)
27	N	1.48	20/6994 (0.3%)	1.58	82/9455 (0.9%)
28	S	1.60	17/3966 (0.4%)	1.65	52/5355 (1.0%)
29	P	1.46	12/3663 (0.3%)	1.62	29/4940 (0.6%)
30	Q	1.47	12/3556 (0.3%)	1.64	49/4787 (1.0%)
31	R	1.58	13/3110 (0.4%)	1.85	74/4193 (1.8%)
32	U	1.46	4/2407 (0.2%)	1.52	27/3258 (0.8%)
33	O	1.50	13/3247 (0.4%)	1.65	38/4380 (0.9%)
34	8	1.72	29/3278 (0.9%)	2.00	90/4402 (2.0%)
All	All	1.64	881/113759 (0.8%)	1.80	2244/153611 (1.5%)

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	7
2	B	0	6
2	b	0	5
3	C	0	10
3	c	0	10
4	D	0	6
4	d	0	8
5	E	0	11
5	e	0	4
6	F	0	7
6	f	0	7
7	G	0	4
7	g	0	5
8	1	0	4
8	h	0	8
9	2	0	6
9	i	0	8

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	3	0	1
10	j	0	6
11	4	0	5
11	k	0	7
12	5	0	4
12	l	0	12
13	6	0	8
13	m	0	9
14	7	0	10
14	n	0	11
15	H	0	6
16	I	0	7
17	K	0	13
18	L	0	12
19	M	0	13
20	J	0	6
21	W	0	4
22	V	0	4
23	T	0	9
24	X	0	4
26	Z	0	3
27	N	0	10
28	S	0	10
29	P	0	10
30	Q	0	6
31	R	0	16
32	U	0	2
33	O	0	7
34	8	0	11
All	All	0	347

All (881) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	S	126	LYS	CA-CB	-39.49	0.67	1.53
27	N	861	TYR	CA-CB	15.62	1.88	1.53
14	7	229	GLY	C-O	-14.51	1.00	1.23
12	5	212	GLY	C-O	-14.49	1.00	1.23
13	6	222	ASP	C-OXT	-12.08	1.00	1.23
17	K	428	LYS	C-OXT	-12.07	1.00	1.23
10	3	204	ASP	C-O	-12.07	1.00	1.23
7	G	244	ASN	C-O	-12.07	1.00	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	89	GLN	C-OXT	-12.07	1.00	1.23
8	1	196	LEU	C-OXT	-12.06	1.00	1.23
25	Y	89	GLN	C-O	-12.06	1.00	1.23
2	B	250	LEU	C-O	-12.06	1.00	1.23
12	5	212	GLY	C-OXT	-12.06	1.00	1.23
30	Q	434	TYR	C-OXT	-12.06	1.00	1.23
18	L	436	LYS	C-O	-12.06	1.00	1.23
4	D	240	GLU	C-O	-12.05	1.00	1.23
16	I	437	LEU	C-OXT	-12.05	1.00	1.23
19	M	434	ALA	C-OXT	-12.05	1.00	1.23
6	F	233	ILE	C-OXT	-12.05	1.00	1.23
10	3	204	ASP	C-OXT	-12.05	1.00	1.23
11	4	195	PHE	C-O	-12.05	1.00	1.23
16	I	437	LEU	C-O	-12.05	1.00	1.23
17	K	428	LYS	C-O	-12.05	1.00	1.23
19	M	434	ALA	C-O	-12.04	1.00	1.23
30	Q	434	TYR	C-O	-12.04	1.00	1.23
2	B	250	LEU	C-OXT	-12.04	1.00	1.23
28	S	492	LYS	C-O	-12.04	1.00	1.23
1	A	242	GLN	C-O	-12.04	1.00	1.23
3	C	244	THR	C-O	-12.04	1.00	1.23
8	1	196	LEU	C-O	-12.04	1.00	1.23
13	6	222	ASP	C-O	-12.04	1.00	1.23
9	2	226	GLU	C-O	-12.03	1.00	1.23
5	E	242	GLU	C-O	-12.03	1.00	1.23
27	N	925	ASP	C-O	-12.03	1.00	1.23
29	P	440	HIS	C-O	-12.03	1.00	1.23
6	F	233	ILE	C-O	-12.03	1.00	1.23
29	P	86	HIS	CA-CB	11.57	1.79	1.53
12	5	69	ARG	NE-CZ	8.94	1.44	1.33
27	N	604	ARG	CD-NE	8.79	1.61	1.46
6	f	148	PRO	N-CA	-8.52	1.32	1.47
14	n	138	SER	CA-CB	8.38	1.65	1.52
14	n	90	SER	CA-CB	8.33	1.65	1.52
29	P	355	GLU	CD-OE2	8.14	1.34	1.25
5	E	107	SER	CA-CB	8.12	1.65	1.52
4	D	47	ARG	CZ-NH2	8.10	1.43	1.33
2	b	236	ARG	CZ-NH1	8.06	1.43	1.33
11	4	149	ARG	CZ-NH1	8.01	1.43	1.33
9	2	207	ARG	CZ-NH2	7.93	1.43	1.33
5	E	85	ARG	CZ-NH2	7.93	1.43	1.33
6	f	23	TYR	CE2-CZ	7.85	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	W	178	PRO	N-CD	-7.84	1.36	1.47
4	d	195	ARG	CZ-NH1	7.80	1.43	1.33
18	L	69	ARG	CZ-NH2	7.77	1.43	1.33
18	L	88	TYR	CG-CD1	7.77	1.49	1.39
7	g	7	SER	CA-CB	7.75	1.64	1.52
11	4	190	ARG	NE-CZ	7.74	1.43	1.33
14	7	41	ARG	NE-CZ	7.72	1.43	1.33
16	I	54	ARG	CZ-NH1	7.71	1.43	1.33
6	f	125	ARG	NE-CZ	7.69	1.43	1.33
19	M	366	ARG	CD-NE	7.67	1.59	1.46
10	3	187	TYR	CZ-OH	7.62	1.50	1.37
9	i	102	GLY	CA-C	-7.62	1.39	1.51
8	1	174	ARG	NE-CZ	7.52	1.42	1.33
14	7	128	ARG	CZ-NH2	7.51	1.42	1.33
4	D	164	ARG	CD-NE	7.50	1.59	1.46
7	g	111	ARG	CZ-NH2	7.48	1.42	1.33
31	R	206	ARG	CZ-NH1	7.48	1.42	1.33
14	7	196	SER	CA-CB	7.46	1.64	1.52
1	a	82	ARG	CZ-NH2	7.43	1.42	1.33
27	N	570	ARG	CZ-NH2	7.42	1.42	1.33
1	a	87	ARG	NE-CZ	7.42	1.42	1.33
15	H	178	ARG	NE-CZ	7.41	1.42	1.33
14	n	137	TYR	CZ-OH	7.41	1.50	1.37
7	g	165	ARG	CZ-NH1	7.35	1.42	1.33
24	X	85	ARG	NE-CZ	7.33	1.42	1.33
14	7	156	ARG	NE-CZ	7.33	1.42	1.33
14	n	182	ARG	CZ-NH2	7.32	1.42	1.33
6	f	106	ARG	NE-CZ	7.31	1.42	1.33
2	B	90	ARG	CZ-NH2	7.28	1.42	1.33
16	I	346	ARG	CD-NE	7.24	1.58	1.46
8	h	174	ARG	NE-CZ	7.24	1.42	1.33
22	V	119	SER	CA-CB	7.23	1.63	1.52
8	1	29	ARG	NE-CZ	7.19	1.42	1.33
30	Q	51	ARG	CD-NE	7.17	1.58	1.46
1	A	235	ARG	NE-CZ	7.15	1.42	1.33
10	j	1	SER	CA-CB	7.14	1.63	1.52
23	T	176	SER	CA-CB	7.13	1.63	1.52
4	D	117	ARG	CZ-NH1	7.08	1.42	1.33
15	H	62	ARG	CZ-NH2	7.08	1.42	1.33
14	7	190	ARG	CZ-NH2	7.07	1.42	1.33
34	8	129	ARG	CZ-NH1	7.06	1.42	1.33
31	R	105	LYS	CA-CB	7.05	1.69	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	153	TYR	CZ-OH	7.04	1.49	1.37
11	4	59	TYR	CZ-OH	7.04	1.49	1.37
2	B	236	ARG	NE-CZ	7.03	1.42	1.33
1	a	3	TYR	CG-CD1	6.99	1.48	1.39
6	f	173	ARG	CZ-NH2	6.98	1.42	1.33
28	S	405	ARG	CZ-NH2	6.98	1.42	1.33
19	M	73	ARG	CZ-NH2	6.98	1.42	1.33
12	l	198	TRP	NE1-CE2	-6.97	1.28	1.37
13	6	134	GLU	CD-OE2	6.96	1.33	1.25
24	X	17	TYR	CG-CD2	6.95	1.48	1.39
3	c	139	TYR	CZ-OH	6.95	1.49	1.37
11	4	149	ARG	NE-CZ	6.91	1.42	1.33
11	k	93	ARG	NE-CZ	6.91	1.42	1.33
22	V	42	ARG	CZ-NH2	6.91	1.42	1.33
13	6	185	ARG	CZ-NH2	6.91	1.42	1.33
20	J	332	SER	CA-CB	6.90	1.63	1.52
15	H	432	ARG	CZ-NH1	6.90	1.42	1.33
7	g	122	TYR	CG-CD1	6.88	1.48	1.39
12	5	61	SER	CA-CB	6.85	1.63	1.52
16	I	300	ARG	CZ-NH2	6.84	1.42	1.33
1	A	111	ARG	NE-CZ	6.84	1.42	1.33
17	K	294	ARG	NE-CZ	6.84	1.42	1.33
7	G	124	SER	CA-CB	6.83	1.63	1.52
24	X	11	ARG	CD-NE	6.82	1.58	1.46
4	D	195	ARG	CZ-NH2	6.82	1.42	1.33
31	R	204	TRP	CG-CD2	6.80	1.55	1.43
10	3	67	ARG	CD-NE	6.79	1.57	1.46
31	R	392	ARG	CZ-NH2	6.79	1.41	1.33
9	i	72	ARG	NE-CZ	6.79	1.41	1.33
4	d	109	ARG	CZ-NH2	6.78	1.41	1.33
8	1	189	TYR	CE2-CZ	6.78	1.47	1.38
18	L	267	PHE	CG-CD1	6.78	1.49	1.38
34	8	234	ARG	CZ-NH2	6.76	1.41	1.33
11	4	45	SER	CA-CB	6.76	1.63	1.52
4	D	181	GLU	CG-CD	6.76	1.62	1.51
1	a	235	ARG	CZ-NH1	6.75	1.41	1.33
10	j	102	TYR	CB-CG	6.75	1.61	1.51
10	3	45	TYR	CZ-OH	6.75	1.49	1.37
9	i	72	ARG	CZ-NH1	6.74	1.41	1.33
10	j	27	ARG	NE-CZ	6.74	1.41	1.33
34	8	287	ARG	CZ-NH2	6.74	1.41	1.33
4	D	170	ARG	NE-CZ	6.73	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	97	TYR	CE1-CZ	6.73	1.47	1.38
2	B	7	PHE	CE2-CZ	6.71	1.50	1.37
15	H	346	ARG	NE-CZ	6.71	1.41	1.33
1	a	62	TYR	CZ-OH	6.71	1.49	1.37
12	l	19	ARG	CZ-NH2	6.70	1.41	1.33
16	I	246	ARG	NE-CZ	6.70	1.41	1.33
6	F	88	ARG	CZ-NH2	6.69	1.41	1.33
4	d	56	ARG	CZ-NH2	6.68	1.41	1.33
2	b	156	TYR	CZ-OH	6.67	1.49	1.37
5	e	114	ARG	CZ-NH1	6.67	1.41	1.33
2	B	99	ARG	NE-CZ	6.67	1.41	1.33
13	m	38	ARG	CZ-NH2	6.64	1.41	1.33
30	Q	123	GLU	CB-CG	-6.63	1.39	1.52
34	8	205	TYR	CE1-CZ	6.63	1.47	1.38
7	g	205	GLU	CD-OE2	6.63	1.32	1.25
6	F	23	TYR	CE1-CZ	6.62	1.47	1.38
10	3	67	ARG	NE-CZ	6.61	1.41	1.33
8	1	42	TRP	CE2-CZ2	-6.60	1.28	1.39
11	4	117	TYR	CE1-CZ	6.60	1.47	1.38
24	X	34	GLU	CG-CD	6.59	1.61	1.51
13	m	5	TYR	CE2-CZ	6.58	1.47	1.38
9	i	75	ARG	CD-NE	6.57	1.57	1.46
13	6	221	ARG	CZ-NH2	6.56	1.41	1.33
26	Z	928	ARG	CZ-NH1	6.55	1.41	1.33
6	f	78	PRO	CA-C	-6.55	1.39	1.52
13	6	137	ARG	CZ-NH1	6.54	1.41	1.33
6	f	100	ARG	CD-NE	6.54	1.57	1.46
7	G	122	TYR	CE1-CZ	6.54	1.47	1.38
5	e	18	TYR	CG-CD2	6.54	1.47	1.39
2	b	120	GLU	CD-OE1	6.53	1.32	1.25
15	H	101	ARG	CZ-NH2	6.53	1.41	1.33
17	K	73	ARG	CZ-NH2	6.53	1.41	1.33
24	X	96	ARG	CZ-NH2	6.53	1.41	1.33
18	L	145	ARG	NE-CZ	6.53	1.41	1.33
2	b	101	TYR	CG-CD1	6.52	1.47	1.39
11	4	148	TYR	CZ-OH	6.51	1.49	1.37
33	O	306	ARG	CZ-NH2	6.50	1.41	1.33
1	a	10	PHE	CG-CD2	6.49	1.48	1.38
34	8	455	GLU	CD-OE2	6.49	1.32	1.25
1	A	82	ARG	CZ-NH1	6.48	1.41	1.33
34	8	331	ARG	NE-CZ	6.48	1.41	1.33
9	i	207	ARG	CZ-NH2	6.48	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	133	ARG	CZ-NH1	6.48	1.41	1.33
5	e	61	GLU	CD-OE1	6.47	1.32	1.25
14	7	156	ARG	CZ-NH2	6.46	1.41	1.33
34	8	494	TYR	CE2-CZ	6.46	1.47	1.38
3	c	128	ARG	CZ-NH1	6.46	1.41	1.33
3	c	163	SER	CA-CB	6.45	1.62	1.52
10	3	97	ARG	CZ-NH2	6.45	1.41	1.33
18	L	359	GLU	CG-CD	6.44	1.61	1.51
31	R	102	LEU	CA-C	-6.44	1.36	1.52
20	J	63	ARG	CZ-NH1	6.44	1.41	1.33
5	e	85	ARG	CZ-NH1	6.43	1.41	1.33
7	g	73	VAL	N-CA	-6.43	1.33	1.46
20	J	371	ARG	NE-CZ	6.42	1.41	1.33
26	Z	841	GLU	CG-CD	-6.41	1.42	1.51
8	h	143	ARG	CZ-NH2	6.39	1.41	1.33
5	E	67	GLY	N-CA	-6.38	1.36	1.46
17	K	281	ARG	CZ-NH1	6.38	1.41	1.33
1	a	96	ARG	NE-CZ	6.38	1.41	1.33
17	K	259	ARG	CD-NE	6.38	1.57	1.46
34	8	234	ARG	CZ-NH1	6.37	1.41	1.33
10	j	98	ARG	NE-CZ	6.37	1.41	1.33
13	6	105	TYR	CE1-CZ	6.37	1.46	1.38
10	j	27	ARG	CD-NE	6.36	1.57	1.46
8	1	182	GLY	CA-C	-6.36	1.41	1.51
14	7	182	ARG	CZ-NH1	6.36	1.41	1.33
34	8	462	TYR	CE1-CZ	6.35	1.46	1.38
7	g	3	GLY	N-CA	-6.34	1.36	1.46
13	6	28	ARG	NE-CZ	6.33	1.41	1.33
32	U	58	GLU	CD-OE1	-6.33	1.18	1.25
14	n	135	VAL	CB-CG1	6.33	1.66	1.52
8	h	143	ARG	CZ-NH1	6.32	1.41	1.33
7	g	87	ARG	CD-NE	6.32	1.57	1.46
7	g	211	GLU	CD-OE1	6.31	1.32	1.25
17	K	350	ARG	CZ-NH2	6.31	1.41	1.33
9	2	150	GLU	CD-OE2	6.31	1.32	1.25
17	K	136	SER	CA-CB	6.30	1.62	1.52
31	R	99	TYR	CE2-CZ	6.30	1.46	1.38
2	b	203	GLU	CG-CD	6.30	1.61	1.51
33	O	279	ILE	N-CA	-6.30	1.33	1.46
17	K	255	ARG	CZ-NH2	6.30	1.41	1.33
8	1	36	ARG	CD-NE	6.29	1.57	1.46
15	H	366	LEU	CA-CB	6.29	1.68	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	133	ARG	NE-CZ	6.29	1.41	1.33
16	I	246	ARG	CD-NE	6.29	1.57	1.46
27	N	15	GLU	CA-CB	6.28	1.67	1.53
1	a	87	ARG	CZ-NH1	6.27	1.41	1.33
1	A	154	TYR	CG-CD2	6.27	1.47	1.39
30	Q	294	ARG	NE-CZ	6.27	1.41	1.33
3	c	142	ARG	NE-CZ	6.26	1.41	1.33
12	5	167	ARG	CZ-NH1	6.26	1.41	1.33
12	5	7	ARG	NE-CZ	6.26	1.41	1.33
14	n	187	ARG	CD-NE	6.26	1.57	1.46
3	C	139	TYR	CB-CG	-6.26	1.42	1.51
3	C	216	ARG	CD-NE	6.26	1.57	1.46
22	V	302	SER	CA-CB	6.25	1.62	1.52
2	b	83	ARG	NE-CZ	6.25	1.41	1.33
8	1	115	LEU	C-N	6.25	1.44	1.33
4	D	146	TYR	CE2-CZ	6.24	1.46	1.38
6	F	109	HIS	CB-CG	-6.23	1.38	1.50
4	d	56	ARG	NE-CZ	6.22	1.41	1.33
7	G	82	ARG	CZ-NH1	6.21	1.41	1.33
10	3	150	GLU	CG-CD	6.20	1.61	1.51
9	i	69	TYR	CB-CG	-6.20	1.42	1.51
10	j	68	TYR	CZ-OH	6.20	1.48	1.37
34	8	198	ARG	CZ-NH1	6.20	1.41	1.33
11	4	171	ARG	CZ-NH1	6.19	1.41	1.33
1	a	6	HIS	CG-CD2	6.19	1.46	1.35
12	l	159	ARG	NE-CZ	6.19	1.41	1.33
13	m	4	PRO	N-CD	-6.19	1.39	1.47
4	D	88	ARG	CD-NE	6.19	1.56	1.46
10	3	187	TYR	CE2-CZ	6.18	1.46	1.38
2	b	110	LEU	N-CA	-6.18	1.33	1.46
7	G	148	GLU	CD-OE2	6.18	1.32	1.25
13	6	144	SER	CA-CB	6.18	1.62	1.52
18	L	132	ARG	NE-CZ	6.17	1.41	1.33
4	d	179	ARG	CZ-NH1	6.17	1.41	1.33
17	K	198	TYR	CB-CG	-6.17	1.42	1.51
5	E	85	ARG	CZ-NH1	6.17	1.41	1.33
21	W	101	ARG	CZ-NH2	6.16	1.41	1.33
21	W	144	PHE	CG-CD1	6.16	1.48	1.38
2	B	4	ARG	NE-CZ	6.15	1.41	1.33
13	6	185	ARG	NE-CZ	6.15	1.41	1.33
1	A	140	GLU	CD-OE2	6.15	1.32	1.25
27	N	526	TYR	C-N	6.15	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	84	SER	CA-CB	6.14	1.62	1.52
6	F	232	TYR	CB-CG	-6.14	1.42	1.51
34	8	357	ARG	NE-CZ	6.14	1.41	1.33
27	N	172	SER	CA-CB	6.14	1.62	1.52
28	S	480	ARG	CZ-NH2	6.14	1.41	1.33
2	B	23	TYR	CG-CD1	6.13	1.47	1.39
19	M	165	SER	CA-CB	6.13	1.62	1.52
33	O	106	PHE	CG-CD1	6.13	1.48	1.38
8	1	102	TYR	CE2-CZ	6.13	1.46	1.38
19	M	47	GLU	CD-OE1	6.12	1.32	1.25
11	k	56	PHE	CG-CD2	6.12	1.48	1.38
18	L	78	ARG	NE-CZ	6.12	1.41	1.33
34	8	316	ARG	NE-CZ	6.12	1.41	1.33
13	m	190	SER	CA-CB	6.11	1.62	1.52
14	7	111	TRP	NE1-CE2	6.11	1.45	1.37
30	Q	356	CYS	CB-SG	-6.10	1.71	1.82
1	A	146	TYR	CE1-CZ	6.10	1.46	1.38
13	m	221	ARG	NE-CZ	6.10	1.41	1.33
14	n	104	ARG	CZ-NH1	6.09	1.41	1.33
26	Z	114	SER	CA-CB	6.09	1.62	1.52
18	L	392	ARG	NE-CZ	6.08	1.41	1.33
1	a	96	ARG	CZ-NH1	6.08	1.41	1.33
18	L	165	PRO	N-CA	-6.08	1.36	1.47
33	O	162	SER	CA-CB	6.08	1.62	1.52
9	i	207	ARG	NE-CZ	6.08	1.41	1.33
3	C	40	SER	CA-CB	6.08	1.62	1.52
26	Z	446	GLU	CG-CD	6.07	1.61	1.51
16	I	256	TYR	CE1-CZ	6.07	1.46	1.38
28	S	126	LYS	CB-CG	6.07	1.69	1.52
6	f	81	ARG	CD-NE	6.07	1.56	1.46
10	j	83	PRO	N-CA	-6.06	1.36	1.47
1	A	175	ASN	CB-CG	6.06	1.65	1.51
11	4	67	TYR	CE2-CZ	6.06	1.46	1.38
2	B	236	ARG	CZ-NH1	6.05	1.41	1.33
2	B	128	ARG	CZ-NH1	6.05	1.41	1.33
10	j	106	PRO	N-CD	-6.05	1.39	1.47
34	8	129	ARG	CD-NE	6.05	1.56	1.46
33	O	12	SER	CA-CB	6.04	1.62	1.52
7	g	52	SER	CA-CB	6.04	1.62	1.52
18	L	345	ARG	NE-CZ	6.04	1.40	1.33
32	U	254	ARG	NE-CZ	6.03	1.40	1.33
8	1	45	ARG	CZ-NH1	6.02	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	182	ARG	CZ-NH2	6.02	1.40	1.33
10	j	97	ARG	CZ-NH2	6.02	1.40	1.33
3	C	225	TYR	CG-CD2	6.01	1.47	1.39
24	X	59	ARG	NE-CZ	6.01	1.40	1.33
6	F	163	ARG	CZ-NH1	6.01	1.40	1.33
11	4	93	ARG	NE-CZ	6.01	1.40	1.33
4	d	4	ARG	NE-CZ	6.00	1.40	1.33
11	4	95	ARG	NE-CZ	6.00	1.40	1.33
34	8	166	ARG	CZ-NH2	6.00	1.40	1.33
7	G	186	ARG	NE-CZ	6.00	1.40	1.33
3	C	144	GLY	CA-C	-6.00	1.42	1.51
21	W	119	SER	CA-CB	5.99	1.61	1.52
1	a	46	SER	CB-OG	5.99	1.50	1.42
27	N	753	PHE	CG-CD1	5.99	1.47	1.38
15	H	385	ARG	CZ-NH1	5.98	1.40	1.33
14	7	103	ARG	CD-NE	5.98	1.56	1.46
8	h	19	ARG	NE-CZ	5.97	1.40	1.33
18	L	200	PRO	N-CD	-5.97	1.39	1.47
14	n	137	TYR	CE1-CZ	5.97	1.46	1.38
2	b	89	SER	CA-CB	5.97	1.61	1.52
2	b	159	TRP	CZ2-CH2	5.96	1.48	1.37
14	n	94	GLU	CD-OE2	5.95	1.32	1.25
5	e	223	TYR	CD1-CE1	5.95	1.48	1.39
1	A	99	TYR	CB-CG	-5.95	1.42	1.51
7	g	153	TYR	CE1-CZ	5.94	1.46	1.38
11	4	95	ARG	CZ-NH2	5.94	1.40	1.33
11	4	130	TYR	CE1-CZ	5.93	1.46	1.38
16	I	372	SER	CA-CB	5.92	1.61	1.52
4	D	166	SER	CA-CB	5.92	1.61	1.52
18	L	339	ARG	CZ-NH2	5.92	1.40	1.33
6	f	23	TYR	CG-CD1	5.92	1.46	1.39
11	k	85	ARG	CZ-NH1	5.92	1.40	1.33
4	D	170	ARG	CZ-NH2	5.91	1.40	1.33
29	P	358	SER	CA-CB	5.91	1.61	1.52
1	a	122	ARG	CZ-NH1	5.91	1.40	1.33
28	S	377	TYR	CE1-CZ	5.91	1.46	1.38
6	F	38	ARG	CZ-NH1	5.90	1.40	1.33
8	1	174	ARG	CZ-NH2	5.90	1.40	1.33
18	L	303	ARG	NE-CZ	5.90	1.40	1.33
19	M	166	ARG	NE-CZ	5.90	1.40	1.33
24	X	75	TRP	CZ2-CH2	5.90	1.48	1.37
4	D	164	ARG	NE-CZ	5.90	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	179	ARG	CZ-NH2	5.89	1.40	1.33
28	S	160	ARG	NE-CZ	5.89	1.40	1.33
15	H	390	ARG	CZ-NH2	5.89	1.40	1.33
3	c	233	GLU	CD-OE1	5.89	1.32	1.25
13	6	28	ARG	CZ-NH2	5.88	1.40	1.33
6	f	201	ARG	NE-CZ	5.88	1.40	1.33
13	m	33	TYR	CG-CD2	5.88	1.46	1.39
8	h	185	ARG	CZ-NH1	5.87	1.40	1.33
1	A	21	TYR	CG-CD1	5.87	1.46	1.39
4	d	157	TRP	NE1-CE2	5.86	1.45	1.37
3	c	216	ARG	NE-CZ	5.86	1.40	1.33
4	d	27	ARG	NE-CZ	5.86	1.40	1.33
2	B	246	ARG	CD-NE	5.86	1.56	1.46
14	n	186	TYR	CG-CD1	5.85	1.46	1.39
13	m	75	TYR	CE1-CZ	5.85	1.46	1.38
9	2	188	ARG	NE-CZ	5.84	1.40	1.33
13	m	215	GLU	CG-CD	5.84	1.60	1.51
32	U	283	ARG	NE-CZ	5.84	1.40	1.33
3	c	139	TYR	CG-CD1	5.84	1.46	1.39
2	B	17	LYS	CD-CE	5.83	1.65	1.51
15	H	331	ARG	NE-CZ	5.83	1.40	1.33
16	I	265	ARG	CZ-NH2	5.83	1.40	1.33
14	n	103	ARG	CZ-NH2	5.83	1.40	1.33
30	Q	55	GLU	CD-OE2	5.82	1.32	1.25
13	m	133	ARG	CD-NE	5.82	1.56	1.46
7	G	126	ARG	CZ-NH2	5.82	1.40	1.33
31	R	345	TYR	CE1-CZ	5.81	1.46	1.38
14	n	190	ARG	CZ-NH2	5.81	1.40	1.33
33	O	187	SER	CA-CB	5.81	1.61	1.52
27	N	740	TRP	CD2-CE3	-5.80	1.31	1.40
16	I	145	CYS	CB-SG	5.79	1.92	1.82
23	T	241	GLU	CG-CD	5.79	1.60	1.51
3	c	17	ARG	NE-CZ	5.79	1.40	1.33
9	i	196	ARG	CD-NE	5.79	1.56	1.46
14	n	51	VAL	CB-CG2	5.78	1.65	1.52
1	a	241	GLU	CD-OE1	5.78	1.32	1.25
5	E	12	ARG	NE-CZ	5.77	1.40	1.33
2	b	75	TYR	CE1-CZ	5.77	1.46	1.38
4	d	177	TYR	CG-CD2	5.76	1.46	1.39
2	B	174	PHE	CG-CD1	5.76	1.47	1.38
23	T	224	ARG	CD-NE	5.76	1.56	1.46
17	K	346	ARG	NE-CZ	5.76	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	261	ARG	NE-CZ	5.76	1.40	1.33
2	b	234	ARG	CD-NE	5.75	1.56	1.46
31	R	110	ILE	C-N	-5.75	1.20	1.34
1	A	37	ARG	CZ-NH2	5.75	1.40	1.33
12	5	146	TRP	CD2-CE2	-5.75	1.34	1.41
4	D	20	TYR	CZ-OH	5.74	1.47	1.37
12	l	144	TYR	CG-CD2	5.74	1.46	1.39
34	8	119	TYR	CD1-CE1	5.74	1.48	1.39
7	G	99	TYR	CG-CD2	5.74	1.46	1.39
15	H	190	ARG	CZ-NH2	5.74	1.40	1.33
19	M	425	ARG	CZ-NH1	5.74	1.40	1.33
12	l	69	ARG	NE-CZ	5.73	1.40	1.33
15	H	346	ARG	CZ-NH1	5.73	1.40	1.33
3	c	148	TYR	CE1-CZ	5.73	1.46	1.38
18	L	392	ARG	CZ-NH1	5.73	1.40	1.33
20	J	42	ARG	CZ-NH2	5.73	1.40	1.33
16	I	398	GLU	CD-OE2	5.73	1.31	1.25
21	W	63	SER	CA-CB	5.73	1.61	1.52
27	N	866	TYR	CE1-CZ	5.73	1.46	1.38
19	M	348	GLU	CD-OE2	5.72	1.31	1.25
29	P	147	LYS	N-CA	-5.72	1.34	1.46
3	c	148	TYR	CG-CD2	5.72	1.46	1.39
23	T	137	GLU	CG-CD	5.72	1.60	1.51
3	C	49	ARG	NE-CZ	5.71	1.40	1.33
7	G	89	ARG	CD-NE	5.71	1.56	1.46
12	5	19	ARG	CD-NE	5.71	1.56	1.46
1	A	43	VAL	CA-CB	-5.71	1.42	1.54
6	f	224	TYR	CZ-OH	5.70	1.47	1.37
19	M	255	TYR	CZ-OH	5.70	1.47	1.37
27	N	394	ARG	NE-CZ	5.70	1.40	1.33
4	d	86	LYS	N-CA	-5.70	1.34	1.46
9	i	19	ARG	NE-CZ	5.70	1.40	1.33
9	i	36	ARG	NE-CZ	5.69	1.40	1.33
11	k	190	ARG	CD-NE	5.69	1.56	1.46
3	C	148	TYR	CE1-CZ	5.68	1.46	1.38
6	F	50	ARG	CZ-NH1	5.68	1.40	1.33
4	D	109	ARG	NE-CZ	5.68	1.40	1.33
29	P	351	ARG	NE-CZ	5.67	1.40	1.33
12	5	19	ARG	CZ-NH1	5.67	1.40	1.33
34	8	119	TYR	CG-CD1	5.67	1.46	1.39
6	f	106	ARG	CZ-NH1	5.67	1.40	1.33
14	7	16	TYR	CG-CD2	5.67	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	139	GLU	CG-CD	5.66	1.60	1.51
33	O	286	PHE	CE1-CZ	5.66	1.48	1.37
26	Z	370	SER	CA-CB	5.66	1.61	1.52
2	b	5	TYR	CG-CD1	5.66	1.46	1.39
5	E	114	ARG	CZ-NH2	5.66	1.40	1.33
12	5	202	GLU	CD-OE2	-5.66	1.19	1.25
13	6	101	ARG	CZ-NH2	5.66	1.40	1.33
1	A	87	ARG	NE-CZ	5.65	1.40	1.33
13	6	5	TYR	CZ-OH	5.65	1.47	1.37
5	E	157	TYR	CB-CG	-5.65	1.43	1.51
11	4	96	ARG	NE-CZ	5.65	1.40	1.33
27	N	14	ARG	CZ-NH2	5.65	1.40	1.33
12	5	159	ARG	CZ-NH1	5.65	1.40	1.33
34	8	458	GLU	CD-OE2	5.64	1.31	1.25
10	3	100	GLY	CA-C	5.64	1.60	1.51
7	G	153	TYR	CB-CG	-5.64	1.43	1.51
4	D	46	ARG	NE-CZ	5.63	1.40	1.33
15	H	211	VAL	C-N	5.63	1.43	1.33
30	Q	51	ARG	CZ-NH2	5.63	1.40	1.33
2	B	5	TYR	CE1-CZ	5.63	1.45	1.38
15	H	62	ARG	CD-NE	5.63	1.56	1.46
1	a	100	GLY	N-CA	-5.63	1.37	1.46
3	c	209	ARG	CZ-NH2	5.63	1.40	1.33
2	b	5	TYR	CE2-CZ	5.62	1.45	1.38
16	I	291	ARG	NE-CZ	5.62	1.40	1.33
34	8	273	ARG	CZ-NH2	5.62	1.40	1.33
12	5	159	ARG	CD-NE	5.62	1.56	1.46
10	j	176	ARG	CZ-NH2	5.61	1.40	1.33
11	k	130	TYR	CG-CD1	5.61	1.46	1.39
6	F	164	SER	CA-CB	5.61	1.61	1.52
20	J	200	ARG	CZ-NH1	5.61	1.40	1.33
14	n	193	ARG	NE-CZ	5.61	1.40	1.33
13	m	194	ARG	CZ-NH1	5.61	1.40	1.33
2	B	128	ARG	CZ-NH2	5.60	1.40	1.33
13	6	67	ARG	CZ-NH1	5.60	1.40	1.33
15	H	88	ARG	NE-CZ	5.60	1.40	1.33
7	g	70	ILE	C-N	5.60	1.43	1.33
6	F	163	ARG	NE-CZ	5.60	1.40	1.33
19	M	198	VAL	CB-CG2	5.59	1.64	1.52
6	F	38	ARG	CZ-NH2	5.59	1.40	1.33
17	K	240	SER	CA-CB	5.59	1.61	1.52
27	N	570	ARG	NE-CZ	5.58	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	68	ARG	CZ-NH2	5.58	1.40	1.33
9	i	203	TYR	CD1-CE1	5.58	1.47	1.39
4	D	4	ARG	CD-NE	5.58	1.55	1.46
5	e	64	ARG	NE-CZ	5.58	1.40	1.33
28	S	304	SER	CA-CB	5.58	1.61	1.52
19	M	42	ARG	CD-NE	5.58	1.55	1.46
9	i	61	SER	CA-CB	5.57	1.61	1.52
20	J	120	TYR	CE2-CZ	5.57	1.45	1.38
4	D	47	ARG	NE-CZ	5.57	1.40	1.33
24	X	10	PHE	CB-CG	-5.57	1.41	1.51
3	c	113	ARG	CZ-NH1	5.57	1.40	1.33
20	J	120	TYR	CZ-OH	5.57	1.47	1.37
34	8	455	GLU	CB-CG	5.57	1.62	1.52
21	W	101	ARG	CZ-NH1	5.56	1.40	1.33
5	E	226	GLU	CG-CD	5.56	1.60	1.51
9	2	190	TYR	CZ-OH	5.56	1.47	1.37
23	T	245	TYR	CG-CD1	5.56	1.46	1.39
19	M	33	ARG	CD-NE	5.56	1.55	1.46
1	A	126	ARG	CZ-NH1	5.56	1.40	1.33
4	D	137	ASP	C-N	5.56	1.44	1.34
18	L	342	ARG	CD-NE	5.56	1.55	1.46
4	d	130	SER	CA-CB	5.55	1.61	1.52
20	J	270	ARG	NE-CZ	5.55	1.40	1.33
1	A	5	ARG	NE-CZ	5.55	1.40	1.33
19	M	345	ARG	NE-CZ	5.55	1.40	1.33
1	a	111	ARG	NE-CZ	5.54	1.40	1.33
13	m	194	ARG	CZ-NH2	5.54	1.40	1.33
10	3	104	VAL	C-N	5.54	1.43	1.33
7	g	68	ARG	CZ-NH2	5.54	1.40	1.33
8	h	124	TYR	CE1-CZ	5.53	1.45	1.38
11	k	141	PHE	CG-CD2	5.53	1.47	1.38
4	D	9	PHE	CB-CG	-5.53	1.42	1.51
12	5	106	ARG	CZ-NH1	5.53	1.40	1.33
22	V	44	GLY	CA-C	-5.53	1.43	1.51
9	i	69	TYR	CG-CD2	5.53	1.46	1.39
26	Z	450	GLY	N-CA	-5.53	1.37	1.46
26	Z	604	GLY	CA-C	-5.53	1.43	1.51
20	J	283	GLU	CD-OE2	5.52	1.31	1.25
13	m	98	TYR	CB-CG	-5.52	1.43	1.51
22	V	100	ARG	CZ-NH2	5.52	1.40	1.33
5	E	45	ARG	CZ-NH1	5.52	1.40	1.33
4	d	125	ARG	CZ-NH2	5.51	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Q	123	GLU	CG-CD	5.51	1.60	1.51
14	n	205	GLY	CA-C	-5.51	1.43	1.51
6	F	98	PHE	CE2-CZ	5.50	1.47	1.37
13	6	101	ARG	CD-NE	5.50	1.55	1.46
16	I	408	ARG	CZ-NH2	5.50	1.40	1.33
13	m	67	ARG	NE-CZ	5.50	1.40	1.33
12	5	40	PHE	CG-CD1	5.50	1.47	1.38
4	D	46	ARG	CD-NE	5.49	1.55	1.46
10	3	153	TYR	CE1-CZ	5.49	1.45	1.38
34	8	376	ARG	CZ-NH1	5.49	1.40	1.33
11	k	95	ARG	CZ-NH2	5.49	1.40	1.33
12	l	19	ARG	NE-CZ	5.48	1.40	1.33
13	m	101	ARG	NE-CZ	5.48	1.40	1.33
34	8	205	TYR	CG-CD1	5.48	1.46	1.39
10	3	27	ARG	CZ-NH1	5.48	1.40	1.33
21	W	43	SER	CB-OG	5.48	1.49	1.42
22	V	171	ARG	CZ-NH2	5.48	1.40	1.33
31	R	331	ARG	NE-CZ	5.48	1.40	1.33
1	A	129	GLY	N-CA	-5.47	1.37	1.46
9	2	193	PRO	N-CD	-5.47	1.40	1.47
4	d	110	TYR	CB-CG	-5.47	1.43	1.51
4	D	127	PHE	CG-CD2	5.47	1.47	1.38
11	k	169	GLU	CG-CD	-5.47	1.43	1.51
2	B	234	ARG	CD-NE	5.46	1.55	1.46
17	K	99	PHE	CB-CG	-5.46	1.42	1.51
11	4	76	SER	CA-CB	5.46	1.61	1.52
20	J	354	SER	CB-OG	5.46	1.49	1.42
13	m	1	GLN	N-CA	5.46	1.57	1.46
8	1	117	GLY	CA-C	-5.46	1.43	1.51
24	X	63	PRO	N-CA	-5.46	1.38	1.47
9	i	188	ARG	CZ-NH2	5.46	1.40	1.33
4	D	230	TYR	CE2-CZ	5.46	1.45	1.38
10	3	198	TYR	CE2-CZ	5.45	1.45	1.38
11	4	6	GLY	N-CA	-5.45	1.37	1.46
4	d	238	LYS	N-CA	-5.45	1.35	1.46
4	D	126	PRO	N-CD	-5.45	1.40	1.47
3	c	148	TYR	CB-CG	-5.45	1.43	1.51
13	m	137	ARG	CD-NE	5.44	1.55	1.46
4	D	67	SER	CB-OG	5.44	1.49	1.42
3	C	128	ARG	NE-CZ	5.44	1.40	1.33
1	A	190	TRP	CZ2-CH2	5.43	1.47	1.37
5	E	117	GLU	CD-OE2	5.43	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	182	ARG	NE-CZ	5.43	1.40	1.33
20	J	371	ARG	CZ-NH1	5.43	1.40	1.33
26	Z	841	GLU	CD-OE2	-5.43	1.19	1.25
16	I	64	ARG	NE-CZ	5.42	1.40	1.33
21	W	122	ARG	NE-CZ	5.42	1.40	1.33
30	Q	181	GLU	CD-OE1	5.42	1.31	1.25
8	1	167	GLY	CA-C	-5.42	1.43	1.51
1	A	146	TYR	CB-CG	-5.42	1.43	1.51
5	E	130	PHE	CG-CD2	5.42	1.46	1.38
5	E	219	GLY	N-CA	-5.42	1.38	1.46
27	N	547	LEU	N-CA	-5.42	1.35	1.46
8	h	70	TYR	CE1-CZ	5.42	1.45	1.38
29	P	319	GLU	CD-OE2	5.41	1.31	1.25
3	C	159	TRP	NE1-CE2	-5.41	1.30	1.37
4	D	81	ARG	NE-CZ	5.41	1.40	1.33
8	1	19	ARG	NE-CZ	5.40	1.40	1.33
26	Z	138	ARG	CZ-NH1	5.40	1.40	1.33
28	S	180	ASN	CB-CG	5.40	1.63	1.51
2	b	99	ARG	NE-CZ	5.40	1.40	1.33
11	k	73	TYR	CE2-CZ	5.40	1.45	1.38
20	J	333	ARG	CZ-NH1	5.40	1.40	1.33
11	4	190	ARG	CZ-NH1	5.39	1.40	1.33
26	Z	394	TYR	CB-CG	5.39	1.59	1.51
16	I	346	ARG	CZ-NH2	5.39	1.40	1.33
1	a	233	GLU	CG-CD	5.39	1.60	1.51
33	O	201	PRO	N-CD	-5.39	1.40	1.47
6	F	100	ARG	CZ-NH2	5.39	1.40	1.33
5	e	2	ARG	NE-CZ	5.39	1.40	1.33
9	i	75	ARG	NE-CZ	5.39	1.40	1.33
27	N	548	ARG	CZ-NH2	5.39	1.40	1.33
1	A	126	ARG	CD-NE	5.38	1.55	1.46
3	C	108	GLU	CD-OE1	5.38	1.31	1.25
7	G	165	ARG	CZ-NH1	5.38	1.40	1.33
21	W	179	ARG	CZ-NH2	5.38	1.40	1.33
34	8	176	PHE	CE1-CZ	5.38	1.47	1.37
13	6	38	ARG	CD-NE	5.38	1.55	1.46
1	a	154	TYR	CB-CG	-5.38	1.43	1.51
3	c	13	SER	CB-OG	5.38	1.49	1.42
14	n	193	ARG	CZ-NH2	5.38	1.40	1.33
17	K	399	ARG	CZ-NH1	5.38	1.40	1.33
27	N	66	SER	CB-OG	-5.37	1.35	1.42
2	b	84	VAL	CB-CG1	5.37	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	91	ARG	NE-CZ	5.37	1.40	1.33
21	W	75	GLY	CA-C	-5.37	1.43	1.51
15	H	53	GLU	CD-OE2	5.37	1.31	1.25
27	N	576	VAL	CB-CG2	-5.37	1.41	1.52
7	g	89	ARG	CZ-NH1	5.36	1.40	1.33
26	Z	801	HIS	N-CA	-5.36	1.35	1.46
32	U	41	ALA	CA-CB	5.36	1.63	1.52
7	g	68	ARG	NE-CZ	5.36	1.40	1.33
11	k	98	TYR	CE1-CZ	5.36	1.45	1.38
15	H	295	PHE	CG-CD2	5.36	1.46	1.38
9	2	8	PHE	CG-CD2	5.36	1.46	1.38
16	I	422	ARG	CZ-NH2	5.35	1.40	1.33
13	6	179	GLU	CD-OE2	5.35	1.31	1.25
16	I	54	ARG	CD-NE	5.35	1.55	1.46
29	P	69	ARG	CZ-NH1	5.35	1.40	1.33
21	W	121	SER	CB-OG	5.35	1.49	1.42
6	F	153	THR	CA-C	-5.34	1.39	1.52
12	5	121	ARG	NE-CZ	5.34	1.40	1.33
28	S	298	ARG	NE-CZ	5.34	1.40	1.33
27	N	345	ASP	N-CA	-5.34	1.35	1.46
6	f	122	TYR	CE2-CZ	5.33	1.45	1.38
11	k	171	ARG	CZ-NH2	5.33	1.40	1.33
11	4	139	TYR	CG-CD1	5.33	1.46	1.39
26	Z	722	ASP	CA-C	-5.33	1.39	1.52
13	m	85	SER	CB-OG	5.33	1.49	1.42
7	G	111	ARG	CD-NE	5.33	1.55	1.46
15	H	164	SER	CA-CB	5.33	1.60	1.52
23	T	24	GLU	CD-OE1	5.33	1.31	1.25
2	B	59	GLU	CD-OE1	-5.33	1.19	1.25
3	C	91	ARG	CZ-NH2	5.33	1.40	1.33
19	M	166	ARG	CZ-NH2	5.33	1.40	1.33
33	O	369	ARG	CZ-NH2	5.33	1.40	1.33
18	L	192	GLU	CD-OE2	5.32	1.31	1.25
22	V	270	TYR	CE1-CZ	5.32	1.45	1.38
10	j	73	TYR	CB-CG	-5.32	1.43	1.51
17	K	112	SER	CB-OG	5.32	1.49	1.42
31	R	141	TYR	CG-CD1	5.32	1.46	1.39
5	E	2	ARG	NE-CZ	5.32	1.40	1.33
17	K	336	ARG	NE-CZ	5.32	1.40	1.33
12	5	64	ARG	CZ-NH1	5.31	1.40	1.33
4	d	139	ARG	CA-C	-5.31	1.39	1.52
9	i	36	ARG	CZ-NH2	5.31	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	49	ARG	NE-CZ	5.31	1.40	1.33
2	b	12	PHE	CG-CD2	5.31	1.46	1.38
4	d	19	GLU	N-CA	-5.31	1.35	1.46
3	C	156	TYR	CG-CD2	5.31	1.46	1.39
16	I	100	ARG	CZ-NH2	5.31	1.40	1.33
15	H	363	PRO	N-CA	-5.30	1.38	1.47
22	V	126	GLN	N-CA	-5.30	1.35	1.46
6	f	88	ARG	NE-CZ	5.30	1.40	1.33
7	g	111	ARG	NE-CZ	5.30	1.40	1.33
16	I	88	LYS	CD-CE	5.29	1.64	1.51
15	H	266	ARG	CZ-NH1	5.29	1.40	1.33
6	f	19	PHE	CG-CD2	5.29	1.46	1.38
8	h	133	PHE	CG-CD2	5.29	1.46	1.38
6	F	86	TYR	CE1-CZ	5.29	1.45	1.38
6	F	88	ARG	NE-CZ	5.29	1.40	1.33
8	1	70	TYR	CE1-CZ	5.29	1.45	1.38
9	2	206	PRO	N-CA	-5.29	1.38	1.47
29	P	318	TYR	CE1-CZ	5.29	1.45	1.38
34	8	391	ARG	NE-CZ	5.29	1.40	1.33
9	i	149	GLU	CB-CG	5.29	1.62	1.52
7	G	74	TYR	CE1-CZ	5.29	1.45	1.38
13	6	35	ILE	N-CA	-5.29	1.35	1.46
8	h	160	SER	CA-CB	5.28	1.60	1.52
26	Z	578	GLY	CA-C	-5.28	1.43	1.51
33	O	372	GLU	CG-CD	5.28	1.59	1.51
34	8	377	ARG	NE-CZ	5.28	1.40	1.33
17	K	349	ARG	CD-NE	5.28	1.55	1.46
3	c	103	GLU	CG-CD	5.28	1.59	1.51
2	B	126	GLY	CA-C	-5.28	1.43	1.51
17	K	171	TYR	CB-CG	-5.28	1.43	1.51
30	Q	36	SER	CA-CB	5.28	1.60	1.52
15	H	289	ARG	CD-NE	5.27	1.55	1.46
18	L	126	ARG	CZ-NH1	5.27	1.40	1.33
4	D	4	ARG	CZ-NH1	5.27	1.39	1.33
18	L	62	ARG	CZ-NH2	5.27	1.39	1.33
14	n	37	ASN	C-N	5.26	1.42	1.33
6	F	224	TYR	CZ-OH	5.26	1.46	1.37
15	H	435	ARG	NE-CZ	5.26	1.39	1.33
19	M	77	TYR	CG-CD1	5.26	1.46	1.39
20	J	312	ARG	CZ-NH2	5.26	1.39	1.33
20	J	329	ARG	CD-NE	5.26	1.55	1.46
9	i	90	TYR	CD1-CE1	5.25	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	23	ARG	NE-CZ	5.25	1.39	1.33
4	d	20	TYR	CG-CD1	5.25	1.46	1.39
9	i	69	TYR	CZ-OH	5.25	1.46	1.37
26	Z	441	TYR	CD1-CE1	5.25	1.47	1.39
33	O	181	PHE	CG-CD1	5.25	1.46	1.38
7	g	147	LEU	CA-CB	5.25	1.65	1.53
17	K	262	ARG	CZ-NH1	5.25	1.39	1.33
6	f	152	VAL	CA-CB	-5.25	1.43	1.54
1	A	96	ARG	NE-CZ	5.25	1.39	1.33
3	C	148	TYR	CZ-OH	5.24	1.46	1.37
18	L	132	ARG	CZ-NH1	5.24	1.39	1.33
31	R	204	TRP	CD2-CE2	-5.24	1.35	1.41
27	N	739	PHE	CG-CD2	5.24	1.46	1.38
1	a	235	ARG	NE-CZ	5.24	1.39	1.33
12	l	167	ARG	NE-CZ	5.24	1.39	1.33
1	a	237	VAL	CA-CB	5.23	1.65	1.54
15	H	420	ARG	CZ-NH2	5.23	1.39	1.33
34	8	135	ASP	CB-CG	5.23	1.62	1.51
14	7	228	TYR	CB-CG	5.23	1.59	1.51
4	d	199	GLU	CD-OE2	-5.22	1.20	1.25
14	7	128	ARG	NE-CZ	5.22	1.39	1.33
7	g	113	GLY	CA-C	-5.22	1.43	1.51
13	6	75	TYR	CZ-OH	5.22	1.46	1.37
16	I	346	ARG	NE-CZ	5.22	1.39	1.33
11	4	36	ARG	CZ-NH2	5.22	1.39	1.33
19	M	320	ARG	NE-CZ	5.22	1.39	1.33
3	C	113	ARG	CZ-NH2	5.22	1.39	1.33
18	L	77	ARG	NE-CZ	5.21	1.39	1.33
4	d	110	TYR	CZ-OH	5.21	1.46	1.37
18	L	407	ARG	CD-NE	5.21	1.55	1.46
11	k	165	VAL	CB-CG2	5.21	1.63	1.52
14	n	128	ARG	CZ-NH1	5.21	1.39	1.33
16	I	64	ARG	CZ-NH1	5.21	1.39	1.33
28	S	439	GLU	CA-CB	5.21	1.65	1.53
1	a	15	ARG	CZ-NH2	5.21	1.39	1.33
13	6	213	ARG	CZ-NH2	5.21	1.39	1.33
5	e	64	ARG	CD-NE	5.20	1.55	1.46
14	n	89	PRO	CA-C	-5.20	1.42	1.52
3	C	66	TYR	CG-CD2	5.20	1.46	1.39
19	M	357	ARG	NE-CZ	5.19	1.39	1.33
1	A	126	ARG	CZ-NH2	5.19	1.39	1.33
34	8	488	SER	CA-CB	5.19	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	16	TYR	CB-CG	-5.19	1.43	1.51
19	M	264	ARG	CZ-NH2	5.19	1.39	1.33
14	n	47	ASP	N-CA	-5.18	1.35	1.46
6	F	50	ARG	NE-CZ	5.18	1.39	1.33
18	L	126	ARG	CD-NE	5.18	1.55	1.46
27	N	325	PHE	CG-CD2	5.18	1.46	1.38
18	L	289	ARG	N-CA	-5.18	1.35	1.46
4	d	36	GLY	N-CA	-5.18	1.38	1.46
7	g	82	ARG	CD-NE	5.18	1.55	1.46
5	E	15	GLN	CG-CD	5.18	1.62	1.51
8	1	70	TYR	CD2-CE2	5.17	1.47	1.39
6	F	7	GLY	CA-C	-5.17	1.43	1.51
17	K	291	GLU	CB-CG	5.17	1.61	1.52
26	Z	244	ARG	NE-CZ	5.17	1.39	1.33
28	S	64	ARG	CD-NE	5.17	1.55	1.46
6	f	232	TYR	CZ-OH	5.17	1.46	1.37
31	R	392	ARG	CZ-NH1	5.17	1.39	1.33
3	c	40	SER	CA-CB	5.16	1.60	1.52
13	m	33	TYR	CZ-OH	5.16	1.46	1.37
6	F	192	GLY	N-CA	-5.16	1.38	1.46
1	a	153	TYR	CB-CG	5.16	1.59	1.51
22	V	135	ARG	CZ-NH2	5.16	1.39	1.33
26	Z	394	TYR	CZ-OH	5.16	1.46	1.37
23	T	51	TYR	CZ-OH	5.16	1.46	1.37
7	G	81	GLY	CA-C	-5.15	1.43	1.51
3	C	145	TYR	CE1-CZ	5.15	1.45	1.38
9	2	200	GLN	CA-CB	5.15	1.65	1.53
26	Z	469	PRO	C-N	5.14	1.45	1.34
28	S	428	ARG	NE-CZ	5.14	1.39	1.33
28	S	491	GLU	CD-OE2	5.14	1.31	1.25
12	l	64	ARG	CZ-NH2	5.14	1.39	1.33
16	I	262	ARG	NE-CZ	5.14	1.39	1.33
8	1	75	THR	N-CA	-5.14	1.36	1.46
14	7	123	GLY	CA-C	-5.14	1.43	1.51
13	m	137	ARG	CZ-NH1	5.13	1.39	1.33
14	7	104	ARG	NE-CZ	5.13	1.39	1.33
12	l	121	ARG	CZ-NH1	5.13	1.39	1.33
16	I	127	ASP	N-CA	-5.13	1.36	1.46
1	A	146	TYR	CZ-OH	5.13	1.46	1.37
34	8	485	GLU	CD-OE1	5.13	1.31	1.25
22	V	48	GLU	CG-CD	5.13	1.59	1.51
33	O	387	ARG	CD-NE	5.13	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	136	CYS	CB-SG	5.13	1.91	1.82
10	j	67	ARG	NE-CZ	5.12	1.39	1.33
17	K	294	ARG	CZ-NH1	5.12	1.39	1.33
19	M	433	TYR	CG-CD1	5.12	1.45	1.39
8	h	29	ARG	CZ-NH2	5.12	1.39	1.33
9	i	142	TRP	CG-CD2	5.12	1.52	1.43
29	P	37	ASP	N-CA	-5.12	1.36	1.46
10	3	115	SER	CA-CB	5.12	1.60	1.52
8	h	174	ARG	CZ-NH1	5.12	1.39	1.33
13	m	105	TYR	CE2-CZ	5.11	1.45	1.38
4	D	225	GLU	CB-CG	5.11	1.61	1.52
11	4	138	PHE	CA-C	-5.11	1.39	1.52
14	n	85	GLU	CD-OE2	5.11	1.31	1.25
11	4	159	ASP	N-CA	-5.11	1.36	1.46
22	V	128	SER	CA-CB	5.11	1.60	1.52
12	5	73	ARG	CD-NE	5.11	1.55	1.46
8	1	36	ARG	CZ-NH2	5.10	1.39	1.33
11	4	8	ARG	NE-CZ	5.10	1.39	1.33
9	i	97	TYR	CE1-CZ	5.10	1.45	1.38
9	2	72	ARG	CZ-NH2	5.10	1.39	1.33
17	K	121	ARG	CZ-NH1	5.10	1.39	1.33
22	V	251	TYR	CE2-CZ	5.10	1.45	1.38
14	n	76	TYR	CZ-OH	5.10	1.46	1.37
30	Q	309	ARG	NE-CZ	5.10	1.39	1.33
5	e	144	GLY	N-CA	-5.09	1.38	1.46
1	A	122	ARG	NE-CZ	5.09	1.39	1.33
1	A	224	PHE	CE1-CZ	5.09	1.47	1.37
14	n	105	SER	CA-CB	5.09	1.60	1.52
2	B	22	ASP	CA-CB	5.09	1.65	1.53
13	6	137	ARG	NE-CZ	5.09	1.39	1.33
14	7	190	ARG	CD-NE	5.09	1.55	1.46
19	M	203	ARG	NE-CZ	5.09	1.39	1.33
10	j	182	TRP	C-N	5.09	1.42	1.33
13	m	185	ARG	CZ-NH2	5.09	1.39	1.33
1	a	117	GLN	CG-CD	5.08	1.62	1.51
14	n	190	ARG	CZ-NH1	5.08	1.39	1.33
4	D	140	ASP	N-CA	-5.08	1.36	1.46
16	I	107	GLY	N-CA	-5.08	1.38	1.46
29	P	232	ARG	CD-NE	5.08	1.55	1.46
12	l	114	TYR	CG-CD1	5.08	1.45	1.39
10	j	29	GLY	N-CA	-5.08	1.38	1.46
11	k	96	ARG	CZ-NH2	5.08	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	91	TYR	CG-CD1	5.08	1.45	1.39
14	n	44	PRO	CA-C	-5.08	1.42	1.52
4	d	74	SER	C-N	5.07	1.42	1.33
8	1	185	ARG	NE-CZ	5.07	1.39	1.33
28	S	384	ARG	CZ-NH1	5.07	1.39	1.33
1	a	57	PRO	CA-CB	-5.07	1.43	1.53
17	K	185	ARG	CZ-NH1	5.07	1.39	1.33
3	c	112	ARG	CZ-NH2	5.07	1.39	1.33
14	n	91	TYR	CE1-CZ	5.06	1.45	1.38
5	e	64	ARG	CZ-NH1	5.06	1.39	1.33
17	K	88	ARG	NE-CZ	5.06	1.39	1.33
19	M	233	ARG	CZ-NH2	5.06	1.39	1.33
26	Z	504	GLU	CB-CG	5.06	1.61	1.52
7	g	16	ARG	CZ-NH1	5.06	1.39	1.33
4	D	110	TYR	CB-CG	-5.06	1.44	1.51
5	E	201	GLU	CB-CG	5.06	1.61	1.52
19	M	299	ARG	CZ-NH2	5.06	1.39	1.33
14	n	41	ARG	CZ-NH2	5.05	1.39	1.33
14	n	65	ARG	CZ-NH2	5.05	1.39	1.33
17	K	349	ARG	CZ-NH2	5.05	1.39	1.33
26	Z	323	TYR	CG-CD2	5.05	1.45	1.39
3	c	112	ARG	CD-NE	5.05	1.55	1.46
6	f	201	ARG	CD-NE	5.05	1.55	1.46
9	2	75	ARG	CZ-NH1	5.05	1.39	1.33
29	P	68	SER	CA-CB	5.05	1.60	1.52
31	R	159	SER	CA-CB	5.05	1.60	1.52
4	d	191	LYS	N-CA	-5.05	1.36	1.46
11	k	73	TYR	CE1-CZ	5.05	1.45	1.38
28	S	25	TYR	N-CA	-5.05	1.36	1.46
3	C	49	ARG	CZ-NH2	5.05	1.39	1.33
14	7	76	TYR	CZ-OH	5.05	1.46	1.37
28	S	246	GLU	CD-OE1	5.04	1.31	1.25
12	5	170	TYR	CZ-OH	5.04	1.46	1.37
15	H	427	GLY	CA-C	-5.04	1.43	1.51
22	V	51	GLY	CA-C	-5.04	1.43	1.51
26	Z	841	GLU	CD-OE1	-5.04	1.20	1.25
2	b	90	ARG	CZ-NH2	5.04	1.39	1.33
13	m	195	HIS	CA-CB	5.04	1.65	1.53
20	J	228	ARG	NE-CZ	5.04	1.39	1.33
2	b	103	GLU	CD-OE2	5.04	1.31	1.25
9	i	77	VAL	CB-CG2	5.04	1.63	1.52
6	f	232	TYR	CG-CD2	5.03	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	165	ASN	CB-CG	5.03	1.62	1.51
5	e	43	GLU	CG-CD	5.03	1.59	1.51
23	T	122	PHE	CG-CD2	5.03	1.46	1.38
15	H	289	ARG	NE-CZ	5.02	1.39	1.33
17	K	139	LEU	N-CA	-5.02	1.36	1.46
9	2	69	TYR	CG-CD2	5.02	1.45	1.39
14	7	228	TYR	CZ-OH	5.02	1.46	1.37
11	4	58	GLU	N-CA	-5.02	1.36	1.46
16	I	242	ALA	CA-CB	5.02	1.62	1.52
2	b	131	GLY	N-CA	-5.02	1.38	1.46
8	h	158	SER	CA-CB	5.02	1.60	1.52
12	l	73	ARG	CZ-NH2	5.02	1.39	1.33
20	J	333	ARG	CZ-NH2	5.02	1.39	1.33
26	Z	147	GLU	CD-OE1	-5.02	1.20	1.25
13	m	215	GLU	CB-CG	5.02	1.61	1.52
34	8	121	ASN	CA-CB	5.02	1.66	1.53
2	B	97	TYR	CG-CD2	5.01	1.45	1.39
17	K	121	ARG	CD-NE	5.01	1.54	1.46
34	8	363	VAL	CB-CG2	5.01	1.63	1.52
7	g	21	GLU	CA-CB	5.01	1.65	1.53
9	i	214	LYS	CA-CB	5.01	1.65	1.53
14	n	41	ARG	CD-NE	5.01	1.54	1.46
1	A	136	SER	CA-CB	5.01	1.60	1.52
22	V	31	SER	CA-CB	5.01	1.60	1.52
1	a	175	ASN	N-CA	-5.01	1.36	1.46
12	l	7	ARG	NE-CZ	5.01	1.39	1.33
13	m	156	PHE	CB-CG	-5.01	1.42	1.51
19	M	124	ARG	NE-CZ	5.01	1.39	1.33
6	f	38	ARG	CZ-NH2	5.00	1.39	1.33
7	G	171	GLU	CB-CG	5.00	1.61	1.52
33	O	131	SER	CA-CB	5.00	1.60	1.52
7	G	71	GLY	N-CA	-5.00	1.38	1.46
17	K	185	ARG	NE-CZ	5.00	1.39	1.33

All (2244) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	P	86	HIS	CB-CA-C	-25.66	59.08	110.40
29	P	86	HIS	N-CA-CB	21.88	149.97	110.60
31	R	70	TYR	CB-CG-CD1	20.53	133.32	121.00
31	R	70	TYR	CB-CG-CD2	-20.08	108.95	121.00
11	k	96	ARG	NE-CZ-NH1	18.02	129.31	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	69	ARG	NE-CZ-NH1	17.69	129.15	120.30
27	N	861	TYR	N-CA-CB	-17.65	78.83	110.60
14	n	35	ARG	NE-CZ-NH2	-17.06	111.77	120.30
3	c	142	ARG	NE-CZ-NH2	-17.05	111.77	120.30
31	R	207	ARG	NE-CZ-NH1	16.84	128.72	120.30
1	A	37	ARG	NE-CZ-NH1	16.82	128.71	120.30
6	F	23	TYR	CB-CG-CD2	-16.77	110.94	121.00
3	c	209	ARG	NE-CZ-NH1	16.20	128.40	120.30
5	E	85	ARG	NE-CZ-NH1	15.98	128.29	120.30
33	O	62	TYR	CB-CG-CD2	-15.86	111.48	121.00
23	T	51	TYR	CB-CG-CD2	-15.83	111.50	121.00
8	1	142	PHE	CB-CG-CD2	-15.73	109.79	120.80
18	L	60	PHE	CB-CG-CD1	15.44	131.61	120.80
5	e	2	ARG	NE-CZ-NH1	15.36	127.98	120.30
34	8	391	ARG	NE-CZ-NH1	15.23	127.91	120.30
6	f	173	ARG	NE-CZ-NH1	15.16	127.88	120.30
27	N	873	ARG	NE-CZ-NH1	15.05	127.83	120.30
19	M	299	ARG	NE-CZ-NH2	-15.03	112.79	120.30
28	S	186	TYR	CB-CG-CD2	-15.01	112.00	121.00
28	S	275	TYR	CB-CG-CD2	14.96	129.98	121.00
8	1	189	TYR	CB-CG-CD1	14.85	129.91	121.00
14	7	128	ARG	NE-CZ-NH1	14.66	127.63	120.30
34	8	337	PHE	CB-CG-CD1	-14.56	110.61	120.80
14	7	161	ARG	NE-CZ-NH2	-14.56	113.02	120.30
7	G	22	TYR	CB-CG-CD2	-14.04	112.58	121.00
33	O	62	TYR	CB-CG-CD1	13.88	129.33	121.00
14	7	95	TYR	CB-CG-CD1	-13.87	112.68	121.00
17	K	212	TYR	CB-CG-CD1	-13.78	112.73	121.00
34	8	128	TYR	CB-CG-CD2	-13.76	112.75	121.00
4	D	195	ARG	NE-CZ-NH1	13.72	127.16	120.30
24	X	91	PHE	CB-CG-CD1	-13.65	111.24	120.80
10	j	45	TYR	CB-CG-CD2	-13.65	112.81	121.00
5	e	78	ARG	NE-CZ-NH2	-13.62	113.49	120.30
3	C	23	TYR	CB-CG-CD1	13.62	129.17	121.00
12	l	88	TYR	CB-CG-CD1	-13.59	112.85	121.00
1	a	15	ARG	NE-CZ-NH2	-13.46	113.57	120.30
33	O	115	ARG	NE-CZ-NH2	-13.44	113.58	120.30
14	7	221	PHE	CB-CG-CD2	-13.42	111.41	120.80
3	c	4	ARG	NE-CZ-NH2	-13.33	113.64	120.30
4	D	88	ARG	NE-CZ-NH2	-13.29	113.66	120.30
16	I	280	PHE	CB-CG-CD2	-13.29	111.50	120.80
1	A	87	ARG	NE-CZ-NH1	13.27	126.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Z	312	TYR	CB-CG-CD2	-13.20	113.08	121.00
3	c	66	TYR	CB-CG-CD2	-13.20	113.08	121.00
22	V	135	ARG	NE-CZ-NH1	13.17	126.88	120.30
29	P	379	TYR	CB-CG-CD2	-13.06	113.17	121.00
2	b	23	TYR	CB-CG-CD2	-13.04	113.18	121.00
3	c	101	TYR	CB-CG-CD1	12.98	128.79	121.00
23	T	186	ARG	NE-CZ-NH1	12.97	126.78	120.30
22	V	171	ARG	NE-CZ-NH1	12.93	126.77	120.30
27	N	873	ARG	NE-CZ-NH2	-12.92	113.84	120.30
18	L	60	PHE	CB-CG-CD2	-12.87	111.79	120.80
34	8	192	TYR	CB-CG-CD1	-12.84	113.29	121.00
5	E	85	ARG	NE-CZ-NH2	-12.80	113.90	120.30
30	Q	409	TYR	CB-CG-CD2	-12.80	113.32	121.00
10	j	45	TYR	CB-CG-CD1	12.79	128.67	121.00
34	8	192	TYR	CB-CG-CD2	12.76	128.66	121.00
26	Z	312	TYR	CB-CG-CD1	12.72	128.63	121.00
5	e	128	ARG	NE-CZ-NH2	-12.67	113.97	120.30
30	Q	398	TYR	CB-CG-CD2	12.66	128.59	121.00
34	8	337	PHE	CB-CG-CD2	12.66	129.66	120.80
10	3	68	TYR	CB-CG-CD2	-12.60	113.44	121.00
7	g	145	TYR	CB-CG-CD1	-12.54	113.47	121.00
14	n	76	TYR	CB-CG-CD2	-12.54	113.47	121.00
34	8	214	PHE	CB-CG-CD1	12.54	129.58	120.80
3	C	49	ARG	NE-CZ-NH1	12.48	126.54	120.30
14	n	193	ARG	NE-CZ-NH2	-12.47	114.07	120.30
9	i	69	TYR	CB-CG-CD2	-12.45	113.53	121.00
8	1	189	TYR	CB-CG-CD2	-12.43	113.55	121.00
17	K	347	ARG	NE-CZ-NH1	12.43	126.51	120.30
8	1	174	ARG	NE-CZ-NH2	-12.42	114.09	120.30
7	G	186	ARG	NE-CZ-NH1	12.41	126.51	120.30
24	X	91	PHE	CB-CG-CD2	12.37	129.46	120.80
4	d	170	ARG	NE-CZ-NH2	-12.35	114.12	120.30
28	S	186	TYR	CB-CG-CD1	12.31	128.39	121.00
13	m	137	ARG	NE-CZ-NH2	12.22	126.41	120.30
11	4	93	ARG	NE-CZ-NH2	-12.18	114.21	120.30
2	b	90	ARG	NE-CZ-NH2	-12.11	114.25	120.30
12	l	6	PHE	CB-CG-CD1	-12.09	112.34	120.80
18	L	420	ARG	NE-CZ-NH1	12.04	126.32	120.30
15	H	353	PHE	CB-CG-CD1	12.02	129.21	120.80
11	4	8	ARG	NE-CZ-NH2	-12.01	114.29	120.30
18	L	88	TYR	CB-CG-CD2	-12.00	113.80	121.00
34	8	233	PHE	CB-CG-CD2	-11.99	112.41	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	8	357	ARG	NE-CZ-NH2	-11.99	114.31	120.30
3	C	145	TYR	CB-CG-CD1	-11.97	113.82	121.00
16	I	208	TYR	CB-CG-CD2	-11.96	113.82	121.00
2	B	75	TYR	CB-CG-CD1	-11.95	113.83	121.00
3	C	216	ARG	NE-CZ-NH1	11.90	126.25	120.30
7	G	22	TYR	CB-CG-CD1	11.83	128.10	121.00
3	C	113	ARG	NE-CZ-NH1	11.82	126.21	120.30
14	7	95	TYR	CB-CG-CD2	11.82	128.09	121.00
13	m	188	PHE	CB-CG-CD2	-11.71	112.61	120.80
1	A	87	ARG	NE-CZ-NH2	-11.68	114.46	120.30
5	e	2	ARG	NE-CZ-NH2	-11.66	114.47	120.30
11	k	117	TYR	CB-CG-CD2	-11.62	114.03	121.00
10	j	153	TYR	CB-CG-CD1	-11.54	114.07	121.00
6	f	38	ARG	NE-CZ-NH1	11.44	126.02	120.30
14	7	91	TYR	CB-CG-CD2	-11.39	114.17	121.00
11	4	95	ARG	NE-CZ-NH1	11.37	125.98	120.30
3	C	23	TYR	CB-CG-CD2	-11.33	114.20	121.00
15	H	318	ARG	NE-CZ-NH1	11.27	125.94	120.30
20	J	112	ARG	NE-CZ-NH1	11.24	125.92	120.30
16	I	54	ARG	NE-CZ-NH1	11.23	125.92	120.30
10	3	176	ARG	NE-CZ-NH1	11.23	125.92	120.30
26	Z	244	ARG	NE-CZ-NH1	-11.23	114.69	120.30
5	e	78	ARG	NE-CZ-NH1	11.21	125.91	120.30
8	1	142	PHE	CB-CG-CD1	11.20	128.64	120.80
8	1	111	TYR	CB-CG-CD1	-11.20	114.28	121.00
14	7	111	TRP	CB-CG-CD1	11.19	141.55	127.00
4	d	146	TYR	CB-CG-CD2	-11.18	114.29	121.00
7	G	126	ARG	NE-CZ-NH1	11.15	125.88	120.30
19	M	73	ARG	NE-CZ-NH1	11.14	125.87	120.30
31	R	70	TYR	CA-CB-CG	11.13	134.54	113.40
4	d	46	ARG	NE-CZ-NH1	11.10	125.85	120.30
13	m	185	ARG	NE-CZ-NH2	-11.08	114.76	120.30
6	f	224	TYR	CB-CG-CD2	-11.05	114.37	121.00
13	m	5	TYR	CB-CG-CD2	-11.05	114.37	121.00
3	c	229	PHE	CB-CG-CD2	-11.04	113.08	120.80
9	i	69	TYR	CB-CG-CD1	11.01	127.61	121.00
34	8	214	PHE	CB-CG-CD2	-10.97	113.12	120.80
8	1	102	TYR	CB-CG-CD2	-10.97	114.42	121.00
13	m	101	ARG	NE-CZ-NH2	-10.95	114.83	120.30
7	G	111	ARG	NE-CZ-NH1	10.94	125.77	120.30
7	G	87	ARG	NE-CZ-NH1	10.93	125.76	120.30
17	K	212	TYR	CB-CG-CD2	10.92	127.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	124	ASP	CB-CG-OD1	-10.90	108.49	118.30
11	k	171	ARG	NE-CZ-NH1	10.88	125.74	120.30
30	Q	51	ARG	NE-CZ-NH2	-10.88	114.86	120.30
10	3	68	TYR	CB-CG-CD1	10.86	127.52	121.00
14	n	161	ARG	NE-CZ-NH1	10.82	125.71	120.30
13	m	137	ARG	NE-CZ-NH1	-10.80	114.90	120.30
5	e	124	ARG	NE-CZ-NH2	-10.79	114.90	120.30
14	7	111	TRP	CB-CG-CD2	-10.79	112.57	126.60
11	4	23	ARG	NE-CZ-NH1	-10.78	114.91	120.30
1	A	17	TYR	CB-CG-CD1	-10.77	114.54	121.00
6	f	224	TYR	CB-CG-CD1	10.76	127.46	121.00
34	8	129	ARG	NE-CZ-NH2	-10.75	114.92	120.30
16	I	280	PHE	CB-CG-CD1	10.75	128.32	120.80
6	F	17	ARG	NE-CZ-NH1	10.72	125.66	120.30
7	g	197	TYR	CB-CG-CD2	-10.72	114.57	121.00
3	c	145	TYR	CB-CG-CD1	-10.70	114.58	121.00
21	W	21	PHE	CB-CG-CD1	10.70	128.29	120.80
28	S	126	LYS	N-CA-CB	10.70	129.86	110.60
27	N	14	ARG	NE-CZ-NH2	-10.69	114.95	120.30
7	G	111	ARG	NE-CZ-NH2	-10.66	114.97	120.30
29	P	379	TYR	CB-CG-CD1	10.65	127.39	121.00
9	2	36	ARG	NE-CZ-NH2	-10.60	115.00	120.30
29	P	220	TYR	CB-CG-CD1	10.58	127.35	121.00
8	h	45	ARG	NE-CZ-NH1	10.56	125.58	120.30
28	S	274	PHE	CB-CG-CD2	-10.55	113.41	120.80
27	N	880	ARG	NE-CZ-NH1	10.55	125.57	120.30
4	d	164	ARG	NE-CZ-NH1	-10.54	115.03	120.30
21	W	60	ARG	NE-CZ-NH2	-10.52	115.04	120.30
1	a	10	PHE	CB-CG-CD2	-10.51	113.44	120.80
10	j	197	ARG	NE-CZ-NH1	10.50	125.55	120.30
3	C	128	ARG	NE-CZ-NH1	10.49	125.55	120.30
18	L	168	TYR	CB-CG-CD1	10.46	127.27	121.00
20	J	48	ARG	NE-CZ-NH1	10.44	125.52	120.30
11	4	95	ARG	NE-CZ-NH2	-10.39	115.10	120.30
11	k	59	TYR	CB-CG-CD2	-10.39	114.76	121.00
19	M	299	ARG	NE-CZ-NH1	10.39	125.50	120.30
20	J	329	ARG	NE-CZ-NH1	10.39	125.50	120.30
3	C	179	TYR	CB-CG-CD2	-10.38	114.77	121.00
34	8	451	PHE	CB-CG-CD1	10.35	128.05	120.80
11	4	141	PHE	CB-CG-CD2	-10.34	113.56	120.80
29	P	13	TYR	CB-CG-CD2	-10.34	114.80	121.00
1	a	82	ARG	NE-CZ-NH2	-10.32	115.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	78	ARG	NE-CZ-NH1	10.31	125.46	120.30
34	8	321	ARG	NE-CZ-NH2	-10.31	115.14	120.30
4	d	164	ARG	NE-CZ-NH2	10.31	125.45	120.30
4	D	95	ARG	NE-CZ-NH1	-10.31	115.15	120.30
17	K	77	ARG	NE-CZ-NH2	-10.28	115.16	120.30
3	c	207	TYR	CB-CG-CD2	10.25	127.15	121.00
18	L	209	ARG	NE-CZ-NH1	-10.25	115.17	120.30
8	h	25	TYR	CB-CG-CD2	-10.23	114.86	121.00
2	b	97	TYR	CB-CG-CD2	-10.23	114.86	121.00
6	f	88	ARG	NE-CZ-NH1	10.22	125.41	120.30
34	8	229	PHE	CB-CG-CD2	-10.22	113.64	120.80
28	S	170	TYR	CA-CB-CG	10.20	132.79	113.40
6	F	93	TYR	CB-CG-CD2	-10.17	114.90	121.00
27	N	861	TYR	CB-CA-C	10.16	130.73	110.40
27	N	896	PHE	CB-CG-CD2	-10.14	113.70	120.80
1	A	95	PHE	CB-CG-CD2	-10.13	113.71	120.80
30	Q	321	TYR	CB-CG-CD2	-10.12	114.92	121.00
12	l	90	TYR	CB-CG-CD2	-10.11	114.94	121.00
12	l	113	TYR	CB-CG-CD2	-10.11	114.94	121.00
32	U	137	TYR	CB-CG-CD2	10.08	127.05	121.00
10	3	123	PHE	CB-CG-CD2	10.07	127.85	120.80
5	E	18	TYR	CB-CG-CD2	-10.07	114.96	121.00
11	k	176	PHE	CB-CG-CD2	-10.05	113.76	120.80
2	B	104	TYR	CB-CG-CD1	10.04	127.02	121.00
5	e	95	TYR	CB-CG-CD1	-10.04	114.98	121.00
34	8	168	PHE	CB-CG-CD1	10.04	127.83	120.80
11	k	190	ARG	NE-CZ-NH2	-10.01	115.30	120.30
5	e	64	ARG	NE-CZ-NH1	-9.98	115.31	120.30
5	e	64	ARG	NE-CZ-NH2	9.97	125.28	120.30
13	m	33	TYR	CB-CG-CD1	9.94	126.97	121.00
4	d	170	ARG	NE-CZ-NH1	9.94	125.27	120.30
1	A	209	PHE	CB-CG-CD1	-9.94	113.84	120.80
34	8	391	ARG	NE-CZ-NH2	-9.93	115.33	120.30
13	m	33	TYR	CB-CG-CD2	-9.93	115.04	121.00
24	X	45	PHE	CB-CG-CD2	-9.90	113.87	120.80
10	j	153	TYR	CB-CG-CD2	9.88	126.93	121.00
13	6	106	TYR	CB-CG-CD1	9.87	126.92	121.00
33	O	60	ARG	NE-CZ-NH2	9.85	125.22	120.30
1	a	146	TYR	CB-CG-CD2	-9.84	115.10	121.00
34	8	129	ARG	NE-CZ-NH1	9.84	125.22	120.30
11	k	72	ASP	CB-CG-OD1	9.83	127.15	118.30
30	Q	355	GLU	N-CA-CB	9.83	128.30	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Z	210	TYR	CB-CG-CD2	-9.82	115.11	121.00
14	7	41	ARG	NE-CZ-NH1	9.82	125.21	120.30
33	O	286	PHE	CB-CG-CD2	-9.82	113.93	120.80
10	3	146	PHE	CB-CG-CD1	9.81	127.67	120.80
12	5	88	TYR	CB-CG-CD1	-9.81	115.12	121.00
14	7	190	ARG	NE-CZ-NH1	9.78	125.19	120.30
9	i	8	PHE	CB-CG-CD1	-9.77	113.96	120.80
27	N	14	ARG	NE-CZ-NH1	9.76	125.18	120.30
19	M	267	PHE	CB-CG-CD1	9.75	127.62	120.80
13	m	101	ARG	NE-CZ-NH1	9.73	125.17	120.30
16	I	208	TYR	CB-CG-CD1	9.72	126.83	121.00
31	R	207	ARG	NE-CZ-NH2	-9.72	115.44	120.30
31	R	102	LEU	N-CA-CB	9.71	129.83	110.40
2	B	148	TYR	CB-CG-CD1	-9.70	115.18	121.00
10	3	197	ARG	NE-CZ-NH1	9.69	125.15	120.30
34	8	297	TYR	CB-CG-CD2	-9.67	115.20	121.00
11	4	85	ARG	NE-CZ-NH1	9.66	125.13	120.30
17	K	73	ARG	NE-CZ-NH1	9.65	125.13	120.30
32	U	137	TYR	CB-CG-CD1	-9.63	115.22	121.00
19	M	166	ARG	NE-CZ-NH1	9.63	125.11	120.30
28	S	399	TYR	CB-CG-CD2	-9.62	115.23	121.00
13	6	221	ARG	NE-CZ-NH1	9.61	125.11	120.30
23	T	73	PHE	CB-CG-CD2	-9.61	114.07	120.80
30	Q	398	TYR	CB-CG-CD1	-9.61	115.23	121.00
11	4	138	PHE	CB-CG-CD2	-9.60	114.08	120.80
15	H	434	ARG	NE-CZ-NH1	9.59	125.10	120.30
14	n	193	ARG	NE-CZ-NH1	9.59	125.09	120.30
29	P	232	ARG	NE-CZ-NH1	9.58	125.09	120.30
27	N	753	PHE	CB-CG-CD2	-9.58	114.09	120.80
6	F	127	TYR	CB-CG-CD1	-9.58	115.25	121.00
27	N	604	ARG	NE-CZ-NH2	-9.54	115.53	120.30
30	Q	321	TYR	CB-CG-CD1	9.54	126.72	121.00
27	N	338	PHE	CB-CG-CD2	-9.52	114.13	120.80
8	h	82	PHE	CB-CG-CD1	-9.52	114.14	120.80
3	C	121	TYR	CB-CG-CD2	-9.51	115.30	121.00
5	E	2	ARG	NE-CZ-NH2	-9.49	115.56	120.30
22	V	188	LEU	N-CA-CB	9.47	129.35	110.40
12	l	144	TYR	CG-CD1-CE1	-9.44	113.75	121.30
19	M	243	PHE	CB-CG-CD1	9.44	127.41	120.80
4	d	4	ARG	NE-CZ-NH2	9.44	125.02	120.30
34	8	287	ARG	NE-CZ-NH1	9.41	125.00	120.30
2	b	157	PHE	CB-CG-CD1	9.38	127.37	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	170	ALA	N-CA-CB	9.37	123.21	110.10
9	i	36	ARG	NE-CZ-NH2	-9.37	115.62	120.30
12	l	8	PHE	CB-CG-CD2	-9.36	114.25	120.80
9	2	51	ASP	CB-CG-OD1	9.35	126.72	118.30
33	O	115	ARG	NE-CZ-NH1	9.35	124.97	120.30
4	d	47	ARG	NE-CZ-NH2	-9.35	115.63	120.30
26	Z	287	ARG	NE-CZ-NH2	-9.34	115.63	120.30
34	8	318	PHE	CB-CG-CD1	9.33	127.33	120.80
10	j	103	PHE	CB-CG-CD1	-9.33	114.27	120.80
16	I	291	ARG	NE-CZ-NH2	-9.31	115.64	120.30
14	7	161	ARG	NE-CZ-NH1	9.30	124.95	120.30
17	K	349	ARG	NE-CZ-NH1	9.29	124.94	120.30
13	m	102	PHE	CB-CG-CD2	-9.28	114.31	120.80
3	c	4	ARG	NE-CZ-NH1	9.28	124.94	120.30
1	A	122	ARG	NE-CZ-NH2	-9.28	115.66	120.30
20	J	329	ARG	NE-CZ-NH2	-9.27	115.67	120.30
4	D	73	PHE	CB-CG-CD2	-9.25	114.32	120.80
16	I	256	TYR	CB-CG-CD1	9.25	126.55	121.00
22	V	171	ARG	NE-CZ-NH2	-9.25	115.67	120.30
15	H	432	ARG	NE-CZ-NH2	9.25	124.92	120.30
34	8	372	ARG	NE-CZ-NH2	-9.24	115.68	120.30
24	X	122	TYR	CB-CG-CD2	-9.23	115.46	121.00
5	E	223	TYR	CB-CG-CD2	-9.22	115.47	121.00
9	2	205	PHE	CB-CG-CD2	-9.22	114.34	120.80
23	T	51	TYR	CB-CG-CD1	9.21	126.53	121.00
13	6	185	ARG	NE-CZ-NH1	9.21	124.90	120.30
18	L	62	ARG	NE-CZ-NH1	9.20	124.90	120.30
34	8	349	TYR	CB-CG-CD1	9.20	126.52	121.00
18	L	132	ARG	NE-CZ-NH2	-9.18	115.71	120.30
13	m	217	TYR	CB-CG-CD1	9.18	126.51	121.00
13	6	185	ARG	NE-CZ-NH2	-9.17	115.72	120.30
33	O	69	PHE	CB-CG-CD1	-9.13	114.41	120.80
14	7	91	TYR	CB-CG-CD1	9.12	126.47	121.00
34	8	451	PHE	CB-CG-CD2	-9.11	114.42	120.80
9	2	36	ARG	NE-CZ-NH1	9.11	124.85	120.30
31	R	110	ILE	O-C-N	-9.10	108.14	122.70
14	7	93	PHE	CB-CG-CD2	-9.10	114.43	120.80
1	a	21	TYR	CB-CG-CD2	-9.09	115.54	121.00
2	B	178	ARG	NE-CZ-NH1	9.09	124.85	120.30
10	j	197	ARG	NE-CZ-NH2	-9.07	115.76	120.30
10	j	187	TYR	CB-CG-CD1	-9.07	115.56	121.00
31	R	357	PHE	CB-CG-CD1	9.06	127.14	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	8	335	PHE	CB-CG-CD2	9.05	127.13	120.80
2	b	90	ARG	NE-CZ-NH1	9.04	124.82	120.30
11	4	23	ARG	NE-CZ-NH2	9.04	124.82	120.30
3	C	8	ARG	NE-CZ-NH2	-9.04	115.78	120.30
4	d	179	ARG	NE-CZ-NH1	9.03	124.81	120.30
4	d	230	TYR	CB-CG-CD2	-9.02	115.59	121.00
13	m	5	TYR	CB-CG-CD1	9.02	126.41	121.00
3	C	41	ASP	CB-CG-OD2	-9.02	110.18	118.30
31	R	394	ASP	CB-CG-OD2	-9.02	110.19	118.30
21	W	179	ARG	NE-CZ-NH2	8.99	124.79	120.30
2	b	101	TYR	CB-CG-CD2	8.97	126.38	121.00
5	E	78	ARG	NE-CZ-NH2	-8.96	115.82	120.30
15	H	353	PHE	CB-CG-CD2	-8.95	114.54	120.80
17	K	262	ARG	NE-CZ-NH1	8.94	124.77	120.30
1	A	126	ARG	NE-CZ-NH2	-8.93	115.83	120.30
3	C	49	ARG	NE-CZ-NH2	-8.91	115.84	120.30
23	T	109	TYR	CB-CG-CD1	8.91	126.34	121.00
9	i	190	TYR	CB-CG-CD2	-8.90	115.66	121.00
6	f	125	ARG	NE-CZ-NH2	-8.89	115.86	120.30
5	e	140	ASP	CB-CG-OD2	-8.88	110.31	118.30
6	f	232	TYR	CB-CG-CD1	-8.88	115.67	121.00
8	1	193	TYR	CB-CG-CD2	8.88	126.33	121.00
30	Q	409	TYR	CB-CG-CD1	8.88	126.33	121.00
11	k	149	ARG	NE-CZ-NH1	8.87	124.74	120.30
26	Z	408	TYR	CB-CG-CD1	-8.87	115.68	121.00
18	L	127	TYR	CB-CG-CD1	-8.83	115.70	121.00
7	G	153	TYR	CB-CG-CD2	-8.83	115.70	121.00
3	c	216	ARG	NE-CZ-NH2	-8.81	115.89	120.30
11	4	59	TYR	CB-CG-CD2	-8.80	115.72	121.00
4	D	81	ARG	NE-CZ-NH2	-8.80	115.90	120.30
24	X	22	ARG	NE-CZ-NH1	8.80	124.70	120.30
14	7	221	PHE	CB-CG-CD1	8.80	126.96	120.80
15	H	101	ARG	NE-CZ-NH1	8.78	124.69	120.30
30	Q	67	THR	C-N-CA	8.78	143.64	121.70
1	A	37	ARG	NE-CZ-NH2	-8.77	115.91	120.30
2	B	7	PHE	CB-CG-CD1	-8.77	114.66	120.80
7	g	156	TYR	CB-CG-CD1	-8.76	115.74	121.00
2	B	156	TYR	CB-CG-CD2	-8.74	115.76	121.00
13	6	174	TYR	CB-CG-CD2	-8.73	115.76	121.00
29	P	220	TYR	CB-CG-CD2	-8.73	115.76	121.00
20	J	374	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	a	3	TYR	CB-CG-CD2	-8.73	115.76	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	127	TYR	CB-CG-CD2	8.72	126.23	121.00
3	c	8	ARG	NE-CZ-NH1	8.72	124.66	120.30
28	S	55	ARG	NE-CZ-NH1	8.72	124.66	120.30
28	S	333	PHE	CB-CG-CD1	8.71	126.90	120.80
1	a	111	ARG	NE-CZ-NH2	-8.71	115.95	120.30
28	S	126	LYS	CA-CB-CG	-8.71	94.25	113.40
12	l	25	TRP	CG-CD2-CE3	-8.69	126.08	133.90
7	G	122	TYR	CB-CG-CD2	-8.68	115.79	121.00
14	7	213	GLN	N-CA-CB	8.65	126.17	110.60
26	Z	210	TYR	CB-CG-CD1	8.65	126.19	121.00
14	n	156	ARG	NE-CZ-NH1	8.65	124.62	120.30
1	a	153	TYR	CB-CG-CD1	-8.64	115.81	121.00
12	l	125	ASP	CB-CG-OD1	8.62	126.06	118.30
10	3	153	TYR	CB-CG-CD1	-8.62	115.83	121.00
3	C	145	TYR	CB-CG-CD2	8.61	126.17	121.00
9	2	8	PHE	CB-CG-CD2	-8.61	114.77	120.80
17	K	374	ARG	NE-CZ-NH2	-8.60	116.00	120.30
2	B	156	TYR	CG-CD2-CE2	-8.59	114.43	121.30
15	H	273	ARG	NE-CZ-NH1	8.59	124.59	120.30
6	f	66	ASP	CB-CG-OD2	-8.59	110.57	118.30
29	P	303	PHE	CB-CG-CD2	-8.58	114.79	120.80
5	e	156	PHE	CB-CG-CD1	-8.58	114.80	120.80
30	Q	123	GLU	C-N-CA	8.57	143.12	121.70
11	4	8	ARG	NE-CZ-NH1	8.55	124.58	120.30
3	c	101	TYR	CB-CG-CD2	-8.54	115.88	121.00
30	Q	65	TYR	CB-CG-CD1	8.52	126.11	121.00
6	F	23	TYR	CG-CD1-CE1	-8.52	114.49	121.30
24	X	17	TYR	CB-CG-CD1	8.51	126.10	121.00
17	K	270	PHE	CB-CG-CD2	-8.50	114.85	120.80
34	8	273	ARG	NE-CZ-NH2	-8.48	116.06	120.30
10	j	198	TYR	CB-CG-CD2	-8.48	115.91	121.00
14	n	187	ARG	NE-CZ-NH1	8.46	124.53	120.30
7	G	108	PHE	CB-CG-CD2	-8.45	114.88	120.80
5	e	95	TYR	CB-CG-CD2	8.45	126.07	121.00
16	I	181	TYR	CB-CG-CD1	-8.44	115.94	121.00
11	4	36	ARG	NE-CZ-NH1	8.44	124.52	120.30
6	f	201	ARG	NE-CZ-NH2	-8.43	116.08	120.30
13	m	194	ARG	NE-CZ-NH2	-8.42	116.09	120.30
6	f	232	TYR	CB-CG-CD2	8.40	126.04	121.00
1	A	102	ASP	CB-CG-OD1	8.40	125.86	118.30
31	R	102	LEU	CB-CG-CD1	8.40	125.27	111.00
3	c	182	ASP	CB-CG-OD1	-8.39	110.75	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	k	107	TYR	CG-CD1-CE1	-8.39	114.59	121.30
9	i	8	PHE	CB-CG-CD2	8.39	126.67	120.80
11	k	107	TYR	CB-CG-CD2	-8.38	115.97	121.00
28	S	421	TYR	CB-CG-CD2	-8.39	115.97	121.00
2	b	130	PHE	CB-CG-CD1	8.37	126.66	120.80
6	f	178	PHE	CB-CG-CD1	8.37	126.66	120.80
11	4	67	TYR	CB-CG-CD2	-8.37	115.98	121.00
3	C	128	ARG	NE-CZ-NH2	-8.37	116.12	120.30
4	D	106	TYR	CB-CG-CD2	8.35	126.01	121.00
14	n	47	ASP	CB-CG-OD2	-8.35	110.79	118.30
9	i	124	TYR	CB-CG-CD2	-8.34	115.99	121.00
22	V	273	ARG	NE-CZ-NH1	8.34	124.47	120.30
27	N	786	ARG	NE-CZ-NH1	-8.34	116.13	120.30
3	C	134	PHE	CB-CG-CD2	-8.32	114.98	120.80
34	8	349	TYR	CB-CG-CD2	-8.31	116.02	121.00
30	Q	65	TYR	CB-CG-CD2	-8.30	116.02	121.00
31	R	110	ILE	N-CA-CB	8.30	129.88	110.80
4	D	56	ARG	NE-CZ-NH2	-8.28	116.16	120.30
14	n	137	TYR	CD1-CE1-CZ	-8.28	112.34	119.80
28	S	480	ARG	NE-CZ-NH1	8.28	124.44	120.30
31	R	49	PHE	CB-CG-CD2	-8.28	115.01	120.80
31	R	394	ASP	CB-CG-OD1	8.28	125.75	118.30
27	N	298	TYR	CB-CG-CD2	-8.27	116.04	121.00
17	K	234	PHE	CB-CG-CD1	8.26	126.58	120.80
6	f	106	ARG	NE-CZ-NH2	-8.26	116.17	120.30
34	8	335	PHE	CB-CG-CD1	-8.26	115.02	120.80
3	c	179	TYR	CB-CG-CD2	-8.23	116.06	121.00
9	2	75	ARG	NE-CZ-NH1	8.23	124.42	120.30
14	7	137	TYR	CD1-CE1-CZ	-8.23	112.39	119.80
16	I	407	ARG	NE-CZ-NH1	8.23	124.42	120.30
23	T	224	ARG	NE-CZ-NH1	-8.23	116.19	120.30
21	W	60	ARG	NE-CZ-NH1	8.22	124.41	120.30
3	C	91	ARG	NE-CZ-NH1	8.22	124.41	120.30
8	1	93	LEU	CB-CG-CD2	8.21	124.96	111.00
34	8	273	ARG	NE-CZ-NH1	8.21	124.41	120.30
3	C	113	ARG	NE-CZ-NH2	-8.21	116.19	120.30
11	4	73	TYR	CG-CD2-CE2	-8.20	114.74	121.30
3	C	66	TYR	CB-CG-CD2	-8.20	116.08	121.00
4	d	88	ARG	NE-CZ-NH1	8.17	124.38	120.30
7	G	145	TYR	CG-CD1-CE1	-8.17	114.77	121.30
2	b	101	TYR	CB-CG-CD1	-8.16	116.10	121.00
2	b	23	TYR	CB-CG-CD1	8.15	125.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	47	ALA	N-CA-CB	8.15	121.51	110.10
19	M	366	ARG	NE-CZ-NH1	8.15	124.38	120.30
2	B	204	PHE	CB-CG-CD2	-8.15	115.10	120.80
9	2	69	TYR	CB-CG-CD2	-8.15	116.11	121.00
19	M	243	PHE	CB-CG-CD2	-8.14	115.10	120.80
23	T	234	TYR	CB-CG-CD2	8.14	125.88	121.00
10	3	66	PHE	CB-CG-CD1	-8.13	115.11	120.80
2	B	104	TYR	CB-CG-CD2	-8.13	116.12	121.00
27	N	861	TYR	CA-CB-CG	8.12	128.84	113.40
19	M	279	PHE	CB-CG-CD1	8.12	126.49	120.80
8	h	166	ASP	CB-CG-OD1	8.12	125.61	118.30
17	K	262	ARG	NE-CZ-NH2	-8.12	116.24	120.30
17	K	340	PHE	CB-CG-CD1	-8.11	115.12	120.80
10	3	73	TYR	CB-CG-CD1	-8.11	116.13	121.00
11	k	135	TYR	CA-CB-CG	-8.10	98.00	113.40
9	2	190	TYR	CD1-CE1-CZ	-8.10	112.51	119.80
4	D	117	ARG	NE-CZ-NH1	8.10	124.35	120.30
9	i	188	ARG	NE-CZ-NH1	8.10	124.35	120.30
32	U	210	TYR	CB-CG-CD2	-8.09	116.15	121.00
8	1	124	TYR	CB-CG-CD1	-8.08	116.15	121.00
11	k	93	ARG	NE-CZ-NH2	8.08	124.34	120.30
14	n	161	ARG	NE-CZ-NH2	-8.06	116.27	120.30
19	M	345	ARG	NE-CZ-NH2	-8.05	116.28	120.30
14	n	65	ARG	NE-CZ-NH1	8.04	124.32	120.30
8	1	174	ARG	NE-CZ-NH1	8.04	124.32	120.30
20	J	238	ARG	NE-CZ-NH2	-8.04	116.28	120.30
13	6	38	ARG	NE-CZ-NH1	8.02	124.31	120.30
15	H	409	ARG	NE-CZ-NH1	8.02	124.31	120.30
8	1	102	TYR	CB-CG-CD1	8.01	125.80	121.00
8	1	135	TYR	CB-CG-CD2	-8.01	116.20	121.00
13	m	67	ARG	NE-CZ-NH2	-8.00	116.30	120.30
24	X	87	PHE	CB-CG-CD1	7.99	126.39	120.80
2	B	82	TYR	CB-CG-CD2	-7.99	116.21	121.00
6	F	170	TYR	CG-CD1-CE1	7.98	127.69	121.30
3	c	143	TYR	CB-CG-CD2	-7.98	116.21	121.00
18	L	303	ARG	NE-CZ-NH2	-7.97	116.31	120.30
13	m	185	ARG	NE-CZ-NH1	7.96	124.28	120.30
14	7	187	ARG	NE-CZ-NH1	7.95	124.28	120.30
26	Z	264	PHE	CB-CG-CD1	7.95	126.36	120.80
17	K	336	ARG	NE-CZ-NH2	-7.94	116.33	120.30
3	c	185	VAL	CA-CB-CG2	7.93	122.80	110.90
6	f	201	ARG	NE-CZ-NH1	7.93	124.26	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	215	THR	CA-CB-CG2	-7.92	101.31	112.40
8	h	25	TYR	CB-CG-CD1	7.92	125.75	121.00
4	D	47	ARG	NE-CZ-NH1	7.92	124.26	120.30
7	G	202	ASP	CB-CG-OD1	7.92	125.43	118.30
13	6	77	PHE	CB-CG-CD2	-7.92	115.25	120.80
30	Q	123	GLU	N-CA-CB	-7.92	96.35	110.60
5	e	128	ARG	NE-CZ-NH1	7.91	124.25	120.30
12	l	69	ARG	NE-CZ-NH2	-7.90	116.35	120.30
13	6	98	TYR	CB-CG-CD1	-7.90	116.26	121.00
12	l	88	TYR	CG-CD1-CE1	-7.89	114.99	121.30
4	d	88	ARG	NE-CZ-NH2	-7.88	116.36	120.30
30	Q	332	ARG	NE-CZ-NH1	7.88	124.24	120.30
18	L	113	SER	N-CA-CB	7.87	122.30	110.50
11	4	117	TYR	CB-CG-CD2	-7.86	116.28	121.00
9	2	72	ARG	NE-CZ-NH1	7.86	124.23	120.30
4	d	146	TYR	CG-CD2-CE2	-7.85	115.02	121.30
18	L	69	ARG	NE-CZ-NH2	-7.85	116.38	120.30
16	I	100	ARG	NE-CZ-NH1	7.84	124.22	120.30
4	D	117	ARG	NE-CZ-NH2	-7.84	116.38	120.30
15	H	370	ARG	NE-CZ-NH2	7.83	124.22	120.30
3	c	113	ARG	CD-NE-CZ	7.83	134.56	123.60
14	7	208	PHE	CB-CG-CD2	-7.83	115.32	120.80
6	F	47	ALA	CB-CA-C	-7.82	98.37	110.10
6	F	98	PHE	CB-CG-CD1	-7.82	115.33	120.80
10	j	97	ARG	N-CA-CB	7.82	124.67	110.60
14	n	221	PHE	CB-CG-CD2	7.82	126.27	120.80
9	i	36	ARG	NE-CZ-NH1	7.81	124.21	120.30
7	G	18	PHE	CB-CG-CD1	7.81	126.27	120.80
7	g	74	TYR	CG-CD1-CE1	-7.81	115.05	121.30
10	3	58	ASP	CB-CG-OD2	-7.81	111.27	118.30
26	Z	272	TYR	CB-CG-CD1	7.80	125.68	121.00
3	C	141	ASP	CB-CG-OD2	7.80	125.32	118.30
2	b	230	ASP	CB-CG-OD1	7.79	125.31	118.30
23	T	199	PHE	CB-CG-CD1	-7.79	115.35	120.80
22	V	21	ASP	CB-CG-OD1	7.79	125.31	118.30
5	E	2	ARG	NE-CZ-NH1	7.78	124.19	120.30
3	c	216	ARG	NE-CZ-NH1	7.78	124.19	120.30
28	S	73	THR	CA-CB-CG2	7.76	123.26	112.40
34	8	128	TYR	CB-CG-CD1	7.76	125.66	121.00
3	C	104	ASP	CB-CG-OD2	-7.75	111.33	118.30
23	T	235	PHE	CB-CG-CD1	7.75	126.22	120.80
7	g	22	TYR	CB-CG-CD2	-7.74	116.36	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	264	ARG	NE-CZ-NH2	-7.74	116.43	120.30
19	M	342	ARG	NE-CZ-NH1	7.74	124.17	120.30
19	M	153	TYR	CB-CG-CD2	7.73	125.64	121.00
27	N	604	ARG	NE-CZ-NH1	7.73	124.16	120.30
2	B	148	TYR	CB-CG-CD2	7.72	125.63	121.00
7	g	74	TYR	CB-CG-CD1	-7.72	116.37	121.00
34	8	189	ARG	NE-CZ-NH1	7.71	124.16	120.30
8	1	36	ARG	NE-CZ-NH1	7.71	124.15	120.30
27	N	436	ASP	CB-CG-OD2	-7.71	111.36	118.30
27	N	887	ASP	CB-CG-OD1	7.71	125.23	118.30
28	S	298	ARG	NE-CZ-NH1	7.70	124.15	120.30
1	A	224	PHE	CB-CG-CD1	-7.70	115.41	120.80
30	Q	297	ASP	CB-CG-OD2	-7.70	111.37	118.30
13	m	131	TYR	CB-CG-CD1	-7.69	116.38	121.00
15	H	448	ASP	CB-CG-OD2	-7.69	111.38	118.30
31	R	214	TYR	CB-CG-CD1	7.68	125.61	121.00
18	L	264	ARG	NE-CZ-NH1	7.67	124.14	120.30
28	S	346	TYR	CB-CG-CD1	-7.67	116.40	121.00
4	d	195	ARG	NE-CZ-NH1	7.66	124.13	120.30
26	Z	502	ASN	N-CA-CB	7.66	124.39	110.60
31	R	70	TYR	CA-C-O	-7.66	104.02	120.10
17	K	427	TYR	CB-CG-CD1	7.65	125.59	121.00
14	n	187	ARG	NE-CZ-NH2	-7.65	116.47	120.30
2	b	128	ARG	NE-CZ-NH1	7.64	124.12	120.30
34	8	135	ASP	CB-CG-OD1	-7.64	111.42	118.30
28	S	170	TYR	CB-CG-CD2	-7.64	116.42	121.00
15	H	448	ASP	CB-CG-OD1	7.64	125.17	118.30
11	k	52	ASP	CB-CG-OD2	7.64	125.17	118.30
12	l	144	TYR	CB-CG-CD1	-7.64	116.42	121.00
12	l	58	TRP	CB-CG-CD2	-7.63	116.68	126.60
10	j	169	ALA	CB-CA-C	-7.63	98.66	110.10
5	e	220	PHE	CB-CG-CD1	-7.62	115.46	120.80
7	g	4	TYR	CG-CD1-CE1	-7.60	115.22	121.30
14	7	101	TYR	CB-CG-CD2	-7.60	116.44	121.00
1	A	23	PHE	CB-CG-CD2	-7.60	115.48	120.80
5	e	12	ARG	NE-CZ-NH1	7.59	124.09	120.30
17	K	349	ARG	NE-CZ-NH2	-7.57	116.51	120.30
7	g	214	TRP	CD1-CG-CD2	-7.57	100.25	106.30
13	m	77	PHE	CB-CG-CD2	-7.57	115.50	120.80
13	6	57	PHE	CB-CG-CD2	-7.57	115.50	120.80
12	l	73	ARG	NE-CZ-NH1	7.56	124.08	120.30
9	i	42	TRP	CB-CG-CD1	7.56	136.83	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	40	ASP	CB-CG-OD1	-7.56	111.50	118.30
21	W	127	ARG	NE-CZ-NH1	7.53	124.07	120.30
19	M	153	TYR	CB-CG-CD1	-7.53	116.48	121.00
19	M	267	PHE	CB-CG-CD2	-7.52	115.54	120.80
7	g	89	ARG	NE-CZ-NH2	7.51	124.06	120.30
24	X	17	TYR	CB-CG-CD2	-7.51	116.49	121.00
4	d	106	TYR	CB-CG-CD1	-7.51	116.50	121.00
2	B	234	ARG	NE-CZ-NH1	7.51	124.05	120.30
12	5	113	TYR	CB-CG-CD1	7.50	125.50	121.00
31	R	102	LEU	CB-CA-C	-7.50	95.96	110.20
22	V	156	PHE	N-CA-CB	7.49	124.09	110.60
6	F	17	ARG	NE-CZ-NH2	-7.49	116.56	120.30
22	V	173	THR	CA-CB-CG2	-7.49	101.92	112.40
14	n	82	ASP	CB-CG-OD1	-7.49	111.56	118.30
22	V	270	TYR	CB-CG-CD1	-7.49	116.51	121.00
8	h	135	TYR	CG-CD2-CE2	-7.48	115.31	121.30
27	N	298	TYR	CB-CG-CD1	7.48	125.49	121.00
1	A	119	TYR	CB-CG-CD1	7.47	125.48	121.00
3	c	147	LEU	CB-CA-C	7.47	124.39	110.20
7	G	95	PHE	CB-CG-CD1	-7.46	115.58	120.80
11	k	139	TYR	CB-CG-CD1	-7.46	116.52	121.00
17	K	258	PHE	CB-CG-CD2	-7.46	115.58	120.80
2	b	83	ARG	NE-CZ-NH1	7.46	124.03	120.30
16	I	256	TYR	CB-CG-CD2	-7.46	116.53	121.00
19	M	298	ASP	CB-CG-OD2	7.46	125.01	118.30
17	K	198	TYR	CB-CG-CD1	-7.46	116.53	121.00
11	4	138	PHE	CB-CG-CD1	7.45	126.02	120.80
11	k	176	PHE	CB-CG-CD1	7.45	126.02	120.80
14	7	65	ARG	NE-CZ-NH1	7.45	124.03	120.30
5	E	159	TYR	CB-CG-CD1	-7.45	116.53	121.00
6	F	100	ARG	NE-CZ-NH1	7.44	124.02	120.30
34	8	205	TYR	CB-CG-CD2	-7.44	116.53	121.00
12	l	144	TYR	CD1-CE1-CZ	7.43	126.49	119.80
19	M	320	ARG	NE-CZ-NH2	-7.43	116.58	120.30
27	N	127	ASP	CB-CG-OD1	-7.43	111.61	118.30
28	S	274	PHE	CB-CG-CD1	7.43	126.00	120.80
34	8	377	ARG	NE-CZ-NH2	-7.43	116.58	120.30
23	T	174	PHE	CB-CG-CD1	7.43	126.00	120.80
20	J	120	TYR	CB-CG-CD2	-7.43	116.54	121.00
15	H	303	ALA	N-CA-CB	7.43	120.50	110.10
34	8	494	TYR	CB-CG-CD1	-7.42	116.55	121.00
10	j	103	PHE	CB-CG-CD2	7.42	126.00	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	k	135	TYR	CB-CG-CD1	-7.42	116.55	121.00
1	A	96	ARG	NE-CZ-NH1	7.41	124.00	120.30
10	3	95	TYR	CG-CD2-CE2	-7.40	115.38	121.30
27	N	599	TYR	CB-CG-CD1	7.40	125.44	121.00
26	Z	253	VAL	CG1-CB-CG2	-7.40	99.06	110.90
10	3	198	TYR	CB-CG-CD2	-7.39	116.56	121.00
16	I	183	ASP	CB-CG-OD2	7.39	124.95	118.30
1	a	62	TYR	CB-CG-CD2	7.38	125.43	121.00
3	c	70	ASP	CB-CG-OD1	7.38	124.94	118.30
1	A	138	ASP	CB-CG-OD2	-7.38	111.66	118.30
2	B	12	PHE	CB-CG-CD1	-7.38	115.64	120.80
4	d	230	TYR	CG-CD1-CE1	-7.37	115.40	121.30
2	b	204	PHE	CB-CG-CD1	-7.37	115.64	120.80
6	f	146	PHE	CB-CG-CD2	-7.37	115.64	120.80
5	E	18	TYR	CB-CG-CD1	7.37	125.42	121.00
8	1	25	TYR	CD1-CE1-CZ	-7.37	113.17	119.80
4	D	139	ARG	NE-CZ-NH2	-7.36	116.62	120.30
25	Y	84	TYR	CB-CG-CD2	-7.36	116.58	121.00
7	g	108	PHE	CB-CG-CD2	-7.36	115.65	120.80
11	k	46	PHE	CB-CG-CD2	-7.36	115.65	120.80
31	R	99	TYR	CB-CG-CD1	-7.36	116.59	121.00
31	R	392	ARG	NE-CZ-NH1	7.36	123.98	120.30
2	b	159	TRP	CB-CG-CD2	-7.35	117.04	126.60
1	A	59	THR	CA-CB-CG2	-7.35	102.11	112.40
14	n	56	ASP	CB-CG-OD1	7.34	124.91	118.30
12	l	6	PHE	CB-CG-CD2	7.34	125.94	120.80
3	C	187	ASP	CB-CG-OD2	7.34	124.90	118.30
26	Z	408	TYR	CB-CG-CD2	7.33	125.40	121.00
12	5	20	ALA	N-CA-CB	7.33	120.37	110.10
12	l	125	ASP	CB-CG-OD2	-7.33	111.70	118.30
3	C	213	ALA	N-CA-CB	7.33	120.36	110.10
2	B	5	TYR	CD1-CE1-CZ	-7.32	113.21	119.80
22	V	251	TYR	CB-CG-CD2	7.31	125.39	121.00
9	2	51	ASP	CB-CG-OD2	-7.31	111.72	118.30
10	3	58	ASP	CB-CG-OD1	7.31	124.88	118.30
27	N	753	PHE	CB-CG-CD1	7.31	125.92	120.80
22	V	135	ARG	NE-CZ-NH2	-7.30	116.65	120.30
6	F	12	PHE	CB-CG-CD2	-7.30	115.69	120.80
27	N	23	TYR	CB-CG-CD2	-7.30	116.62	121.00
32	U	254	ARG	NE-CZ-NH1	-7.30	116.65	120.30
13	6	106	TYR	CB-CG-CD2	-7.29	116.62	121.00
15	H	268	ASP	CB-CG-OD1	7.29	124.86	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	J	365	ALA	CB-CA-C	-7.29	99.17	110.10
18	L	245	PHE	CB-CG-CD1	-7.29	115.70	120.80
31	R	70	TYR	CB-CA-C	7.29	124.97	110.40
1	a	10	PHE	CB-CG-CD1	7.27	125.89	120.80
26	Z	133	ASP	CB-CG-OD1	7.27	124.84	118.30
34	8	448	TYR	CD1-CE1-CZ	-7.26	113.26	119.80
19	M	315	PHE	CB-CG-CD2	-7.25	115.72	120.80
8	1	185	ARG	NE-CZ-NH1	7.25	123.93	120.30
23	T	197	TYR	CB-CG-CD2	-7.25	116.65	121.00
6	F	208	ASP	CB-CG-OD1	7.24	124.82	118.30
10	j	175	ASP	CB-CG-OD1	-7.24	111.79	118.30
15	H	367	ARG	NE-CZ-NH1	7.22	123.91	120.30
6	f	173	ARG	NH1-CZ-NH2	-7.21	111.46	119.40
10	j	43	PHE	CB-CG-CD1	-7.21	115.75	120.80
1	A	154	TYR	CB-CG-CD2	7.21	125.33	121.00
18	L	339	ARG	NE-CZ-NH1	7.21	123.90	120.30
17	K	198	TYR	CB-CG-CD2	7.20	125.32	121.00
26	Z	272	TYR	CB-CG-CD2	-7.20	116.68	121.00
7	g	138	ASP	CB-CG-OD2	-7.19	111.83	118.30
27	N	325	PHE	CB-CG-CD2	-7.19	115.77	120.80
27	N	880	ARG	NE-CZ-NH2	-7.18	116.71	120.30
31	R	338	TYR	CB-CG-CD2	-7.17	116.69	121.00
19	M	75	LEU	CB-CG-CD2	7.17	123.19	111.00
27	N	560	ALA	CB-CA-C	-7.17	99.35	110.10
17	K	58	TYR	CB-CG-CD2	-7.16	116.70	121.00
18	L	329	ARG	NE-CZ-NH1	7.16	123.88	120.30
32	U	80	CYS	O-C-N	7.16	134.16	122.70
10	j	202	ARG	NE-CZ-NH2	7.16	123.88	120.30
12	l	139	VAL	CB-CA-C	-7.16	97.80	111.40
10	j	176	ARG	NE-CZ-NH1	7.15	123.88	120.30
30	Q	146	TYR	CB-CG-CD1	7.15	125.29	121.00
10	j	161	ASP	CB-CG-OD2	-7.15	111.87	118.30
8	h	183	VAL	CA-CB-CG1	7.15	121.62	110.90
7	g	187	GLU	O-C-N	7.14	134.13	122.70
10	3	97	ARG	NE-CZ-NH1	7.14	123.87	120.30
14	7	128	ARG	NE-CZ-NH2	-7.14	116.73	120.30
3	c	156	TYR	CB-CG-CD2	-7.13	116.72	121.00
4	d	140	ASP	CB-CG-OD2	-7.13	111.88	118.30
30	Q	123	GLU	CA-C-N	7.13	132.88	117.20
30	Q	146	TYR	CB-CG-CD2	-7.12	116.72	121.00
3	c	8	ARG	NE-CZ-NH2	-7.12	116.74	120.30
1	A	119	TYR	CB-CG-CD2	-7.12	116.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	4	56	PHE	CB-CG-CD2	-7.12	115.82	120.80
12	5	114	TYR	CB-CG-CD1	-7.10	116.74	121.00
29	P	179	PHE	CB-CG-CD2	-7.10	115.83	120.80
2	B	75	TYR	CG-CD1-CE1	-7.09	115.62	121.30
4	D	105	GLU	N-CA-CB	-7.09	97.84	110.60
23	T	92	ASN	N-CA-CB	7.09	123.36	110.60
5	e	140	ASP	CB-CG-OD1	7.09	124.68	118.30
27	N	576	VAL	CB-CA-C	-7.09	97.94	111.40
27	N	784	TYR	CB-CG-CD1	7.09	125.25	121.00
28	S	275	TYR	CB-CG-CD1	-7.09	116.75	121.00
3	c	23	TYR	CB-CG-CD1	7.08	125.25	121.00
31	R	371	PHE	CB-CG-CD2	-7.08	115.84	120.80
2	B	199	SER	N-CA-CB	7.07	121.11	110.50
6	F	88	ARG	NE-CZ-NH1	7.07	123.83	120.30
11	4	108	ASP	CB-CG-OD2	-7.07	111.94	118.30
34	8	287	ARG	NE-CZ-NH2	-7.06	116.77	120.30
13	6	200	ASP	N-CA-CB	7.06	123.31	110.60
11	4	141	PHE	CB-CG-CD1	7.06	125.74	120.80
9	i	186	TYR	CB-CG-CD2	-7.05	116.77	121.00
8	1	111	TYR	CB-CG-CD2	7.05	125.23	121.00
5	E	114	ARG	NE-CZ-NH1	-7.05	116.78	120.30
30	Q	299	MET	CG-SD-CE	-7.04	88.94	100.20
34	8	229	PHE	CB-CG-CD1	7.04	125.73	120.80
9	2	123	TYR	CB-CG-CD2	-7.03	116.78	121.00
3	c	49	ARG	NE-CZ-NH2	-7.02	116.79	120.30
3	c	207	TYR	CB-CG-CD1	-7.02	116.79	121.00
3	c	181	ASP	CB-CG-OD1	7.01	124.61	118.30
8	1	25	TYR	CG-CD2-CE2	-7.01	115.69	121.30
19	M	319	ASP	CB-CG-OD1	7.01	124.61	118.30
20	J	199	ALA	CB-CA-C	-7.01	99.58	110.10
33	O	92	PHE	CB-CG-CD1	-7.01	115.89	120.80
2	b	20	GLN	CB-CA-C	-7.01	96.39	110.40
2	b	145	PHE	CB-CG-CD2	7.00	125.70	120.80
8	1	193	TYR	CB-CG-CD1	-7.00	116.80	121.00
31	R	109	LYS	CB-CA-C	7.00	124.41	110.40
24	X	45	PHE	CB-CG-CD1	7.00	125.70	120.80
33	O	328	VAL	CA-CB-CG2	-7.00	100.40	110.90
14	n	82	ASP	CB-CG-OD2	7.00	124.60	118.30
7	g	226	PHE	CB-CG-CD1	6.99	125.69	120.80
12	5	73	ARG	NE-CZ-NH2	-6.99	116.81	120.30
9	2	196	ARG	NE-CZ-NH1	6.99	123.79	120.30
5	e	145	TYR	CB-CG-CD1	6.97	125.18	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	401	PHE	CB-CG-CD1	6.97	125.68	120.80
14	n	56	ASP	CB-CG-OD2	-6.97	112.03	118.30
31	R	210	TYR	CB-CG-CD2	-6.97	116.82	121.00
31	R	345	TYR	CB-CG-CD1	-6.97	116.82	121.00
8	h	102	TYR	CB-CG-CD2	-6.96	116.83	121.00
4	d	145	LEU	CB-CG-CD1	6.96	122.82	111.00
3	C	209	ARG	NE-CZ-NH1	6.96	123.78	120.30
26	Z	264	PHE	CB-CG-CD2	-6.96	115.93	120.80
20	J	42	ARG	NE-CZ-NH1	6.95	123.78	120.30
24	X	96	ARG	NE-CZ-NH1	6.95	123.78	120.30
23	T	250	MET	CG-SD-CE	-6.94	89.09	100.20
22	V	269	ARG	NE-CZ-NH1	6.94	123.77	120.30
10	3	98	ARG	NE-CZ-NH2	6.93	123.77	120.30
19	M	77	TYR	CB-CG-CD2	6.93	125.16	121.00
30	Q	116	PHE	CB-CG-CD2	-6.93	115.95	120.80
4	d	110	TYR	CB-CG-CD1	6.93	125.16	121.00
1	a	17	TYR	CG-CD2-CE2	-6.92	115.76	121.30
31	R	69	GLU	CB-CA-C	-6.92	96.56	110.40
6	F	47	ALA	N-CA-CB	6.92	119.79	110.10
18	L	269	TYR	CB-CG-CD2	-6.92	116.85	121.00
2	B	178	ARG	NE-CZ-NH2	-6.91	116.84	120.30
30	Q	232	TYR	CB-CG-CD1	-6.91	116.85	121.00
11	k	138	PHE	CB-CG-CD1	6.91	125.64	120.80
19	M	77	TYR	CB-CG-CD1	-6.91	116.86	121.00
2	b	128	ARG	NE-CZ-NH2	6.90	123.75	120.30
4	D	10	SER	N-CA-CB	6.90	120.85	110.50
11	k	95	ARG	NE-CZ-NH2	-6.90	116.85	120.30
9	2	54	ALA	N-CA-CB	6.90	119.76	110.10
7	G	153	TYR	CB-CG-CD1	6.90	125.14	121.00
8	1	75	THR	CA-CB-CG2	-6.89	102.75	112.40
8	1	25	TYR	CB-CG-CD2	-6.89	116.86	121.00
6	F	5	TYR	CB-CG-CD2	-6.89	116.87	121.00
12	5	178	TYR	CB-CG-CD2	-6.89	116.87	121.00
18	L	88	TYR	CB-CG-CD1	6.88	125.13	121.00
30	Q	123	GLU	N-CA-C	6.88	129.59	111.00
17	K	270	PHE	CB-CG-CD1	6.88	125.62	120.80
5	E	155	THR	CA-CB-CG2	-6.88	102.78	112.40
17	K	347	ARG	NE-CZ-NH2	-6.87	116.86	120.30
3	c	121	TYR	CB-CA-C	-6.87	96.66	110.40
4	D	179	ARG	NE-CZ-NH1	6.87	123.73	120.30
23	T	10	SER	N-CA-CB	6.86	120.79	110.50
17	K	171	TYR	CB-CG-CD1	-6.85	116.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	273	PHE	CB-CG-CD1	6.85	125.59	120.80
7	G	87	ARG	NE-CZ-NH2	-6.85	116.88	120.30
4	d	179	ARG	NE-CZ-NH2	-6.84	116.88	120.30
3	c	181	ASP	CB-CG-OD2	-6.84	112.14	118.30
16	I	128	TYR	CB-CG-CD1	-6.84	116.90	121.00
15	H	354	ALA	N-CA-CB	6.84	119.67	110.10
4	d	81	ARG	NE-CZ-NH2	-6.83	116.88	120.30
27	N	784	TYR	CG-CD1-CE1	6.83	126.77	121.30
19	M	201	MET	CG-SD-CE	-6.83	89.28	100.20
23	T	60	ARG	NE-CZ-NH1	6.83	123.71	120.30
7	g	238	PHE	CB-CG-CD1	-6.82	116.03	120.80
12	5	90	TYR	CB-CG-CD1	6.82	125.09	121.00
3	c	148	TYR	CZ-CE2-CD2	-6.82	113.67	119.80
11	4	159	ASP	CB-CG-OD2	6.82	124.44	118.30
18	L	161	ARG	NE-CZ-NH2	6.82	123.71	120.30
18	L	401	PHE	CB-CG-CD2	-6.82	116.03	120.80
4	d	125	ARG	NE-CZ-NH1	6.81	123.71	120.30
8	h	42	TRP	CG-CD2-CE3	-6.81	127.77	133.90
17	K	258	PHE	CB-CG-CD1	6.81	125.57	120.80
7	G	16	ARG	NE-CZ-NH2	-6.80	116.90	120.30
34	8	317	PHE	CB-CG-CD1	6.80	125.56	120.80
8	1	29	ARG	NE-CZ-NH1	6.80	123.70	120.30
14	7	60	MET	CG-SD-CE	-6.79	89.33	100.20
26	Z	199	ASP	CB-CG-OD2	6.79	124.41	118.30
29	P	186	LEU	CB-CG-CD2	6.79	122.54	111.00
7	g	145	TYR	CB-CG-CD2	6.79	125.07	121.00
13	m	102	PHE	CB-CG-CD1	6.79	125.55	120.80
14	n	35	ARG	NH1-CZ-NH2	6.79	126.86	119.40
23	T	235	PHE	CB-CG-CD2	-6.79	116.05	120.80
13	m	160	TYR	CB-CG-CD2	6.78	125.07	121.00
11	k	117	TYR	CG-CD1-CE1	-6.78	115.88	121.30
18	L	132	ARG	NE-CZ-NH1	6.78	123.69	120.30
6	f	163	ARG	NE-CZ-NH2	6.78	123.69	120.30
2	b	81	ASP	CB-CG-OD2	6.77	124.40	118.30
5	e	12	ARG	NE-CZ-NH2	-6.77	116.91	120.30
15	H	101	ARG	CD-NE-CZ	6.77	133.08	123.60
11	4	98	TYR	CB-CG-CD1	-6.77	116.94	121.00
31	R	357	PHE	CB-CG-CD2	-6.77	116.06	120.80
5	E	180	HIS	N-CA-CB	6.77	122.78	110.60
6	F	127	TYR	CB-CG-CD2	6.76	125.06	121.00
12	5	167	ARG	NE-CZ-NH2	6.76	123.68	120.30
28	S	111	ARG	NE-CZ-NH1	-6.76	116.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	186	ARG	NE-CZ-NH2	-6.75	116.92	120.30
24	X	85	ARG	NE-CZ-NH1	-6.75	116.92	120.30
27	N	117	TYR	CB-CG-CD1	-6.75	116.95	121.00
32	U	132	LEU	CB-CG-CD2	6.74	122.46	111.00
34	8	237	PHE	CB-CG-CD1	-6.74	116.08	120.80
14	n	95	TYR	CB-CG-CD2	6.74	125.04	121.00
9	2	17	ASP	CB-CG-OD2	6.73	124.36	118.30
15	H	178	ARG	NE-CZ-NH2	-6.73	116.93	120.30
13	6	7	ASP	CB-CG-OD2	-6.73	112.24	118.30
18	L	416	MET	CG-SD-CE	-6.73	89.44	100.20
27	N	310	ASP	CB-CG-OD1	-6.72	112.25	118.30
31	R	335	ARG	NE-CZ-NH2	-6.72	116.94	120.30
13	m	222	ASP	CB-CG-OD1	6.71	124.34	118.30
19	M	415	PHE	CB-CG-CD1	-6.71	116.10	120.80
34	8	357	ARG	NE-CZ-NH1	6.71	123.66	120.30
13	6	98	TYR	CZ-CE2-CD2	-6.71	113.76	119.80
14	7	5	ILE	O-C-N	-6.71	111.97	122.70
16	I	340	ARG	NE-CZ-NH2	-6.71	116.94	120.30
27	N	325	PHE	CB-CG-CD1	6.71	125.50	120.80
34	8	189	ARG	NE-CZ-NH2	-6.71	116.95	120.30
10	3	119	PHE	CB-CG-CD2	-6.71	116.11	120.80
33	O	286	PHE	N-CA-CB	6.70	122.67	110.60
17	K	333	ARG	NE-CZ-NH2	-6.70	116.95	120.30
27	N	465	ALA	N-CA-CB	6.70	119.48	110.10
14	7	228	TYR	CA-CB-CG	-6.70	100.68	113.40
31	R	324	ARG	NE-CZ-NH2	6.69	123.65	120.30
19	M	345	ARG	NE-CZ-NH1	6.69	123.65	120.30
31	R	304	TYR	CB-CG-CD2	-6.69	116.99	121.00
33	O	58	ARG	NE-CZ-NH2	-6.69	116.95	120.30
23	T	109	TYR	CB-CG-CD2	-6.69	116.99	121.00
7	g	214	TRP	CG-CD2-CE3	-6.69	127.88	133.90
1	a	235	ARG	NE-CZ-NH2	-6.68	116.96	120.30
8	h	114	PRO	O-C-N	6.68	133.40	122.70
9	2	123	TYR	CB-CG-CD1	6.68	125.01	121.00
22	V	196	TYR	CA-CB-CG	-6.68	100.70	113.40
2	b	245	ASP	CB-CG-OD1	6.68	124.31	118.30
3	c	83	ALA	N-CA-CB	6.68	119.45	110.10
8	1	143	ARG	NE-CZ-NH2	-6.68	116.96	120.30
34	8	232	ASP	CB-CG-OD2	-6.68	112.29	118.30
12	l	64	ARG	NE-CZ-NH2	-6.68	116.96	120.30
30	Q	232	TYR	CB-CG-CD2	6.67	125.00	121.00
16	I	316	PHE	CB-CG-CD1	6.67	125.47	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	109	LYS	CA-CB-CG	6.67	128.07	113.40
12	l	170	TYR	CB-CG-CD1	-6.67	117.00	121.00
17	K	252	ARG	NE-CZ-NH1	6.67	123.63	120.30
28	S	272	TYR	CB-CG-CD2	-6.67	117.00	121.00
17	K	374	ARG	NE-CZ-NH1	6.67	123.63	120.30
4	D	9	PHE	CB-CG-CD2	6.66	125.46	120.80
25	Y	68	GLU	N-CA-CB	6.66	122.58	110.60
26	Z	936	VAL	CA-CB-CG2	-6.66	100.92	110.90
13	m	131	TYR	CB-CG-CD2	6.65	124.99	121.00
6	f	106	ARG	NE-CZ-NH1	6.65	123.62	120.30
17	K	63	LEU	CB-CG-CD2	6.65	122.30	111.00
5	e	124	ARG	NE-CZ-NH1	6.65	123.62	120.30
6	f	136	TYR	CG-CD2-CE2	-6.64	115.98	121.30
5	e	104	LEU	CB-CG-CD1	6.64	122.29	111.00
34	8	168	PHE	CB-CG-CD2	-6.64	116.15	120.80
16	I	114	ASP	CB-CG-OD1	-6.64	112.32	118.30
33	O	81	TYR	CG-CD2-CE2	-6.64	115.99	121.30
7	G	137	VAL	CA-CB-CG1	-6.63	100.95	110.90
2	B	75	TYR	CB-CG-CD2	6.63	124.98	121.00
10	3	27	ARG	NE-CZ-NH2	-6.63	116.98	120.30
17	K	168	ASP	CB-CG-OD2	-6.63	112.33	118.30
11	4	149	ARG	NE-CZ-NH1	-6.62	116.99	120.30
2	b	128	ARG	NH1-CZ-NH2	-6.62	112.12	119.40
3	C	148	TYR	CB-CG-CD2	-6.62	117.03	121.00
31	R	105	LYS	CB-CA-C	6.62	123.63	110.40
12	l	40	PHE	CB-CA-C	-6.61	97.17	110.40
4	D	170	ARG	CD-NE-CZ	6.61	132.86	123.60
5	E	159	TYR	CG-CD1-CE1	-6.61	116.01	121.30
13	m	160	TYR	CA-CB-CG	-6.61	100.84	113.40
6	F	224	TYR	CB-CG-CD1	-6.61	117.04	121.00
7	g	138	ASP	CB-CG-OD1	6.60	124.24	118.30
1	A	106	ASP	CB-CG-OD1	-6.60	112.36	118.30
6	F	221	PHE	CB-CG-CD2	-6.60	116.18	120.80
8	h	179	THR	CA-CB-CG2	-6.60	103.16	112.40
4	d	169	VAL	CA-CB-CG1	6.59	120.79	110.90
26	Z	287	ARG	NE-CZ-NH1	6.59	123.60	120.30
4	D	195	ARG	NE-CZ-NH2	-6.59	117.00	120.30
10	3	202	ARG	NE-CZ-NH1	6.59	123.59	120.30
34	8	119	TYR	CB-CG-CD2	-6.59	117.05	121.00
2	B	92	VAL	CA-CB-CG2	-6.59	101.02	110.90
33	O	288	ARG	NE-CZ-NH1	-6.58	117.01	120.30
3	C	41	ASP	CB-CG-OD1	6.58	124.22	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	J	371	ARG	NE-CZ-NH2	-6.58	117.01	120.30
5	E	64	ARG	NE-CZ-NH2	6.57	123.59	120.30
20	J	234	PHE	CB-CG-CD2	-6.57	116.20	120.80
13	6	133	ARG	NE-CZ-NH2	-6.57	117.02	120.30
1	A	154	TYR	N-CA-CB	6.57	122.42	110.60
13	6	188	PHE	CB-CG-CD1	6.55	125.39	120.80
10	j	12	VAL	CG1-CB-CG2	6.55	121.38	110.90
10	3	187	TYR	CB-CG-CD2	-6.55	117.07	121.00
12	l	135	PHE	CB-CG-CD1	6.55	125.38	120.80
13	6	19	ASP	CB-CG-OD1	-6.54	112.41	118.30
3	c	136	TYR	CB-CG-CD2	-6.54	117.08	121.00
7	g	156	TYR	CB-CG-CD2	6.54	124.92	121.00
2	B	130	PHE	CB-CG-CD1	-6.54	116.22	120.80
15	H	457	PHE	CB-CG-CD1	6.54	125.38	120.80
31	R	335	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	b	151	ASP	CB-CG-OD2	-6.54	112.42	118.30
5	e	179	TRP	CB-CG-CD1	6.53	135.49	127.00
2	b	130	PHE	CB-CG-CD2	-6.53	116.23	120.80
14	n	224	ASP	CB-CG-OD2	-6.53	112.42	118.30
20	J	230	VAL	CA-CB-CG1	-6.53	101.11	110.90
11	4	59	TYR	CG-CD2-CE2	-6.53	116.08	121.30
14	7	30	TYR	CB-CG-CD2	-6.53	117.08	121.00
8	1	135	TYR	CB-CG-CD1	6.52	124.92	121.00
15	H	187	LEU	CB-CG-CD2	6.52	122.08	111.00
34	8	464	PHE	CB-CG-CD2	-6.52	116.24	120.80
2	b	4	ARG	NE-CZ-NH1	6.51	123.56	120.30
1	A	93	ALA	CB-CA-C	-6.51	100.33	110.10
26	Z	231	ASP	CB-CG-OD1	6.51	124.16	118.30
13	m	188	PHE	CB-CG-CD1	6.51	125.36	120.80
4	d	54	ASP	N-CA-CB	6.51	122.31	110.60
18	L	434	TYR	CG-CD2-CE2	-6.51	116.09	121.30
1	a	124	TYR	CB-CG-CD2	-6.50	117.10	121.00
9	i	142	TRP	CB-CG-CD1	6.50	135.45	127.00
7	G	77	LEU	CB-CG-CD2	6.50	122.05	111.00
27	N	418	ASP	CB-CG-OD1	-6.50	112.45	118.30
11	k	4	ILE	N-CA-CB	6.49	125.73	110.80
27	N	622	ALA	N-CA-CB	6.49	119.18	110.10
12	5	4	LEU	CB-CG-CD2	6.49	122.03	111.00
3	c	111	VAL	CG1-CB-CG2	-6.48	100.53	110.90
10	j	143	ASP	CB-CG-OD1	6.48	124.13	118.30
4	d	231	VAL	CG1-CB-CG2	6.48	121.27	110.90
15	H	45	TYR	CB-CG-CD2	6.48	124.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Z	269	TYR	CB-CG-CD1	-6.47	117.12	121.00
15	H	409	ARG	NE-CZ-NH2	-6.47	117.06	120.30
32	U	254	ARG	NE-CZ-NH2	-6.47	117.06	120.30
28	S	171	TYR	CB-CG-CD1	-6.47	117.12	121.00
13	6	174	TYR	CG-CD1-CE1	-6.47	116.13	121.30
4	d	4	ARG	NE-CZ-NH1	-6.46	117.07	120.30
16	I	384	LYS	N-CA-CB	6.46	122.24	110.60
10	j	83	PRO	N-CA-CB	6.46	111.05	103.30
20	J	56	ARG	NE-CZ-NH2	-6.46	117.07	120.30
6	F	5	TYR	CD1-CE1-CZ	-6.46	113.99	119.80
13	6	72	VAL	CA-CB-CG2	-6.46	101.21	110.90
27	N	622	ALA	CB-CA-C	-6.46	100.42	110.10
18	L	243	PHE	CB-CG-CD1	6.46	125.32	120.80
6	f	206	THR	CA-CB-CG2	-6.45	103.36	112.40
31	R	49	PHE	CB-CG-CD1	6.45	125.32	120.80
32	U	72	TYR	CB-CG-CD1	-6.45	117.13	121.00
12	5	212	GLY	CA-C-O	-6.44	109.00	120.60
13	6	91	ARG	NE-CZ-NH2	-6.44	117.08	120.30
14	7	229	GLY	CA-C-O	-6.44	109.01	120.60
31	R	204	TRP	CE2-CD2-CE3	6.44	126.43	118.70
20	J	357	ASP	CB-CG-OD2	6.44	124.09	118.30
27	N	162	ARG	NE-CZ-NH1	6.44	123.52	120.30
31	R	62	TYR	CB-CG-CD1	6.44	124.86	121.00
32	U	277	TYR	CB-CG-CD1	6.44	124.86	121.00
14	n	104	ARG	NE-CZ-NH1	6.44	123.52	120.30
8	1	93	LEU	CB-CG-CD1	-6.43	100.07	111.00
17	K	58	TYR	CB-CG-CD1	6.43	124.86	121.00
34	8	227	ASP	CB-CG-OD1	-6.43	112.51	118.30
13	m	216	PHE	CB-CG-CD1	-6.43	116.30	120.80
5	E	205	ASP	CB-CG-OD1	6.43	124.09	118.30
27	N	560	ALA	N-CA-CB	6.43	119.10	110.10
16	I	391	ASP	CB-CG-OD2	-6.42	112.52	118.30
34	8	462	TYR	N-CA-CB	6.42	122.17	110.60
12	5	207	PHE	CB-CG-CD2	-6.42	116.31	120.80
13	m	26	ASP	CB-CG-OD1	-6.42	112.52	118.30
15	H	439	THR	CA-CB-CG2	-6.42	103.41	112.40
18	L	412	PRO	N-CA-CB	6.42	111.00	103.30
13	m	149	PHE	CB-CG-CD2	-6.41	116.31	120.80
16	I	124	THR	CA-CB-CG2	-6.41	103.42	112.40
30	Q	45	SER	N-CA-CB	6.41	120.12	110.50
6	F	186	ASP	CB-CG-OD1	6.41	124.07	118.30
15	H	343	PHE	CB-CG-CD2	-6.41	116.31	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	386	PHE	CB-CG-CD2	-6.41	116.31	120.80
11	k	20	ALA	CB-CA-C	-6.40	100.50	110.10
31	R	69	GLU	N-CA-CB	6.40	122.12	110.60
4	D	179	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	146	TYR	CB-CG-CD1	-6.40	117.16	121.00
5	E	169	GLU	N-CA-CB	6.40	122.11	110.60
31	R	338	TYR	CB-CG-CD1	6.40	124.84	121.00
6	F	66	ASP	CB-CG-OD2	6.39	124.06	118.30
10	3	45	TYR	CB-CG-CD2	-6.39	117.17	121.00
5	e	156	PHE	CG-CD1-CE1	-6.39	113.77	120.80
8	h	115	LEU	CB-CG-CD1	-6.39	100.14	111.00
6	f	214	ILE	CG1-CB-CG2	6.38	125.44	111.40
3	C	116	ASP	CB-CG-OD1	6.38	124.05	118.30
26	Z	295	ARG	NE-CZ-NH2	-6.38	117.11	120.30
27	N	599	TYR	CB-CG-CD2	-6.38	117.17	121.00
6	F	125	ARG	NE-CZ-NH2	-6.38	117.11	120.30
14	n	180	ALA	CB-CA-C	-6.38	100.53	110.10
2	B	22	ASP	CB-CG-OD1	-6.37	112.56	118.30
3	C	207	TYR	CB-CG-CD1	6.37	124.82	121.00
17	K	145	ALA	CB-CA-C	-6.37	100.55	110.10
10	j	98	ARG	NE-CZ-NH1	-6.37	117.12	120.30
27	N	418	ASP	CB-CG-OD2	6.37	124.03	118.30
27	N	696	LYS	N-CA-CB	6.36	122.05	110.60
6	f	126	PRO	N-CA-CB	6.36	110.93	103.30
27	N	549	TYR	CB-CG-CD2	-6.36	117.19	121.00
12	l	159	ARG	NE-CZ-NH2	-6.35	117.12	120.30
9	2	203	TYR	CG-CD1-CE1	6.35	126.38	121.30
28	S	281	ALA	N-CA-CB	6.35	118.99	110.10
30	Q	182	SER	N-CA-CB	6.35	120.02	110.50
13	6	33	TYR	CZ-CE2-CD2	6.35	125.51	119.80
24	X	11	ARG	NE-CZ-NH2	-6.34	117.13	120.30
8	h	124	TYR	CB-CG-CD1	-6.34	117.20	121.00
1	a	96	ARG	NE-CZ-NH2	-6.34	117.13	120.30
1	a	222	ASP	CB-CG-OD2	-6.34	112.60	118.30
32	U	158	PRO	CA-N-CD	6.34	120.57	111.70
8	h	166	ASP	CB-CG-OD2	-6.33	112.60	118.30
3	C	101	TYR	CG-CD2-CE2	-6.33	116.23	121.30
7	g	45	ALA	N-CA-CB	6.33	118.96	110.10
1	A	235	ARG	NE-CZ-NH2	-6.33	117.14	120.30
15	H	173	ARG	NE-CZ-NH2	-6.33	117.14	120.30
5	e	71	SER	N-CA-CB	6.33	119.99	110.50
11	k	96	ARG	NH1-CZ-NH2	-6.32	112.44	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2	111	PHE	CB-CA-C	-6.32	97.75	110.40
7	g	146	MET	CG-SD-CE	-6.32	90.09	100.20
8	h	138	CYS	N-CA-CB	6.31	121.96	110.60
15	H	190	ARG	NE-CZ-NH2	-6.31	117.14	120.30
31	R	408	ASP	CB-CG-OD1	6.30	123.97	118.30
14	n	117	ALA	N-CA-CB	6.30	118.92	110.10
12	5	7	ARG	NE-CZ-NH1	-6.30	117.15	120.30
27	N	120	ASP	CB-CG-OD2	6.30	123.97	118.30
28	S	326	ASP	CB-CG-OD2	-6.30	112.63	118.30
11	k	138	PHE	CB-CG-CD2	-6.30	116.39	120.80
21	W	142	ILE	N-CA-C	-6.30	93.99	111.00
22	V	22	ASP	CB-CG-OD2	-6.30	112.63	118.30
5	E	180	HIS	CB-CA-C	-6.30	97.80	110.40
12	5	106	ARG	NE-CZ-NH2	6.30	123.45	120.30
13	m	105	TYR	CB-CG-CD2	-6.30	117.22	121.00
13	6	91	ARG	NE-CZ-NH1	6.30	123.45	120.30
20	J	145	SER	N-CA-CB	6.29	119.94	110.50
10	j	68	TYR	CB-CG-CD1	-6.29	117.22	121.00
1	A	20	GLU	OE1-CD-OE2	6.29	130.85	123.30
9	2	160	GLN	N-CA-CB	6.29	121.93	110.60
34	8	361	ARG	N-CA-CB	6.29	121.92	110.60
11	k	174	MET	CA-CB-CG	6.29	123.99	113.30
14	n	45	VAL	CA-CB-CG2	-6.29	101.47	110.90
31	R	158	LEU	N-CA-CB	6.29	122.98	110.40
31	R	321	TYR	CB-CG-CD2	-6.29	117.23	121.00
32	U	283	ARG	NE-CZ-NH1	6.29	123.44	120.30
3	C	156	TYR	CB-CG-CD2	-6.28	117.23	121.00
18	L	342	ARG	NE-CZ-NH2	-6.28	117.16	120.30
4	d	224	SER	N-CA-CB	6.28	119.92	110.50
20	J	282	PHE	CB-CA-C	-6.28	97.84	110.40
15	H	83	ASP	CB-CG-OD2	-6.28	112.65	118.30
20	J	87	LYS	N-CA-C	-6.28	94.06	111.00
13	6	75	TYR	CB-CG-CD2	6.27	124.77	121.00
1	A	111	ARG	NE-CZ-NH1	-6.27	117.17	120.30
26	Z	209	PRO	N-CA-CB	6.27	110.82	103.30
30	Q	77	PHE	CB-CA-C	-6.27	97.86	110.40
33	O	190	TYR	CB-CG-CD1	6.27	124.76	121.00
10	j	150	GLU	OE1-CD-OE2	6.26	130.82	123.30
2	B	225	THR	CA-CB-CG2	-6.26	103.63	112.40
7	G	74	TYR	CB-CG-CD2	-6.26	117.24	121.00
23	T	97	SER	N-CA-CB	6.26	119.89	110.50
27	N	208	ARG	NE-CZ-NH1	6.26	123.43	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	J	234	PHE	CB-CG-CD1	6.26	125.18	120.80
31	R	59	MET	CG-SD-CE	-6.26	90.19	100.20
32	U	189	ARG	NE-CZ-NH2	-6.25	117.17	120.30
7	G	161	THR	CA-CB-OG1	6.25	122.13	109.00
8	h	135	TYR	CZ-CE2-CD2	6.25	125.42	119.80
34	8	376	ARG	NE-CZ-NH1	6.25	123.42	120.30
4	D	56	ARG	NE-CZ-NH1	6.25	123.42	120.30
33	O	137	TYR	CB-CG-CD2	-6.25	117.25	121.00
34	8	494	TYR	CB-CG-CD2	6.25	124.75	121.00
1	a	37	ARG	NE-CZ-NH2	-6.24	117.18	120.30
5	e	95	TYR	CG-CD1-CE1	-6.24	116.31	121.30
20	J	283	GLU	N-CA-CB	6.24	121.83	110.60
4	D	106	TYR	CG-CD1-CE1	6.24	126.29	121.30
9	2	190	TYR	CG-CD2-CE2	-6.24	116.31	121.30
20	J	201	ALA	N-CA-CB	6.24	118.83	110.10
26	Z	439	TYR	CB-CG-CD1	-6.24	117.26	121.00
6	f	71	LEU	CB-CG-CD1	6.23	121.59	111.00
6	f	5	TYR	CB-CG-CD1	6.23	124.74	121.00
13	m	44	PHE	CG-CD1-CE1	-6.22	113.96	120.80
3	c	142	ARG	NH1-CZ-NH2	6.22	126.24	119.40
28	S	421	TYR	CB-CG-CD1	6.22	124.73	121.00
12	l	115	VAL	CA-CB-CG1	6.21	120.22	110.90
12	l	55	TRP	CB-CG-CD2	-6.21	118.53	126.60
27	N	559	TYR	CG-CD2-CE2	6.21	126.27	121.30
6	f	86	TYR	CB-CG-CD2	-6.21	117.28	121.00
1	a	37	ARG	NE-CZ-NH1	6.21	123.40	120.30
10	j	68	TYR	CB-CG-CD2	6.21	124.72	121.00
13	m	91	ARG	NE-CZ-NH1	6.21	123.40	120.30
17	K	82	ALA	N-CA-CB	6.21	118.79	110.10
27	N	557	LEU	CB-CG-CD2	6.21	121.55	111.00
2	B	25	LEU	CB-CG-CD2	6.21	121.55	111.00
3	C	148	TYR	N-CA-CB	6.20	121.76	110.60
33	O	248	TYR	CB-CG-CD1	6.20	124.72	121.00
1	a	101	TYR	CD1-CE1-CZ	-6.20	114.22	119.80
5	e	40	LEU	CB-CG-CD2	6.20	121.54	111.00
2	b	111	VAL	CA-CB-CG1	6.20	120.19	110.90
8	h	41	ILE	N-CA-C	-6.20	94.27	111.00
3	C	143	TYR	CB-CG-CD1	6.20	124.72	121.00
17	K	67	TYR	CB-CG-CD1	-6.20	117.28	121.00
11	4	70	ARG	NE-CZ-NH1	6.19	123.40	120.30
17	K	396	ARG	NE-CZ-NH2	6.19	123.39	120.30
25	Y	42	THR	CA-CB-CG2	-6.19	103.74	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	182	TRP	CB-CG-CD2	-6.19	118.56	126.60
19	M	433	TYR	CB-CG-CD1	6.18	124.71	121.00
23	T	162	ASP	CB-CG-OD1	6.18	123.87	118.30
33	O	65	PHE	CB-CG-CD2	6.18	125.13	120.80
2	b	111	VAL	CA-CB-CG2	-6.18	101.64	110.90
4	d	189	CYS	CA-CB-SG	-6.18	102.88	114.00
11	k	144	LEU	CB-CG-CD2	6.17	121.50	111.00
31	R	70	TYR	CG-CD1-CE1	-6.17	116.36	121.30
17	K	426	PHE	CB-CG-CD1	-6.17	116.48	120.80
7	G	238	PHE	CB-CG-CD1	-6.17	116.48	120.80
17	K	63	LEU	N-CA-CB	6.17	122.73	110.40
12	5	114	TYR	CB-CG-CD2	6.17	124.70	121.00
34	8	134	ARG	NE-CZ-NH1	6.16	123.38	120.30
2	B	103	GLU	N-CA-CB	6.16	121.69	110.60
7	G	68	ARG	NE-CZ-NH2	-6.16	117.22	120.30
10	3	142	SER	N-CA-CB	6.16	119.73	110.50
8	1	45	ARG	CB-CA-C	-6.16	98.09	110.40
19	M	61	LYS	CB-CA-C	-6.15	98.09	110.40
34	8	176	PHE	CB-CG-CD1	6.15	125.11	120.80
3	C	70	ASP	CB-CG-OD1	-6.15	112.76	118.30
18	L	168	TYR	CB-CG-CD2	-6.15	117.31	121.00
9	2	32	ALA	N-CA-CB	6.15	118.71	110.10
15	H	45	TYR	CB-CG-CD1	-6.15	117.31	121.00
27	N	896	PHE	CB-CG-CD1	6.15	125.10	120.80
11	4	98	TYR	CG-CD2-CE2	-6.15	116.38	121.30
18	L	303	ARG	NE-CZ-NH1	6.14	123.37	120.30
27	N	741	TYR	CZ-CE2-CD2	-6.14	114.27	119.80
4	d	46	ARG	NE-CZ-NH2	-6.14	117.23	120.30
7	G	244	ASN	CB-CA-C	-6.14	98.12	110.40
34	8	324	ASN	N-CA-CB	6.13	121.64	110.60
6	F	136	TYR	CG-CD1-CE1	-6.13	116.39	121.30
9	2	97	TYR	CD1-CE1-CZ	-6.13	114.28	119.80
27	N	598	ASP	N-CA-C	-6.13	94.45	111.00
4	D	107	LEU	CB-CG-CD1	6.13	121.42	111.00
6	f	152	VAL	CA-CB-CG2	6.12	120.07	110.90
3	c	61	SER	N-CA-CB	6.11	119.67	110.50
31	R	246	TYR	CB-CG-CD1	-6.11	117.33	121.00
12	5	64	ARG	NE-CZ-NH1	6.11	123.36	120.30
12	5	144	TYR	CB-CG-CD2	-6.11	117.33	121.00
4	d	237	GLU	OE1-CD-OE2	-6.11	115.97	123.30
20	J	150	VAL	CA-CB-CG1	-6.11	101.74	110.90
7	g	116	VAL	CA-CB-CG2	-6.11	101.74	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	8	321	ARG	NE-CZ-NH1	6.11	123.35	120.30
19	M	425	ARG	NE-CZ-NH2	-6.10	117.25	120.30
23	T	224	ARG	NH1-CZ-NH2	6.10	126.11	119.40
3	c	139	TYR	CG-CD1-CE1	-6.10	116.42	121.30
21	W	182	TYR	CB-CG-CD2	-6.10	117.34	121.00
3	c	148	TYR	CB-CG-CD2	-6.09	117.34	121.00
12	l	97	MET	CG-SD-CE	-6.09	90.45	100.20
28	S	44	THR	O-C-N	-6.09	112.95	122.70
10	3	119	PHE	CB-CG-CD1	6.09	125.06	120.80
1	A	153	TYR	CB-CG-CD2	-6.08	117.35	121.00
31	R	334	ARG	NE-CZ-NH2	-6.08	117.26	120.30
31	R	410	LEU	CB-CG-CD1	6.08	121.33	111.00
11	4	16	ALA	CB-CA-C	-6.08	100.98	110.10
13	m	28	ARG	NE-CZ-NH2	6.08	123.34	120.30
32	U	72	TYR	CG-CD1-CE1	-6.08	116.44	121.30
18	L	62	ARG	NH1-CZ-NH2	-6.07	112.72	119.40
22	V	194	ARG	NE-CZ-NH1	-6.07	117.27	120.30
30	Q	9	GLU	OE1-CD-OE2	-6.07	116.02	123.30
8	h	61	TYR	CB-CG-CD2	-6.07	117.36	121.00
13	m	65	VAL	CA-CB-CG1	6.07	120.00	110.90
1	A	235	ARG	NE-CZ-NH1	6.07	123.33	120.30
19	M	45	ARG	NE-CZ-NH1	-6.06	117.27	120.30
30	Q	185	TYR	CB-CG-CD2	-6.06	117.36	121.00
12	5	178	TYR	CB-CG-CD1	6.06	124.64	121.00
10	3	146	PHE	CB-CG-CD2	-6.06	116.56	120.80
28	S	425	ARG	NE-CZ-NH1	6.06	123.33	120.30
2	B	214	ILE	N-CA-C	-6.06	94.65	111.00
16	I	292	TYR	CB-CG-CD1	6.06	124.63	121.00
5	E	121	GLY	O-C-N	-6.05	113.01	122.70
28	S	46	LEU	C-N-CA	6.05	136.84	121.70
1	a	31	ILE	CB-CA-C	-6.05	99.50	111.60
21	W	109	ARG	NE-CZ-NH2	-6.05	117.27	120.30
23	T	54	ASP	CB-CG-OD2	-6.05	112.85	118.30
26	Z	916	LEU	CB-CG-CD2	6.05	121.29	111.00
12	l	90	TYR	CG-CD1-CE1	-6.05	116.46	121.30
4	D	110	TYR	CB-CG-CD1	-6.05	117.37	121.00
5	E	223	TYR	CG-CD1-CE1	-6.05	116.46	121.30
1	a	49	LYS	N-CA-CB	6.05	121.49	110.60
2	b	80	PRO	O-C-N	6.05	132.37	122.70
26	Z	117	ASP	CB-CG-OD2	-6.04	112.86	118.30
1	a	21	TYR	CG-CD1-CE1	-6.04	116.47	121.30
7	g	27	VAL	CG1-CB-CG2	-6.04	101.23	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	O	63	ASP	CB-CG-OD1	-6.04	112.86	118.30
13	6	174	TYR	CD1-CE1-CZ	6.04	125.23	119.80
1	a	62	TYR	CB-CG-CD1	-6.04	117.38	121.00
5	E	156	PHE	CB-CG-CD2	-6.04	116.57	120.80
9	i	186	TYR	CG-CD2-CE2	-6.04	116.47	121.30
4	D	97	THR	CA-CB-CG2	-6.04	103.95	112.40
32	U	254	ARG	NH1-CZ-NH2	6.04	126.04	119.40
1	A	23	PHE	CB-CG-CD1	6.03	125.02	120.80
9	2	145	ASP	N-CA-CB	6.03	121.46	110.60
18	L	310	THR	CA-CB-CG2	-6.03	103.95	112.40
34	8	334	VAL	CG1-CB-CG2	-6.03	101.25	110.90
2	b	179	TRP	CB-CG-CD2	-6.03	118.76	126.60
4	D	110	TYR	CB-CG-CD2	6.03	124.62	121.00
4	D	79	ASP	CB-CG-OD1	6.03	123.73	118.30
28	S	137	PHE	CB-CG-CD1	6.03	125.02	120.80
5	E	96	ASP	CB-CG-OD2	6.03	123.72	118.30
18	L	345	ARG	NE-CZ-NH1	-6.03	117.29	120.30
27	N	881	TYR	CB-CG-CD2	-6.03	117.38	121.00
4	d	127	PHE	CB-CG-CD1	-6.03	116.58	120.80
13	m	205	LEU	CB-CG-CD1	6.03	121.24	111.00
12	5	25	TRP	CG-CD2-CE3	-6.03	128.48	133.90
30	Q	252	HIS	CA-CB-CG	6.03	123.84	113.60
7	g	11	PHE	N-CA-CB	6.02	121.44	110.60
34	8	388	MET	CG-SD-CE	-6.02	90.56	100.20
6	f	225	ASP	CB-CG-OD2	6.02	123.72	118.30
8	h	102	TYR	CB-CG-CD1	6.02	124.61	121.00
30	Q	339	TYR	CB-CG-CD2	-6.01	117.39	121.00
10	3	132	ALA	N-CA-CB	6.01	118.52	110.10
26	Z	437	ASP	CB-CG-OD2	6.01	123.71	118.30
12	5	7	ARG	N-CA-CB	6.01	121.42	110.60
18	L	279	PHE	CB-CG-CD1	6.01	125.01	120.80
33	O	81	TYR	CD1-CE1-CZ	6.01	125.21	119.80
3	c	139	TYR	CB-CG-CD2	-6.01	117.40	121.00
7	g	71	GLY	N-CA-C	-6.01	98.08	113.10
9	2	19	ARG	NE-CZ-NH2	-6.01	117.30	120.30
14	7	17	ASP	CB-CG-OD1	6.01	123.71	118.30
4	D	41	VAL	CB-CA-C	-6.00	100.00	111.40
26	Z	407	VAL	CA-CB-CG2	-6.00	101.90	110.90
5	E	95	TYR	CB-CG-CD2	-6.00	117.40	121.00
5	E	128	ARG	NE-CZ-NH2	-6.00	117.30	120.30
7	G	122	TYR	CG-CD1-CE1	-6.00	116.50	121.30
18	L	406	ASP	N-CA-CB	6.00	121.39	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	127	THR	N-CA-CB	6.00	121.69	110.30
3	c	12	PHE	CB-CG-CD2	5.99	125.00	120.80
21	W	35	PHE	CB-CG-CD1	5.99	125.00	120.80
17	K	323	THR	CA-CB-CG2	-5.99	104.02	112.40
4	D	54	ASP	CB-CG-OD1	-5.99	112.91	118.30
5	e	94	TYR	CB-CG-CD2	-5.99	117.41	121.00
13	m	217	TYR	CB-CG-CD2	-5.99	117.41	121.00
14	7	83	ALA	CB-CA-C	-5.99	101.12	110.10
9	i	42	TRP	CB-CG-CD2	-5.98	118.82	126.60
1	a	101	TYR	CZ-CE2-CD2	-5.98	114.42	119.80
13	6	5	TYR	CB-CG-CD2	-5.98	117.41	121.00
34	8	358	ASP	CB-CG-OD2	5.98	123.68	118.30
14	n	183	VAL	CA-CB-CG1	5.97	119.86	110.90
17	K	363	ALA	N-CA-CB	5.97	118.46	110.10
28	S	137	PHE	CB-CG-CD2	-5.97	116.62	120.80
34	8	128	TYR	CG-CD2-CE2	-5.97	116.53	121.30
14	7	190	ARG	NE-CZ-NH2	-5.97	117.32	120.30
17	K	400	TYR	CB-CG-CD2	5.97	124.58	121.00
28	S	272	TYR	CB-CG-CD1	5.97	124.58	121.00
6	F	103	ALA	CB-CA-C	-5.96	101.15	110.10
13	6	213	ARG	NE-CZ-NH1	5.96	123.28	120.30
27	N	280	GLN	C-N-CA	5.96	134.81	122.30
1	a	134	PHE	CB-CG-CD1	5.96	124.97	120.80
5	e	16	VAL	CA-CB-CG2	-5.96	101.96	110.90
4	D	78	ALA	N-CA-CB	5.96	118.44	110.10
32	U	58	GLU	N-CA-CB	5.96	121.32	110.60
9	2	120	ASP	CB-CG-OD2	5.96	123.66	118.30
18	L	241	ALA	N-CA-CB	5.96	118.44	110.10
34	8	361	ARG	NE-CZ-NH1	5.96	123.28	120.30
34	8	465	ASN	CA-C-N	-5.96	104.10	117.20
13	6	44	PHE	CB-CG-CD1	5.95	124.97	120.80
4	d	81	ARG	NE-CZ-NH1	5.95	123.28	120.30
12	5	25	TRP	CZ3-CH2-CZ2	-5.95	114.46	121.60
6	F	57	SER	N-CA-CB	5.95	119.42	110.50
16	I	262	ARG	NE-CZ-NH2	-5.95	117.33	120.30
2	B	22	ASP	CB-CG-OD2	5.95	123.65	118.30
10	j	168	GLN	N-CA-CB	5.94	121.30	110.60
6	F	116	GLN	O-C-N	-5.94	113.20	122.70
34	8	376	ARG	NE-CZ-NH2	-5.94	117.33	120.30
10	j	79	ARG	CD-NE-CZ	5.93	131.91	123.60
34	8	202	GLY	CA-C-O	-5.93	109.92	120.60
12	5	113	TYR	CG-CD1-CE1	5.93	126.05	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	T	249	MET	N-CA-CB	5.93	121.27	110.60
8	1	185	ARG	NE-CZ-NH2	-5.92	117.34	120.30
12	l	158	LYS	N-CA-CB	5.92	121.26	110.60
6	f	111	LEU	CB-CA-C	-5.92	98.96	110.20
34	8	430	TYR	CB-CG-CD1	5.91	124.55	121.00
30	Q	278	VAL	CG1-CB-CG2	-5.91	101.45	110.90
6	f	17	ARG	NE-CZ-NH2	5.91	123.25	120.30
3	C	5	TYR	CZ-CE2-CD2	5.91	125.12	119.80
14	n	103	ARG	NE-CZ-NH1	5.90	123.25	120.30
13	6	63	ALA	N-CA-CB	5.90	118.36	110.10
16	I	222	TYR	N-CA-CB	5.90	121.22	110.60
30	Q	151	TYR	CB-CG-CD2	-5.90	117.46	121.00
3	c	236	ASP	CB-CG-OD1	5.90	123.61	118.30
10	j	135	PHE	CD1-CE1-CZ	-5.90	113.02	120.10
16	I	163	ASP	CB-CG-OD1	-5.90	112.99	118.30
16	I	340	ARG	NE-CZ-NH1	5.90	123.25	120.30
28	S	64	ARG	NE-CZ-NH1	5.90	123.25	120.30
14	n	91	TYR	CZ-CE2-CD2	5.90	125.11	119.80
1	A	126	ARG	NE-CZ-NH1	5.89	123.25	120.30
14	7	16	TYR	CB-CG-CD1	-5.89	117.46	121.00
26	Z	321	PHE	CB-CG-CD2	-5.89	116.68	120.80
30	Q	380	MET	CG-SD-CE	5.89	109.62	100.20
28	S	281	ALA	CB-CA-C	-5.88	101.27	110.10
4	d	126	PRO	N-CA-CB	5.88	110.36	103.30
2	B	239	THR	N-CA-CB	5.88	121.48	110.30
4	D	172	PHE	CB-CG-CD2	-5.88	116.68	120.80
34	8	368	ASN	CB-CA-C	-5.88	98.64	110.40
1	a	149	ASP	CB-CG-OD1	5.88	123.59	118.30
4	d	204	GLY	N-CA-C	-5.88	98.40	113.10
1	A	225	PHE	CB-CG-CD1	-5.88	116.69	120.80
7	G	220	THR	N-CA-CB	5.88	121.47	110.30
11	k	185	ASP	CB-CG-OD2	-5.87	113.02	118.30
16	I	100	ARG	NE-CZ-NH2	-5.87	117.36	120.30
34	8	108	PRO	N-CD-CG	5.87	112.01	103.20
9	i	97	TYR	CB-CG-CD1	-5.87	117.48	121.00
29	P	277	GLN	C-N-CA	5.87	136.37	121.70
6	F	2	ARG	NE-CZ-NH2	-5.87	117.37	120.30
9	i	132	LEU	CB-CG-CD2	5.87	120.97	111.00
7	G	18	PHE	CB-CG-CD2	-5.87	116.69	120.80
32	U	210	TYR	CB-CG-CD1	5.86	124.52	121.00
27	N	578	ASP	CB-CG-OD1	-5.86	113.03	118.30
1	A	69	THR	N-CA-CB	5.86	121.43	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	147	LEU	CB-CG-CD1	5.86	120.96	111.00
1	a	21	TYR	CB-CG-CD1	5.86	124.52	121.00
6	f	38	ARG	NE-CZ-NH2	-5.86	117.37	120.30
27	N	58	ARG	N-CA-CB	-5.86	100.06	110.60
14	n	129	TYR	CB-CG-CD2	5.86	124.51	121.00
12	5	104	TYR	CG-CD2-CE2	-5.86	116.61	121.30
17	K	171	TYR	CZ-CE2-CD2	5.85	125.07	119.80
33	O	81	TYR	CB-CG-CD2	-5.85	117.49	121.00
22	V	197	TYR	CB-CG-CD1	-5.85	117.49	121.00
7	g	16	ARG	NE-CZ-NH1	5.85	123.22	120.30
31	R	102	LEU	C-N-CA	5.85	136.32	121.70
17	K	110	VAL	CA-CB-CG1	5.85	119.67	110.90
20	J	374	ARG	NE-CZ-NH2	-5.85	117.38	120.30
27	N	540	LEU	CB-CG-CD1	5.84	120.93	111.00
12	l	7	ARG	NE-CZ-NH2	-5.84	117.38	120.30
6	F	208	ASP	CB-CG-OD2	-5.83	113.05	118.30
13	m	28	ARG	NE-CZ-NH1	-5.83	117.38	120.30
14	7	102	GLN	N-CA-CB	5.83	121.10	110.60
2	B	139	HIS	N-CA-CB	5.83	121.10	110.60
6	F	201	ARG	NE-CZ-NH1	5.83	123.22	120.30
24	X	11	ARG	NE-CZ-NH1	5.83	123.22	120.30
3	c	186	ASP	CB-CG-OD1	-5.83	113.06	118.30
1	A	124	TYR	CG-CD2-CE2	-5.82	116.64	121.30
1	a	97	TYR	CB-CG-CD1	-5.82	117.51	121.00
1	a	215	GLU	N-CA-C	-5.82	95.28	111.00
2	B	220	ASP	CB-CA-C	-5.82	98.76	110.40
3	C	181	ASP	CB-CG-OD2	-5.82	113.06	118.30
24	X	96	ARG	NE-CZ-NH2	-5.82	117.39	120.30
14	7	219	TRP	CG-CD2-CE3	-5.82	128.67	133.90
31	R	347	THR	N-CA-CB	5.82	121.35	110.30
30	Q	328	ASP	CB-CG-OD2	-5.81	113.07	118.30
31	R	159	SER	CB-CA-C	-5.81	99.05	110.10
7	G	156	TYR	CD1-CE1-CZ	5.81	125.03	119.80
28	S	333	PHE	CB-CG-CD2	-5.81	116.73	120.80
20	J	43	ARG	NE-CZ-NH1	5.81	123.20	120.30
31	R	181	TYR	CB-CG-CD2	-5.81	117.51	121.00
16	I	370	ASN	N-CA-C	-5.81	95.32	111.00
2	b	5	TYR	CB-CG-CD2	-5.80	117.52	121.00
7	g	160	ALA	N-CA-CB	5.80	118.22	110.10
18	L	243	PHE	CB-CG-CD2	-5.80	116.74	120.80
1	a	183	ASP	CB-CG-OD1	5.80	123.52	118.30
10	3	102	TYR	CB-CG-CD2	5.80	124.48	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	I	346	ARG	NE-CZ-NH2	-5.80	117.40	120.30
26	Z	253	VAL	CA-C-N	5.80	133.34	117.10
13	m	74	TRP	CG-CD2-CE3	-5.80	128.68	133.90
3	C	116	ASP	CB-CG-OD2	-5.80	113.08	118.30
14	7	182	ARG	NE-CZ-NH2	5.80	123.20	120.30
16	I	405	ARG	NE-CZ-NH1	-5.80	117.40	120.30
3	c	23	TYR	CD1-CE1-CZ	-5.80	114.58	119.80
18	L	267	PHE	CB-CG-CD2	-5.80	116.74	120.80
18	L	392	ARG	NE-CZ-NH2	5.80	123.20	120.30
6	F	202	ASP	N-CA-CB	5.79	121.03	110.60
3	c	12	PHE	CD1-CE1-CZ	5.79	127.05	120.10
9	i	142	TRP	CB-CG-CD2	-5.79	119.07	126.60
12	l	198	TRP	CB-CG-CD1	5.79	134.53	127.00
34	8	166	ARG	NE-CZ-NH2	-5.79	117.40	120.30
28	S	98	SER	N-CA-CB	5.79	119.18	110.50
12	5	86	LEU	CB-CG-CD1	5.79	120.84	111.00
9	i	31	CYS	N-CA-CB	5.79	121.01	110.60
2	B	81	ASP	CB-CG-OD2	-5.79	113.09	118.30
11	4	103	LEU	N-CA-C	-5.79	95.38	111.00
8	h	98	ILE	N-CA-C	-5.78	95.39	111.00
5	E	96	ASP	CB-CG-OD1	-5.78	113.10	118.30
1	a	209	PHE	CB-CG-CD2	5.78	124.84	120.80
30	Q	384	LYS	N-CA-CB	5.78	121.00	110.60
1	A	176	HIS	O-C-N	5.78	131.94	122.70
15	H	106	ILE	N-CA-C	-5.78	95.40	111.00
28	S	74	LEU	CB-CG-CD1	5.78	120.82	111.00
7	G	72	CYS	CA-CB-SG	-5.77	103.61	114.00
11	k	193	ASP	CB-CG-OD2	5.76	123.49	118.30
11	k	2	ASP	CB-CG-OD1	-5.76	113.11	118.30
19	M	336	ALA	CB-CA-C	-5.76	101.46	110.10
10	j	148	MET	CB-CA-C	-5.76	98.89	110.40
12	5	104	TYR	CZ-CE2-CD2	5.76	124.98	119.80
32	U	100	ARG	NE-CZ-NH1	5.76	123.18	120.30
27	N	887	ASP	CB-CG-OD2	-5.75	113.12	118.30
28	S	425	ARG	NE-CZ-NH2	-5.75	117.42	120.30
6	f	113	ASP	CB-CG-OD2	-5.75	113.12	118.30
12	l	58	TRP	CB-CG-CD1	5.75	134.48	127.00
6	F	215	VAL	CG1-CB-CG2	-5.75	101.70	110.90
14	7	172	VAL	CG1-CB-CG2	-5.75	101.70	110.90
10	3	71	ASN	N-CA-CB	5.75	120.94	110.60
8	h	142	PHE	CB-CG-CD1	5.74	124.82	120.80
21	W	21	PHE	CB-CG-CD2	-5.74	116.78	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	345	ARG	NE-CZ-NH2	-5.74	117.43	120.30
19	M	350	PRO	N-CA-CB	5.74	110.19	103.30
3	c	112	ARG	CD-NE-CZ	5.74	131.64	123.60
34	8	416	PHE	CB-CA-C	-5.74	98.92	110.40
1	a	128	LEU	CB-CG-CD2	5.74	120.75	111.00
8	1	154	PHE	CB-CG-CD1	5.74	124.81	120.80
33	O	215	TYR	CB-CG-CD2	5.74	124.44	121.00
4	d	91	ALA	CB-CA-C	-5.73	101.50	110.10
5	e	18	TYR	CZ-CE2-CD2	5.73	124.96	119.80
34	8	140	TYR	N-CA-CB	5.73	120.92	110.60
14	n	221	PHE	CB-CG-CD1	-5.73	116.79	120.80
7	G	221	ASN	N-CA-CB	5.73	120.92	110.60
28	S	285	ASP	CB-CG-OD1	-5.73	113.14	118.30
8	1	27	ALA	CB-CA-C	-5.73	101.51	110.10
9	i	19	ARG	NE-CZ-NH1	5.73	123.16	120.30
8	h	111	TYR	CD1-CE1-CZ	-5.72	114.65	119.80
17	K	422	ASP	CB-CG-OD1	-5.72	113.15	118.30
21	W	144	PHE	CB-CG-CD1	-5.72	116.80	120.80
26	Z	145	ASP	CB-CG-OD1	-5.72	113.15	118.30
18	L	375	ASP	CB-CG-OD2	-5.72	113.15	118.30
7	g	214	TRP	CB-CG-CD1	5.71	134.43	127.00
13	m	57	PHE	CB-CG-CD2	-5.71	116.80	120.80
26	Z	941	ARG	NE-CZ-NH2	-5.71	117.44	120.30
26	Z	195	PHE	CB-CG-CD1	-5.71	116.80	120.80
8	1	188	PHE	CB-CG-CD1	-5.71	116.80	120.80
6	f	171	LEU	CB-CG-CD2	5.71	120.70	111.00
8	1	82	PHE	CZ-CE2-CD2	-5.71	113.25	120.10
26	Z	221	VAL	CG1-CB-CG2	5.71	120.03	110.90
29	P	326	ASP	C-N-CA	5.70	135.96	121.70
14	n	137	TYR	N-CA-CB	5.70	120.86	110.60
26	Z	928	ARG	NE-CZ-NH1	5.70	123.15	120.30
27	N	140	MET	CG-SD-CE	-5.70	91.08	100.20
1	a	52	ASP	CB-CG-OD1	-5.70	113.17	118.30
1	a	5	ARG	NE-CZ-NH2	-5.70	117.45	120.30
10	3	12	VAL	CG1-CB-CG2	5.70	120.01	110.90
18	L	174	GLU	N-CA-CB	5.70	120.85	110.60
26	Z	103	TYR	CB-CG-CD1	-5.69	117.58	121.00
16	I	222	TYR	CB-CG-CD2	5.69	124.42	121.00
16	I	337	ALA	CB-CA-C	-5.69	101.56	110.10
7	G	4	TYR	CG-CD2-CE2	5.69	125.85	121.30
7	g	42	VAL	CG1-CB-CG2	-5.69	101.80	110.90
18	L	157	ARG	NE-CZ-NH1	5.69	123.14	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	17	GLN	CB-CA-C	-5.68	99.03	110.40
7	G	47	GLU	CB-CG-CD	-5.68	98.85	114.20
11	k	46	PHE	CB-CG-CD1	5.68	124.78	120.80
14	n	110	LEU	N-CA-C	-5.68	95.66	111.00
5	e	153	SER	CA-C-N	5.68	127.56	116.20
7	g	186	ARG	NE-CZ-NH1	-5.68	117.46	120.30
21	W	179	ARG	NH1-CZ-NH2	-5.67	113.16	119.40
5	E	129	PRO	N-CA-C	5.67	126.85	112.10
5	e	69	ALA	N-CA-CB	5.67	118.04	110.10
23	T	88	TYR	CB-CG-CD1	5.67	124.40	121.00
23	T	177	PHE	CB-CG-CD2	-5.67	116.83	120.80
17	K	171	TYR	CG-CD2-CE2	-5.67	116.77	121.30
31	R	147	LYS	N-CA-CB	5.67	120.80	110.60
4	d	141	ASP	CB-CG-OD1	-5.66	113.20	118.30
4	d	157	TRP	CG-CD2-CE3	-5.66	128.80	133.90
30	Q	387	TYR	CB-CG-CD1	5.66	124.40	121.00
23	T	110	LEU	CB-CG-CD2	5.66	120.62	111.00
5	e	201	GLU	CG-CD-OE2	-5.66	106.98	118.30
7	g	165	ARG	NE-CZ-NH2	5.66	123.13	120.30
19	M	87	ASP	N-CA-CB	5.66	120.78	110.60
8	h	36	ARG	NE-CZ-NH1	5.66	123.13	120.30
1	A	50	VAL	CA-CB-CG2	-5.66	102.42	110.90
18	L	88	TYR	CD1-CE1-CZ	-5.66	114.71	119.80
29	P	168	TYR	CB-CG-CD2	-5.66	117.61	121.00
3	c	121	TYR	CB-CG-CD2	5.65	124.39	121.00
4	d	212	VAL	CB-CA-C	-5.65	100.66	111.40
8	h	134	ILE	CA-CB-CG1	5.65	121.74	111.00
22	V	100	ARG	NE-CZ-NH2	-5.65	117.47	120.30
30	Q	116	PHE	CB-CG-CD1	5.65	124.76	120.80
16	I	282	ASP	CB-CG-OD1	5.65	123.39	118.30
9	i	124	TYR	CD1-CE1-CZ	5.65	124.88	119.80
9	2	190	TYR	CG-CD1-CE1	5.65	125.82	121.30
34	8	204	PHE	N-CA-CB	5.65	120.77	110.60
5	e	220	PHE	N-CA-CB	5.65	120.76	110.60
2	B	236	ARG	N-CA-C	-5.65	95.75	111.00
1	A	224	PHE	CB-CG-CD2	5.64	124.75	120.80
18	L	346	LYS	N-CA-C	-5.64	95.77	111.00
4	d	2	TYR	CG-CD2-CE2	5.64	125.81	121.30
29	P	267	PHE	CB-CG-CD1	5.64	124.75	120.80
20	J	296	ARG	N-CA-CB	5.64	120.75	110.60
12	5	181	THR	C-N-CA	5.64	135.79	121.70
18	L	344	ASP	CB-CG-OD1	-5.64	113.23	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	136	PHE	CB-CG-CD1	-5.63	116.86	120.80
13	m	189	THR	CA-CB-CG2	-5.63	104.51	112.40
5	e	205	ASP	N-CA-CB	5.63	120.74	110.60
9	i	32	ALA	N-CA-CB	5.63	117.98	110.10
11	4	135	TYR	O-C-N	5.63	131.70	122.70
7	G	160	ALA	CB-CA-C	-5.63	101.66	110.10
6	F	182	ASP	CB-CG-OD1	-5.62	113.24	118.30
5	e	183	LEU	CB-CG-CD2	5.62	120.56	111.00
14	n	45	VAL	CA-CB-CG1	-5.62	102.47	110.90
1	A	24	LYS	N-CA-CB	5.62	120.72	110.60
12	5	145	LYS	N-CA-CB	5.62	120.72	110.60
1	a	196	PHE	CB-CG-CD2	-5.62	116.87	120.80
14	n	214	VAL	CA-CB-CG2	-5.62	102.47	110.90
14	7	208	PHE	CB-CG-CD1	5.62	124.73	120.80
24	X	48	PHE	N-CA-CB	5.62	120.71	110.60
7	G	115	TYR	CB-CG-CD1	5.62	124.37	121.00
15	H	454	TYR	CG-CD2-CE2	-5.62	116.81	121.30
26	Z	561	ASP	CB-CG-OD2	-5.61	113.25	118.30
31	R	114	ASN	N-CA-CB	5.61	120.71	110.60
4	D	141	ASP	CB-CG-OD2	-5.61	113.25	118.30
19	M	318	ASP	CB-CG-OD1	5.61	123.35	118.30
27	N	50	TYR	CB-CG-CD1	-5.61	117.64	121.00
13	6	28	ARG	NE-CZ-NH1	5.60	123.10	120.30
8	h	100	ALA	N-CA-CB	5.60	117.94	110.10
22	V	104	VAL	CA-CB-CG1	-5.60	102.50	110.90
10	3	176	ARG	NE-CZ-NH2	-5.60	117.50	120.30
17	K	367	ASP	CB-CG-OD1	5.60	123.34	118.30
2	b	247	LEU	CB-CA-C	-5.60	99.56	110.20
4	D	109	ARG	NE-CZ-NH1	-5.60	117.50	120.30
21	W	112	ALA	N-CA-CB	5.59	117.93	110.10
28	S	75	CYS	CA-CB-SG	-5.59	103.93	114.00
11	k	161	LEU	CB-CG-CD1	5.59	120.51	111.00
6	F	206	THR	CA-CB-CG2	-5.59	104.57	112.40
15	H	159	LEU	CB-CG-CD1	5.59	120.50	111.00
9	i	56	THR	N-CA-CB	5.59	120.92	110.30
3	C	212	PHE	CB-CG-CD2	-5.59	116.89	120.80
13	6	148	PRO	N-CA-CB	5.59	110.01	103.30
1	a	15	ARG	NH1-CZ-NH2	5.59	125.54	119.40
1	a	195	GLU	N-CA-CB	5.59	120.66	110.60
4	d	139	ARG	NE-CZ-NH1	5.59	123.09	120.30
11	4	175	ASP	CB-CG-OD1	5.58	123.33	118.30
6	f	11	THR	N-CA-CB	5.58	120.90	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	174	TYR	CB-CG-CD2	-5.58	117.65	121.00
13	6	189	THR	CA-CB-CG2	5.58	120.22	112.40
20	J	85	LEU	N-CA-C	-5.58	95.93	111.00
7	g	124	SER	N-CA-CB	-5.58	102.13	110.50
13	6	102	PHE	CB-CG-CD2	-5.58	116.89	120.80
27	N	127	ASP	CB-CG-OD2	5.58	123.32	118.30
26	Z	551	LEU	CB-CG-CD2	5.58	120.48	111.00
33	O	246	SER	N-CA-CB	5.58	118.87	110.50
26	Z	415	MET	CG-SD-CE	-5.57	91.28	100.20
22	V	76	THR	C-N-CA	5.57	133.99	122.30
5	E	61	GLU	N-CA-C	-5.57	95.98	111.00
34	8	222	SER	N-CA-CB	5.57	118.85	110.50
14	n	65	ARG	NE-CZ-NH2	-5.56	117.52	120.30
17	K	256	ASP	CB-CG-OD1	-5.56	113.30	118.30
6	F	81	ARG	NE-CZ-NH1	5.56	123.08	120.30
7	G	187	GLU	N-CA-CB	5.56	120.61	110.60
12	5	17	ASP	CB-CG-OD2	-5.56	113.30	118.30
21	W	188	SER	N-CA-CB	5.56	118.84	110.50
9	i	57	GLN	O-C-N	-5.56	113.81	122.70
10	j	25	ASP	CB-CG-OD2	-5.56	113.30	118.30
10	3	115	SER	N-CA-CB	5.56	118.84	110.50
14	7	23	ALA	N-CA-CB	5.56	117.88	110.10
26	Z	142	ASP	CA-CB-CG	-5.55	101.18	113.40
13	6	132	GLU	CB-CA-C	-5.55	99.30	110.40
20	J	312	ARG	NE-CZ-NH2	-5.55	117.52	120.30
31	R	246	TYR	CZ-CE2-CD2	-5.55	114.80	119.80
7	g	156	TYR	CZ-CE2-CD2	-5.55	114.81	119.80
5	E	119	ALA	N-CA-CB	5.55	117.87	110.10
20	J	238	ARG	NE-CZ-NH1	5.55	123.07	120.30
1	A	82	ARG	NE-CZ-NH2	-5.54	117.53	120.30
2	b	204	PHE	CB-CG-CD2	5.54	124.68	120.80
3	c	112	ARG	NE-CZ-NH1	-5.54	117.53	120.30
13	m	136	CYS	CA-CB-SG	-5.54	104.03	114.00
1	A	153	TYR	CG-CD1-CE1	-5.54	116.87	121.30
12	5	93	ALA	N-CA-CB	5.54	117.85	110.10
14	7	130	VAL	CG1-CB-CG2	5.54	119.76	110.90
26	Z	67	SER	CB-CA-C	-5.54	99.58	110.10
14	n	224	ASP	CB-CG-OD1	5.53	123.28	118.30
11	4	148	TYR	CG-CD1-CE1	-5.53	116.88	121.30
31	R	63	TYR	CG-CD2-CE2	5.53	125.72	121.30
4	d	106	TYR	O-C-N	5.53	131.54	122.70
2	b	159	TRP	CB-CG-CD1	5.53	134.18	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	4	67	TYR	CD1-CG-CD2	5.53	123.98	117.90
20	J	129	LYS	CB-CA-C	-5.53	99.35	110.40
26	Z	710	SER	N-CA-CB	5.53	118.79	110.50
1	A	203	ASP	CB-CG-OD1	-5.52	113.33	118.30
6	F	125	ARG	NE-CZ-NH1	5.52	123.06	120.30
34	8	412	TYR	CB-CG-CD2	-5.52	117.69	121.00
4	d	117	ARG	CD-NE-CZ	5.52	131.33	123.60
12	5	127	PHE	CB-CG-CD2	-5.52	116.94	120.80
11	4	190	ARG	N-CA-CB	5.52	120.53	110.60
1	A	201	MET	CG-SD-CE	-5.51	91.38	100.20
18	L	365	THR	CA-CB-CG2	-5.51	104.68	112.40
20	J	316	PHE	CB-CG-CD1	5.51	124.66	120.80
6	f	37	LEU	N-CA-CB	5.51	121.42	110.40
20	J	199	ALA	N-CA-CB	5.51	117.82	110.10
34	8	119	TYR	CG-CD1-CE1	-5.51	116.89	121.30
3	C	143	TYR	CB-CG-CD2	-5.51	117.69	121.00
33	O	356	ARG	NE-CZ-NH2	-5.51	117.55	120.30
11	k	100	VAL	O-C-N	5.51	131.51	122.70
2	B	60	THR	CA-CB-CG2	-5.51	104.69	112.40
28	S	95	PHE	N-CA-CB	-5.51	100.69	110.60
3	c	147	LEU	CB-CG-CD2	5.50	120.36	111.00
1	A	223	LYS	N-CA-CB	5.50	120.51	110.60
7	g	134	PHE	CB-CG-CD1	5.50	124.65	120.80
5	E	12	ARG	NE-CZ-NH2	-5.50	117.55	120.30
3	C	62	THR	N-CA-C	-5.50	96.16	111.00
15	H	429	PHE	CB-CA-C	-5.50	99.40	110.40
16	I	329	ASN	C-N-CA	5.50	135.44	121.70
31	R	112	GLU	N-CA-CB	5.50	120.49	110.60
3	c	157	THR	CA-CB-CG2	-5.49	104.71	112.40
8	h	135	TYR	CB-CG-CD1	5.49	124.30	121.00
10	j	121	ALA	N-CA-CB	5.49	117.79	110.10
8	h	135	TYR	CB-CG-CD2	-5.49	117.71	121.00
14	n	69	ASP	CB-CG-OD1	5.49	123.24	118.30
4	d	29	THR	CA-CB-CG2	-5.49	104.72	112.40
12	5	207	PHE	N-CA-CB	5.48	120.47	110.60
17	K	48	TYR	CA-CB-CG	-5.48	102.98	113.40
4	D	151	SER	CB-CA-C	5.48	120.52	110.10
34	8	430	TYR	CB-CG-CD2	-5.48	117.71	121.00
2	b	229	THR	N-CA-CB	5.48	120.71	110.30
22	V	195	HIS	N-CA-CB	5.48	120.46	110.60
28	S	138	MET	CG-SD-CE	-5.48	91.43	100.20
8	h	175	MET	N-CA-CB	5.48	120.46	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	j	135	PHE	CG-CD1-CE1	5.48	126.83	120.80
3	c	124	HIS	CB-CA-C	-5.48	99.45	110.40
19	M	298	ASP	CB-CG-OD1	-5.47	113.37	118.30
20	J	251	ASP	N-CA-CB	5.47	120.45	110.60
10	j	198	TYR	CD1-CG-CD2	5.47	123.92	117.90
31	R	109	LYS	CG-CD-CE	5.47	128.32	111.90
11	k	149	ARG	NH1-CZ-NH2	-5.47	113.38	119.40
7	g	22	TYR	CB-CG-CD1	5.47	124.28	121.00
13	6	39	TYR	CB-CG-CD1	5.47	124.28	121.00
2	b	157	PHE	CB-CG-CD2	-5.46	116.98	120.80
24	X	122	TYR	CB-CG-CD1	5.46	124.28	121.00
12	5	18	SER	N-CA-CB	5.46	118.69	110.50
17	K	98	GLN	CG-CD-OE1	5.46	132.52	121.60
33	O	62	TYR	CG-CD1-CE1	-5.46	116.93	121.30
12	5	27	ALA	N-CA-CB	5.46	117.74	110.10
12	5	203	GLU	O-C-N	-5.46	113.97	122.70
15	H	216	ASP	CB-CG-OD1	5.46	123.21	118.30
1	a	133	THR	CA-CB-CG2	-5.46	104.76	112.40
23	T	264	MET	CG-SD-CE	-5.46	91.47	100.20
6	f	156	TYR	CB-CA-C	-5.46	99.49	110.40
10	3	169	ALA	CB-CA-C	-5.46	101.92	110.10
4	D	70	VAL	CG1-CB-CG2	5.45	119.63	110.90
3	c	73	ALA	N-CA-CB	5.45	117.73	110.10
6	F	176	ASP	CB-CG-OD2	5.45	123.21	118.30
20	J	147	TYR	CE1-CZ-OH	-5.45	105.39	120.10
11	k	107	TYR	CD1-CG-CD2	5.45	123.89	117.90
18	L	374	PHE	CB-CG-CD1	5.45	124.61	120.80
26	Z	202	ARG	CD-NE-CZ	5.45	131.23	123.60
31	R	204	TRP	CB-CG-CD2	-5.45	119.52	126.60
2	b	81	ASP	CB-CG-OD1	-5.45	113.40	118.30
7	g	186	ARG	NE-CZ-NH2	5.45	123.02	120.30
15	H	373	ARG	NE-CZ-NH1	5.45	123.02	120.30
9	2	175	VAL	CA-CB-CG1	-5.45	102.73	110.90
18	L	112	LEU	CB-CG-CD1	5.45	120.26	111.00
31	R	252	TYR	CB-CG-CD2	-5.45	117.73	121.00
13	6	174	TYR	CB-CG-CD1	5.44	124.27	121.00
8	h	111	TYR	CZ-CE2-CD2	-5.44	114.90	119.80
7	G	143	HIS	CB-CA-C	-5.44	99.52	110.40
22	V	83	VAL	CA-CB-CG2	5.44	119.06	110.90
32	U	245	ASP	CB-CG-OD2	5.44	123.20	118.30
10	j	35	VAL	N-CA-CB	5.44	123.47	111.50
14	n	208	PHE	CG-CD1-CE1	-5.44	114.82	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	45	ARG	NE-CZ-NH1	5.44	123.02	120.30
23	T	72	THR	CA-CB-CG2	-5.44	104.78	112.40
34	8	376	ARG	O-C-N	5.44	131.41	122.70
1	a	130	VAL	CA-CB-CG1	-5.44	102.74	110.90
2	B	179	TRP	CG-CD2-CE3	-5.44	129.00	133.90
7	g	208	PHE	CB-CG-CD2	-5.44	116.99	120.80
9	i	147	THR	N-CA-CB	5.44	120.63	110.30
14	n	44	PRO	N-CA-CB	5.44	109.82	103.30
3	C	24	ALA	CB-CA-C	5.43	118.25	110.10
7	g	237	ASP	CB-CG-OD2	5.43	123.19	118.30
8	1	144	GLU	N-CA-CB	5.43	120.38	110.60
10	3	175	ASP	CB-CG-OD1	-5.43	113.41	118.30
27	N	162	ARG	NE-CZ-NH2	-5.43	117.58	120.30
29	P	138	ARG	NE-CZ-NH2	-5.43	117.58	120.30
11	k	8	ARG	NE-CZ-NH1	5.43	123.02	120.30
16	I	54	ARG	NH1-CZ-NH2	-5.43	113.43	119.40
8	1	19	ARG	NE-CZ-NH2	-5.43	117.59	120.30
5	e	85	ARG	NE-CZ-NH2	-5.42	117.59	120.30
13	m	41	PRO	CA-N-CD	-5.42	103.91	111.50
18	L	375	ASP	CB-CG-OD1	5.42	123.18	118.30
31	R	96	GLN	N-CA-CB	5.42	120.37	110.60
10	j	21	ALA	CB-CA-C	-5.42	101.97	110.10
6	f	96	LEU	CB-CG-CD2	5.42	120.22	111.00
3	C	170	ALA	N-CA-CB	5.42	117.69	110.10
17	K	80	LYS	N-CA-CB	5.42	120.36	110.60
8	h	29	ARG	CA-CB-CG	5.42	125.32	113.40
8	h	112	THR	N-CA-CB	5.42	120.59	110.30
32	U	277	TYR	CB-CG-CD2	-5.42	117.75	121.00
7	g	181	GLU	OE1-CD-OE2	5.42	129.80	123.30
27	N	282	TYR	CB-CG-CD1	-5.42	117.75	121.00
30	Q	290	THR	CA-CB-CG2	-5.42	104.82	112.40
11	k	194	ASP	CB-CG-OD1	-5.41	113.43	118.30
6	F	106	ARG	NE-CZ-NH2	-5.41	117.59	120.30
17	K	81	ARG	NE-CZ-NH2	-5.41	117.59	120.30
20	J	227	SER	N-CA-CB	5.41	118.62	110.50
26	Z	137	TYR	CB-CG-CD1	5.41	124.25	121.00
29	P	328	ALA	N-CA-CB	5.41	117.68	110.10
30	Q	123	GLU	CA-C-O	-5.41	108.73	120.10
26	Z	502	ASN	CB-CA-C	-5.41	99.58	110.40
10	j	155	PRO	C-N-CA	5.41	135.22	121.70
3	C	101	TYR	CB-CG-CD2	-5.41	117.75	121.00
17	K	259	ARG	NE-CZ-NH1	-5.41	117.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	T	89	TYR	CB-CG-CD1	-5.41	117.75	121.00
7	g	77	LEU	N-CA-CB	5.41	121.21	110.40
19	M	279	PHE	CB-CG-CD2	-5.41	117.02	120.80
8	h	188	PHE	CB-CG-CD1	-5.40	117.02	120.80
3	C	63	GLU	CA-CB-CG	5.40	125.29	113.40
5	E	196	LEU	CB-CG-CD2	-5.40	101.82	111.00
7	g	74	TYR	CD1-CG-CD2	5.40	123.84	117.90
9	i	196	ARG	NE-CZ-NH2	-5.40	117.60	120.30
4	D	205	ALA	N-CA-CB	5.40	117.66	110.10
33	O	135	ARG	NE-CZ-NH1	5.40	123.00	120.30
4	D	95	ARG	N-CA-CB	5.40	120.32	110.60
33	O	98	TYR	CG-CD2-CE2	-5.40	116.98	121.30
20	J	101	ASP	CB-CG-OD1	-5.40	113.44	118.30
3	c	23	TYR	CB-CG-CD2	-5.39	117.76	121.00
12	l	127	PHE	CD1-CE1-CZ	-5.39	113.63	120.10
8	1	42	TRP	CG-CD2-CE3	-5.39	129.04	133.90
5	e	70	MET	CA-CB-CG	5.39	122.47	113.30
14	n	30	TYR	N-CA-C	-5.39	96.44	111.00
7	G	110	ASP	CB-CG-OD2	5.39	123.15	118.30
3	C	5	TYR	CG-CD2-CE2	-5.39	116.99	121.30
14	7	195	PHE	CB-CG-CD1	-5.39	117.03	120.80
15	H	202	GLU	N-CA-CB	5.39	120.30	110.60
31	R	331	ARG	NE-CZ-NH2	5.39	123.00	120.30
10	j	30	SER	N-CA-CB	5.39	118.58	110.50
3	c	224	VAL	CA-CB-CG2	-5.39	102.82	110.90
10	j	18	ASP	N-CA-CB	5.39	120.30	110.60
10	j	177	ASP	CB-CG-OD1	5.39	123.15	118.30
18	L	324	ILE	N-CA-C	-5.39	96.46	111.00
20	J	274	GLU	CB-CA-C	-5.39	99.62	110.40
21	W	83	GLY	O-C-N	-5.39	114.08	122.70
31	R	36	SER	CB-CA-C	-5.39	99.86	110.10
2	b	136	ILE	N-CA-CB	5.38	123.18	110.80
4	d	2	TYR	CZ-CE2-CD2	-5.38	114.95	119.80
9	2	200	GLN	OE1-CD-NE2	5.38	134.28	121.90
24	X	30	GLN	N-CA-C	-5.38	96.47	111.00
3	C	139	TYR	CG-CD1-CE1	-5.38	117.00	121.30
17	K	153	ASP	CB-CG-OD1	-5.38	113.46	118.30
11	k	117	TYR	CA-CB-CG	-5.38	103.18	113.40
12	l	42	LEU	N-CA-CB	5.38	121.16	110.40
4	D	103	THR	N-CA-CB	5.38	120.52	110.30
33	O	371	VAL	CA-CB-CG2	-5.38	102.83	110.90
2	b	80	PRO	N-CD-CG	5.38	111.26	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	J	180	ALA	N-CA-CB	5.38	117.63	110.10
22	V	269	ARG	NE-CZ-NH2	-5.38	117.61	120.30
8	h	43	CYS	O-C-N	5.37	131.30	122.70
1	a	61	SER	N-CA-CB	5.37	118.56	110.50
1	a	62	TYR	CD1-CE1-CZ	-5.37	114.97	119.80
1	A	13	GLU	N-CA-CB	5.37	120.27	110.60
3	C	141	ASP	CB-CG-OD1	-5.37	113.47	118.30
9	2	146	LEU	CB-CG-CD2	5.37	120.13	111.00
13	m	142	ALA	N-CA-CB	5.37	117.62	110.10
3	C	203	SER	N-CA-CB	5.37	118.56	110.50
21	W	186	ALA	CB-CA-C	-5.37	102.05	110.10
13	m	32	ASP	CB-CG-OD2	5.37	123.13	118.30
4	D	139	ARG	NE-CZ-NH1	5.37	122.98	120.30
34	8	430	TYR	CG-CD1-CE1	5.37	125.59	121.30
4	D	215	PRO	N-CD-CG	5.37	111.25	103.20
8	1	51	ASP	CB-CG-OD1	5.37	123.13	118.30
20	J	187	LEU	N-CA-C	-5.37	96.52	111.00
23	T	21	ALA	N-CA-CB	5.37	117.61	110.10
27	N	630	ALA	CB-CA-C	-5.36	102.05	110.10
20	J	280	ASP	N-CA-CB	5.36	120.25	110.60
20	J	323	ALA	CB-CA-C	-5.36	102.06	110.10
1	a	86	LEU	CB-CG-CD1	5.36	120.11	111.00
19	M	432	PHE	CB-CG-CD2	5.36	124.55	120.80
6	f	184	ASN	N-CA-CB	5.36	120.24	110.60
27	N	437	GLU	OE1-CD-OE2	-5.36	116.87	123.30
30	Q	64	LEU	CB-CG-CD2	5.36	120.11	111.00
17	K	198	TYR	CZ-CE2-CD2	5.36	124.62	119.80
28	S	176	LEU	CB-CG-CD2	5.36	120.11	111.00
3	c	213	ALA	N-CA-CB	5.35	117.59	110.10
9	i	207	ARG	NE-CZ-NH1	5.35	122.98	120.30
18	L	261	ARG	NE-CZ-NH2	-5.35	117.62	120.30
3	C	139	TYR	CB-CG-CD1	-5.35	117.79	121.00
2	B	201	GLU	CB-CA-C	-5.35	99.71	110.40
26	Z	959	HIS	N-CA-CB	5.35	120.23	110.60
8	h	64	GLU	CB-CA-C	-5.34	99.71	110.40
20	J	138	MET	CG-SD-CE	-5.34	91.65	100.20
27	N	756	THR	CA-CB-CG2	-5.34	104.92	112.40
13	m	160	TYR	CG-CD1-CE1	5.34	125.58	121.30
6	F	202	ASP	CB-CG-OD2	-5.34	113.49	118.30
12	5	137	TYR	CB-CG-CD1	-5.34	117.79	121.00
27	N	90	ASP	CB-CG-OD2	-5.34	113.49	118.30
18	L	345	ARG	NH1-CZ-NH2	5.34	125.28	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	42	GLY	C-N-CA	5.34	135.05	121.70
2	B	159	TRP	CB-CG-CD2	-5.34	119.66	126.60
10	3	192	ASP	CB-CG-OD1	-5.34	113.49	118.30
27	N	412	TYR	CB-CG-CD2	-5.34	117.80	121.00
29	P	266	TYR	CG-CD1-CE1	5.34	125.57	121.30
34	8	439	GLN	N-CA-CB	5.34	120.21	110.60
4	D	76	LEU	CB-CG-CD2	5.33	120.07	111.00
9	2	88	PHE	CB-CG-CD2	-5.33	117.07	120.80
28	S	204	ASP	CB-CG-OD1	5.33	123.10	118.30
29	P	79	LEU	N-CA-C	5.33	125.40	111.00
7	g	68	ARG	NE-CZ-NH2	-5.33	117.64	120.30
5	E	36	GLU	OE1-CD-OE2	5.33	129.70	123.30
32	U	218	GLU	N-CA-CB	5.33	120.20	110.60
33	O	12	SER	O-C-N	-5.33	114.17	122.70
9	i	98	LEU	N-CA-CB	5.33	121.06	110.40
3	c	138	GLY	O-C-N	5.33	131.22	122.70
7	g	112	LEU	CB-CA-C	-5.33	100.08	110.20
1	A	96	ARG	NH1-CZ-NH2	-5.33	113.54	119.40
17	K	98	GLN	CB-CA-C	5.33	121.05	110.40
26	Z	770	GLU	N-CA-CB	5.33	120.19	110.60
10	3	134	ASP	CB-CG-OD2	-5.32	113.51	118.30
19	M	273	LYS	N-CA-CB	5.32	120.18	110.60
30	Q	271	MET	CG-SD-CE	-5.32	91.68	100.20
11	k	73	TYR	CD1-CE1-CZ	-5.32	115.01	119.80
34	8	494	TYR	CZ-CE2-CD2	-5.32	115.01	119.80
30	Q	434	TYR	CB-CG-CD1	-5.32	117.81	121.00
12	5	61	SER	N-CA-CB	5.32	118.48	110.50
2	b	23	TYR	CG-CD2-CE2	-5.32	117.05	121.30
2	B	82	TYR	CD1-CG-CD2	5.32	123.75	117.90
5	E	79	SER	CB-CA-C	-5.32	100.00	110.10
13	6	203	GLU	OE1-CD-OE2	-5.32	116.92	123.30
29	P	95	TYR	CB-CG-CD2	-5.31	117.81	121.00
2	b	249	ALA	N-CA-CB	5.31	117.53	110.10
17	K	225	ALA	N-CA-CB	5.31	117.53	110.10
22	V	212	MET	N-CA-CB	5.31	120.16	110.60
3	c	97	TYR	CB-CG-CD2	-5.31	117.82	121.00
34	8	289	ASP	CB-CG-OD1	5.31	123.08	118.30
31	R	100	ASN	CA-CB-CG	-5.30	101.73	113.40
4	d	159	ALA	N-CA-CB	5.30	117.52	110.10
14	n	41	ARG	NE-CZ-NH2	-5.30	117.65	120.30
17	K	46	ASP	CB-CG-OD1	5.30	123.07	118.30
23	T	122	PHE	CB-CG-CD2	5.30	124.51	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Y	89	GLN	CA-C-O	-5.30	108.97	120.10
34	8	391	ARG	CD-NE-CZ	-5.30	116.18	123.60
11	4	108	ASP	CB-CG-OD1	5.30	123.07	118.30
10	3	204	ASP	CA-C-O	-5.29	108.99	120.10
29	P	440	HIS	CA-C-O	-5.29	108.99	120.10
1	a	154	TYR	CB-CG-CD2	-5.29	117.83	121.00
6	F	233	ILE	CA-C-O	-5.29	108.99	120.10
9	2	200	GLN	CG-CD-OE1	-5.29	111.02	121.60
9	2	226	GLU	CA-C-O	-5.29	108.99	120.10
10	3	67	ARG	NE-CZ-NH1	5.29	122.94	120.30
11	4	117	TYR	N-CA-CB	5.29	120.12	110.60
11	4	195	PHE	CA-C-O	-5.29	108.99	120.10
15	H	88	ARG	NE-CZ-NH1	5.29	122.94	120.30
13	6	222	ASP	CA-C-O	-5.29	109.00	120.10
27	N	811	LYS	CB-CA-C	-5.29	99.82	110.40
30	Q	405	GLN	N-CA-CB	5.29	120.12	110.60
16	I	437	LEU	CA-C-O	-5.29	109.00	120.10
26	Z	253	VAL	O-C-N	-5.29	111.06	121.10
1	a	56	ASP	CB-CG-OD2	-5.29	113.54	118.30
15	H	373	ARG	NE-CZ-NH2	5.29	122.94	120.30
19	M	318	ASP	CB-CG-OD2	-5.29	113.54	118.30
19	M	434	ALA	CA-C-O	-5.29	109.00	120.10
27	N	925	ASP	CA-C-O	-5.29	109.00	120.10
28	S	152	LEU	C-N-CA	5.29	134.91	121.70
30	Q	434	TYR	CA-C-O	-5.29	109.00	120.10
33	O	92	PHE	N-CA-CB	5.29	120.11	110.60
1	A	222	ASP	CB-CG-OD1	-5.28	113.55	118.30
4	D	240	GLU	CA-C-O	-5.28	109.01	120.10
33	O	48	PHE	CB-CG-CD2	-5.28	117.10	120.80
28	S	492	LYS	CA-C-O	-5.28	109.01	120.10
29	P	39	LEU	CB-CA-C	-5.28	100.17	110.20
31	R	243	LEU	CB-CA-C	-5.28	100.16	110.20
2	b	241	GLN	CA-CB-CG	5.28	125.02	113.40
5	e	45	ARG	NE-CZ-NH2	-5.28	117.66	120.30
2	B	250	LEU	CA-C-O	-5.28	109.01	120.10
7	G	244	ASN	CA-C-O	-5.28	109.01	120.10
26	Z	498	ALA	CB-CA-C	5.28	118.02	110.10
26	Z	928	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
18	L	436	LYS	CA-C-O	-5.28	109.02	120.10
27	N	157	ALA	CB-CA-C	-5.28	102.18	110.10
8	1	196	LEU	CA-C-O	-5.28	109.02	120.10
30	Q	229	ASP	CB-CG-OD1	5.28	123.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	242	GLN	CA-C-O	-5.28	109.02	120.10
5	E	242	GLU	CA-C-O	-5.28	109.02	120.10
34	8	267	GLY	N-CA-C	-5.28	99.91	113.10
17	K	306	PHE	CB-CG-CD2	-5.27	117.11	120.80
17	K	428	LYS	CA-C-O	-5.27	109.03	120.10
7	g	44	PHE	CB-CG-CD1	5.27	124.49	120.80
9	2	56	THR	O-C-N	5.27	131.13	122.70
9	i	157	ASP	CB-CG-OD2	-5.27	113.56	118.30
3	C	244	THR	CA-C-O	-5.27	109.03	120.10
4	D	148	THR	CA-CB-CG2	-5.27	105.02	112.40
13	6	131	TYR	CB-CG-CD2	-5.27	117.84	121.00
26	Z	928	ARG	N-CA-CB	5.27	120.08	110.60
31	R	312	TYR	CB-CG-CD1	5.27	124.16	121.00
18	L	255	TYR	CB-CG-CD1	-5.26	117.84	121.00
6	f	207	VAL	CA-CB-CG2	5.26	118.79	110.90
8	1	4	MET	N-CA-CB	5.26	120.07	110.60
12	5	88	TYR	CG-CD1-CE1	-5.26	117.09	121.30
17	K	127	ASP	CB-CG-OD2	5.26	123.03	118.30
12	l	7	ARG	CB-CA-C	-5.26	99.89	110.40
8	1	122	LEU	CB-CA-C	-5.26	100.21	110.20
19	M	124	ARG	N-CA-CB	5.26	120.06	110.60
11	k	32	ASP	O-C-N	5.26	131.11	122.70
14	n	107	MET	N-CA-CB	5.26	120.06	110.60
4	D	35	LYS	N-CA-CB	5.26	120.06	110.60
4	D	200	VAL	CA-CB-CG2	5.25	118.78	110.90
9	2	31	CYS	N-CA-C	-5.25	96.82	111.00
26	Z	441	TYR	CB-CA-C	-5.25	99.90	110.40
13	6	141	ALA	N-CA-CB	5.25	117.45	110.10
1	a	109	ALA	CB-CA-C	-5.25	102.23	110.10
12	l	167	ARG	NE-CZ-NH2	-5.25	117.68	120.30
3	C	151	ASN	CA-CB-CG	-5.25	101.86	113.40
13	6	188	PHE	N-CA-CB	5.25	120.04	110.60
18	L	329	ARG	NE-CZ-NH2	-5.25	117.68	120.30
3	c	162	ILE	CA-CB-CG1	5.24	120.96	111.00
5	E	130	PHE	CB-CG-CD1	5.24	124.47	120.80
18	L	221	TYR	CB-CG-CD1	-5.24	117.85	121.00
33	O	81	TYR	CG-CD1-CE1	-5.24	117.11	121.30
7	g	131	SER	N-CA-CB	5.24	118.36	110.50
11	4	5	LEU	CB-CA-C	-5.24	100.24	110.20
13	6	125	PHE	CB-CG-CD1	5.24	124.47	120.80
3	c	191	LEU	CB-CG-CD1	5.24	119.91	111.00
4	d	117	ARG	NE-CZ-NH2	-5.24	117.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	k	135	TYR	CB-CG-CD2	5.24	124.14	121.00
12	l	104	TYR	CA-CB-CG	5.24	123.35	113.40
8	h	82	PHE	CB-CG-CD2	5.24	124.47	120.80
16	I	61	ARG	NE-CZ-NH1	-5.24	117.68	120.30
13	m	52	MET	CG-SD-CE	-5.23	91.83	100.20
7	g	134	PHE	CB-CG-CD2	-5.23	117.14	120.80
11	k	45	SER	CB-CA-C	-5.23	100.16	110.10
6	F	38	ARG	CD-NE-CZ	5.23	130.92	123.60
14	7	137	TYR	N-CA-CB	5.23	120.01	110.60
17	K	45	SER	N-CA-CB	5.23	118.35	110.50
17	K	361	SER	O-C-N	-5.23	114.33	122.70
31	R	363	PHE	N-CA-CB	5.23	120.02	110.60
17	K	146	LEU	CB-CG-CD2	5.23	119.89	111.00
32	U	52	PHE	CB-CG-CD2	-5.23	117.14	120.80
7	g	44	PHE	CB-CG-CD2	-5.23	117.14	120.80
8	h	147	SER	N-CA-CB	5.23	118.34	110.50
19	M	85	VAL	CA-CB-CG1	-5.23	103.06	110.90
6	f	50	ARG	N-CA-CB	5.22	120.00	110.60
14	7	23	ALA	O-C-N	5.22	131.06	122.70
31	R	99	TYR	N-CA-CB	5.22	120.01	110.60
32	U	187	SER	N-CA-CB	5.22	118.34	110.50
6	f	151	ASN	N-CA-CB	5.22	120.00	110.60
23	T	224	ARG	NE-CZ-NH2	-5.22	117.69	120.30
24	X	79	LYS	N-CA-CB	5.22	120.00	110.60
8	h	102	TYR	N-CA-CB	5.22	119.99	110.60
13	m	140	GLY	O-C-N	5.22	131.05	122.70
17	K	253	MET	CG-SD-CE	-5.22	91.85	100.20
23	T	234	TYR	N-CA-C	-5.22	96.91	111.00
34	8	373	GLU	O-C-N	-5.22	114.35	122.70
8	h	102	TYR	N-CA-C	-5.22	96.91	111.00
10	j	95	TYR	CB-CG-CD1	5.22	124.13	121.00
1	A	68	ARG	CD-NE-CZ	5.22	130.90	123.60
29	P	268	LEU	CB-CG-CD2	5.22	119.87	111.00
32	U	100	ARG	NE-CZ-NH2	5.22	122.91	120.30
5	e	48	SER	CB-CA-C	-5.21	100.19	110.10
1	A	95	PHE	CB-CG-CD1	5.21	124.45	120.80
13	6	214	LYS	N-CA-CB	5.21	119.98	110.60
20	J	403	LEU	CB-CG-CD1	5.21	119.86	111.00
26	Z	149	TRP	CB-CA-C	-5.21	99.97	110.40
19	M	372	ASP	CB-CG-OD1	-5.21	113.61	118.30
12	l	188	HIS	CA-C-N	5.21	126.62	116.20
22	V	153	ILE	N-CA-C	-5.21	96.93	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	79	PRO	N-CA-CB	5.21	109.55	103.30
13	6	160	TYR	CB-CG-CD1	-5.21	117.87	121.00
27	N	279	ALA	N-CA-CB	5.21	117.39	110.10
3	c	90	ALA	N-CA-CB	5.21	117.39	110.10
18	L	82	ARG	NE-CZ-NH1	5.21	122.91	120.30
19	M	130	PRO	N-CD-CG	5.21	111.01	103.20
21	W	127	ARG	NE-CZ-NH2	-5.21	117.70	120.30
1	a	75	ASN	N-CA-C	-5.21	96.94	111.00
3	c	66	TYR	CD1-CG-CD2	5.21	123.63	117.90
4	d	47	ARG	NE-CZ-NH1	5.21	122.90	120.30
12	l	144	TYR	CD1-CG-CD2	5.21	123.63	117.90
3	C	137	ALA	CB-CA-C	-5.21	102.29	110.10
13	6	138	ALA	N-CA-CB	5.21	117.39	110.10
26	Z	968	ASP	N-CA-C	-5.21	96.94	111.00
3	C	221	ASP	CB-CG-OD1	5.20	122.98	118.30
4	D	212	VAL	CB-CA-C	-5.20	101.52	111.40
19	M	303	ARG	NE-CZ-NH2	-5.20	117.70	120.30
28	S	487	THR	CA-CB-CG2	-5.20	105.11	112.40
30	Q	308	ASN	CA-CB-CG	-5.20	101.95	113.40
16	I	436	TYR	CZ-CE2-CD2	5.20	124.48	119.80
31	R	391	ASN	CA-CB-CG	-5.20	101.96	113.40
6	f	178	PHE	CB-CG-CD2	-5.20	117.16	120.80
14	n	142	LEU	O-C-N	5.20	131.02	122.70
25	Y	72	ASP	CB-CG-OD1	-5.20	113.62	118.30
15	H	272	ILE	N-CA-C	-5.20	96.97	111.00
32	U	100	ARG	NH1-CZ-NH2	-5.20	113.69	119.40
7	g	166	GLN	N-CA-CB	5.19	119.95	110.60
7	g	208	PHE	CB-CG-CD1	5.19	124.44	120.80
11	4	73	TYR	CB-CG-CD1	-5.19	117.89	121.00
17	K	66	ASP	CB-CG-OD1	-5.19	113.63	118.30
2	B	29	LYS	N-CA-CB	5.19	119.94	110.60
13	m	182	LYS	N-CA-CB	5.19	119.94	110.60
5	E	57	GLU	N-CA-CB	5.19	119.94	110.60
31	R	195	ASN	O-C-N	-5.19	114.40	122.70
3	c	156	TYR	CG-CD1-CE1	-5.18	117.15	121.30
14	7	193	ARG	NE-CZ-NH1	5.18	122.89	120.30
16	I	220	ILE	CB-CA-C	-5.18	101.23	111.60
12	l	55	TRP	N-CA-CB	5.18	119.93	110.60
30	Q	109	ASP	N-CA-CB	5.18	119.93	110.60
8	h	45	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
5	E	128	ARG	N-CA-CB	5.18	119.92	110.60
20	J	16	GLU	CB-CA-C	-5.18	100.05	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	79	SER	N-CA-CB	5.18	118.27	110.50
27	N	14	ARG	N-CA-CB	5.18	119.92	110.60
7	g	184	SER	N-CA-CB	5.17	118.26	110.50
10	3	45	TYR	CB-CG-CD1	5.17	124.11	121.00
11	4	135	TYR	CD1-CE1-CZ	-5.17	115.14	119.80
19	M	405	ASN	N-CA-CB	5.17	119.92	110.60
28	S	142	VAL	CA-CB-CG2	-5.17	103.14	110.90
3	c	66	TYR	CG-CD1-CE1	-5.17	117.16	121.30
3	c	130	PHE	CB-CG-CD1	5.17	124.42	120.80
12	l	32	LYS	O-C-N	5.17	130.97	122.70
8	1	74	SER	N-CA-CB	5.17	118.25	110.50
26	Z	180	ASP	CB-CG-OD2	-5.17	113.65	118.30
27	N	388	PRO	CA-N-CD	5.17	118.93	111.70
30	Q	297	ASP	CB-CG-OD1	5.17	122.95	118.30
7	g	106	PRO	N-CA-CB	5.17	109.50	103.30
33	O	92	PHE	CB-CG-CD2	5.17	124.42	120.80
1	A	5	ARG	NE-CZ-NH2	-5.16	117.72	120.30
4	D	174	GLU	OE1-CD-OE2	-5.16	117.10	123.30
7	G	15	GLY	O-C-N	-5.16	114.44	122.70
22	V	251	TYR	CB-CG-CD1	-5.16	117.90	121.00
26	Z	339	PHE	CB-CG-CD1	5.16	124.42	120.80
29	P	6	PRO	N-CA-CB	5.16	109.50	103.30
34	8	271	PHE	CB-CG-CD1	5.16	124.42	120.80
21	W	105	VAL	CG1-CB-CG2	-5.16	102.64	110.90
33	O	98	TYR	CZ-CE2-CD2	5.16	124.45	119.80
3	c	82	ASP	CB-CG-OD1	-5.16	113.66	118.30
15	H	91	LEU	CB-CG-CD1	5.16	119.77	111.00
34	8	291	THR	O-C-N	-5.16	114.43	123.20
2	b	17	LYS	CA-CB-CG	5.16	124.75	113.40
1	A	104	PRO	O-C-N	5.16	130.95	122.70
9	2	18	THR	CA-CB-CG2	-5.16	105.18	112.40
8	h	189	TYR	CB-CG-CD1	-5.16	117.91	121.00
14	n	99	VAL	CA-CB-CG2	-5.16	103.17	110.90
18	L	342	ARG	NE-CZ-NH1	5.16	122.88	120.30
19	M	221	TYR	CB-CG-CD1	-5.16	117.91	121.00
18	L	88	TYR	CG-CD2-CE2	-5.15	117.18	121.30
26	Z	952	SER	CB-CA-C	-5.15	100.31	110.10
10	j	31	GLN	N-CA-CB	5.15	119.88	110.60
13	m	198	VAL	CA-CB-CG2	-5.15	103.17	110.90
28	S	443	ILE	O-C-N	5.15	130.94	122.70
29	P	253	ASP	CB-CG-OD2	5.15	122.94	118.30
4	d	57	ILE	C-N-CA	5.15	134.58	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	116	GLN	CB-CA-C	-5.15	100.10	110.40
5	E	145	TYR	O-C-N	-5.15	114.46	122.70
3	c	209	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
12	l	20	ALA	N-CA-CB	5.14	117.30	110.10
18	L	392	ARG	NH1-CZ-NH2	-5.14	113.74	119.40
24	X	92	SER	C-N-CA	5.14	134.56	121.70
1	a	168	GLU	OE1-CD-OE2	5.14	129.47	123.30
5	E	159	TYR	CD1-CG-CD2	5.14	123.56	117.90
18	L	107	GLU	N-CA-CB	5.14	119.86	110.60
28	S	300	ALA	N-CA-CB	5.14	117.30	110.10
34	8	271	PHE	CB-CG-CD2	-5.14	117.20	120.80
3	C	213	ALA	CB-CA-C	-5.14	102.39	110.10
26	Z	861	THR	O-C-N	-5.14	114.47	122.70
5	e	68	CYS	N-CA-CB	5.14	119.85	110.60
6	f	211	SER	O-C-N	5.14	130.92	122.70
2	B	25	LEU	CB-CG-CD1	-5.14	102.26	111.00
3	C	19	TYR	CB-CG-CD2	-5.14	117.92	121.00
4	D	50	LEU	N-CA-CB	5.14	120.68	110.40
17	K	363	ALA	CB-CA-C	-5.14	102.39	110.10
18	L	138	SER	N-CA-CB	5.14	118.21	110.50
4	d	16	PHE	CB-CG-CD1	-5.14	117.20	120.80
4	D	50	LEU	CB-CG-CD1	5.14	119.73	111.00
3	c	141	ASP	CB-CG-OD1	5.14	122.92	118.30
7	g	11	PHE	CB-CG-CD2	5.14	124.39	120.80
7	g	171	GLU	OE1-CD-OE2	-5.14	117.14	123.30
9	2	104	ASP	CB-CG-OD2	-5.13	113.68	118.30
27	N	559	TYR	CZ-CE2-CD2	-5.13	115.18	119.80
7	g	23	ALA	CB-CA-C	-5.13	102.40	110.10
13	m	41	PRO	N-CD-CG	5.13	110.90	103.20
14	n	91	TYR	CB-CG-CD2	-5.13	117.92	121.00
6	F	200	LEU	CB-CG-CD2	5.13	119.72	111.00
6	F	202	ASP	CB-CG-OD1	5.13	122.92	118.30
27	N	881	TYR	CA-CB-CG	-5.13	103.65	113.40
2	b	157	PHE	CG-CD2-CE2	5.13	126.44	120.80
15	H	443	PHE	CB-CG-CD1	-5.13	117.21	120.80
17	K	194	GLN	O-C-N	-5.13	114.50	122.70
28	S	165	PRO	N-CD-CG	5.13	110.89	103.20
3	c	145	TYR	CD1-CG-CD2	5.12	123.54	117.90
1	A	240	ALA	CB-CA-C	-5.12	102.42	110.10
33	O	71	ASP	CB-CG-OD2	-5.12	113.69	118.30
27	N	461	GLU	OE1-CD-OE2	5.12	129.44	123.30
32	U	157	LEU	CB-CA-C	-5.12	100.47	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	8	186	ASN	CB-CG-OD1	5.12	131.84	121.60
3	C	23	TYR	O-C-N	-5.12	114.51	122.70
5	E	212	SER	CB-CA-C	-5.12	100.37	110.10
9	2	133	ALA	CB-CA-C	-5.12	102.42	110.10
14	7	65	ARG	NH1-CZ-NH2	-5.12	113.77	119.40
31	R	239	THR	N-CA-C	-5.12	97.18	111.00
12	l	178	TYR	CB-CG-CD2	-5.12	117.93	121.00
16	I	220	ILE	N-CA-CB	5.12	122.57	110.80
28	S	51	ARG	CB-CA-C	-5.12	100.17	110.40
29	P	245	TYR	CB-CG-CD2	5.12	124.07	121.00
31	R	342	LEU	CB-CG-CD2	5.12	119.70	111.00
5	e	179	TRP	CG-CD2-CE3	-5.12	129.30	133.90
6	F	37	LEU	CB-CG-CD2	5.12	119.70	111.00
20	J	147	TYR	OH-CZ-CE2	5.12	133.91	120.10
15	H	395	SER	N-CA-CB	5.11	118.17	110.50
18	L	159	LEU	CB-CA-C	-5.11	100.49	110.20
23	T	186	ARG	NE-CZ-NH2	-5.11	117.74	120.30
27	N	890	PHE	CB-CG-CD1	-5.11	117.22	120.80
27	N	916	LEU	CB-CA-C	-5.11	100.48	110.20
32	U	273	LEU	CB-CA-C	-5.11	100.48	110.20
10	j	95	TYR	CB-CG-CD2	-5.11	117.93	121.00
18	L	145	ARG	NE-CZ-NH2	5.11	122.86	120.30
6	f	72	SER	N-CA-CB	5.11	118.16	110.50
7	g	110	ASP	CB-CG-OD2	-5.11	113.70	118.30
10	j	49	PHE	CB-CG-CD2	-5.11	117.22	120.80
3	C	121	TYR	CB-CA-C	-5.11	100.19	110.40
26	Z	859	LYS	C-N-CA	5.11	133.02	122.30
27	N	338	PHE	CB-CG-CD1	5.11	124.37	120.80
31	R	63	TYR	CZ-CE2-CD2	-5.11	115.20	119.80
12	l	163	ALA	N-CA-CB	5.10	117.25	110.10
17	K	316	MET	CG-SD-CE	-5.10	92.03	100.20
15	H	202	GLU	C-N-CA	5.10	134.46	121.70
26	Z	142	ASP	N-CA-C	5.10	124.78	111.00
27	N	91	ILE	C-N-CA	5.10	134.46	121.70
31	R	110	ILE	CG1-CB-CG2	-5.10	100.17	111.40
33	O	307	MET	N-CA-CB	5.10	119.78	110.60
1	A	214	LEU	CB-CA-C	-5.10	100.51	110.20
6	F	12	PHE	CB-CG-CD1	5.10	124.37	120.80
20	J	354	SER	N-CA-C	-5.10	97.23	111.00
12	5	187	TYR	CB-CG-CD2	-5.10	117.94	121.00
8	h	124	TYR	CB-CG-CD2	5.09	124.06	121.00
8	h	193	TYR	CG-CD2-CE2	-5.09	117.22	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	147	ASP	CB-CG-OD1	-5.09	113.72	118.30
15	H	246	ILE	N-CA-C	-5.09	97.25	111.00
34	8	318	PHE	CB-CG-CD2	-5.09	117.23	120.80
3	C	25	LEU	CB-CG-CD2	-5.09	102.35	111.00
17	K	399	ARG	NE-CZ-NH2	-5.09	117.76	120.30
29	P	21	PHE	CB-CG-CD1	-5.09	117.24	120.80
2	b	87	ASP	CB-CG-OD1	5.09	122.88	118.30
10	j	45	TYR	N-CA-C	-5.09	97.27	111.00
20	J	390	MET	CA-CB-CG	5.09	121.95	113.30
7	g	216	SER	N-CA-CB	5.08	118.13	110.50
3	C	159	TRP	N-CA-CB	5.08	119.75	110.60
13	6	164	THR	CA-CB-CG2	-5.08	105.28	112.40
19	M	163	PHE	CG-CD2-CE2	-5.08	115.21	120.80
20	J	48	ARG	NE-CZ-NH2	-5.08	117.76	120.30
32	U	30	ASN	N-CA-CB	5.08	119.75	110.60
14	n	152	ASN	CA-C-N	5.08	131.33	117.10
9	2	203	TYR	CD1-CE1-CZ	-5.08	115.23	119.80
16	I	207	LEU	CB-CG-CD1	5.08	119.64	111.00
15	H	266	ARG	NE-CZ-NH1	5.08	122.84	120.30
5	e	143	ASP	CB-CG-OD1	5.08	122.87	118.30
8	h	159	LEU	N-CA-CB	5.08	120.56	110.40
8	h	193	TYR	CZ-CE2-CD2	5.08	124.37	119.80
9	i	22	GLN	N-CA-C	-5.08	97.29	111.00
12	l	8	PHE	N-CA-CB	5.08	119.74	110.60
12	l	113	TYR	CD1-CG-CD2	5.08	123.49	117.90
2	b	147	LEU	O-C-N	-5.08	114.58	122.70
4	D	88	ARG	NH1-CZ-NH2	5.08	124.98	119.40
10	3	49	PHE	CG-CD2-CE2	-5.08	115.22	120.80
13	6	48	ASP	N-CA-CB	5.08	119.74	110.60
15	H	270	THR	CA-CB-CG2	-5.08	105.30	112.40
16	I	86	GLU	N-CA-CB	5.08	119.73	110.60
5	e	147	LEU	CB-CA-C	-5.07	100.56	110.20
6	F	229	VAL	CA-CB-CG2	5.07	118.51	110.90
7	g	122	TYR	CG-CD2-CE2	-5.07	117.24	121.30
8	1	51	ASP	CB-CA-C	-5.07	100.26	110.40
22	V	180	LEU	N-CA-C	-5.07	97.31	111.00
27	N	328	PHE	CB-CG-CD2	-5.07	117.25	120.80
30	Q	264	TYR	CB-CG-CD1	5.07	124.04	121.00
34	8	436	ILE	CG1-CB-CG2	5.07	122.56	111.40
7	g	82	ARG	NE-CZ-NH1	5.07	122.83	120.30
6	f	66	ASP	CB-CG-OD1	5.07	122.86	118.30
7	g	197	TYR	CG-CD1-CE1	-5.07	117.25	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	76	TYR	CB-CG-CD1	5.07	124.04	121.00
4	D	212	VAL	CA-CB-CG1	5.07	118.50	110.90
19	M	218	ALA	N-CA-CB	5.07	117.19	110.10
12	l	54	PHE	CG-CD1-CE1	-5.07	115.23	120.80
13	m	75	TYR	CG-CD2-CE2	5.06	125.35	121.30
33	O	286	PHE	CB-CA-C	-5.06	100.27	110.40
5	E	75	ALA	N-CA-CB	5.06	117.19	110.10
22	V	45	VAL	CA-CB-CG1	5.06	118.49	110.90
5	e	220	PHE	CG-CD2-CE2	-5.06	115.23	120.80
6	f	130	GLY	N-CA-C	-5.06	100.45	113.10
34	8	133	LEU	CB-CG-CD2	5.06	119.60	111.00
34	8	346	THR	CA-CB-CG2	-5.06	105.32	112.40
3	c	97	TYR	CG-CD2-CE2	-5.06	117.25	121.30
4	d	91	ALA	N-CA-CB	5.06	117.18	110.10
11	k	89	ALA	CB-CA-C	-5.06	102.52	110.10
23	T	51	TYR	CG-CD2-CE2	-5.06	117.25	121.30
10	3	28	LEU	N-CA-C	-5.05	97.36	111.00
11	4	110	LYS	CB-CA-C	-5.05	100.29	110.40
18	L	72	ASP	CB-CG-OD2	-5.05	113.75	118.30
2	b	212	ALA	CB-CA-C	-5.05	102.52	110.10
9	2	186	TYR	N-CA-C	-5.05	97.36	111.00
23	T	151	TRP	CE2-CD2-CE3	5.05	124.76	118.70
8	h	13	ILE	CB-CA-C	-5.05	101.50	111.60
13	m	174	TYR	CZ-CE2-CD2	5.05	124.34	119.80
17	K	252	ARG	NE-CZ-NH2	-5.05	117.78	120.30
20	J	86	VAL	CA-CB-CG1	5.05	118.47	110.90
8	h	42	TRP	CE3-CZ3-CH2	-5.05	115.65	121.20
3	c	213	ALA	CB-CA-C	-5.05	102.53	110.10
6	f	88	ARG	NE-CZ-NH2	-5.05	117.78	120.30
7	G	177	ASP	CB-CG-OD1	-5.05	113.76	118.30
9	2	193	PRO	N-CA-CB	5.05	109.36	103.30
31	R	109	LYS	CA-C-O	-5.05	109.50	120.10
34	8	399	ALA	N-CA-CB	5.05	117.17	110.10
5	e	209	ALA	N-CA-CB	5.04	117.16	110.10
9	i	31	CYS	N-CA-C	-5.04	97.38	111.00
13	m	32	ASP	CB-CG-OD1	-5.04	113.76	118.30
21	W	144	PHE	CB-CG-CD2	5.04	124.33	120.80
4	d	106	TYR	CG-CD1-CE1	-5.04	117.27	121.30
11	k	159	ASP	CB-CG-OD1	-5.04	113.76	118.30
17	K	333	ARG	NE-CZ-NH1	5.04	122.82	120.30
24	X	51	ARG	CD-NE-CZ	5.04	130.66	123.60
26	Z	575	MET	CG-SD-CE	-5.04	92.14	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	N	786	ARG	NE-CZ-NH2	5.04	122.82	120.30
15	H	362	ASP	CB-CG-OD1	-5.04	113.77	118.30
3	c	69	ASN	N-CA-CB	5.04	119.66	110.60
26	Z	785	VAL	CA-CB-CG1	-5.04	103.35	110.90
3	c	68	LEU	CB-CG-CD1	-5.03	102.44	111.00
8	h	31	THR	CA-CB-CG2	-5.03	105.35	112.40
10	3	123	PHE	N-CA-CB	5.03	119.66	110.60
15	H	190	ARG	NE-CZ-NH1	5.03	122.82	120.30
17	K	233	ALA	N-CA-CB	5.03	117.15	110.10
29	P	371	LEU	CB-CG-CD1	-5.03	102.44	111.00
7	g	65	VAL	N-CA-CB	5.03	122.57	111.50
14	7	14	MET	CB-CG-SD	5.03	127.49	112.40
29	P	69	ARG	NE-CZ-NH2	-5.03	117.78	120.30
9	2	79	ALA	N-CA-CB	5.03	117.14	110.10
17	K	427	TYR	CB-CG-CD2	-5.03	117.98	121.00
27	N	517	LEU	CB-CG-CD2	5.03	119.55	111.00
12	l	118	ASP	CB-CG-OD2	5.03	122.83	118.30
13	m	38	ARG	NE-CZ-NH2	-5.03	117.79	120.30
20	J	352	GLY	N-CA-C	-5.03	100.54	113.10
27	N	648	PRO	CA-N-CD	5.03	118.74	111.70
4	d	176	ASN	O-C-N	-5.02	114.66	122.70
4	d	54	ASP	CB-CG-OD2	5.02	122.82	118.30
1	A	199	THR	CA-CB-CG2	-5.02	105.37	112.40
6	F	193	VAL	CA-CB-CG2	-5.02	103.36	110.90
6	F	221	PHE	CB-CG-CD1	5.02	124.32	120.80
14	7	146	PHE	CB-CG-CD1	5.02	124.32	120.80
15	H	196	THR	CA-CB-CG2	-5.02	105.37	112.40
33	O	56	PRO	C-N-CA	5.02	134.25	121.70
24	X	62	ASP	N-CA-CB	5.02	119.64	110.60
2	b	195	THR	CA-CB-CG2	-5.02	105.38	112.40
10	3	156	ASN	CA-CB-CG	-5.02	102.36	113.40
16	I	98	GLU	CB-CG-CD	-5.02	100.65	114.20
1	a	56	ASP	CB-CG-OD1	5.02	122.81	118.30
33	O	106	PHE	CB-CG-CD2	-5.02	117.29	120.80
9	i	143	LYS	CB-CA-C	-5.01	100.37	110.40
12	l	139	VAL	CA-CB-CG2	-5.01	103.38	110.90
14	7	90	SER	CB-CA-C	-5.01	100.57	110.10
18	L	111	GLU	OE1-CD-OE2	5.01	129.32	123.30
31	R	222	ARG	NE-CZ-NH2	-5.01	117.79	120.30
3	C	10	THR	CA-CB-CG2	5.01	119.42	112.40
14	n	10	SER	CB-CA-C	5.01	119.62	110.10
27	N	314	LEU	CB-CA-C	-5.01	100.68	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	215	VAL	CG1-CB-CG2	5.01	118.91	110.90
14	n	124	ASP	CB-CG-OD2	5.01	122.81	118.30
2	B	23	TYR	CB-CG-CD1	-5.01	117.99	121.00
18	L	267	PHE	CB-CG-CD1	5.01	124.31	120.80
26	Z	242	PHE	CB-CG-CD2	-5.01	117.29	120.80
5	E	68	CYS	N-CA-CB	5.01	119.61	110.60
6	F	97	VAL	CA-CB-CG2	-5.01	103.39	110.90
5	E	171	ALA	N-CA-CB	5.00	117.10	110.10
14	7	223	LYS	N-CA-CB	5.00	119.61	110.60
18	L	280	MET	N-CA-CB	5.00	119.61	110.60
23	T	266	TYR	CB-CG-CD1	5.00	124.00	121.00
24	X	113	GLU	N-CA-CB	5.00	119.61	110.60
20	J	119	SER	N-CA-CB	5.00	118.00	110.50

There are no chirality outliers.

All (347) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	193	TYR	Sidechain
8	1	25	TYR	Sidechain
8	1	70	TYR	Sidechain
8	1	87	TYR	Sidechain
9	2	123	TYR	Sidechain
9	2	124	TYR	Sidechain
9	2	19	ARG	Sidechain
9	2	69	TYR	Sidechain
9	2	72	ARG	Sidechain
9	2	75	ARG	Sidechain
10	3	197	ARG	Sidechain
11	4	146	HIS	Sidechain
11	4	148	TYR	Sidechain
11	4	149	ARG	Sidechain
11	4	176	PHE	Sidechain
11	4	36	ARG	Sidechain
12	5	144	TYR	Sidechain
12	5	167	ARG	Sidechain
12	5	187	TYR	Sidechain
12	5	88	TYR	Sidechain
13	6	108	HIS	Sidechain
13	6	137	ARG	Sidechain
13	6	160	TYR	Sidechain
13	6	174	TYR	Sidechain

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Mol	Chain	Res	Type	Group
13	6	2	PHE	Sidechain
13	6	5	TYR	Sidechain
13	6	68	PHE	Sidechain
13	6	75	TYR	Sidechain
14	7	101	TYR	Sidechain
14	7	103	ARG	Sidechain
14	7	128	ARG	Sidechain
14	7	129	TYR	Sidechain
14	7	16	TYR	Sidechain
14	7	193	ARG	Sidechain
14	7	195	PHE	Sidechain
14	7	76	TYR	Sidechain
14	7	91	TYR	Sidechain
14	7	93	PHE	Sidechain
34	8	128	TYR	Sidechain
34	8	205	TYR	Sidechain
34	8	218	PHE	Sidechain
34	8	229	PHE	Sidechain
34	8	273	ARG	Sidechain
34	8	321	ARG	Sidechain
34	8	372	ARG	Sidechain
34	8	385	GLU	Peptide
34	8	394	TYR	Sidechain
34	8	430	TYR	Sidechain
34	8	494	TYR	Sidechain
1	A	101	TYR	Sidechain
1	A	153	TYR	Sidechain
1	A	21	TYR	Sidechain
1	A	62	TYR	Sidechain
1	A	96	ARG	Sidechain
2	B	105	PRO	Peptide
2	B	134	LEU	Peptide
2	B	156	TYR	Sidechain
2	B	235	PHE	Sidechain
2	B	82	TYR	Sidechain
2	B	90	ARG	Sidechain
3	C	101	TYR	Sidechain
3	C	112	ARG	Sidechain
3	C	134	PHE	Sidechain
3	C	139	TYR	Sidechain
3	C	148	TYR	Sidechain
3	C	156	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	C	225	TYR	Sidechain
3	C	23	TYR	Sidechain
3	C	8	ARG	Sidechain
3	C	97	TYR	Sidechain
4	D	109	ARG	Sidechain
4	D	117	ARG	Sidechain
4	D	16	PHE	Sidechain
4	D	2	TYR	Sidechain
4	D	56	ARG	Sidechain
4	D	95	ARG	Sidechain
5	E	114	ARG	Sidechain
5	E	115	PHE	Sidechain
5	E	128	ARG	Peptide
5	E	14	PHE	Sidechain
5	E	145	TYR	Sidechain
5	E	157	TYR	Sidechain
5	E	158	ARG	Sidechain
5	E	159	TYR	Sidechain
5	E	7	PHE	Sidechain
5	E	94	TYR	Sidechain
5	E	95	TYR	Sidechain
6	F	125	ARG	Sidechain
6	F	170	TYR	Sidechain
6	F	173	ARG	Sidechain
6	F	38	ARG	Sidechain
6	F	58	TYR	Sidechain
6	F	86	TYR	Sidechain
6	F	88	ARG	Sidechain
7	G	134	PHE	Sidechain
7	G	186	ARG	Sidechain
7	G	87	ARG	Sidechain
7	G	89	ARG	Sidechain
15	H	145	TYR	Sidechain
15	H	178	ARG	Sidechain
15	H	367	ARG	Peptide
15	H	390	ARG	Sidechain
15	H	400	ARG	Sidechain
15	H	420	ARG	Sidechain
16	I	100	ARG	Peptide
16	I	128	TYR	Sidechain
16	I	179	GLU	Peptide
16	I	199	GLU	Peptide

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Mol	Chain	Res	Type	Group
16	I	223	GLY	Peptide
16	I	291	ARG	Sidechain
16	I	319	ARG	Sidechain
20	J	144	ASP	Peptide
20	J	154	THR	Peptide
20	J	231	ARG	Sidechain
20	J	368	TYR	Sidechain
20	J	71	TYR	Peptide
20	J	94	TYR	Sidechain
17	K	103	ILE	Peptide
17	K	118	TYR	Sidechain
17	K	121	ARG	Sidechain
17	K	212	TYR	Peptide
17	K	231	LYS	Peptide
17	K	255	ARG	Sidechain
17	K	262	ARG	Sidechain
17	K	329	LEU	Peptide
17	K	333	ARG	Peptide,Sidechain
17	K	346	ARG	Sidechain
17	K	426	PHE	Sidechain
17	K	67	TYR	Sidechain
18	L	191	ARG	Sidechain
18	L	207	PHE	Sidechain
18	L	290	ARG	Sidechain
18	L	342	ARG	Peptide,Sidechain
18	L	345	ARG	Sidechain
18	L	361	PHE	Sidechain
18	L	400	PHE	Sidechain
18	L	407	ARG	Sidechain
18	L	420	ARG	Sidechain
18	L	62	ARG	Sidechain
18	L	78	ARG	Sidechain
19	M	128	PHE	Sidechain
19	M	166	ARG	Sidechain
19	M	175	LYS	Peptide
19	M	229	THR	Peptide
19	M	279	PHE	Sidechain
19	M	281	ASP	Peptide
19	M	303	ARG	Sidechain
19	M	42	ARG	Sidechain
19	M	433	TYR	Sidechain
19	M	44	PHE	Sidechain

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Mol	Chain	Res	Type	Group
19	M	45	ARG	Sidechain
19	M	50	ARG	Sidechain
19	M	73	ARG	Sidechain
27	N	117	TYR	Sidechain
27	N	412	TYR	Sidechain
27	N	422	TYR	Sidechain
27	N	548	ARG	Sidechain
27	N	580	ASN	Peptide
27	N	599	TYR	Sidechain
27	N	75	TYR	Sidechain
27	N	786	ARG	Sidechain
27	N	866	TYR	Sidechain
27	N	908	ARG	Sidechain
33	O	115	ARG	Sidechain
33	O	210	ARG	Sidechain
33	O	248	TYR	Sidechain
33	O	283	HIS	Sidechain
33	O	310	PHE	Sidechain
33	O	48	PHE	Sidechain
33	O	62	TYR	Sidechain
29	P	109	SER	Peptide
29	P	21	PHE	Sidechain
29	P	221	TYR	Sidechain
29	P	234	TYR	Sidechain
29	P	273	TYR	Sidechain
29	P	274	GLY	Peptide
29	P	286	ASN	Peptide
29	P	390	TYR	Sidechain
29	P	79	LEU	Mainchain,Peptide
30	Q	146	TYR	Sidechain
30	Q	161	LEU	Peptide
30	Q	240	PHE	Sidechain
30	Q	246	TYR	Sidechain
30	Q	255	TYR	Sidechain
30	Q	50	ARG	Sidechain
31	R	123	ASP	Peptide
31	R	186	TYR	Sidechain
31	R	213	TYR	Sidechain
31	R	217	HIS	Sidechain
31	R	24	TYR	Sidechain
31	R	246	TYR	Sidechain
31	R	305	PHE	Sidechain

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Mol	Chain	Res	Type	Group
31	R	307	TYR	Sidechain
31	R	338	TYR	Sidechain
31	R	345	TYR	Sidechain
31	R	62	TYR	Sidechain
31	R	63	TYR	Sidechain
31	R	65	TYR	Sidechain
31	R	68	GLU	Peptide
31	R	70	TYR	Sidechain
31	R	99	TYR	Sidechain
28	S	111	ARG	Sidechain
28	S	170	TYR	Sidechain
28	S	173	LEU	Peptide
28	S	174	ARG	Sidechain
28	S	185	PHE	Sidechain
28	S	259	TYR	Sidechain
28	S	292	TYR	Sidechain
28	S	377	TYR	Sidechain
28	S	399	TYR	Sidechain
28	S	428	ARG	Sidechain
23	T	129	LEU	Peptide
23	T	197	TYR	Sidechain
23	T	199	PHE	Sidechain
23	T	233	VAL	Peptide
23	T	251	HIS	Peptide
23	T	266	TYR	Sidechain
23	T	91	SER	Mainchain,Peptide
23	T	96	LEU	Peptide
32	U	179	ARG	Sidechain
32	U	72	TYR	Sidechain
22	V	100	ARG	Sidechain
22	V	157	ARG	Sidechain
22	V	254	ARG	Sidechain
22	V	270	TYR	Sidechain
21	W	101	ARG	Sidechain
21	W	25	ARG	Sidechain
21	W	26	PHE	Sidechain
21	W	65	PHE	Sidechain
24	X	22	ARG	Sidechain
24	X	27	ILE	Peptide
24	X	48	PHE	Sidechain
24	X	85	ARG	Sidechain
26	Z	394	TYR	Sidechain

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Mol	Chain	Res	Type	Group
26	Z	408	TYR	Sidechain
26	Z	426	TYR	Sidechain
1	a	15	ARG	Sidechain
1	a	157	TYR	Sidechain
1	a	235	ARG	Sidechain
1	a	3	TYR	Sidechain
1	a	62	TYR	Sidechain
1	a	82	ARG	Sidechain
1	a	96	ARG	Sidechain
2	b	148	TYR	Sidechain
2	b	178	ARG	Sidechain
2	b	23	TYR	Sidechain
2	b	4	ARG	Sidechain
2	b	83	ARG	Sidechain
3	c	101	TYR	Sidechain
3	c	112	ARG	Sidechain
3	c	113	ARG	Sidechain
3	c	128	ARG	Sidechain
3	c	142	ARG	Sidechain
3	c	179	TYR	Sidechain
3	c	216	ARG	Sidechain
3	c	5	TYR	Sidechain
3	c	66	TYR	Sidechain
3	c	97	TYR	Sidechain
4	d	106	TYR	Sidechain
4	d	110	TYR	Sidechain
4	d	164	ARG	Sidechain
4	d	170	ARG	Sidechain
4	d	177	TYR	Sidechain
4	d	195	ARG	Sidechain
4	d	73	PHE	Sidechain
4	d	95	ARG	Sidechain
5	e	124	ARG	Sidechain
5	e	128	ARG	Peptide
5	e	2	ARG	Sidechain
5	e	95	TYR	Sidechain
6	f	100	ARG	Sidechain
6	f	125	ARG	Sidechain
6	f	146	PHE	Sidechain
6	f	156	TYR	Sidechain
6	f	163	ARG	Sidechain
6	f	50	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	f	58	TYR	Sidechain
7	g	108	PHE	Sidechain
7	g	156	TYR	Sidechain
7	g	16	ARG	Sidechain
7	g	197	TYR	Sidechain
7	g	69	HIS	Sidechain
8	h	185	ARG	Sidechain
8	h	189	TYR	Sidechain
8	h	36	ARG	Sidechain
8	h	45	ARG	Sidechain
8	h	70	TYR	Sidechain
8	h	8	PHE	Sidechain
8	h	82	PHE	Sidechain
8	h	87	TYR	Sidechain
9	i	111	PHE	Sidechain
9	i	123	TYR	Sidechain
9	i	124	TYR	Sidechain
9	i	141	HIS	Sidechain
9	i	186	TYR	Sidechain
9	i	75	ARG	Sidechain
9	i	8	PHE	Sidechain
9	i	97	TYR	Sidechain
10	j	103	PHE	Sidechain
10	j	146	PHE	Sidechain
10	j	27	ARG	Sidechain
10	j	73	TYR	Sidechain
10	j	79	ARG	Sidechain
10	j	99	PHE	Sidechain
11	k	107	TYR	Sidechain
11	k	121	TYR	Sidechain
11	k	59	TYR	Sidechain
11	k	67	TYR	Sidechain
11	k	70	ARG	Sidechain
11	k	73	TYR	Sidechain
11	k	93	ARG	Sidechain
12	l	114	TYR	Sidechain
12	l	121	ARG	Sidechain
12	l	135	PHE	Sidechain
12	l	144	TYR	Sidechain
12	l	170	TYR	Sidechain
12	l	188	HIS	Sidechain
12	l	40	PHE	Sidechain

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Mol	Chain	Res	Type	Group
12	l	54	PHE	Sidechain
12	l	6	PHE	Sidechain
12	l	7	ARG	Sidechain
12	l	73	ARG	Sidechain
12	l	88	TYR	Sidechain
13	m	106	TYR	Sidechain
13	m	133	ARG	Sidechain
13	m	174	TYR	Sidechain
13	m	194	ARG	Sidechain
13	m	213	ARG	Sidechain
13	m	221	ARG	Sidechain
13	m	39	TYR	Sidechain
13	m	75	TYR	Sidechain
13	m	98	TYR	Sidechain
14	n	103	ARG	Sidechain
14	n	126	PHE	Sidechain
14	n	146	PHE	Sidechain
14	n	182	ARG	Sidechain
14	n	185	TYR	Sidechain
14	n	190	ARG	Sidechain
14	n	228	TYR	Sidechain
14	n	35	ARG	Sidechain
14	n	41	ARG	Sidechain
14	n	91	TYR	Sidechain
14	n	95	TYR	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	239/252 (95%)	227 (95%)	11 (5%)	1 (0%)	34 72
1	a	239/252 (95%)	231 (97%)	8 (3%)	0	100 100
2	B	248/250 (99%)	236 (95%)	11 (4%)	1 (0%)	34 72
2	b	248/250 (99%)	234 (94%)	11 (4%)	3 (1%)	13 50
3	C	242/258 (94%)	228 (94%)	11 (4%)	3 (1%)	13 50
3	c	242/258 (94%)	227 (94%)	12 (5%)	3 (1%)	13 50
4	D	238/254 (94%)	222 (93%)	12 (5%)	4 (2%)	9 42
4	d	238/254 (94%)	219 (92%)	16 (7%)	3 (1%)	12 48
5	E	240/260 (92%)	227 (95%)	11 (5%)	2 (1%)	19 60
5	e	240/260 (92%)	228 (95%)	10 (4%)	2 (1%)	19 60
6	F	231/234 (99%)	220 (95%)	9 (4%)	2 (1%)	17 57
6	f	229/234 (98%)	221 (96%)	8 (4%)	0	100 100
7	G	241/288 (84%)	228 (95%)	12 (5%)	1 (0%)	34 72
7	g	241/288 (84%)	230 (95%)	10 (4%)	1 (0%)	34 72
8	1	194/215 (90%)	184 (95%)	8 (4%)	2 (1%)	15 55
8	h	194/215 (90%)	189 (97%)	5 (3%)	0	100 100
9	2	224/261 (86%)	213 (95%)	9 (4%)	2 (1%)	17 57
9	i	224/261 (86%)	214 (96%)	10 (4%)	0	100 100
10	3	202/205 (98%)	190 (94%)	10 (5%)	2 (1%)	15 55
10	j	202/205 (98%)	187 (93%)	12 (6%)	3 (2%)	10 46
11	4	193/198 (98%)	187 (97%)	6 (3%)	0	100 100
11	k	193/198 (98%)	188 (97%)	4 (2%)	1 (0%)	29 69
12	5	210/287 (73%)	201 (96%)	9 (4%)	0	100 100
12	l	210/287 (73%)	202 (96%)	7 (3%)	1 (0%)	29 69
13	6	220/241 (91%)	205 (93%)	13 (6%)	2 (1%)	17 57
13	m	220/241 (91%)	203 (92%)	17 (8%)	0	100 100
14	7	227/266 (85%)	209 (92%)	16 (7%)	2 (1%)	17 57
14	n	230/266 (86%)	214 (93%)	14 (6%)	2 (1%)	17 57
15	H	376/467 (80%)	340 (90%)	23 (6%)	13 (4%)	3 25
16	I	383/437 (88%)	346 (90%)	27 (7%)	10 (3%)	5 31
17	K	387/428 (90%)	351 (91%)	24 (6%)	12 (3%)	4 27
18	L	386/437 (88%)	353 (92%)	26 (7%)	7 (2%)	8 40

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
19	M	377/434 (87%)	350 (93%)	19 (5%)	8 (2%)	7 36
20	J	391/405 (96%)	360 (92%)	21 (5%)	10 (3%)	5 31
21	W	195/268 (73%)	180 (92%)	11 (6%)	4 (2%)	7 36
22	V	287/306 (94%)	263 (92%)	20 (7%)	4 (1%)	11 46
23	T	264/274 (96%)	240 (91%)	19 (7%)	5 (2%)	8 38
24	X	125/156 (80%)	101 (81%)	15 (12%)	9 (7%)	1 14
25	Y	47/89 (53%)	44 (94%)	1 (2%)	2 (4%)	2 22
26	Z	902/993 (91%)	824 (91%)	52 (6%)	26 (3%)	4 29
27	N	886/945 (94%)	850 (96%)	25 (3%)	11 (1%)	13 50
28	S	473/523 (90%)	435 (92%)	18 (4%)	20 (4%)	3 22
29	P	438/445 (98%)	417 (95%)	13 (3%)	8 (2%)	8 40
30	Q	432/434 (100%)	387 (90%)	28 (6%)	17 (4%)	3 23
31	R	377/429 (88%)	355 (94%)	18 (5%)	4 (1%)	14 52
32	U	296/338 (88%)	284 (96%)	9 (3%)	3 (1%)	15 55
33	O	386/393 (98%)	368 (95%)	16 (4%)	2 (0%)	29 69
34	8	393/499 (79%)	366 (93%)	21 (5%)	6 (2%)	10 46
All	All	14100/15638 (90%)	13178 (94%)	698 (5%)	224 (2%)	13 44

All (224) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
5	e	129	PRO
10	j	182	TRP
5	E	128	ARG
5	E	129	PRO
6	F	162	ALA
15	H	77	ALA
16	I	79	SER
16	I	115	ASP
16	I	224	ALA
16	I	330	LYS
17	K	244	HIS
17	K	334	LEU
18	L	174	GLU
19	M	229	THR
19	M	230	LEU

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Mol	Chain	Res	Type
19	M	296	SER
19	M	345	ARG
20	J	72	VAL
20	J	145	SER
23	T	92	ASN
23	T	234	TYR
25	Y	31	GLU
26	Z	19	SER
26	Z	83	THR
26	Z	939	ALA
27	N	856	PHE
27	N	857	TYR
27	N	862	SER
28	S	44	THR
28	S	47	THR
28	S	102	SER
28	S	150	LYS
28	S	174	ARG
29	P	110	LEU
29	P	397	ALA
30	Q	68	MET
30	Q	170	ASP
30	Q	354	PHE
30	Q	387	TYR
31	R	245	SER
31	R	280	ILE
33	O	199	LEU
2	b	20	GLN
2	b	200	VAL
4	d	52	LEU
4	D	203	THR
15	H	78	PRO
15	H	94	GLU
15	H	280	VAL
15	H	344	ASP
15	H	434	ARG
15	H	456	LYS
17	K	127	ASP
17	K	232	ALA
17	K	274	VAL
17	K	314	VAL
17	K	398	ASN

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Mol	Chain	Res	Type
18	L	101	ILE
18	L	188	GLU
20	J	117	SER
20	J	353	CYS
22	V	143	PRO
23	T	97	SER
23	T	138	ASP
24	X	29	VAL
24	X	38	ASN
24	X	44	GLY
24	X	59	ARG
24	X	110	PRO
26	Z	8	LYS
26	Z	237	VAL
26	Z	825	ALA
26	Z	887	GLY
27	N	666	GLN
27	N	895	LYS
28	S	132	ALA
29	P	130	ILE
29	P	327	LEU
29	P	328	ALA
30	Q	40	ALA
30	Q	44	ALA
30	Q	286	TYR
30	Q	309	ARG
34	8	383	SER
2	b	19	GLY
10	j	156	ASN
10	j	191	LYS
14	n	81	ALA
1	A	187	GLU
4	D	29	THR
4	D	102	VAL
6	F	4	ASN
8	1	107	LYS
9	2	171	SER
13	6	130	SER
13	6	200	ASP
16	I	136	VAL
17	K	248	GLY
17	K	344	ARG

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Mol	Chain	Res	Type
17	K	419	ASN
18	L	291	PHE
18	L	343	LEU
20	J	207	ASP
21	W	179	ARG
22	V	61	TYR
22	V	215	ASN
22	V	259	LYS
24	X	42	GLU
24	X	114	LEU
26	Z	82	MET
26	Z	84	ALA
26	Z	174	GLU
26	Z	309	GLN
26	Z	463	HIS
26	Z	728	LYS
26	Z	913	ILE
27	N	739	PHE
28	S	69	LEU
28	S	83	PRO
28	S	97	THR
28	S	117	SER
28	S	153	GLU
29	P	79	LEU
30	Q	45	SER
30	Q	51	ARG
30	Q	75	ARG
30	Q	355	GLU
31	R	102	LEU
32	U	30	ASN
34	8	205	TYR
34	8	385	GLU
3	c	53	SER
3	c	205	LEU
3	c	206	THR
4	d	203	THR
5	e	27	SER
12	l	95	LEU
2	B	225	THR
3	C	6	ASP
3	C	183	MET
4	D	10	SER

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Mol	Chain	Res	Type
7	G	69	HIS
15	H	415	THR
16	I	175	LYS
16	I	339	ILE
16	I	411	VAL
17	K	104	ASP
17	K	421	VAL
18	L	221	TYR
19	M	151	ASP
20	J	152	GLY
20	J	155	LYS
20	J	309	ARG
21	W	3	LEU
21	W	136	ASN
21	W	144	PHE
23	T	96	LEU
24	X	22	ARG
25	Y	69	VAL
26	Z	70	ALA
26	Z	76	LYS
26	Z	142	ASP
26	Z	429	ASN
26	Z	444	GLU
26	Z	926	ASN
26	Z	963	ALA
27	N	395	ALA
27	N	790	GLU
28	S	101	LYS
28	S	126	LYS
28	S	263	ASP
30	Q	18	LYS
30	Q	46	VAL
30	Q	384	LYS
31	R	58	GLU
34	8	206	LYS
34	8	316	ARG
34	8	386	ASN
7	g	221	ASN
11	k	178	GLY
14	n	10	SER
3	C	220	ASN
9	2	193	PRO

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Mol	Chain	Res	Type
10	3	156	ASN
14	7	77	ASP
14	7	83	ALA
15	H	190	ARG
15	H	203	LYS
15	H	314	VAL
16	I	340	ARG
19	M	124	ARG
19	M	186	LEU
20	J	335	MET
24	X	28	PRO
26	Z	789	GLN
26	Z	940	GLY
27	N	631	GLY
28	S	65	ASN
28	S	118	PHE
28	S	152	LEU
28	S	198	SER
29	P	3	ARG
29	P	92	SER
30	Q	110	SER
30	Q	253	ASN
32	U	146	ASP
33	O	243	VAL
8	1	172	VAL
15	H	152	ILE
18	L	179	THR
19	M	172	VAL
26	Z	366	LYS
27	N	176	GLN
32	U	5	HIS
4	d	36	GLY
10	3	183	GLY
16	I	176	SER
20	J	308	GLY
15	H	412	PRO
26	Z	233	LEU
26	Z	85	VAL
27	N	432	GLY
28	S	301	PRO
28	S	96	ILE

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/210 (98%)	199 (97%)	7 (3%)	37	60
1	a	206/210 (98%)	192 (93%)	14 (7%)	16	41
2	B	209/209 (100%)	205 (98%)	4 (2%)	57	75
2	b	209/209 (100%)	199 (95%)	10 (5%)	25	51
3	C	203/216 (94%)	195 (96%)	8 (4%)	32	56
3	c	203/216 (94%)	192 (95%)	11 (5%)	22	47
4	D	212/226 (94%)	204 (96%)	8 (4%)	33	57
4	d	212/226 (94%)	205 (97%)	7 (3%)	38	61
5	E	198/215 (92%)	191 (96%)	7 (4%)	36	59
5	e	198/215 (92%)	188 (95%)	10 (5%)	24	48
6	F	192/193 (100%)	187 (97%)	5 (3%)	46	66
6	f	190/193 (98%)	183 (96%)	7 (4%)	34	58
7	G	201/239 (84%)	195 (97%)	6 (3%)	41	63
7	g	201/239 (84%)	199 (99%)	2 (1%)	76	86
8	1	162/178 (91%)	161 (99%)	1 (1%)	86	92
8	h	162/178 (91%)	160 (99%)	2 (1%)	71	83
9	2	185/214 (86%)	185 (100%)	0	100	100
9	i	185/214 (86%)	181 (98%)	4 (2%)	52	71
10	3	172/173 (99%)	167 (97%)	5 (3%)	42	64
10	j	172/173 (99%)	168 (98%)	4 (2%)	50	70
11	4	173/175 (99%)	167 (96%)	6 (4%)	36	59
11	k	173/175 (99%)	168 (97%)	5 (3%)	42	64
12	5	169/235 (72%)	161 (95%)	8 (5%)	26	51
12	l	169/235 (72%)	164 (97%)	5 (3%)	41	63
13	6	185/201 (92%)	179 (97%)	6 (3%)	39	61
13	m	185/201 (92%)	181 (98%)	4 (2%)	52	71

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
14	7	195/224 (87%)	186 (95%)	9 (5%)	27	52
14	n	198/224 (88%)	191 (96%)	7 (4%)	36	59
15	H	320/399 (80%)	307 (96%)	13 (4%)	30	55
16	I	342/385 (89%)	326 (95%)	16 (5%)	26	51
17	K	342/374 (91%)	336 (98%)	6 (2%)	59	77
18	L	332/377 (88%)	321 (97%)	11 (3%)	38	61
19	M	329/375 (88%)	322 (98%)	7 (2%)	53	72
20	J	342/352 (97%)	328 (96%)	14 (4%)	30	55
21	W	171/230 (74%)	170 (99%)	1 (1%)	86	92
22	V	253/268 (94%)	251 (99%)	2 (1%)	81	89
23	T	249/256 (97%)	244 (98%)	5 (2%)	55	74
24	X	116/144 (81%)	110 (95%)	6 (5%)	23	48
25	Y	50/81 (62%)	49 (98%)	1 (2%)	55	74
26	Z	773/850 (91%)	766 (99%)	7 (1%)	78	87
27	N	745/797 (94%)	740 (99%)	5 (1%)	84	90
28	S	447/489 (91%)	439 (98%)	8 (2%)	59	77
29	P	412/415 (99%)	408 (99%)	4 (1%)	76	86
30	Q	391/391 (100%)	385 (98%)	6 (2%)	65	80
31	R	333/379 (88%)	327 (98%)	6 (2%)	59	77
32	U	271/308 (88%)	270 (100%)	1 (0%)	91	94
33	O	363/368 (99%)	360 (99%)	3 (1%)	81	89
34	8	359/449 (80%)	353 (98%)	6 (2%)	60	78
All	All	12265/13503 (91%)	11965 (98%)	300 (2%)	51	69

All (300) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	10	PHE
1	a	16	LEU
1	a	82	ARG
1	a	96	ARG
1	a	114	ASN
1	a	117	GLN
1	a	135	VAL

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Mol	Chain	Res	Type
1	a	150	PRO
1	a	160	THR
1	a	162	THR
1	a	176	HIS
1	a	200	HIS
1	a	231	ASN
1	a	235	ARG
2	b	12	PHE
2	b	23	TYR
2	b	33	THR
2	b	35	LEU
2	b	38	LYS
2	b	80	PRO
2	b	98	LYS
2	b	181	ASP
2	b	204	PHE
2	b	233	PRO
3	c	5	TYR
3	c	12	PHE
3	c	18	LEU
3	c	48	GLU
3	c	63	GLU
3	c	65	LEU
3	c	113	ARG
3	c	141	ASP
3	c	157	THR
3	c	172	GLN
3	c	210	LEU
4	d	4	ARG
4	d	53	GLN
4	d	63	SER
4	d	76	LEU
4	d	92	GLN
4	d	116	GLN
4	d	200	VAL
5	e	17	GLU
5	e	70	MET
5	e	80	MET
5	e	94	TYR
5	e	115	PHE
5	e	128	ARG
5	e	187	GLU

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Mol	Chain	Res	Type
5	e	201	GLU
5	e	206	GLU
5	e	215	THR
6	f	66	ASP
6	f	71	LEU
6	f	73	LEU
6	f	116	GLN
6	f	178	PHE
6	f	188	LEU
6	f	204	SER
7	g	39	ASN
7	g	214	TRP
8	h	31	THR
8	h	118	SER
9	i	204	LYS
9	i	207	ARG
9	i	215	GLU
9	i	218	VAL
10	j	77	GLU
10	j	88	GLN
10	j	146	PHE
10	j	158	GLU
11	k	7	ILE
11	k	37	GLN
11	k	40	PRO
11	k	118	GLN
11	k	193	ASP
12	l	4	LEU
12	l	8	PHE
12	l	34	VAL
12	l	90	TYR
12	l	104	TYR
13	m	18	GLU
13	m	19	ASP
13	m	213	ARG
13	m	222	ASP
14	n	9	THR
14	n	30	TYR
14	n	102	GLN
14	n	132	LEU
14	n	187	ARG
14	n	208	PHE

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Mol	Chain	Res	Type
14	n	221	PHE
1	A	19	VAL
1	A	41	CYS
1	A	117	GLN
1	A	139	GLU
1	A	143	PRO
1	A	221	LYS
1	A	223	LYS
2	B	35	LEU
2	B	84	VAL
2	B	119	GLN
2	B	179	TRP
3	C	3	ARG
3	C	4	ARG
3	C	33	THR
3	C	63	GLU
3	C	82	ASP
3	C	88	ASN
3	C	194	LYS
3	C	231	PRO
4	D	50	LEU
4	D	79	ASP
4	D	103	THR
4	D	107	LEU
4	D	116	GLN
4	D	147	GLN
4	D	161	THR
4	D	229	GLN
5	E	1	ASP
5	E	63	ASP
5	E	70	MET
5	E	110	ASP
5	E	125	LEU
5	E	201	GLU
5	E	224	ASP
6	F	1	PHE
6	F	4	ASN
6	F	71	LEU
6	F	122	TYR
6	F	152	VAL
7	G	11	PHE
7	G	127	PRO

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Mol	Chain	Res	Type
7	G	175	LEU
7	G	208	PHE
7	G	214	TRP
7	G	220	THR
8	1	74	SER
10	3	12	VAL
10	3	25	ASP
10	3	85	THR
10	3	135	PHE
10	3	146	PHE
11	4	29	LYS
11	4	68	SER
11	4	110	LYS
11	4	126	VAL
11	4	186	LYS
11	4	191	GLN
12	5	4	LEU
12	5	72	GLU
12	5	100	MET
12	5	104	TYR
12	5	106	ARG
12	5	137	TYR
12	5	152	ASP
12	5	181	THR
13	6	76	HIS
13	6	92	ASN
13	6	107	VAL
13	6	207	VAL
13	6	209	LYS
13	6	222	ASP
14	7	25	ASP
14	7	35	ARG
14	7	47	ASP
14	7	49	THR
14	7	104	ARG
14	7	140	PRO
14	7	187	ARG
14	7	188	ASP
14	7	221	PHE
15	H	94	GLU
15	H	162	ARG
15	H	172	MET

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Mol	Chain	Res	Type
15	H	178	ARG
15	H	191	ILE
15	H	208	TYR
15	H	267	THR
15	H	300	THR
15	H	307	PHE
15	H	320	ASP
15	H	341	ASP
15	H	367	ARG
15	H	419	LEU
16	I	69	LEU
16	I	80	GLU
16	I	85	PHE
16	I	86	GLU
16	I	105	SER
16	I	123	PRO
16	I	155	SER
16	I	216	PRO
16	I	261	PRO
16	I	280	PHE
16	I	310	LEU
16	I	324	VAL
16	I	339	ILE
16	I	341	PRO
16	I	416	PHE
16	I	433	GLU
17	K	121	ARG
17	K	281	ARG
17	K	324	LEU
17	K	325	ASP
17	K	330	ARG
17	K	360	MET
18	L	148	LEU
18	L	174	GLU
18	L	177	GLU
18	L	192	GLU
18	L	216	LYS
18	L	228	LYS
18	L	243	PHE
18	L	279	PHE
18	L	309	LEU
18	L	361	PHE

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Mol	Chain	Res	Type
18	L	406	ASP
19	M	83	VAL
19	M	315	PHE
19	M	318	ASP
19	M	340	SER
19	M	343	LEU
19	M	373	ASP
19	M	403	LEU
20	J	37	LYS
20	J	84	VAL
20	J	131	ASP
20	J	144	ASP
20	J	153	LEU
20	J	218	LEU
20	J	230	VAL
20	J	240	HIS
20	J	243	SER
20	J	257	ARG
20	J	296	ARG
20	J	343	LEU
20	J	354	SER
20	J	403	LEU
21	W	194	GLU
22	V	50	MET
22	V	156	PHE
23	T	109	TYR
23	T	197	TYR
23	T	198	ASP
23	T	213	ASN
23	T	257	THR
24	X	11	ARG
24	X	17	TYR
24	X	47	ASP
24	X	81	SER
24	X	111	LEU
24	X	115	SER
25	Y	32	ASP
26	Z	1	MET
26	Z	133	ASP
26	Z	185	ASP
26	Z	354	PRO
26	Z	367	SER

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Mol	Chain	Res	Type
26	Z	406	TRP
26	Z	577	GLN
27	N	509	GLN
27	N	603	PRO
27	N	739	PHE
27	N	770	LYS
27	N	873	ARG
28	S	46	LEU
28	S	72	GLU
28	S	82	TYR
28	S	101	LYS
28	S	119	TYR
28	S	157	GLU
28	S	207	ASN
28	S	405	ARG
29	P	38	GLN
29	P	277	GLN
29	P	285	GLN
29	P	362	LEU
30	Q	2	SER
30	Q	29	SER
30	Q	50	ARG
30	Q	94	VAL
30	Q	111	LEU
30	Q	207	SER
31	R	70	TYR
31	R	99	TYR
31	R	109	LYS
31	R	122	GLU
31	R	137	LEU
31	R	199	GLU
32	U	115	GLN
33	O	51	ASP
33	O	163	ILE
33	O	387	ARG
34	8	128	TYR
34	8	201	GLN
34	8	321	ARG
34	8	335	PHE
34	8	343	ASP
34	8	415	HIS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102)

such sidechains are listed below:

Mol	Chain	Res	Type
1	a	6	HIS
2	b	30	GLN
2	b	190	HIS
2	b	218	ASN
3	c	172	GLN
4	d	147	GLN
4	d	202	GLN
5	e	65	HIS
6	f	30	GLN
6	f	68	HIS
6	f	116	GLN
7	g	83	HIS
7	g	119	HIS
7	g	143	HIS
7	g	203	ASN
8	h	38	HIS
8	h	157	HIS
9	i	114	HIS
9	i	144	GLN
10	j	71	ASN
10	j	172	ASN
11	k	101	ASN
12	l	166	HIS
12	l	179	HIS
12	l	188	HIS
13	m	76	HIS
13	m	79	HIS
13	m	153	GLN
14	n	74	ASN
14	n	194	ASN
14	n	213	GLN
1	A	18	GLN
2	B	94	HIS
2	B	190	HIS
4	D	116	GLN
4	D	120	GLN
5	E	91	HIS
5	E	210	GLN
6	F	4	ASN
7	G	200	HIS
7	G	244	ASN
9	2	30	ASN

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Mol	Chain	Res	Type
9	2	66	HIS
10	3	37	ASN
10	3	71	ASN
11	4	133	HIS
11	4	146	HIS
11	4	147	HIS
13	6	108	HIS
13	6	152	ASN
13	6	159	GLN
13	6	197	GLN
14	7	194	ASN
14	7	213	GLN
15	H	98	GLN
16	I	95	GLN
16	I	117	HIS
17	K	72	GLN
17	K	140	HIS
17	K	142	HIS
17	K	144	ASN
17	K	164	ASN
17	K	228	ASN
18	L	50	GLN
19	M	81	ASN
19	M	189	GLN
19	M	253	GLN
19	M	405	ASN
20	J	28	GLN
20	J	277	ASN
20	J	278	GLN
21	W	106	GLN
22	V	111	HIS
22	V	204	HIS
24	X	18	ASN
26	Z	132	HIS
27	N	182	ASN
27	N	506	GLN
27	N	679	ASN
27	N	703	GLN
27	N	859	ASN
28	S	65	ASN
28	S	191	HIS
28	S	225	HIS

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Mol	Chain	Res	Type
29	P	289	ASN
29	P	334	ASN
30	Q	37	GLN
31	R	132	GLN
31	R	397	ASN
31	R	401	HIS
32	U	5	HIS
32	U	84	ASN
32	U	216	ASN
32	U	234	ASN
32	U	262	GLN
33	O	186	ASN
34	8	144	GLN
34	8	148	ASN
34	8	264	HIS
34	8	415	HIS
34	8	447	HIS
34	8	465	ASN

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	$\#\|Z\| > 2$
35	ATP	J	501	36	26,33,33	1.26	3 (11%)	31,52,52	1.88	4 (12%)
35	ATP	M	501	36	26,33,33	1.24	2 (7%)	31,52,52	1.82	6 (19%)
37	ADP	K	501	36	24,29,29	1.28	3 (12%)	29,45,45	2.34	7 (24%)
35	ATP	I	501	36	26,33,33	1.60	4 (15%)	31,52,52	2.37	7 (22%)
37	ADP	L	501	36	24,29,29	1.39	2 (8%)	29,45,45	1.74	5 (17%)
35	ATP	H	501	36	26,33,33	1.52	6 (23%)	31,52,52	1.83	5 (16%)

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

All (20) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	M	501	ATP	C8-N7	-4.25	1.27	1.34
35	I	501	ATP	C8-N7	-3.56	1.28	1.34
35	I	501	ATP	O4'-C1'	3.44	1.45	1.41
37	L	501	ADP	C8-N7	-3.12	1.29	1.34
35	J	501	ATP	C8-N7	-3.08	1.29	1.34
35	I	501	ATP	O4'-C4'	3.02	1.51	1.45
37	L	501	ADP	O4'-C4'	-2.98	1.38	1.45
35	H	501	ATP	C4-N3	-2.71	1.31	1.35
35	H	501	ATP	C2'-C1'	-2.70	1.49	1.53
35	H	501	ATP	C8-N7	-2.64	1.30	1.34
37	K	501	ADP	C8-N7	-2.61	1.30	1.34
35	H	501	ATP	O4'-C1'	2.60	1.44	1.41
37	K	501	ADP	C2-N3	2.57	1.36	1.32
35	J	501	ATP	O4'-C1'	2.51	1.44	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	I	501	ATP	C2-N3	2.49	1.36	1.32
37	K	501	ADP	C3'-C4'	2.33	1.58	1.53
35	J	501	ATP	C2-N3	2.29	1.35	1.32
35	H	501	ATP	C2'-C3'	2.23	1.59	1.53
35	H	501	ATP	C2-N3	2.10	1.35	1.32
35	M	501	ATP	C2-N3	2.03	1.35	1.32

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	K	501	ADP	PA-O3A-PB	9.57	165.66	132.83
35	I	501	ATP	PB-O3B-PG	7.73	159.35	132.83
35	H	501	ATP	PB-O3B-PG	6.70	155.82	132.83
35	J	501	ATP	PB-O3B-PG	6.66	155.66	132.83
35	I	501	ATP	PA-O3A-PB	6.64	155.61	132.83
35	M	501	ATP	PB-O3B-PG	5.54	151.84	132.83
37	L	501	ADP	PA-O3A-PB	4.75	149.12	132.83
35	J	501	ATP	PA-O3A-PB	4.49	148.25	132.83
35	I	501	ATP	C1'-N9-C4	4.12	133.89	126.64
35	H	501	ATP	PA-O3A-PB	4.10	146.89	132.83
35	M	501	ATP	N6-C6-N1	3.91	126.69	118.57
35	J	501	ATP	N6-C6-N1	3.91	126.69	118.57
37	L	501	ADP	N3-C2-N1	3.64	134.36	128.68
37	K	501	ADP	N3-C2-N1	3.48	134.11	128.68
35	M	501	ATP	PA-O3A-PB	3.37	144.40	132.83
37	K	501	ADP	O3B-PB-O2B	3.28	120.15	107.64
35	M	501	ATP	C5-C6-N1	-3.14	113.24	120.35
37	K	501	ADP	C5-C6-N1	-2.88	113.82	120.35
35	H	501	ATP	C5-C6-N1	-2.87	113.84	120.35
37	K	501	ADP	N6-C6-N1	2.75	124.29	118.57
35	I	501	ATP	O2A-PA-O1A	2.59	125.06	112.24
37	K	501	ADP	C1'-N9-C4	2.57	131.16	126.64
37	L	501	ADP	C1'-N9-C4	-2.47	122.30	126.64
37	L	501	ADP	O5'-C5'-C4'	2.41	117.29	108.99
35	H	501	ATP	N6-C6-N1	2.36	123.46	118.57
35	I	501	ATP	O4'-C1'-C2'	-2.34	103.51	106.93
35	H	501	ATP	C4-C5-N7	2.33	111.83	109.40
37	L	501	ADP	C2-N1-C6	-2.30	114.82	118.75
35	J	501	ATP	C5-C6-N6	-2.26	116.92	120.35
35	M	501	ATP	C4-C5-N7	2.22	111.71	109.40
37	K	501	ADP	C2'-C3'-C4'	2.20	106.91	102.64
35	I	501	ATP	O5'-C5'-C4'	2.14	116.36	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	M	501	ATP	O3'-C3'-C2'	2.12	118.67	111.82
35	I	501	ATP	O2B-PB-O1B	2.01	122.18	112.24

There are no chirality outliers.

All (26) torsion outliers are listed below:

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

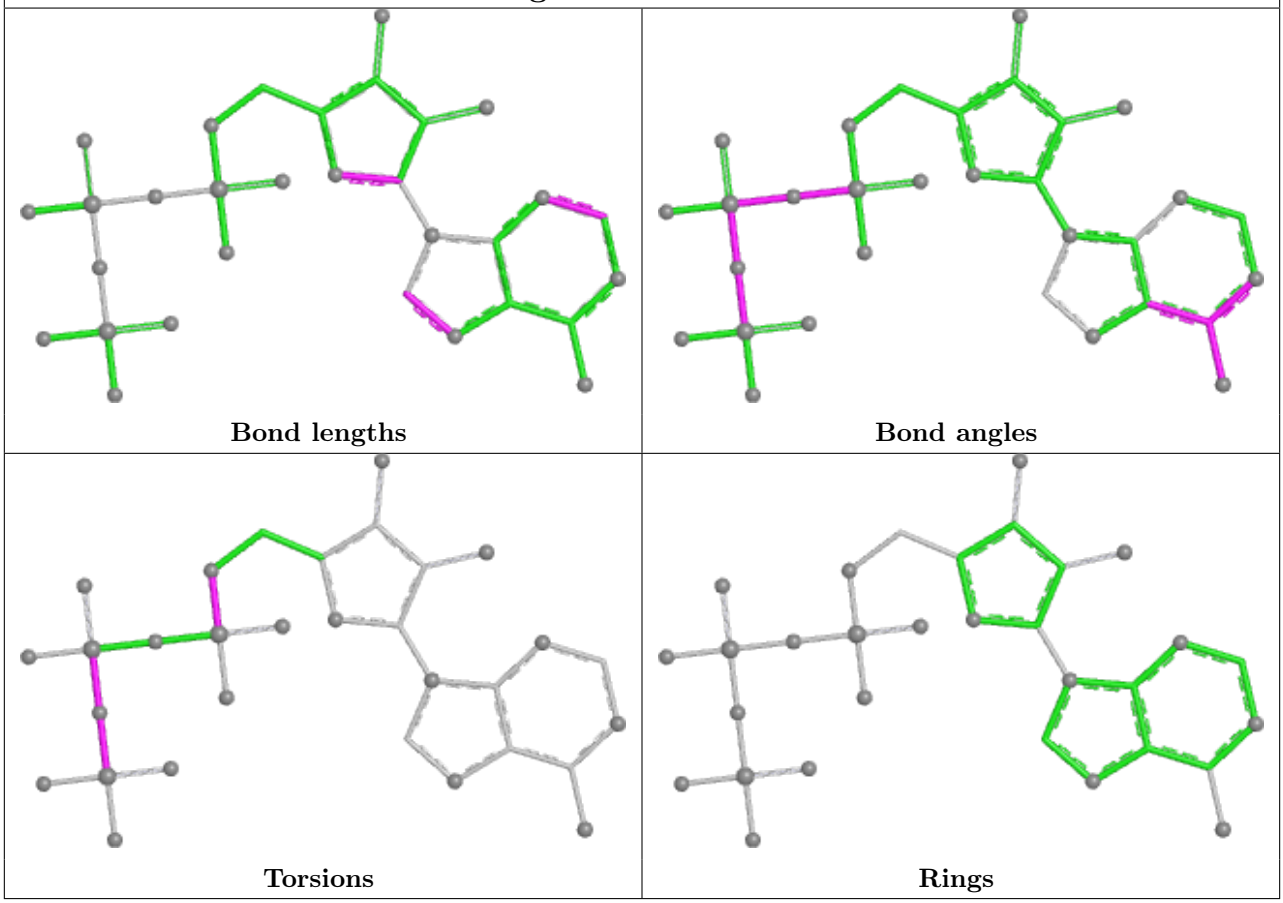
There are no ring outliers.

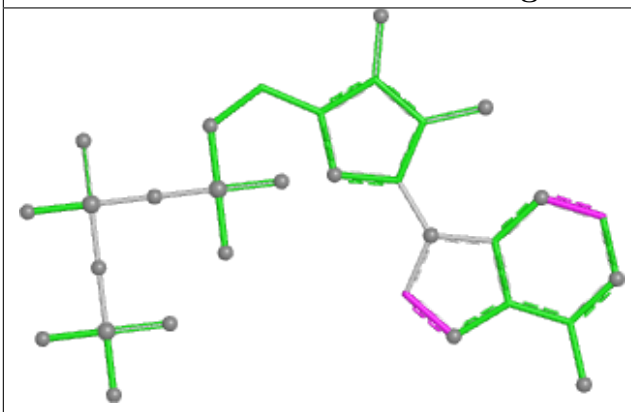
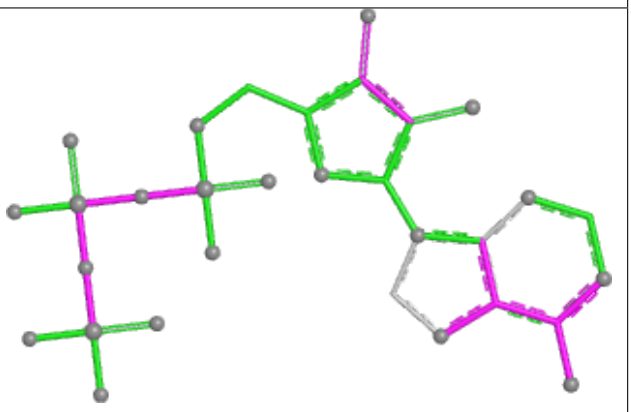
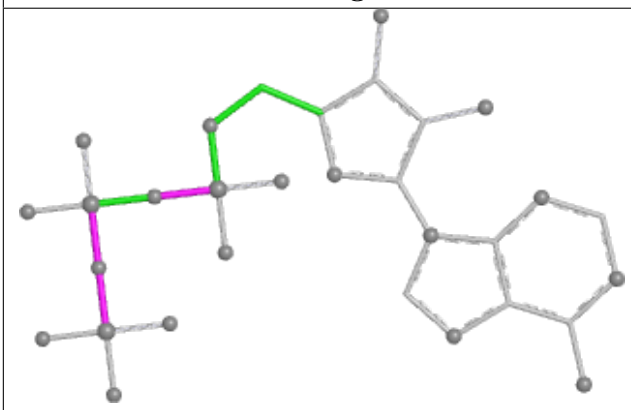
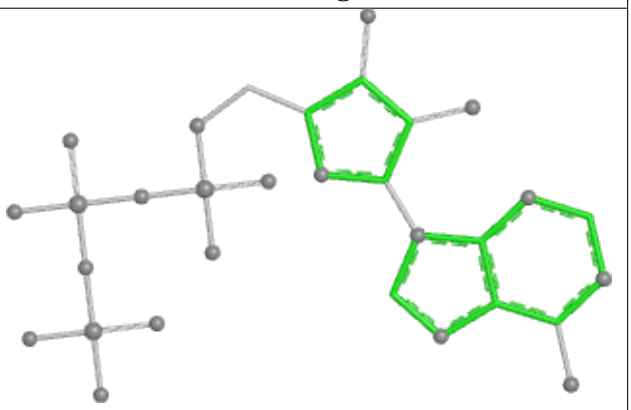
No monomer is involved in short contacts.

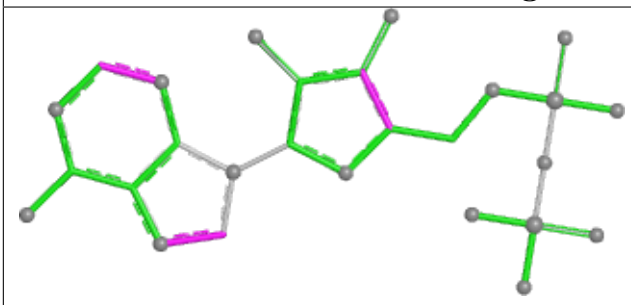
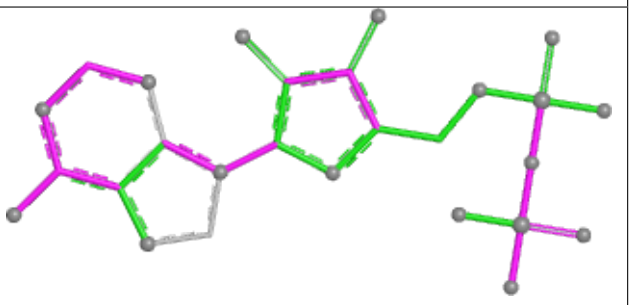
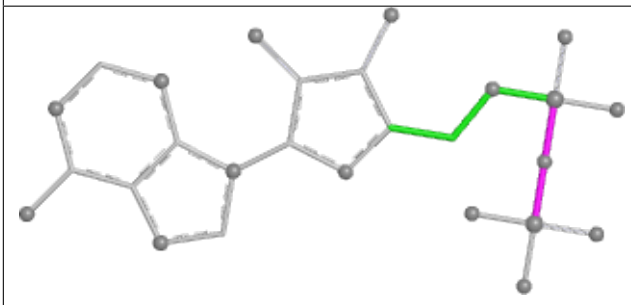
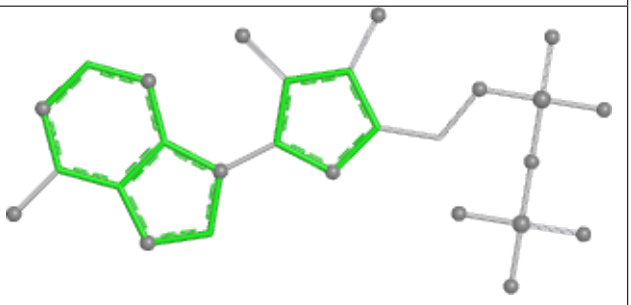
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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.

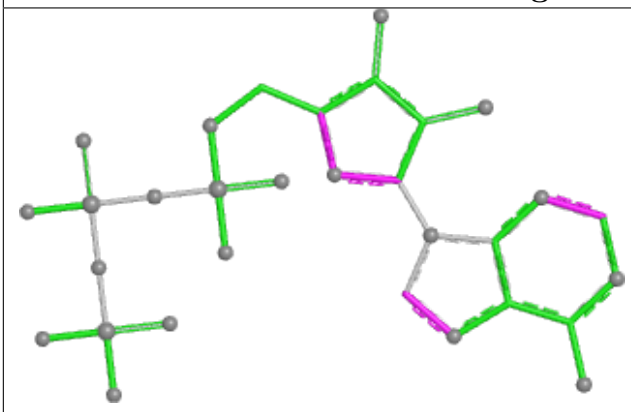
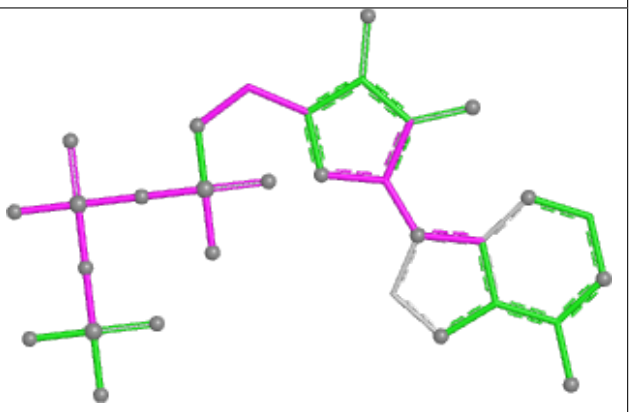
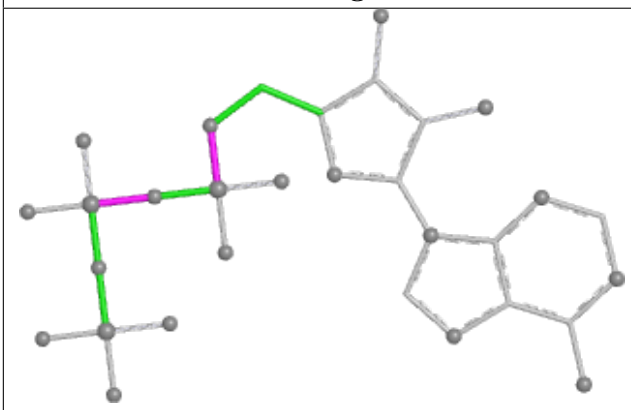
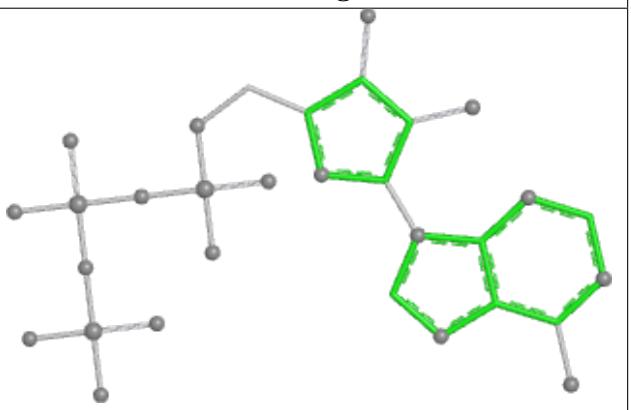
Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD 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.

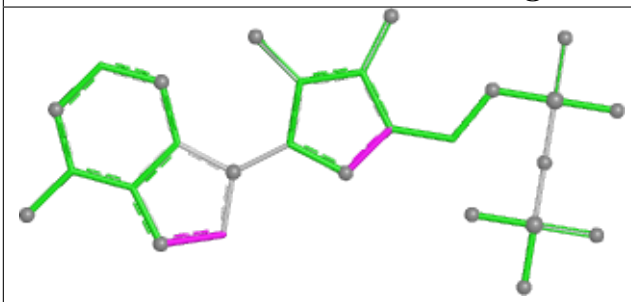
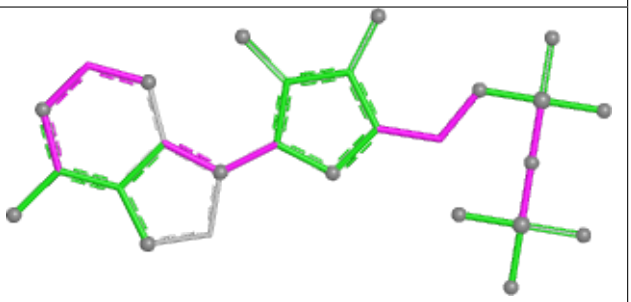
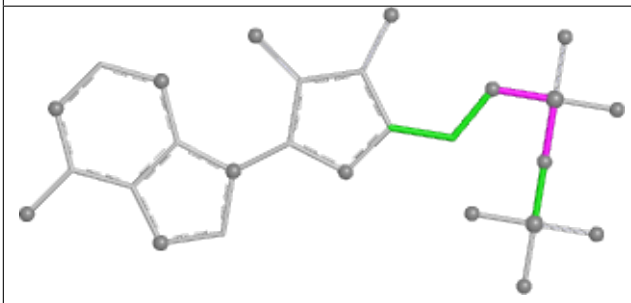
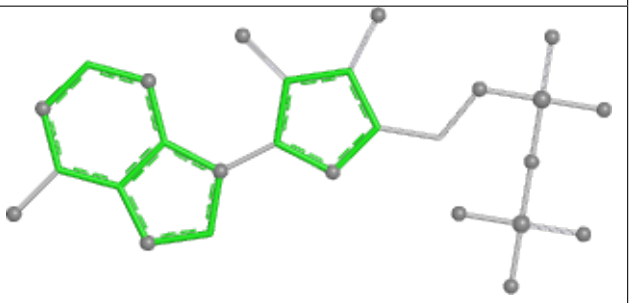
Ligand ATP J 501

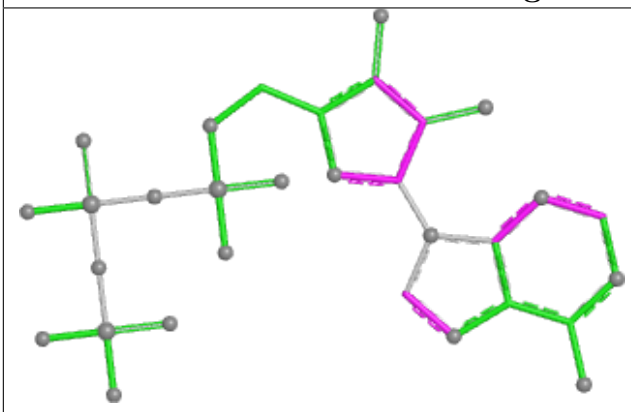
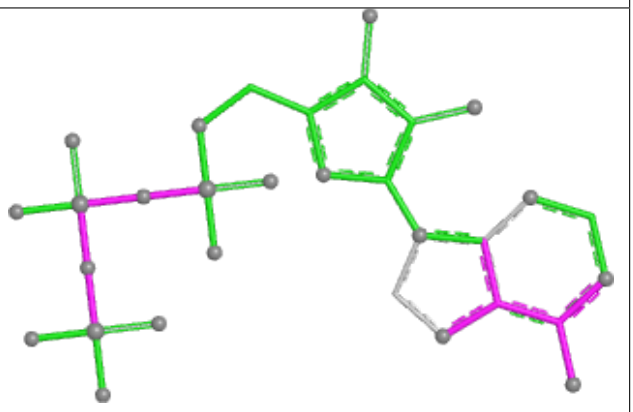
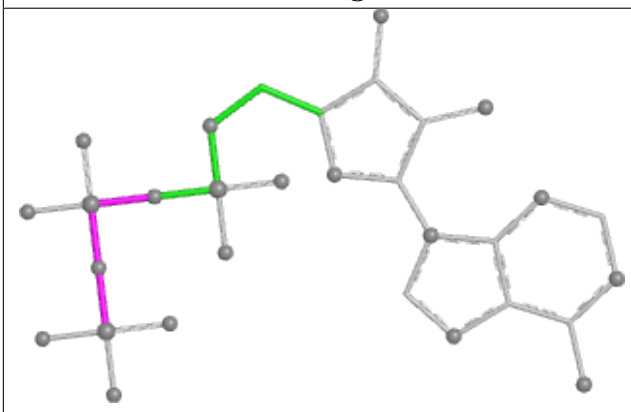
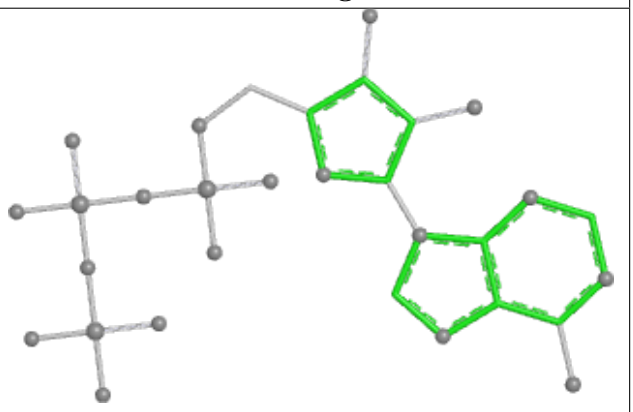


Ligand ATP M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP K 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP I 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP L 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP H 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

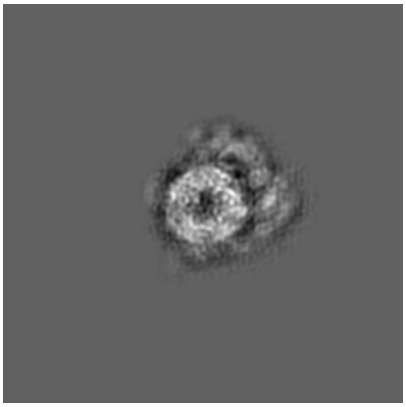
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3537. These allow visual inspection of the internal detail of the map and identification of artifacts.

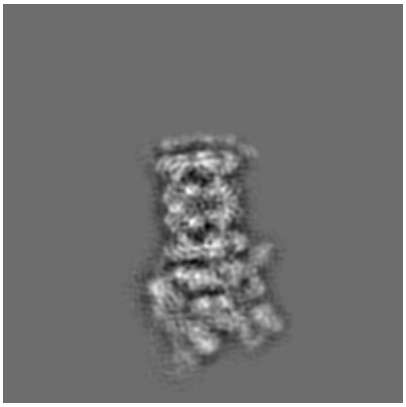
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

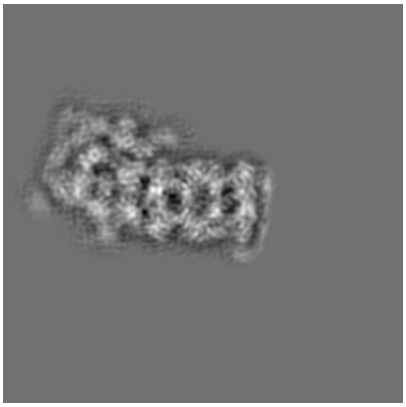
6.1.1 Primary map



X



Y

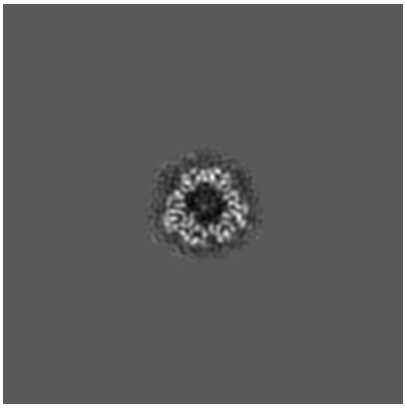


Z

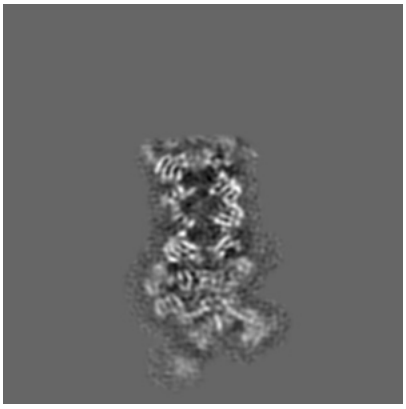
The images above show the map projected in three orthogonal directions.

6.2 Central slices

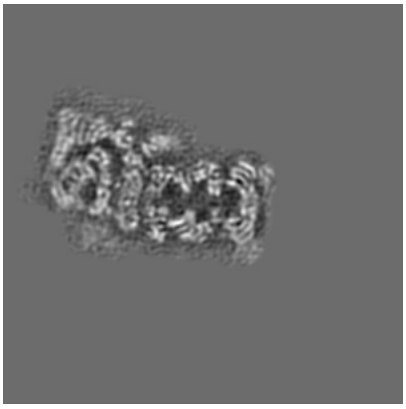
6.2.1 Primary map



X Index: 208



Y Index: 208

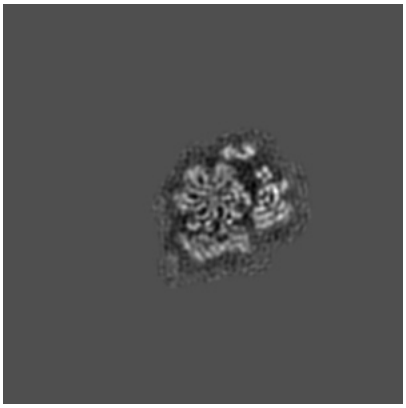


Z Index: 208

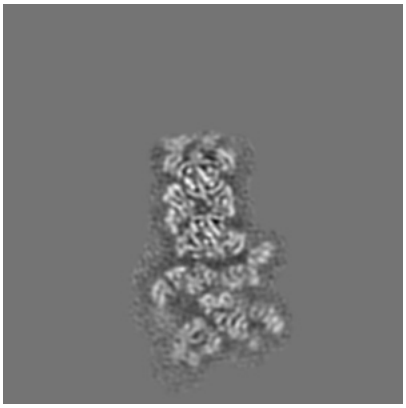
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

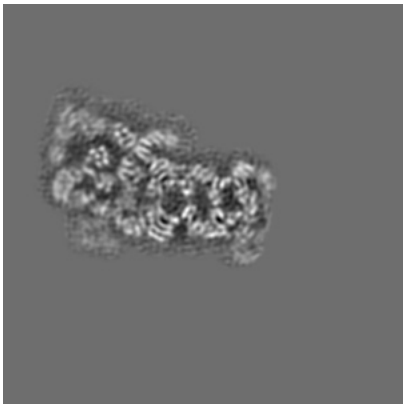
6.3.1 Primary map



X Index: 126



Y Index: 230

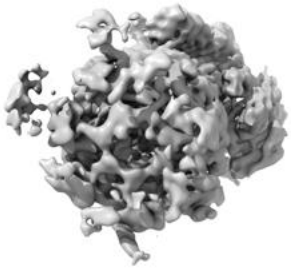


Z Index: 216

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

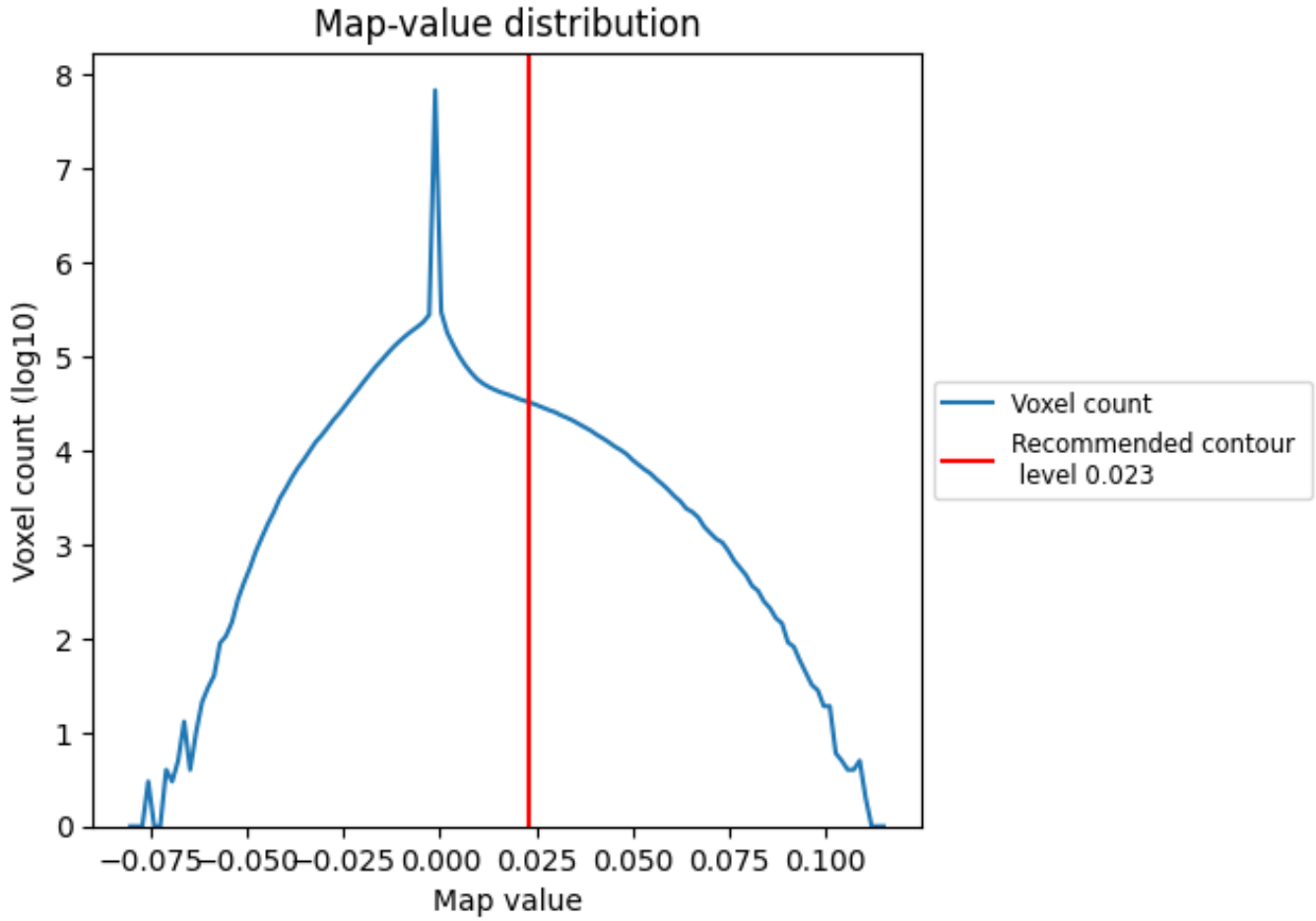
6.5 Mask visualisation (i)

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

7 Map analysis

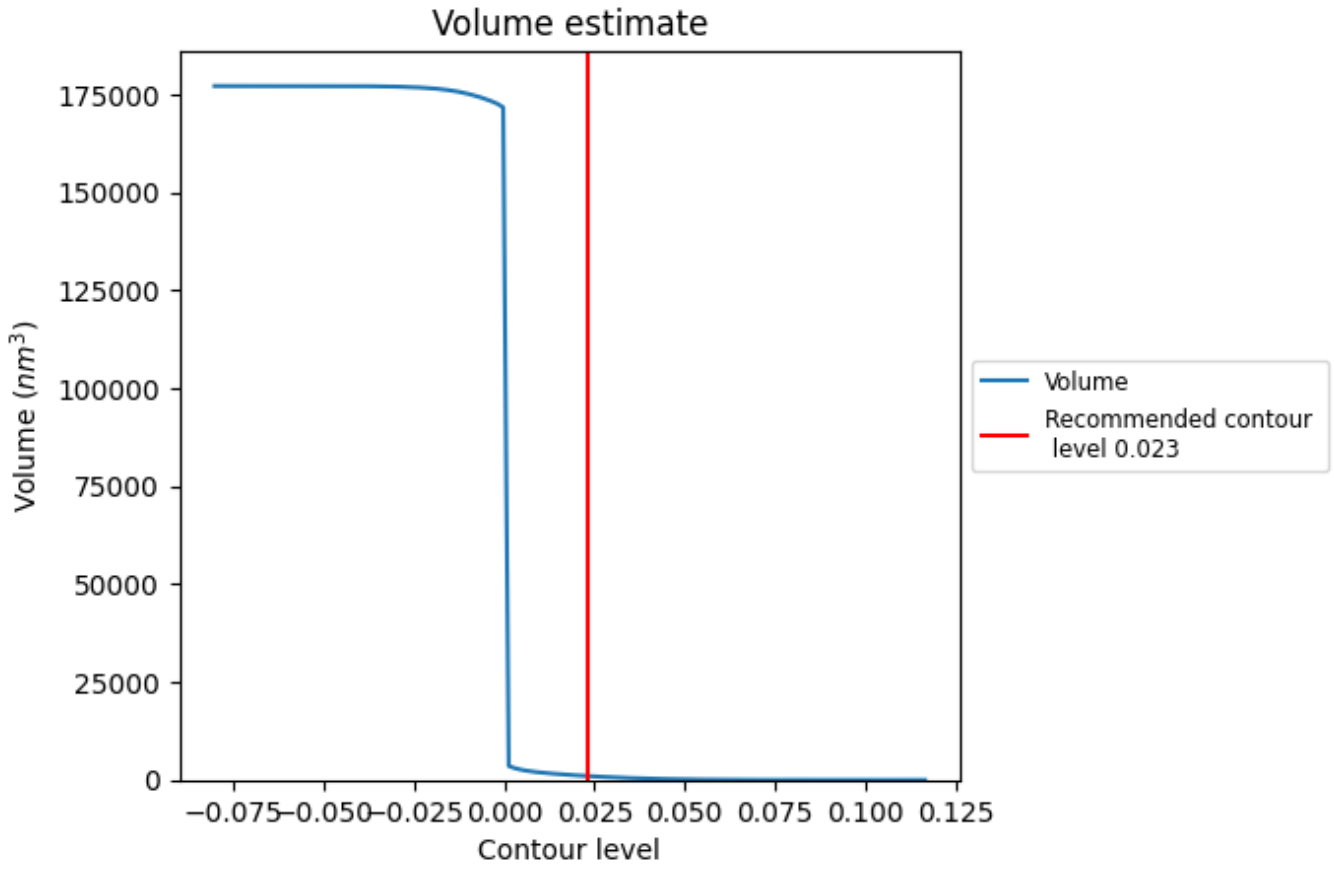
This section contains the results of statistical analysis of the map.

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.

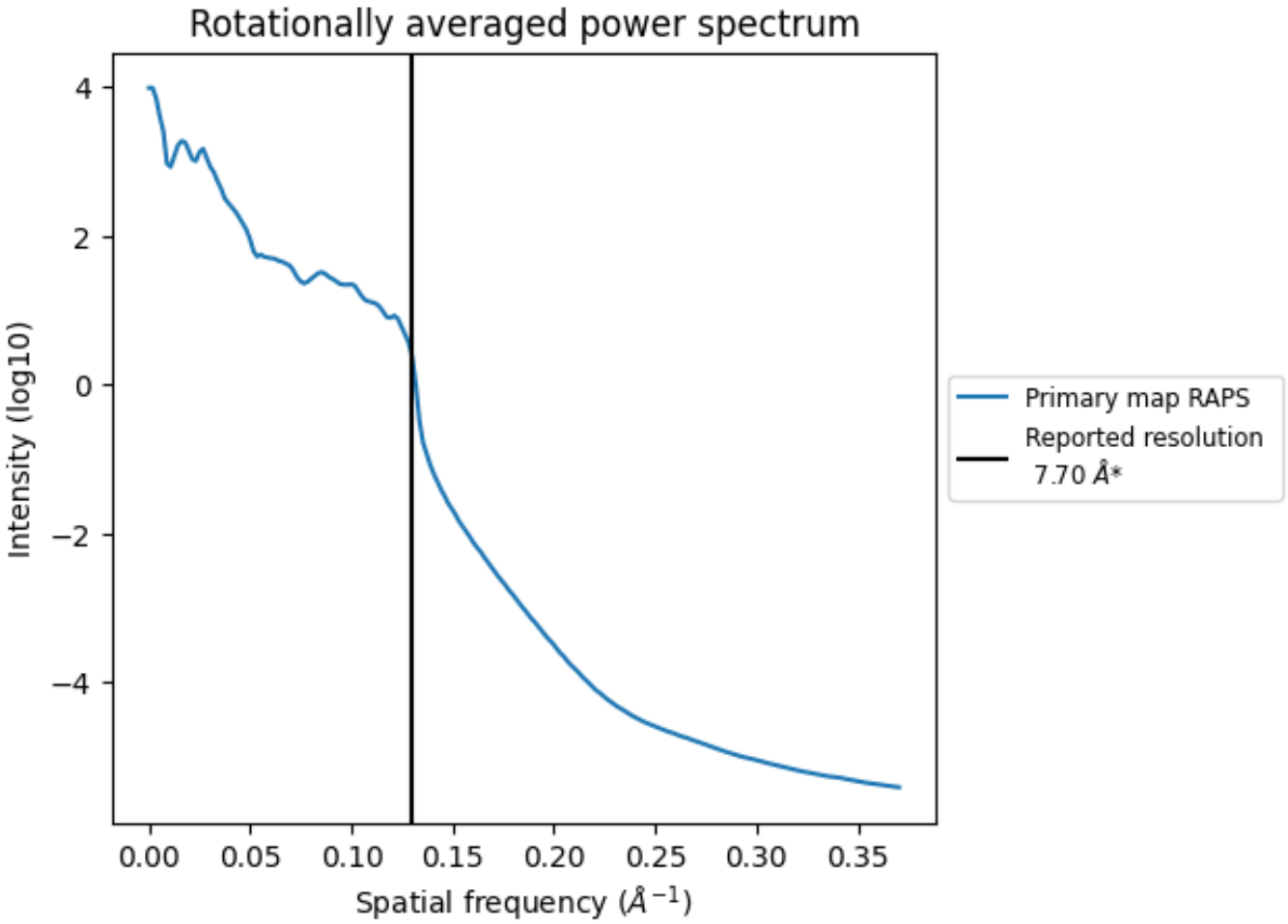
7.2 Volume estimate



The volume at the recommended contour level is 1008 nm^3; this corresponds to an approximate mass of 911 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 0.130 Å^{-1}

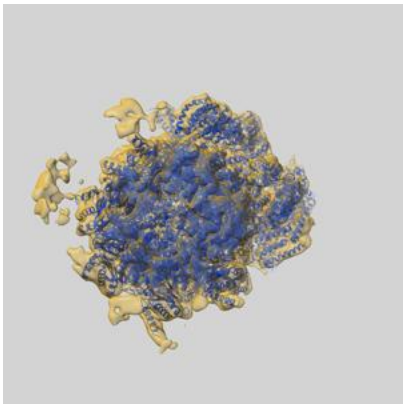
8 Fourier-Shell correlation (i)

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

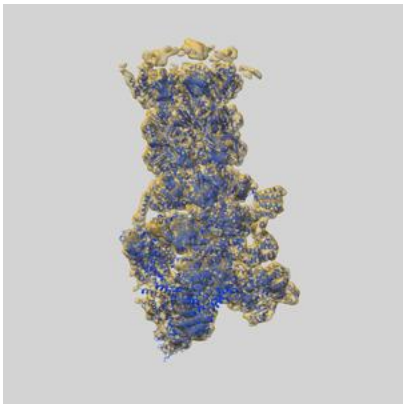
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3537 and PDB model 5MPC. Per-residue inclusion information can be found in section 3 on page 13.

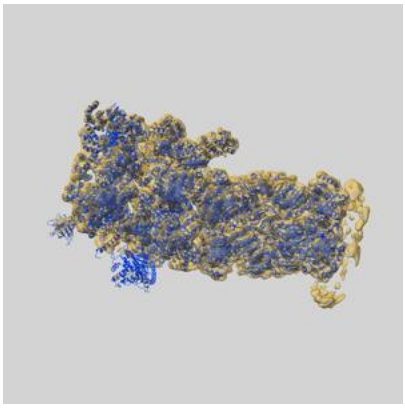
9.1 Map-model overlay



X



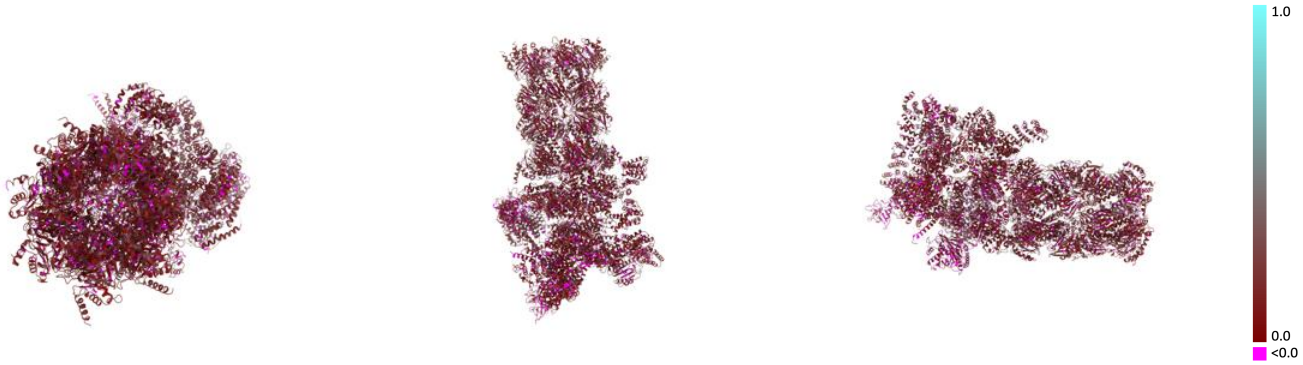
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.023 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

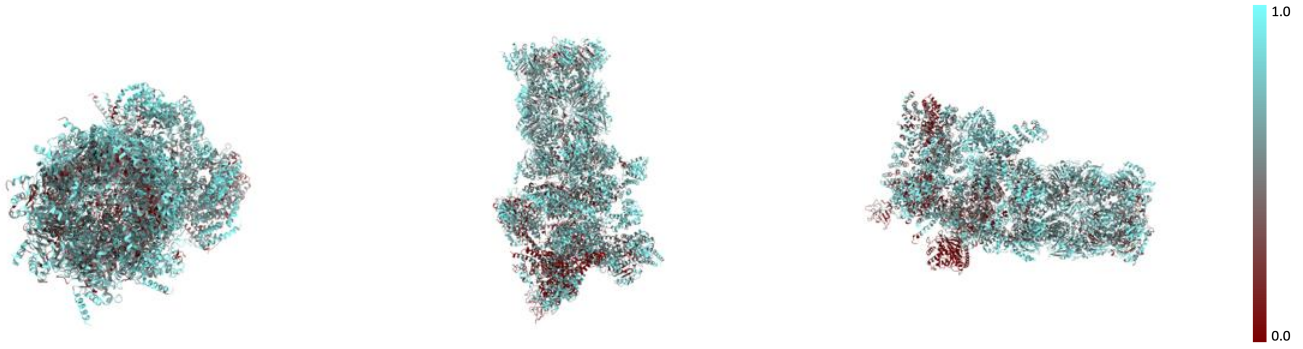
9.2 Q-score mapped to coordinate model (i)



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.

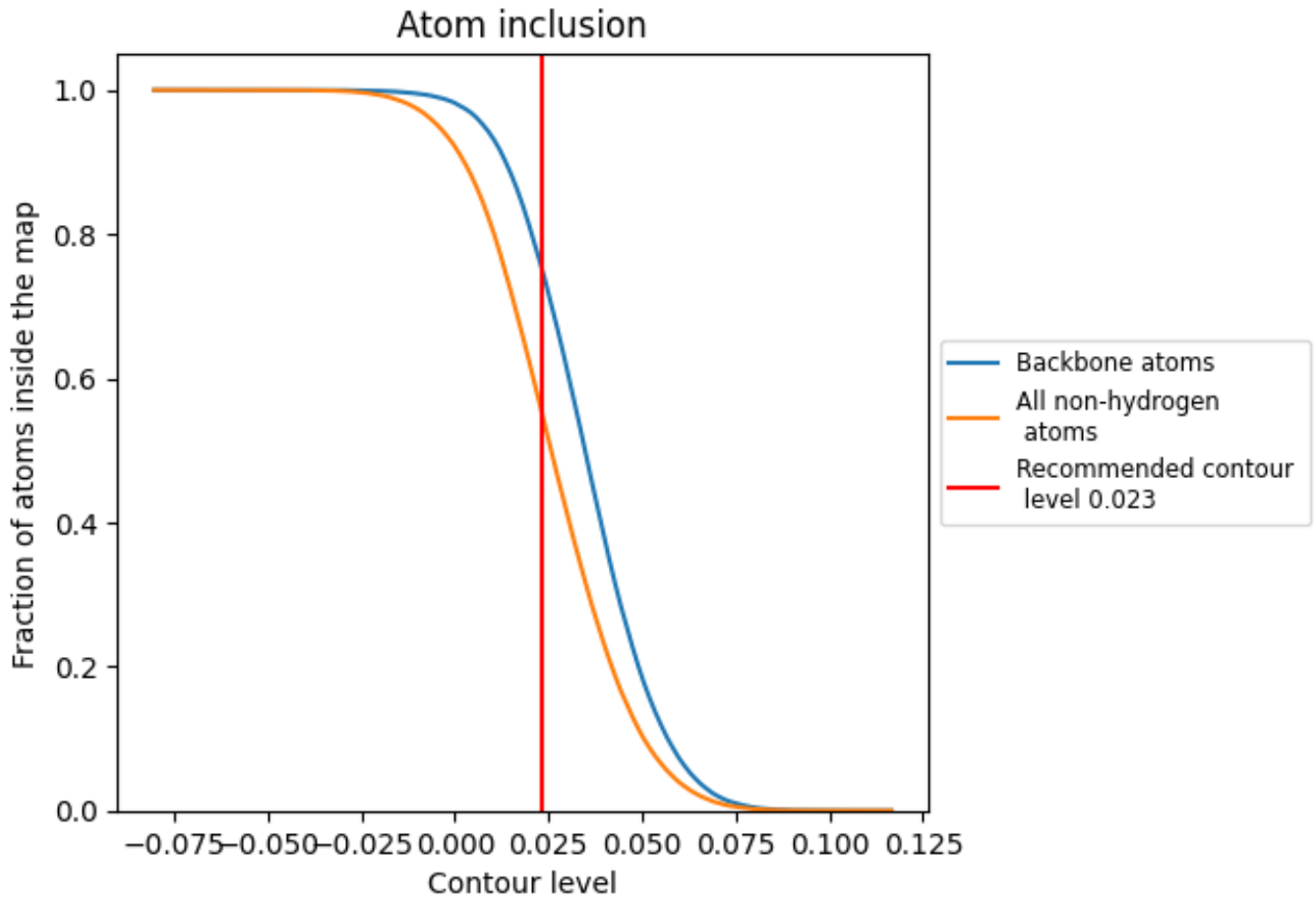
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.023).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 56% 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 (0.023) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5573	0.1350
1	0.6671	0.1510
2	0.6505	0.1520
3	0.5713	0.1440
4	0.6584	0.1530
5	0.6911	0.1510
6	0.6632	0.1460
7	0.6783	0.1580
8	0.0202	0.0730
A	0.6408	0.1500
B	0.5857	0.1460
C	0.5733	0.1450
D	0.6101	0.1450
E	0.6034	0.1480
F	0.6418	0.1480
G	0.6633	0.1450
H	0.5287	0.1280
I	0.4631	0.1340
J	0.4632	0.1230
K	0.4847	0.1240
L	0.4995	0.1200
M	0.5329	0.1350
N	0.5010	0.1310
O	0.6040	0.1470
P	0.7570	0.1490
Q	0.7037	0.1430
R	0.6903	0.1460
S	0.4410	0.1290
T	0.3330	0.1250
U	0.5107	0.1410
V	0.5203	0.1350
W	0.5483	0.1110
X	0.1510	0.0710
Y	0.4116	0.0880
Z	0.5139	0.1040

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Chain	Atom inclusion	Q-score
a	0.6211	0.1460
b	0.5427	0.1380
c	0.5561	0.1380
d	0.6150	0.1420
e	0.5985	0.1440
f	0.6199	0.1400
g	0.6445	0.1500
h	0.6509	0.1420
i	0.6257	0.1470
j	0.5848	0.1390
k	0.6479	0.1410
l	0.6781	0.1490
m	0.6551	0.1510
n	0.6395	0.1430