Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 02:01 pm GMT

PDB ID	:	5MPB
EMDB ID	:	EMD-3536
Title	:	26S proteasome in presence of AMP-PNP (s3)
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	:	7.80 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:

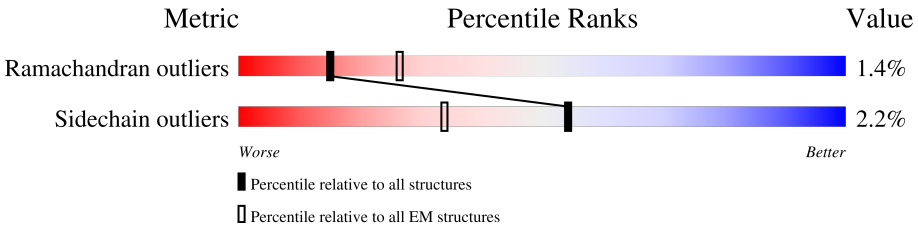
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance

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

The reported resolution of this entry is 7.80 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	21% 77% 17%
1	a	252	20% 74% 18%
2	B	250	26% 84% 14%
2	b	250	26% 80% 16%
3	C	258	18% 83% 11% 5%
3	c	258	22% 74% 17% 5%
4	D	254	13% 80% 13% 6%
4	d	254	16% 74% 18% 6%
5	E	260	17% 77% 15% 7%

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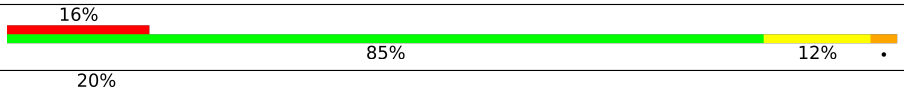
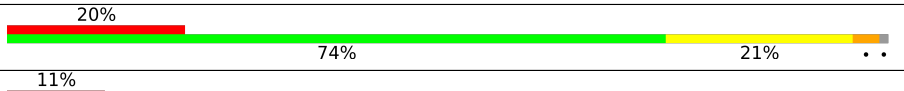
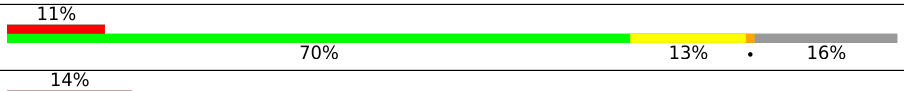
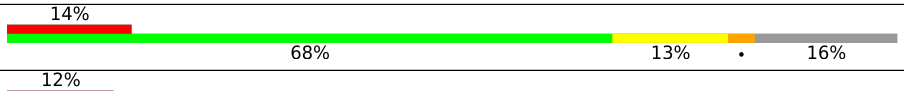
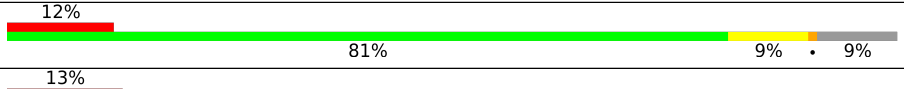
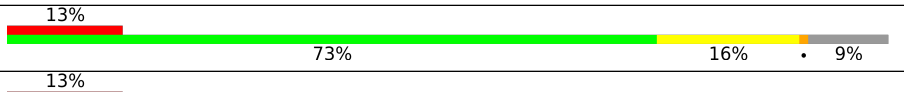
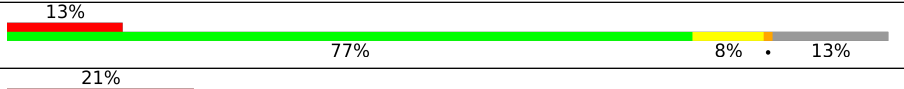
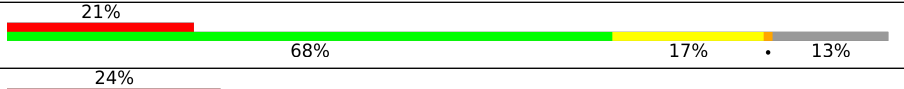
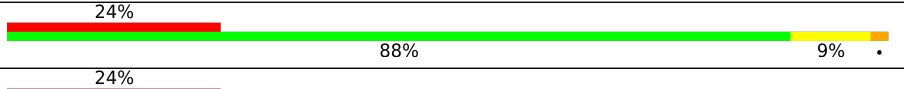
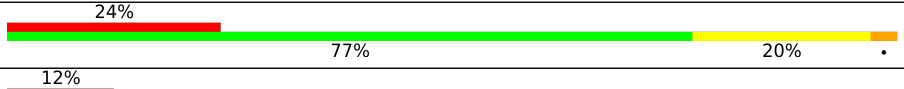
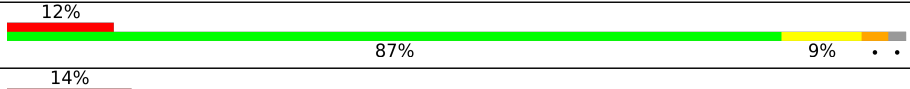
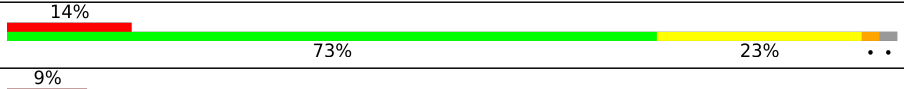
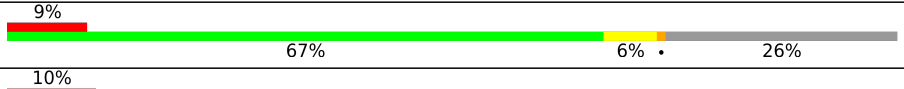
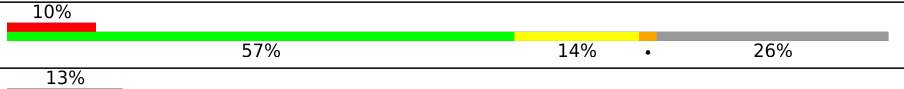
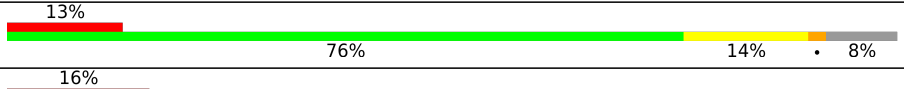
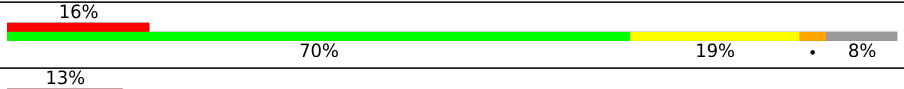
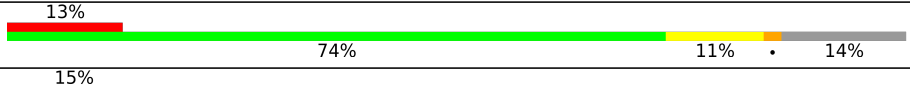
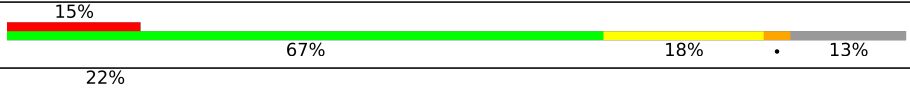
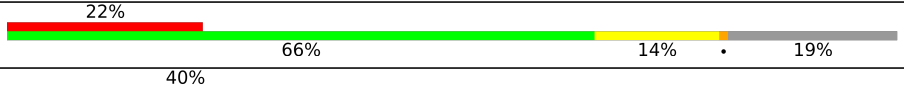
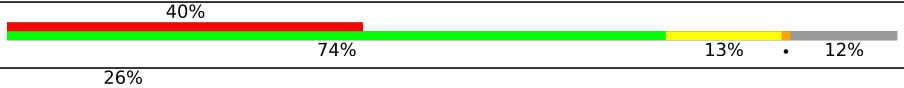
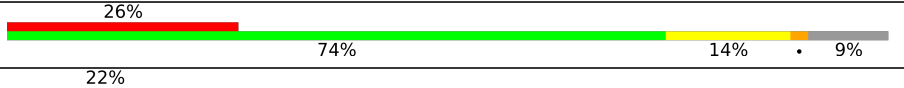
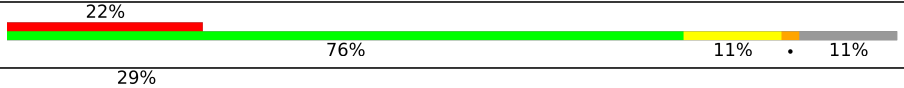
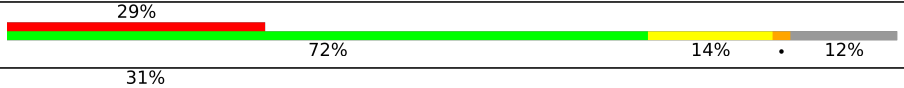
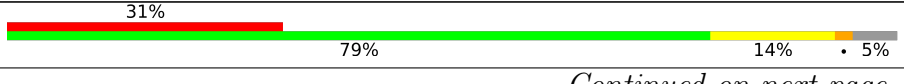
Mol	Chain	Length	Quality of chain
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	1	215	
8	h	215	
9	2	261	
9	i	261	
10	3	205	
10	j	205	
11	4	198	
11	k	198	
12	5	287	
12	l	287	
13	6	241	
13	m	241	
14	7	266	
14	n	266	
15	H	467	
16	I	437	
17	K	428	
18	L	437	
19	M	434	
20	J	405	

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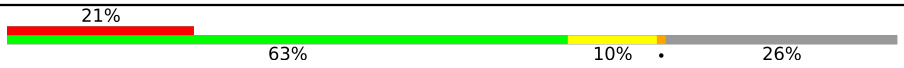
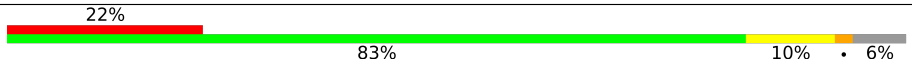
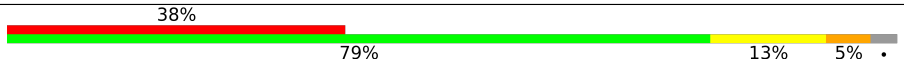
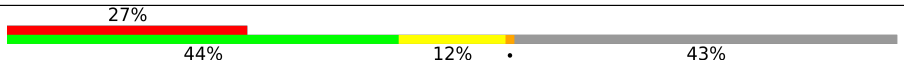
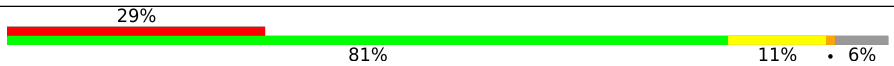
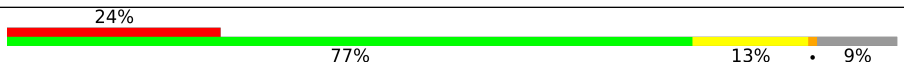
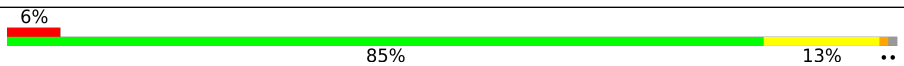
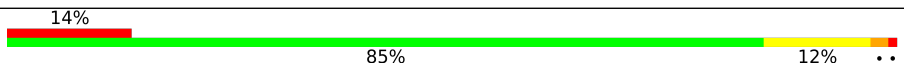
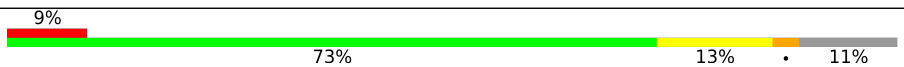
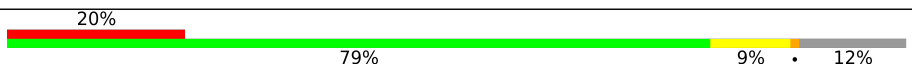
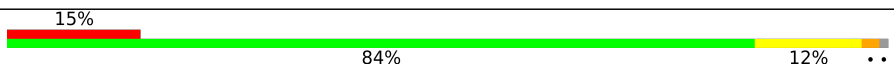
Mol	Chain	Length	Quality of chain
21	W	268	
22	V	306	
23	T	274	
24	X	156	
25	Y	89	
26	Z	993	
27	N	945	
28	S	523	
29	P	445	
30	Q	434	
31	R	429	
32	U	338	
33	O	393	

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 108771 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	386	Total	C	N	O	S	0	0
			3033	1906	543	567	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		

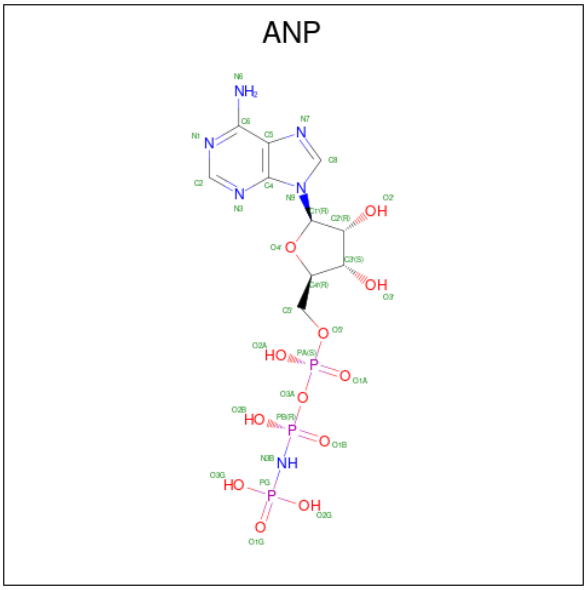
- Molecule 32 is a protein called 26S proteasome regulatory subunit RPN8.

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 PHOSPHOAMINOPHOSPHONIC ACID-ADENYLATE ESTER (three-letter code: ANP) (formula: $C_{10}H_{17}N_6O_{12}P_3$).



Mol	Chain	Residues	Atoms					AltConf
34	H	1	Total	C	N	O	P	0
			31	10	6	12	3	

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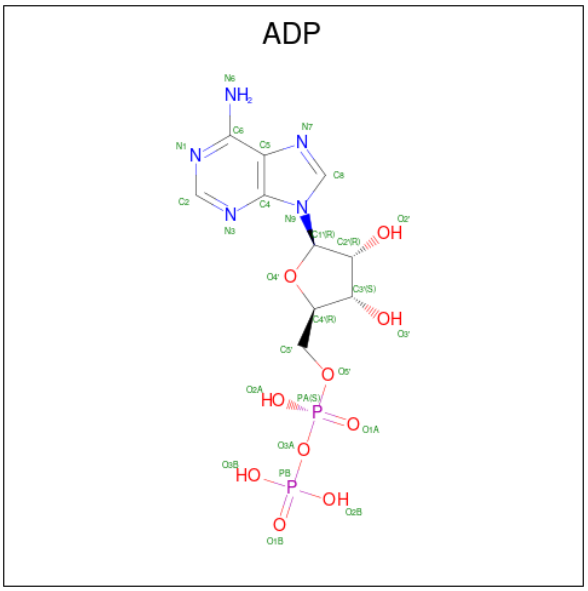
Mol	Chain	Residues	Atoms					AltConf
34	I	1	Total	C	N	O	P	0
			31	10	6	12	3	
34	K	1	Total	C	N	O	P	0
			31	10	6	12	3	
34	L	1	Total	C	N	O	P	0
			31	10	6	12	3	
34	J	1	Total	C	N	O	P	0
			31	10	6	12	3	

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

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

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



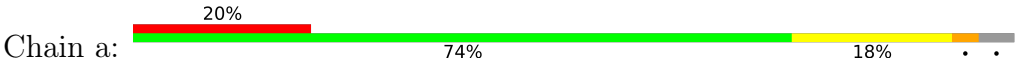
Mol	Chain	Residues	Atoms					AltConf
36	M	1	Total	C	N	O	P	0
			27	10	5	10	2	

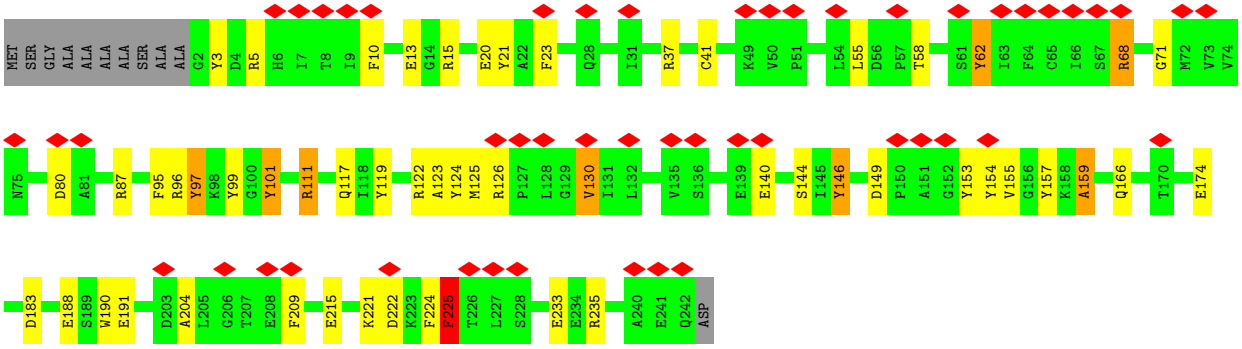
3 Residue-property plots (i)

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

• Molecule 1: Proteasome subunit alpha type-1

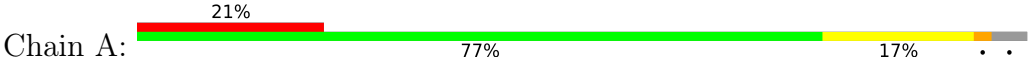
Chain a:

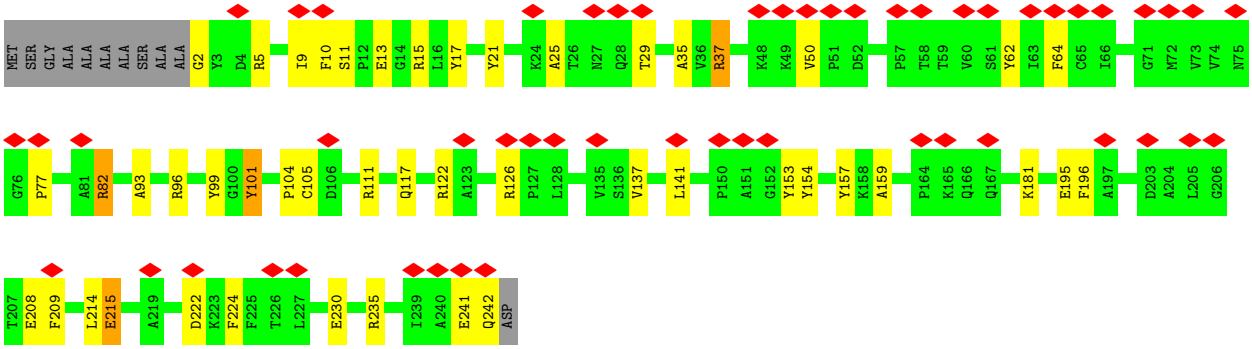




• Molecule 1: Proteasome subunit alpha type-1

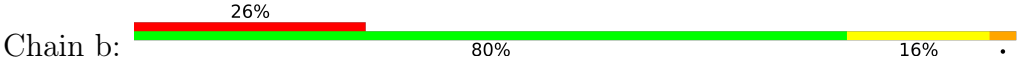
Chain A:

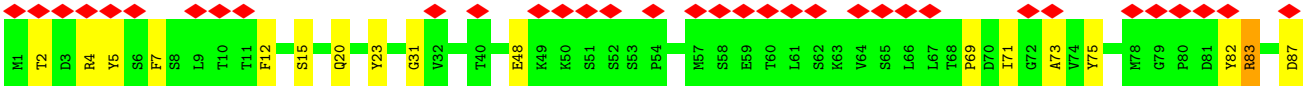


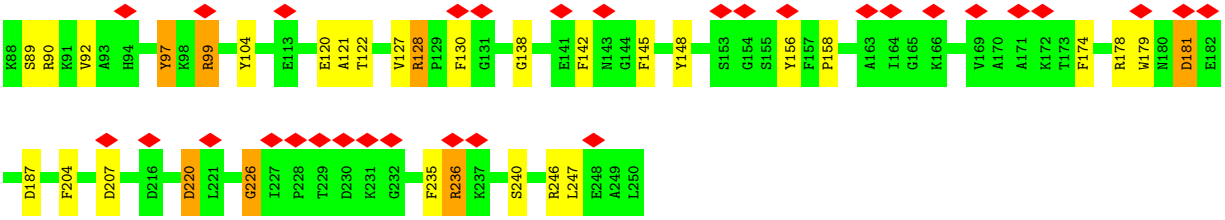


• Molecule 2: Proteasome subunit alpha type-2

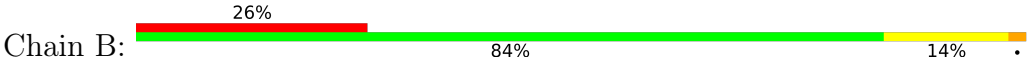
Chain b:

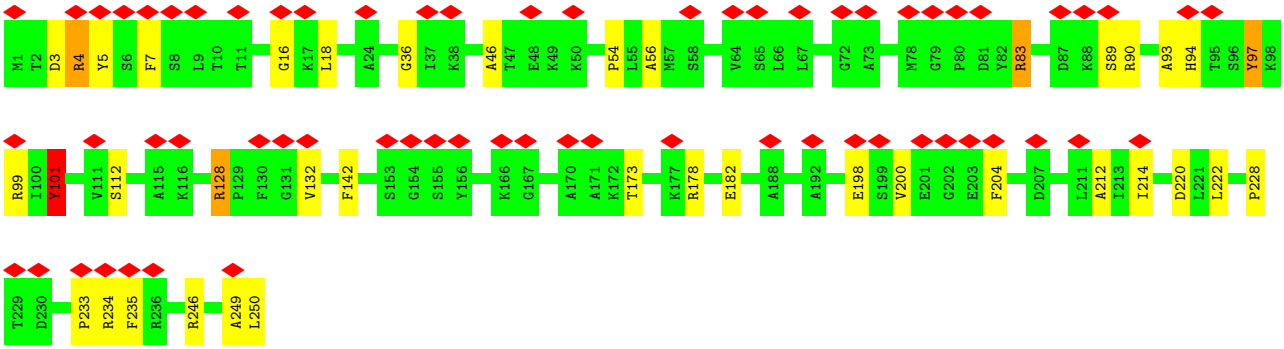




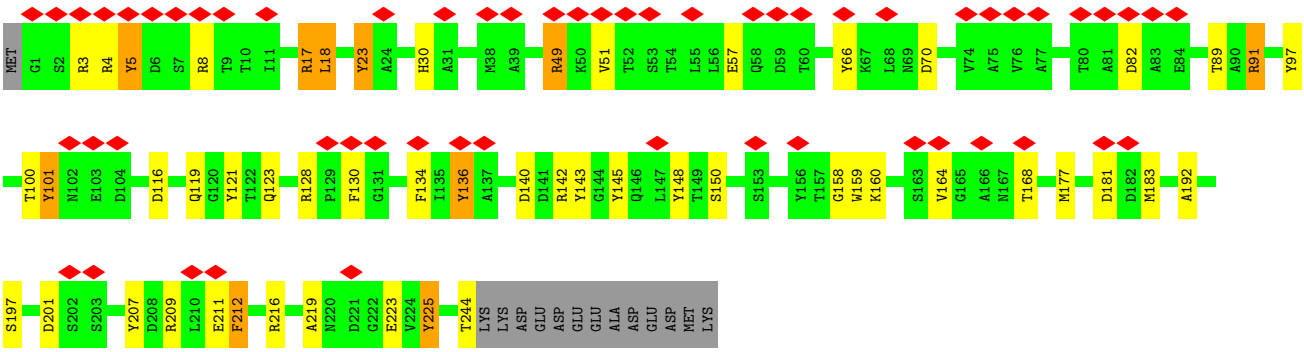


• Molecule 2: Proteasome subunit alpha type-2

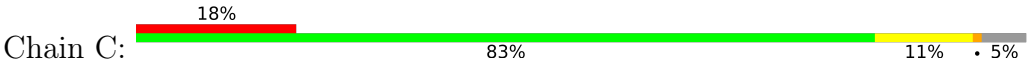


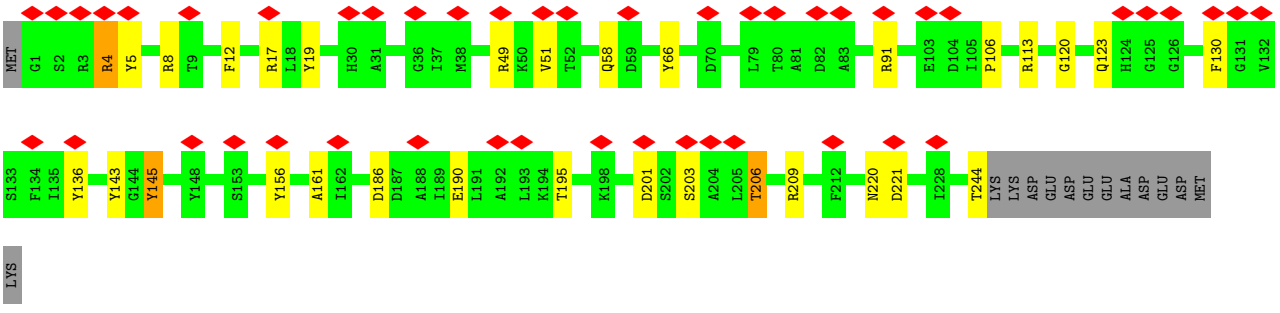


• Molecule 3: Proteasome subunit alpha type-3



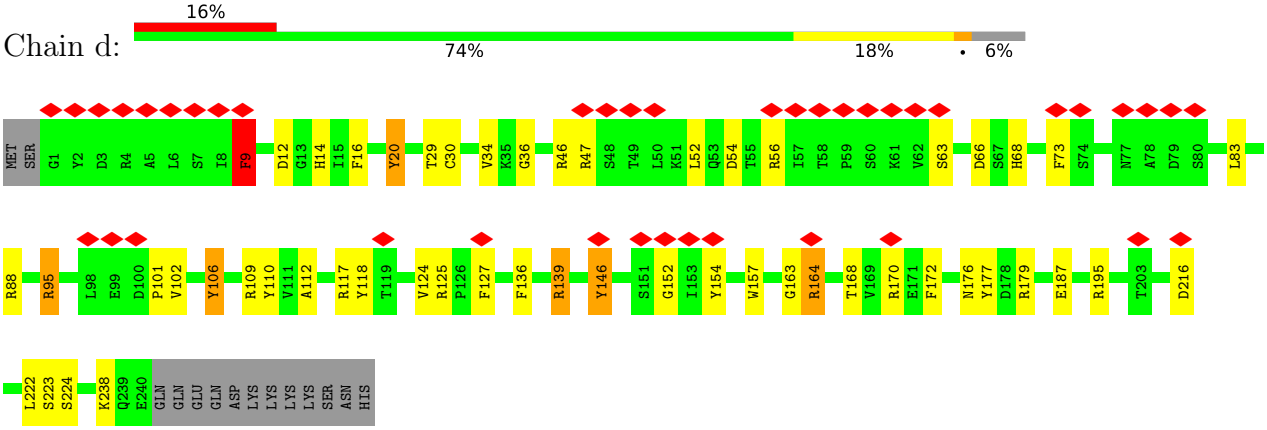
• Molecule 3: Proteasome subunit alpha type-3





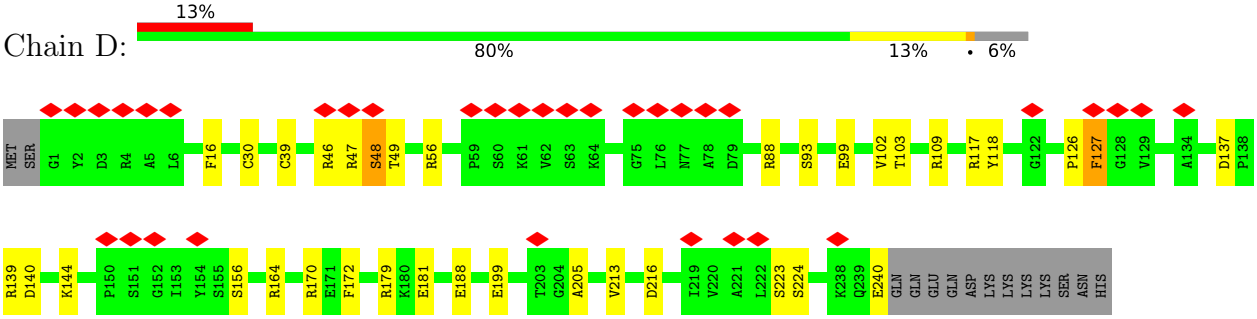
• Molecule 4: Proteasome subunit alpha type-4

Chain d:



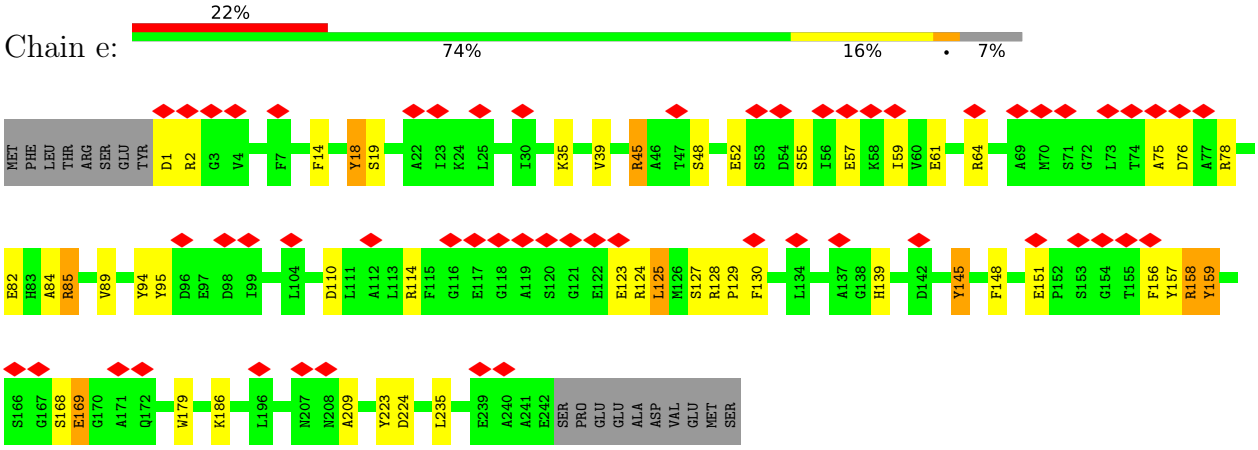
• Molecule 4: Proteasome subunit alpha type-4

Chain D:



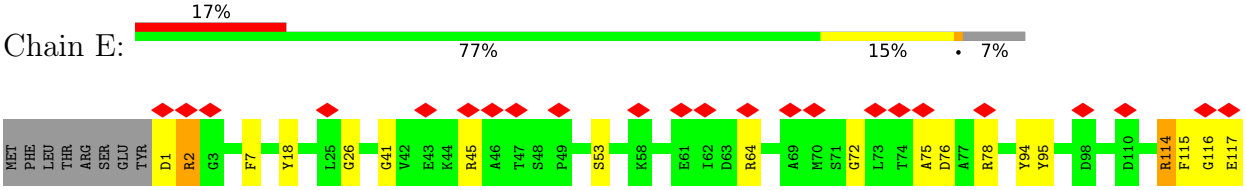
• Molecule 5: Proteasome subunit alpha type-5

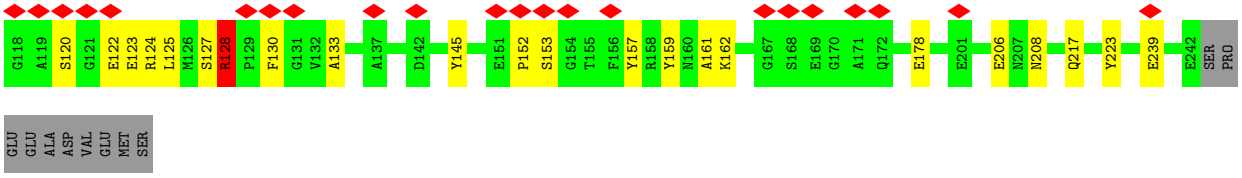
Chain e:



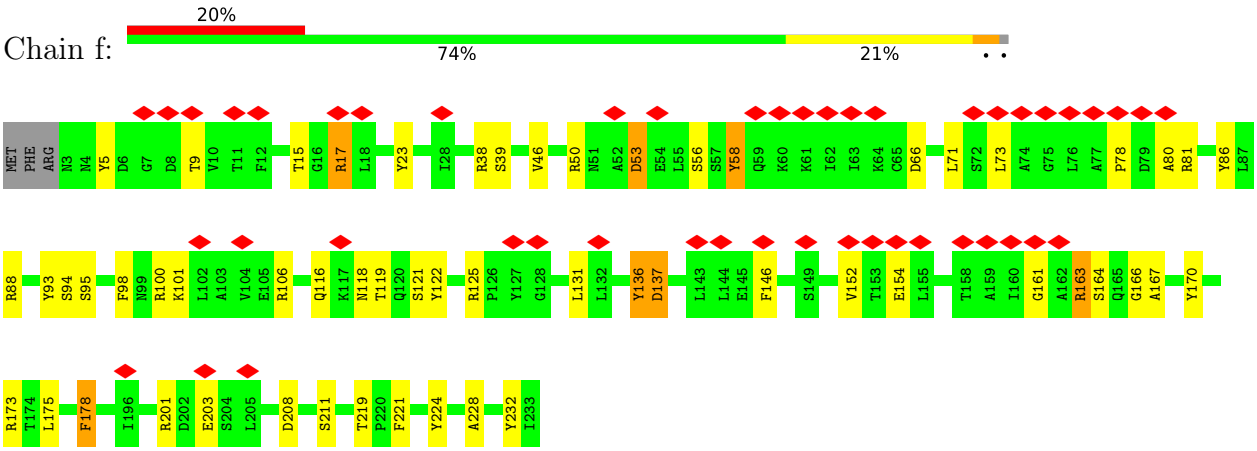
• Molecule 5: Proteasome subunit alpha type-5

Chain E:

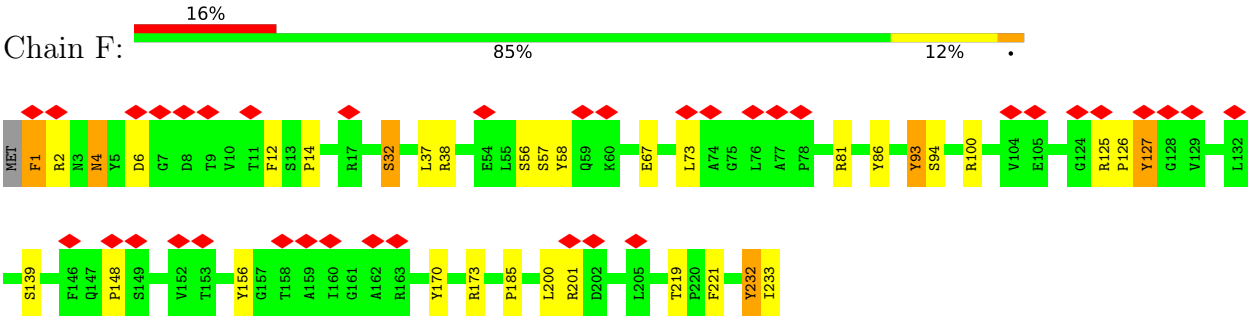




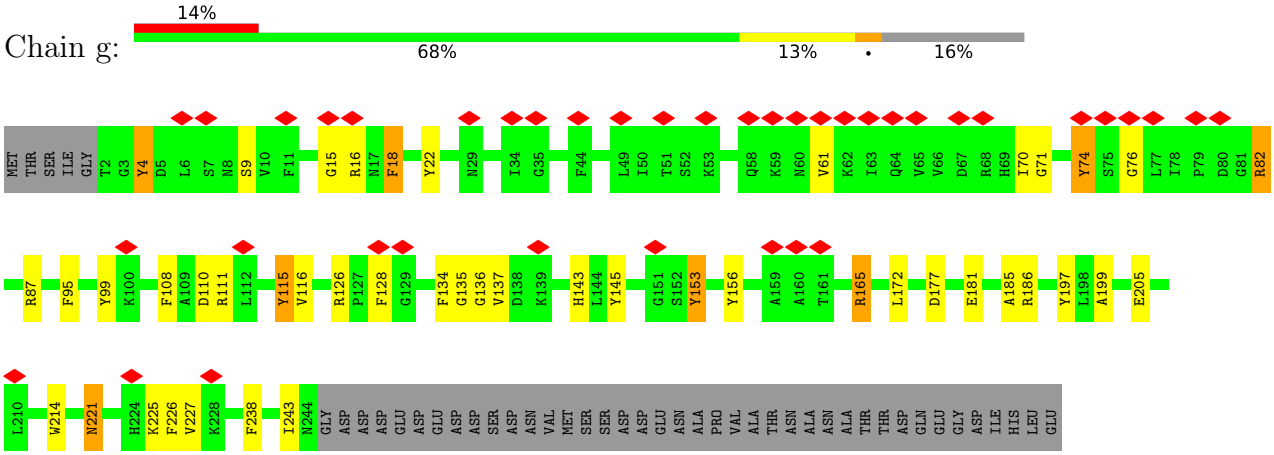
• Molecule 6: Proteasome subunit alpha type-6



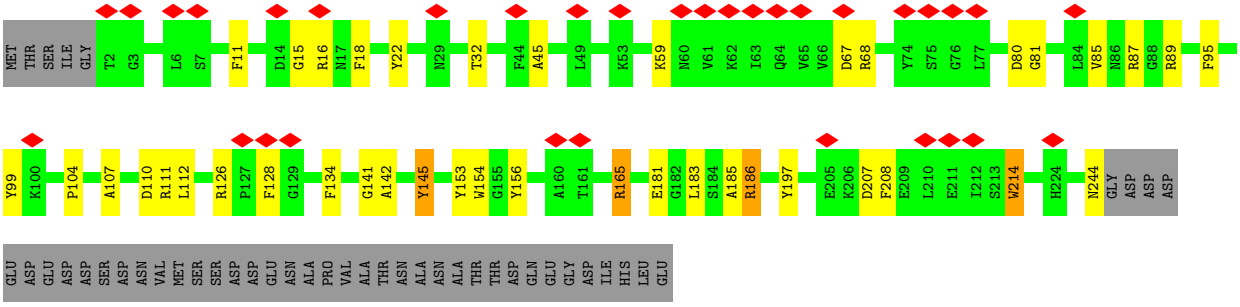
• Molecule 6: Proteasome subunit alpha type-6



• Molecule 7: Probable proteasome subunit alpha type-7

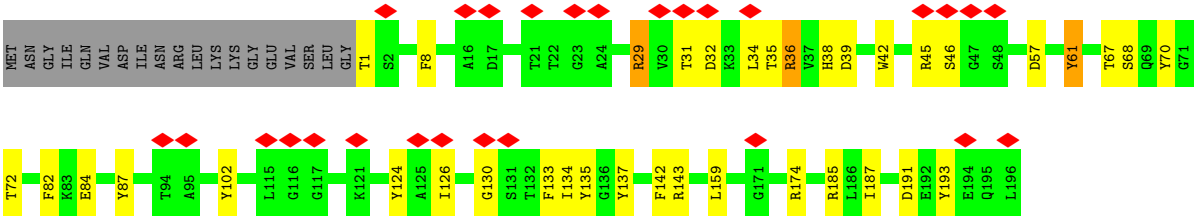


• Molecule 7: Probable proteasome subunit alpha type-7



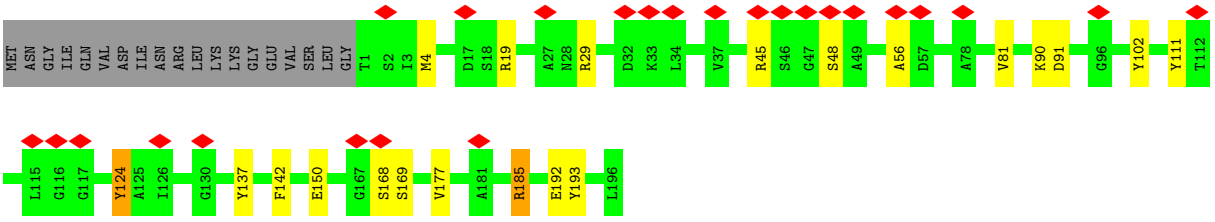
• Molecule 8: Proteasome subunit beta type-1

Chain h:



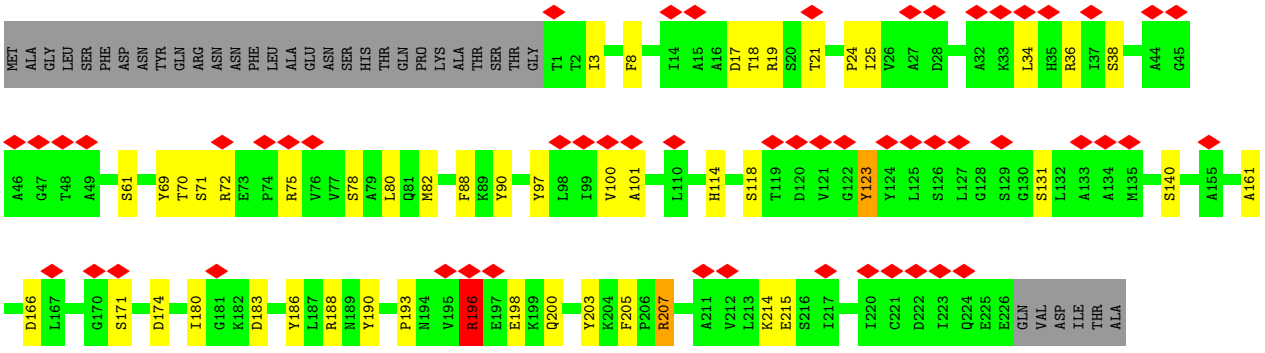
• Molecule 8: Proteasome subunit beta type-1

Chain 1:



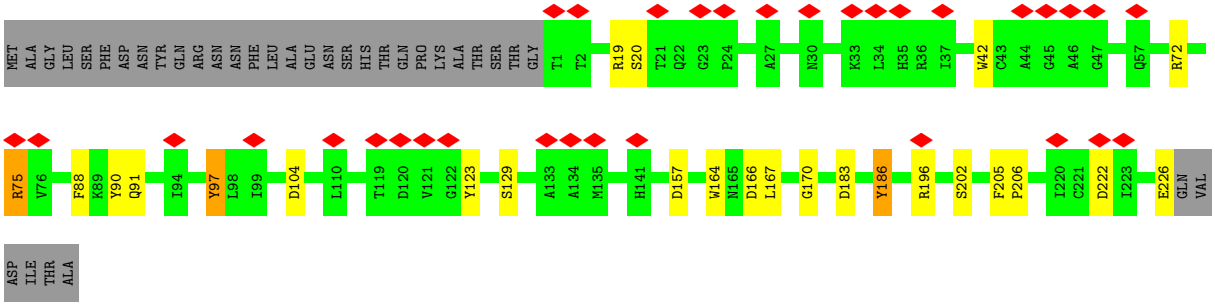
• Molecule 9: Proteasome subunit beta type-2

Chain i:

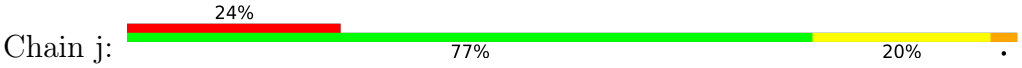


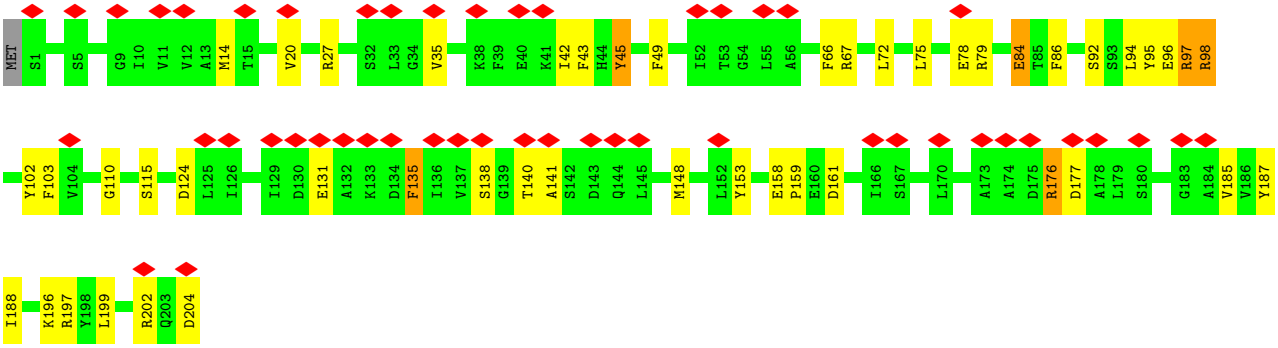
• Molecule 9: Proteasome subunit beta type-2

Chain 2:

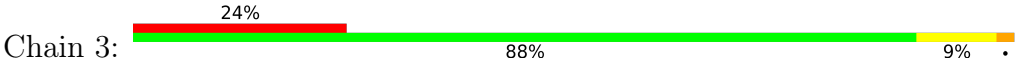


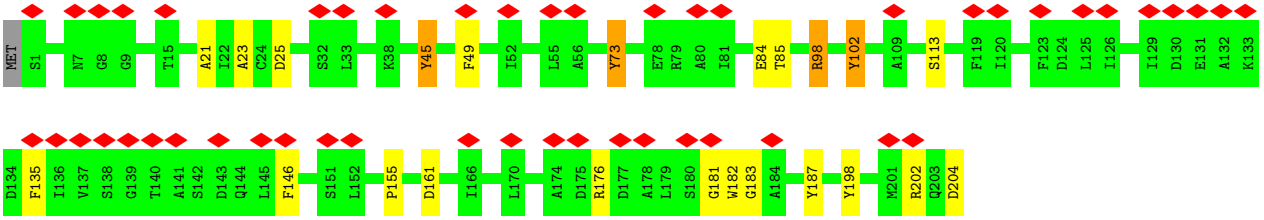
• Molecule 10: Proteasome subunit beta type-3



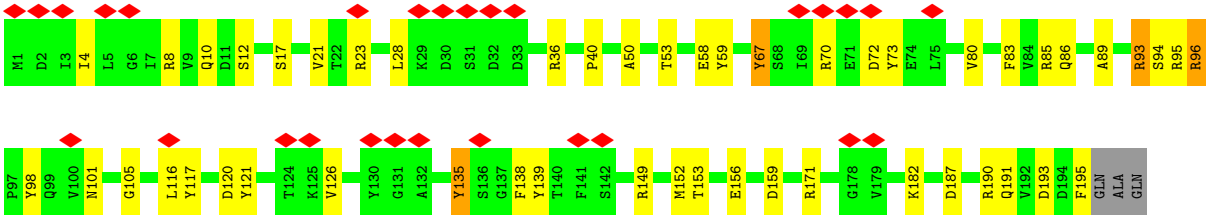


• Molecule 10: Proteasome subunit beta type-3

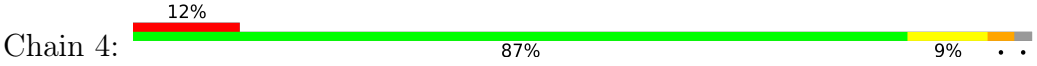


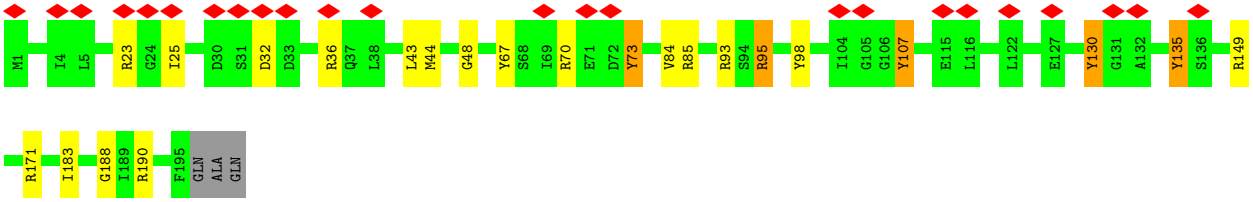


• Molecule 11: Proteasome subunit beta type-4

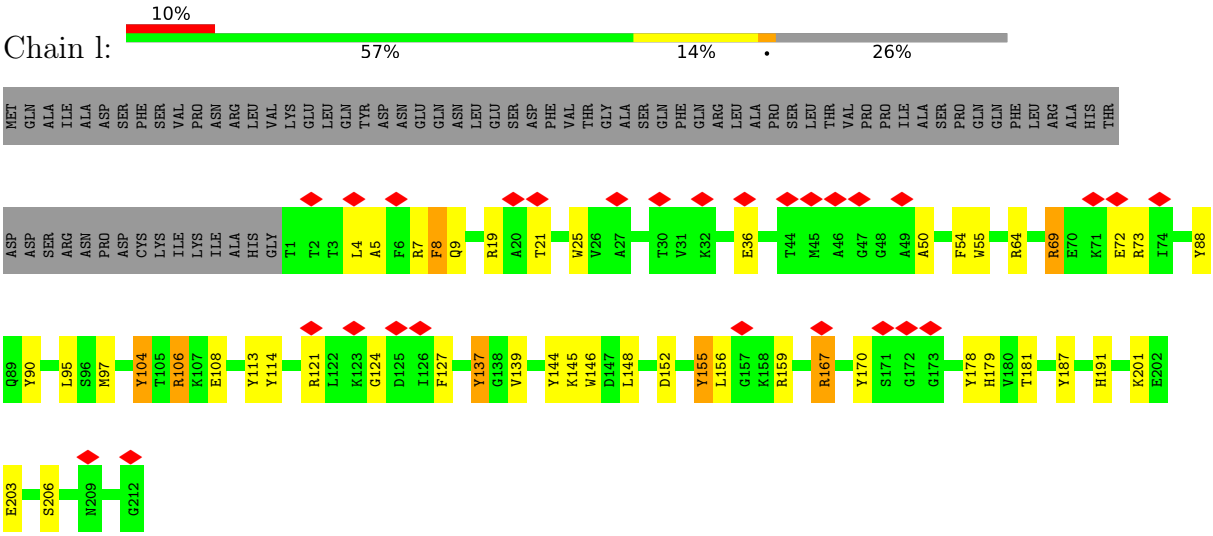


• Molecule 11: Proteasome subunit beta type-4

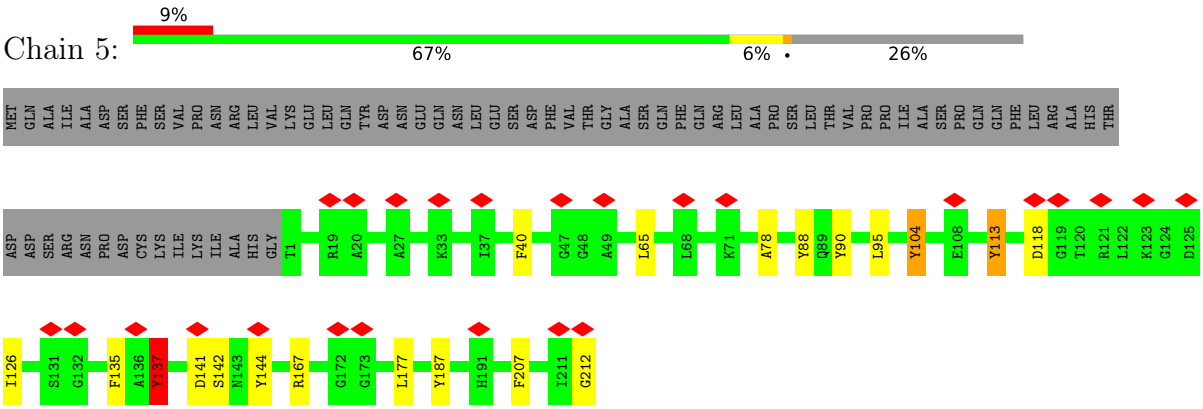




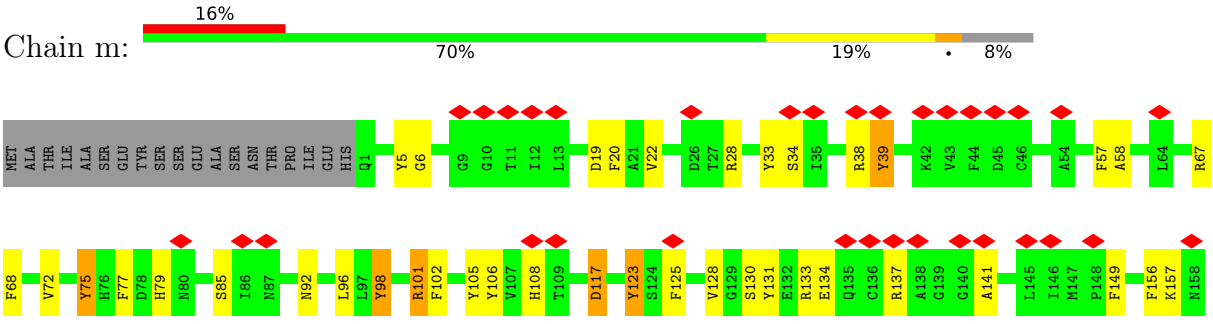
• Molecule 12: Proteasome subunit beta type-5

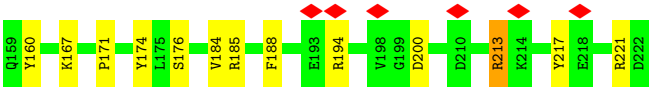


• Molecule 12: Proteasome subunit beta type-5

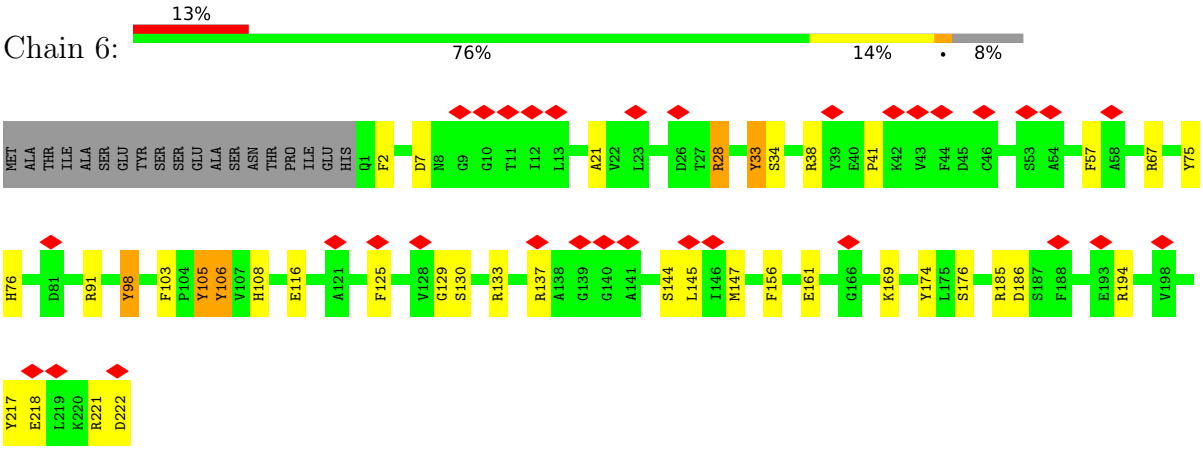


• Molecule 13: Proteasome subunit beta type-6

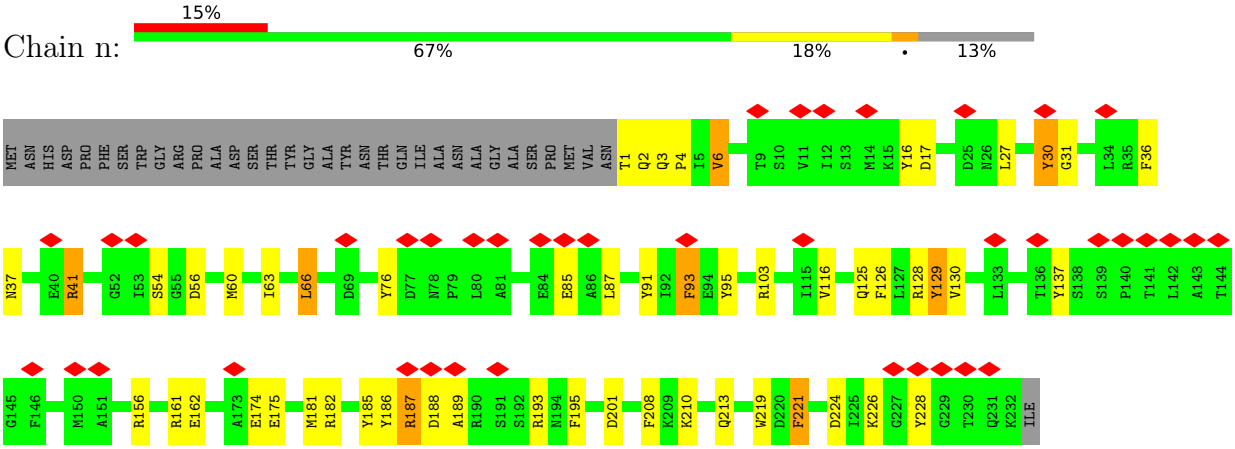




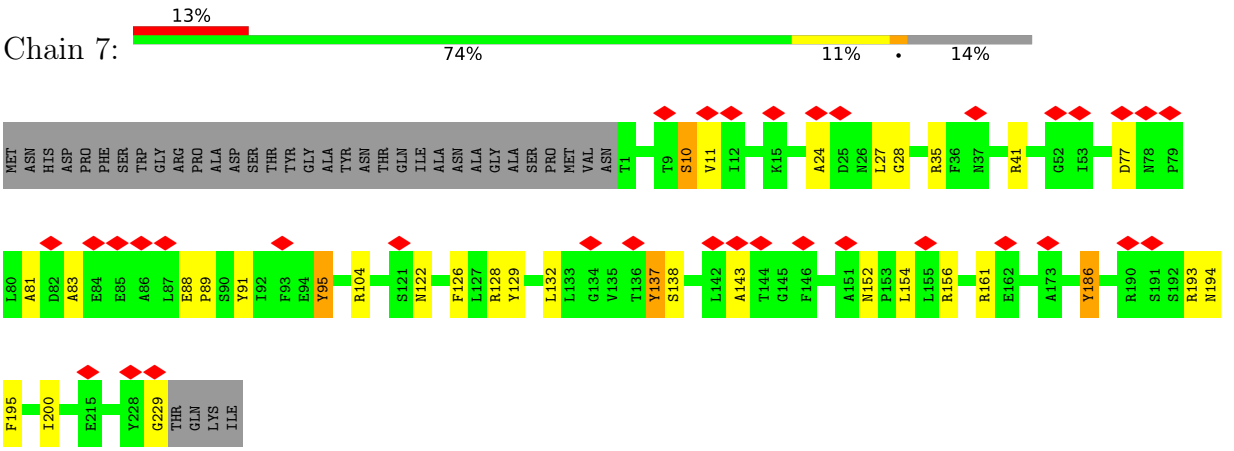
• Molecule 13: Proteasome subunit beta type-6



• Molecule 14: Proteasome subunit beta type-7

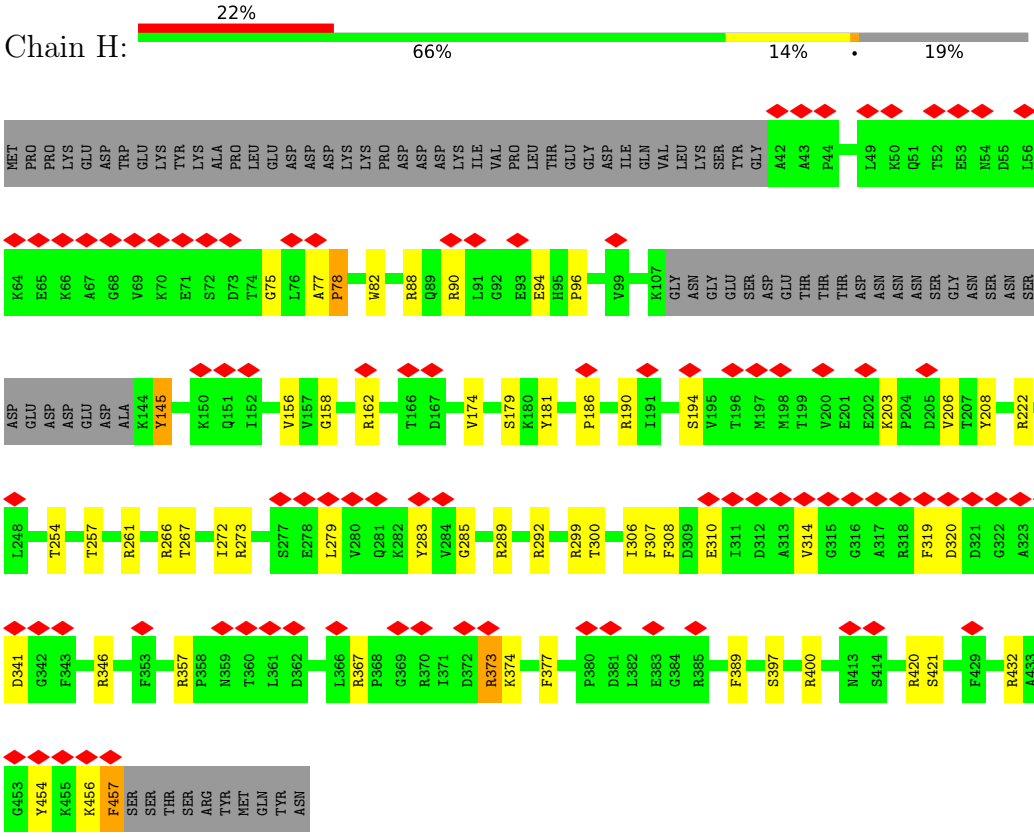


• Molecule 14: Proteasome subunit beta type-7



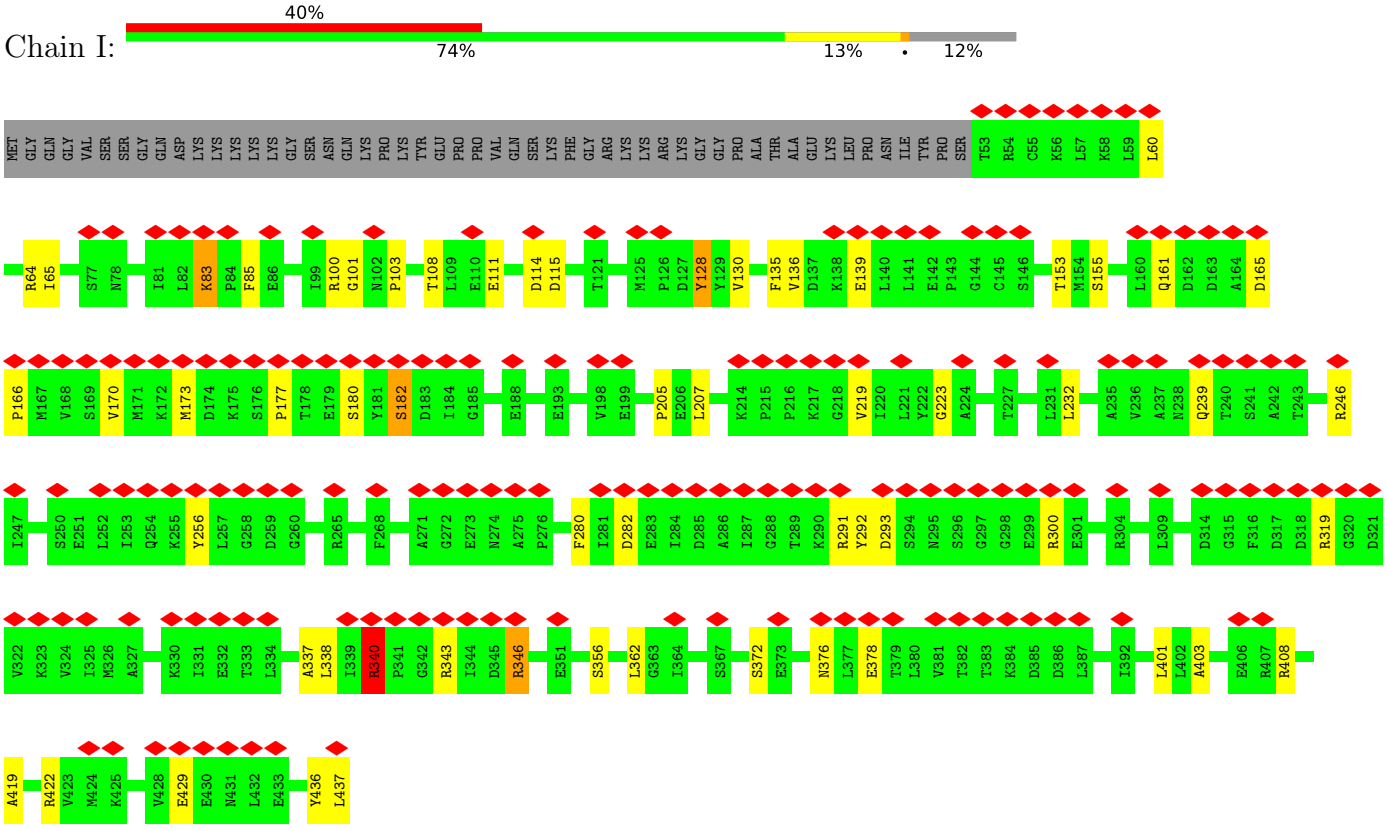
• Molecule 15: 26S protease regulatory subunit 7 homolog

Chain H:



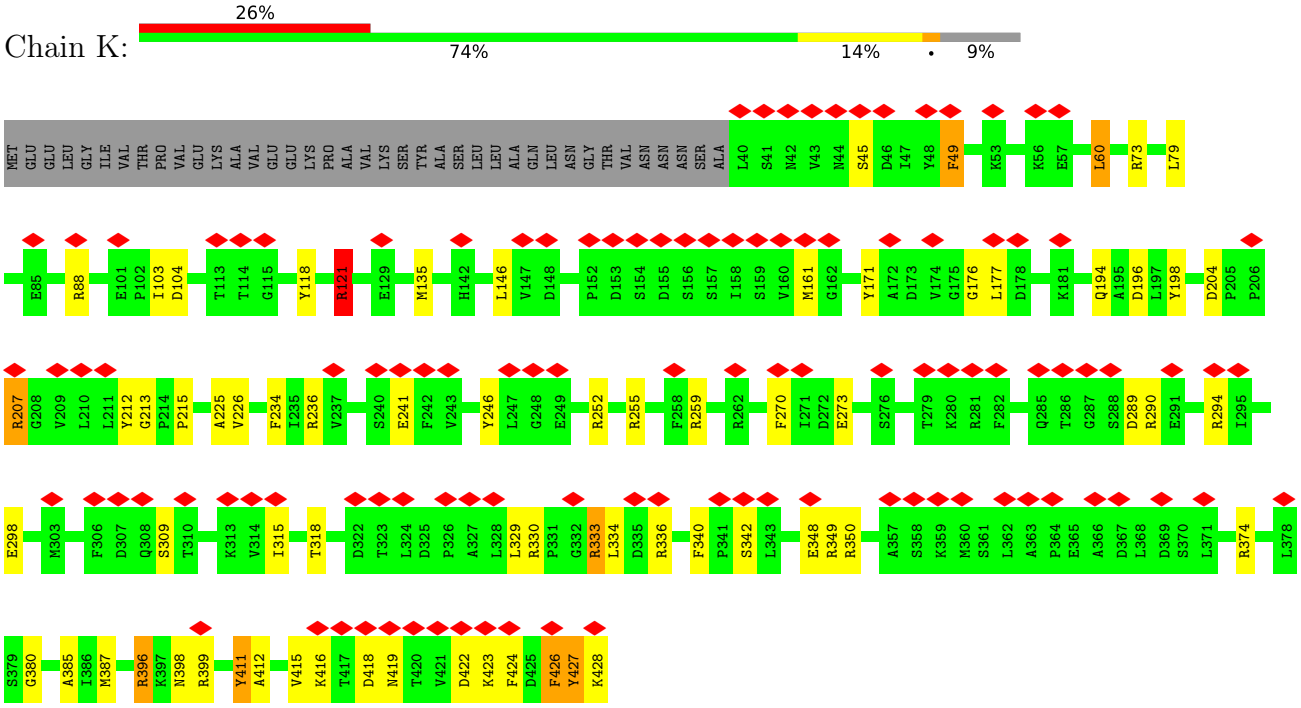
• Molecule 16: 26S protease regulatory subunit 4 homolog

Chain I:



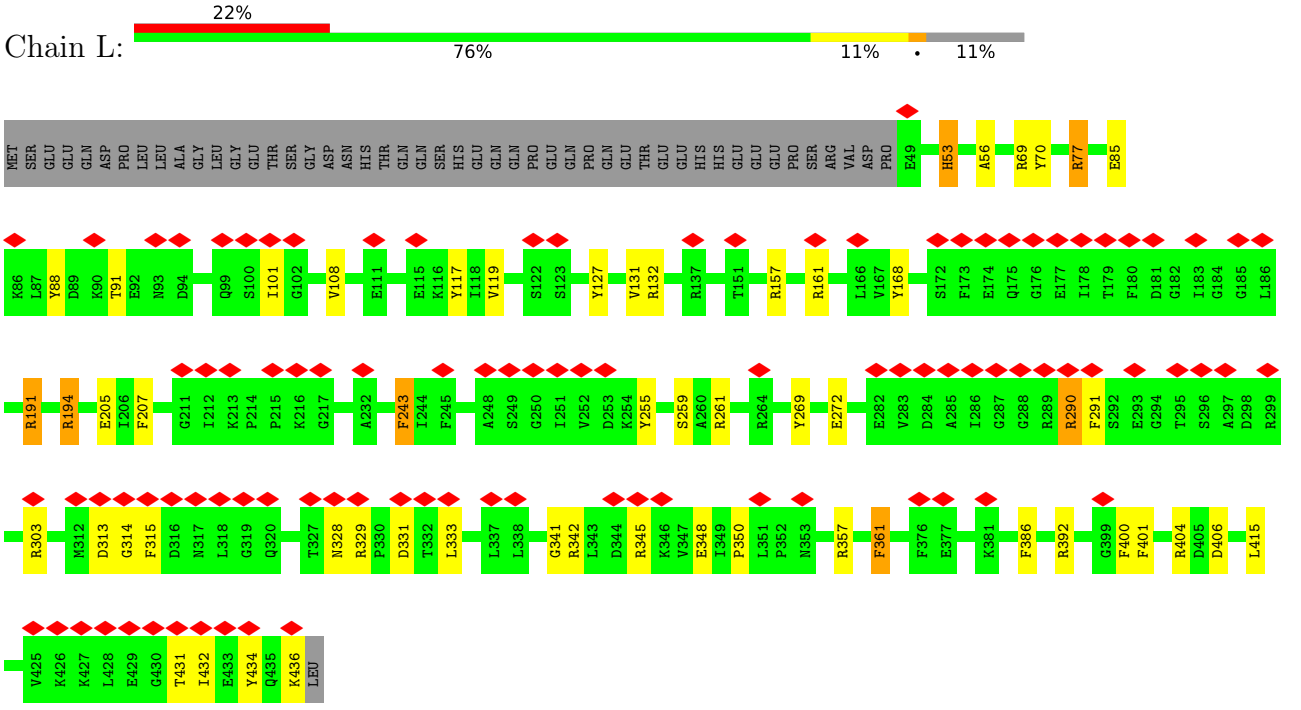
• Molecule 17: 26S protease regulatory subunit 6B homolog

Chain K:



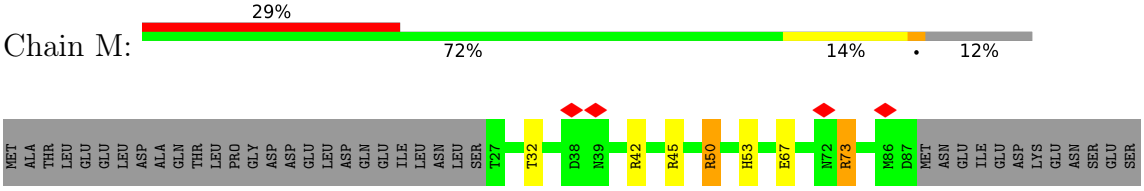
• Molecule 18: 26S protease subunit RPT4

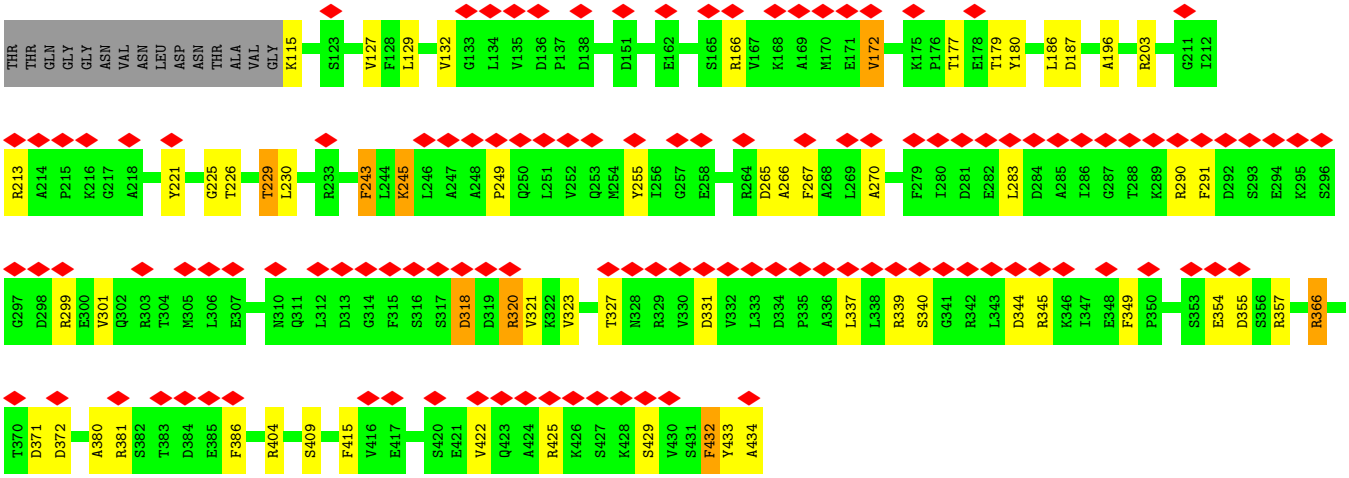
Chain L:



• Molecule 19: 26S protease regulatory subunit 6A

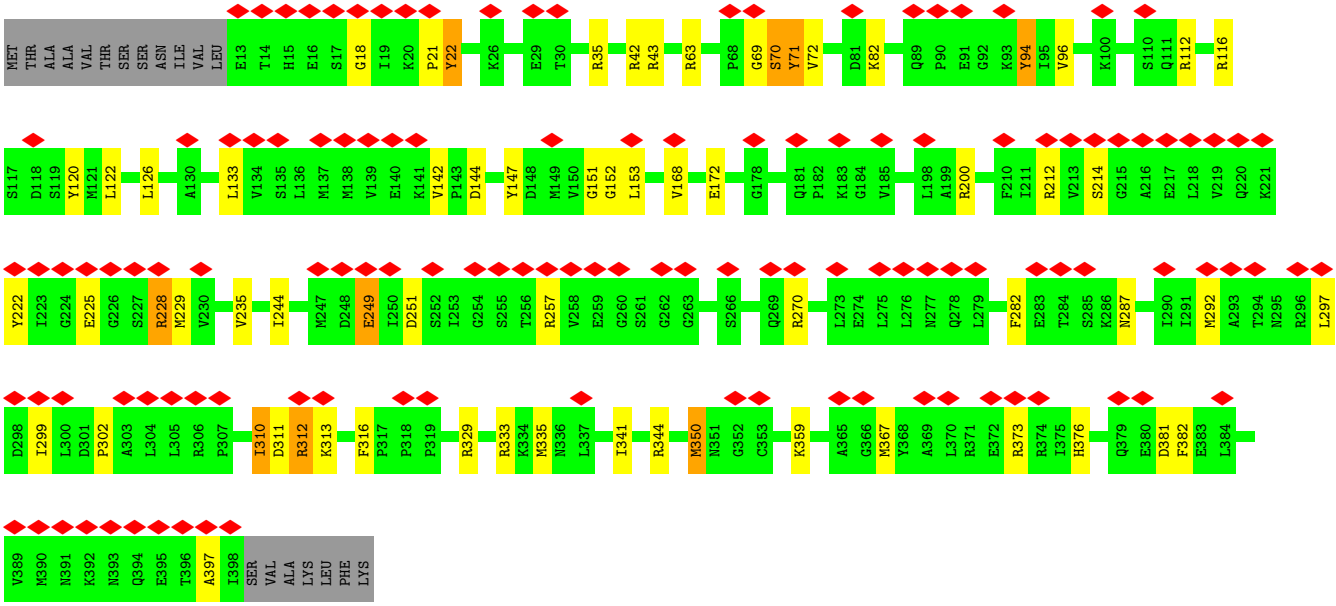
Chain M:





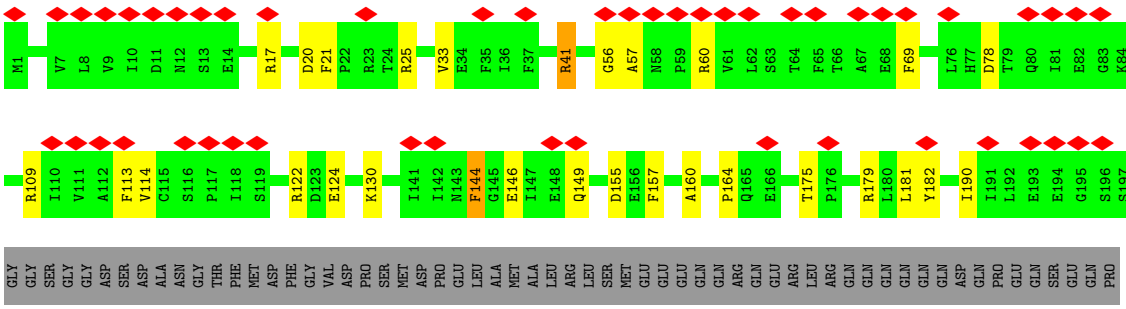
• Molecule 20: 26S protease regulatory subunit 8 homolog

Chain J:



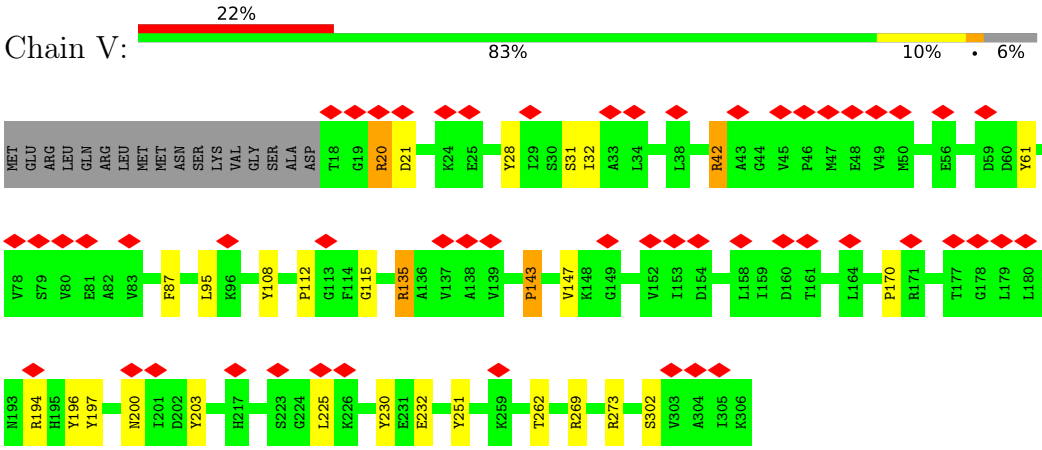
• Molecule 21: 26S proteasome regulatory subunit RPN10

Chain W:



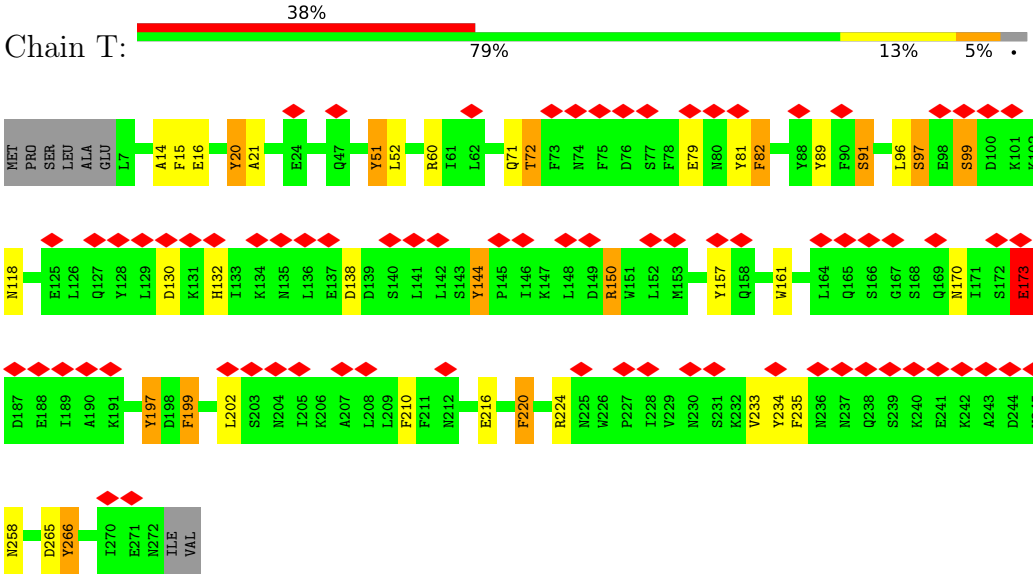
• Molecule 22: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:



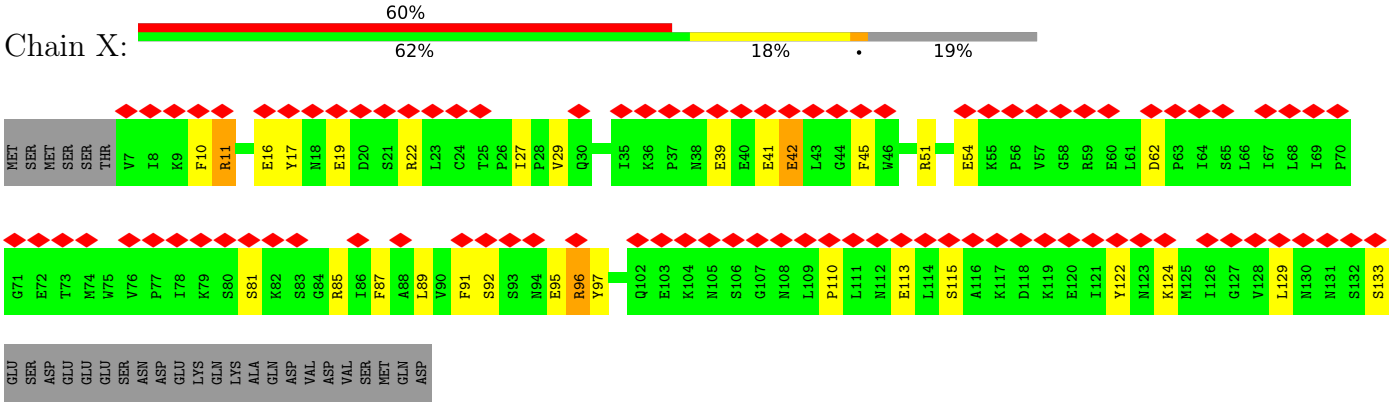
• Molecule 23: 26S proteasome regulatory subunit RPN12

Chain T:



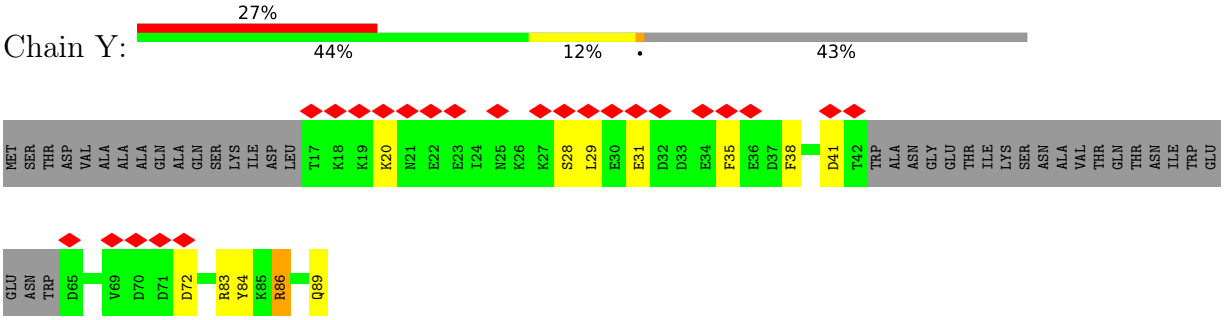
• Molecule 24: 26S proteasome regulatory subunit RPN13

Chain X:



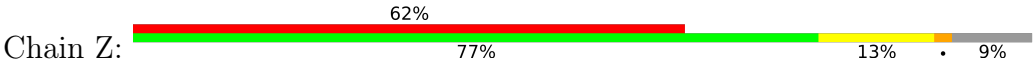
• Molecule 25: 26S proteasome complex subunit SEM1

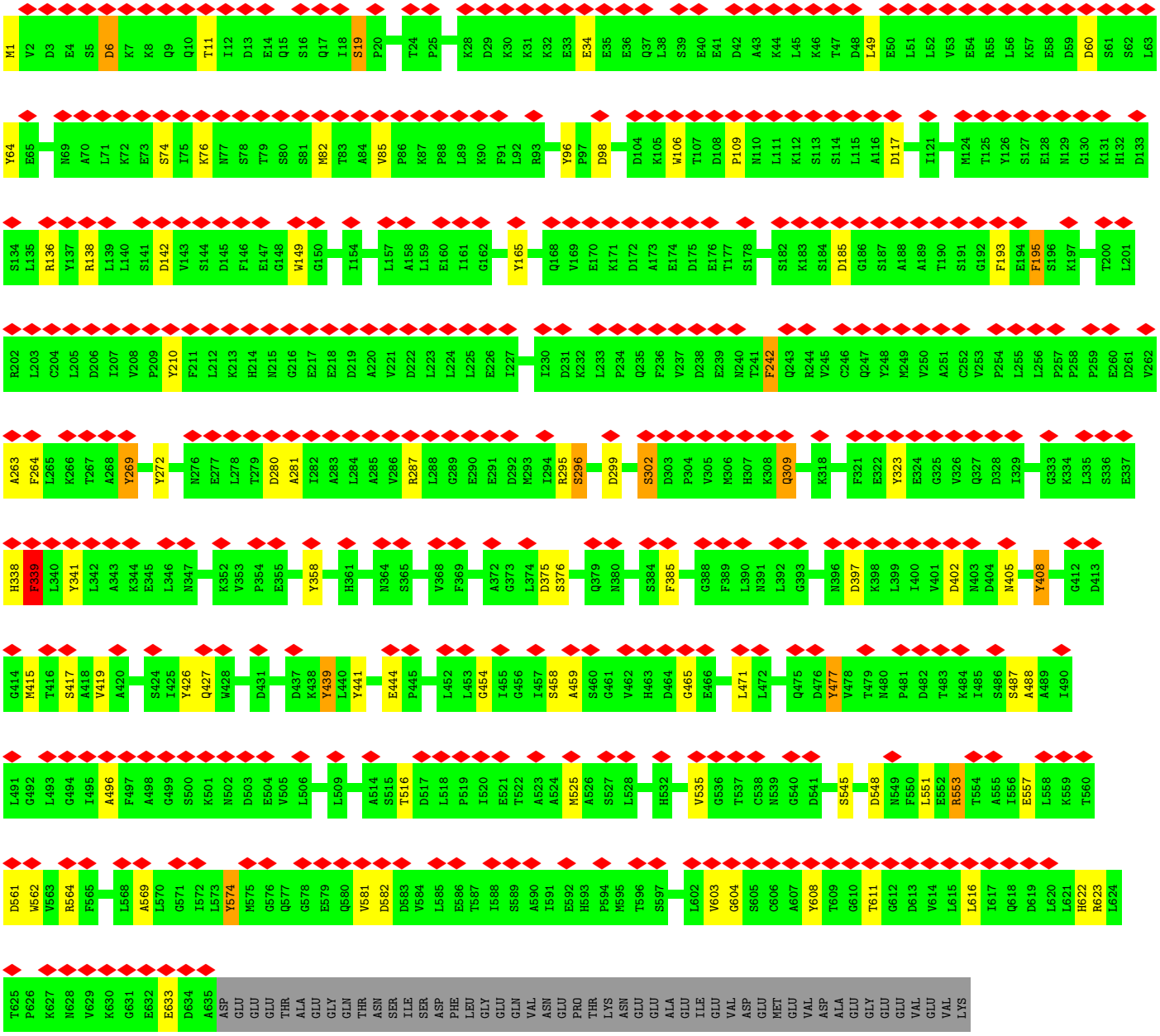
Chain Y:

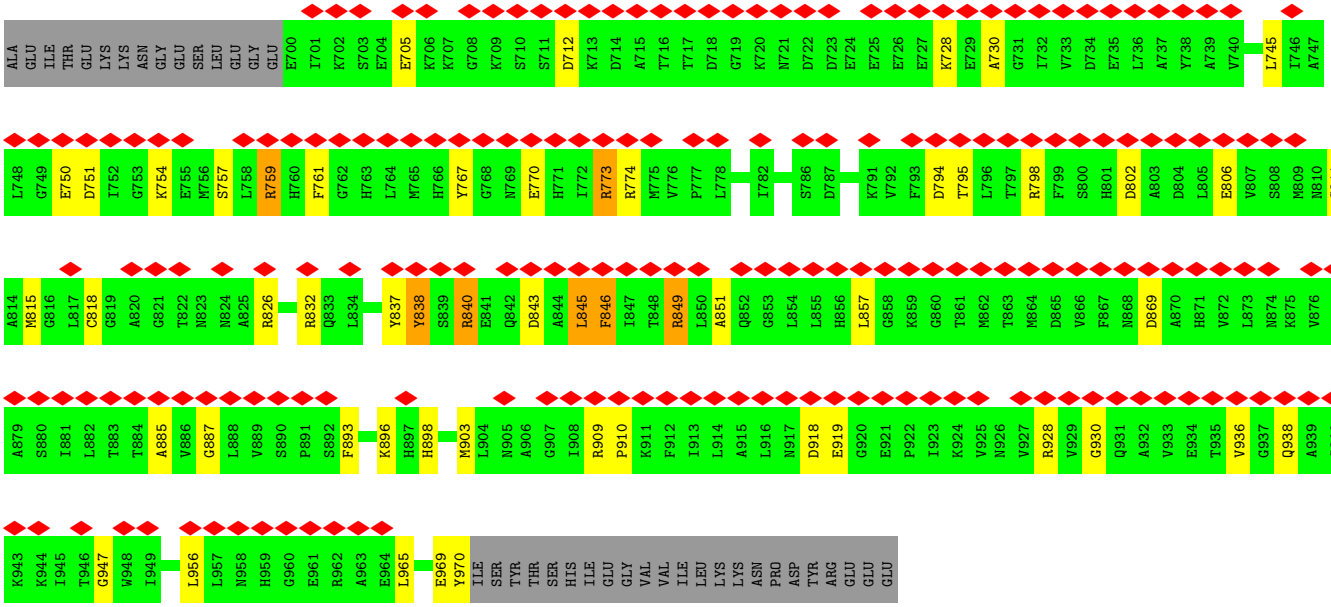


• Molecule 26: 26S proteasome regulatory subunit RPN1

Chain Z:

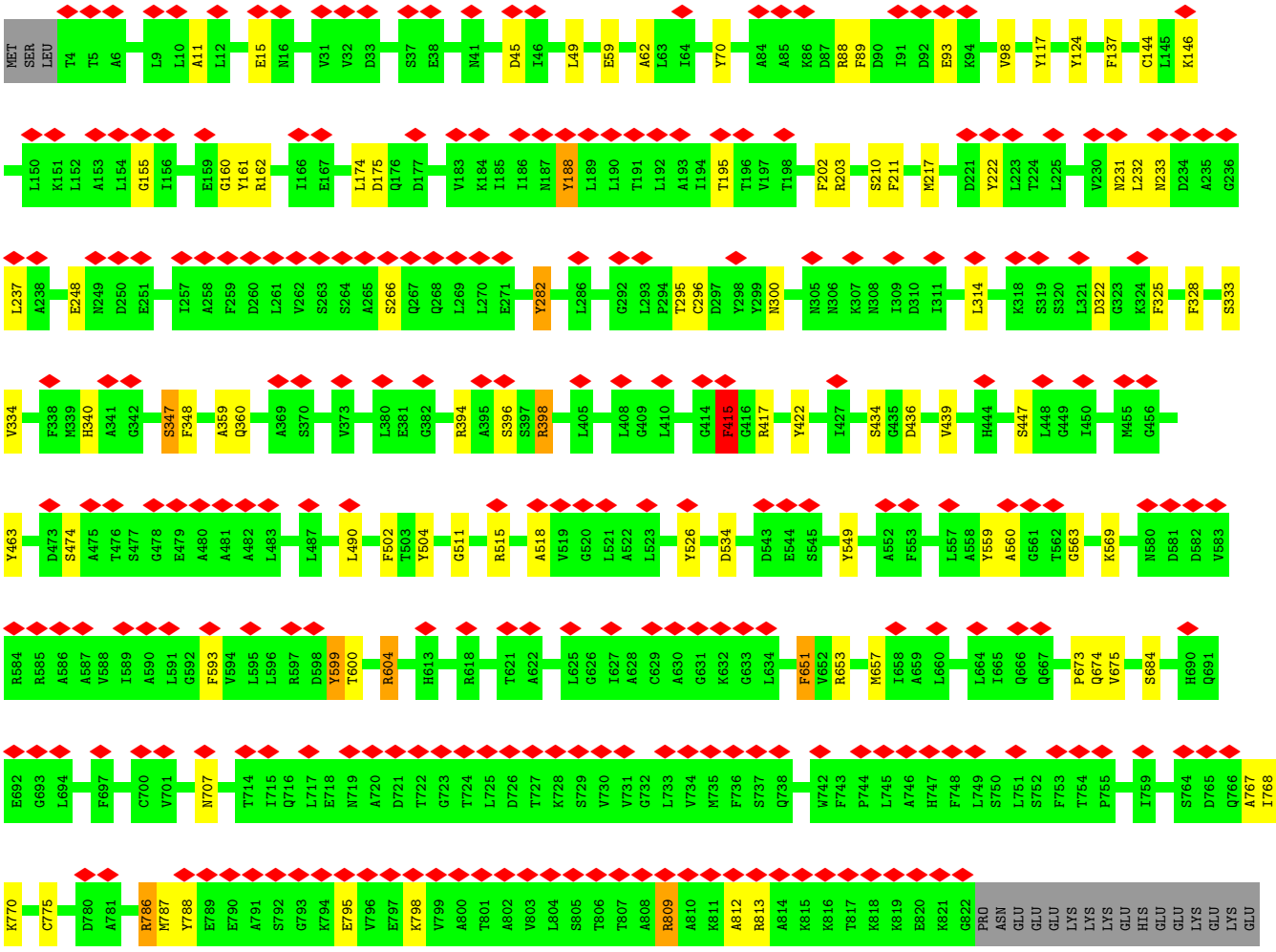


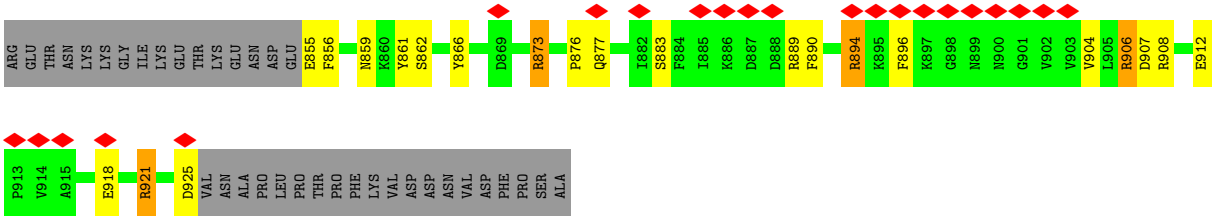




• Molecule 27: 26S proteasome regulatory subunit RPN2

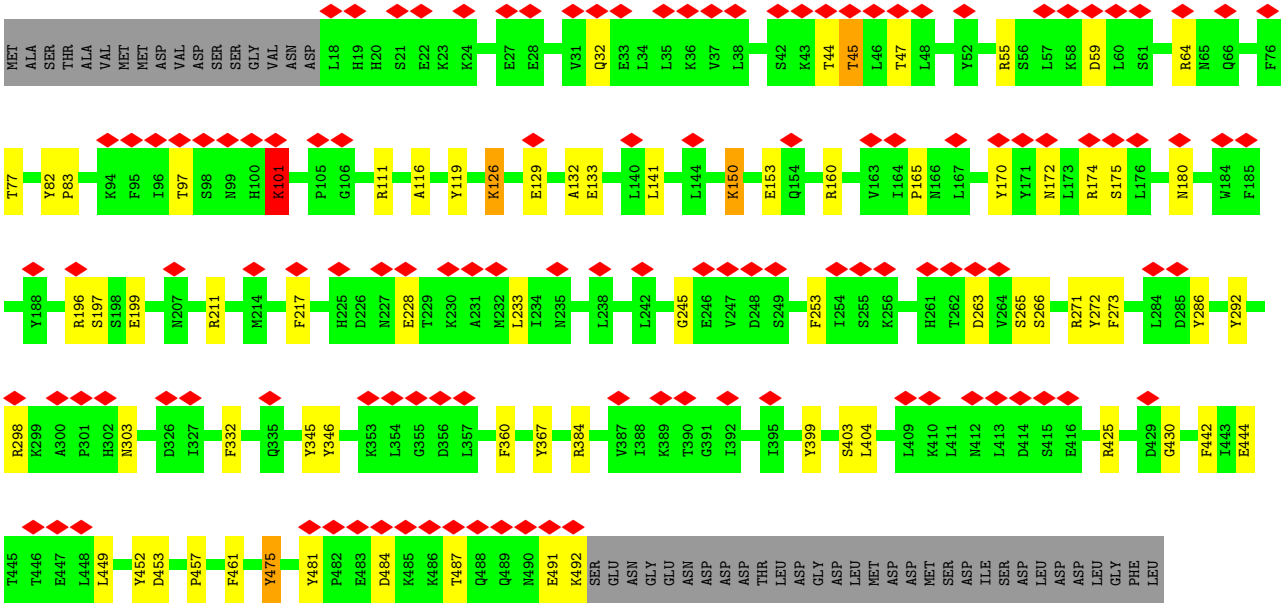
Chain N:





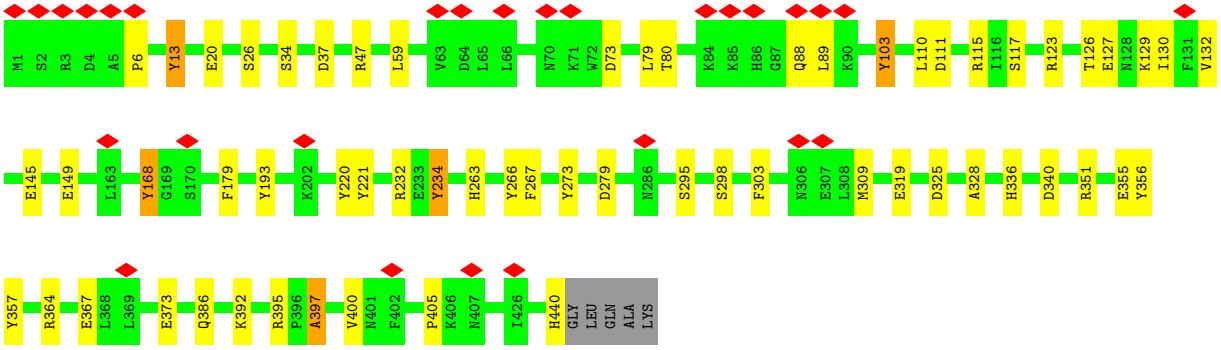
• Molecule 28: 26S proteasome regulatory subunit RPN3

Chain S:



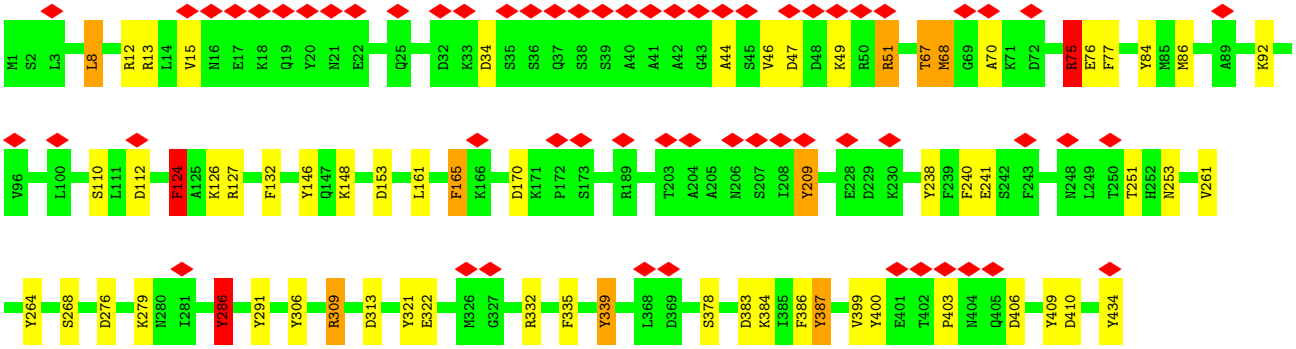
• Molecule 29: 26S proteasome regulatory subunit RPN5

Chain P:



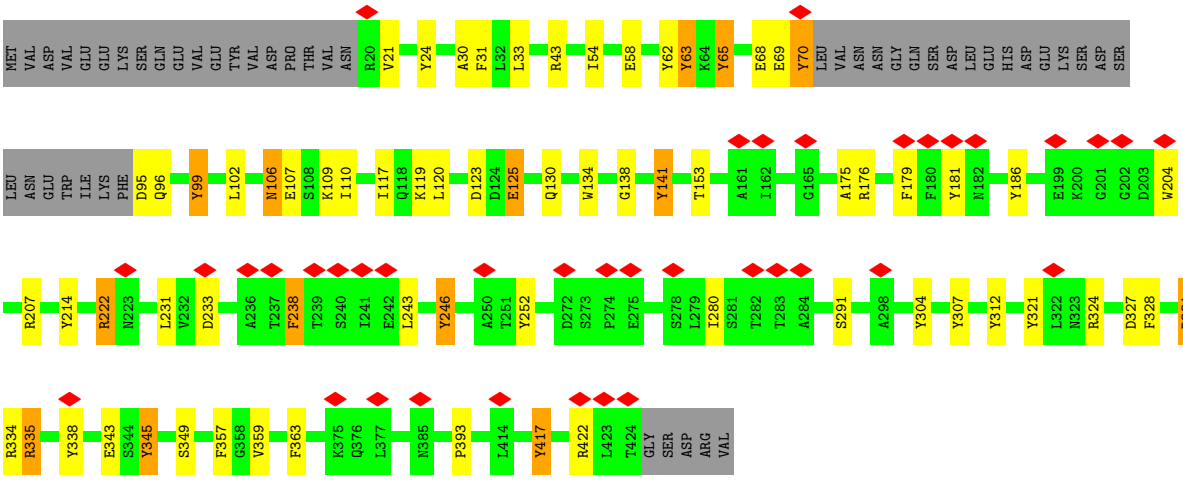
• Molecule 30: 26S proteasome regulatory subunit RPN6

Chain Q:



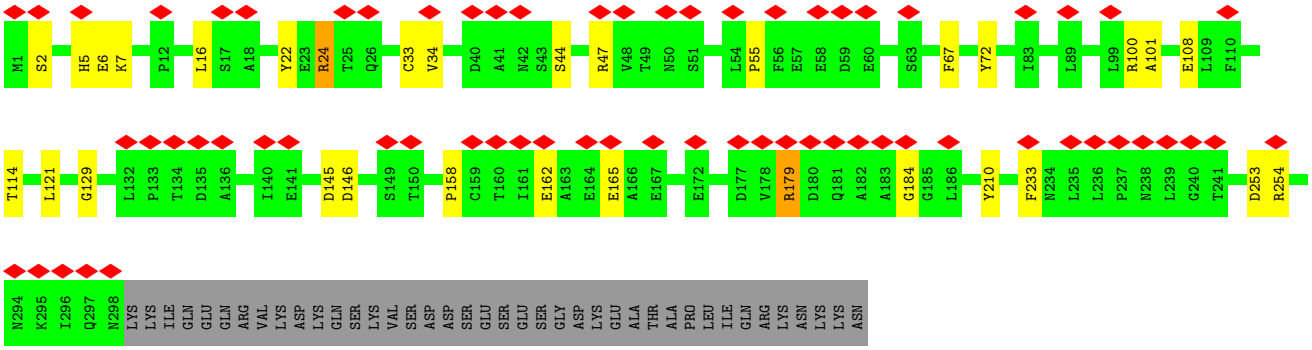
• Molecule 31: 26S proteasome regulatory subunit RPN7

Chain R:



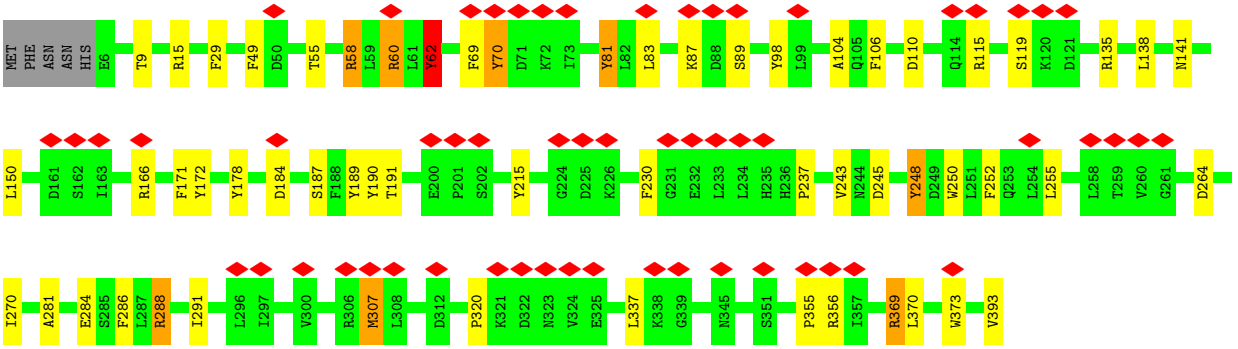
• Molecule 32: 26S proteasome regulatory subunit RPN8

Chain U:



• Molecule 33: 26S proteasome regulatory subunit RPN9

Chain O:


MET PHE ASN ASN HIS E6 T9 R15 F29 F49 D50 T55 R58 L59 R60 L61 Y62 F69 Y70 D71 K72 I73 Y81 L82 L83 K87 D88 S89 Y98 L99 A104 Q105 F106 D110 Q114 R115 S119 K120 D121 R135 L138 N141
L150 D161 S162 I163 R166 F171 Y172 Y178 D184 S187 F188 Y189 Y190 T191 E200 P201 S202 Y215 G224 D225 K226 F230 G231 E232 L233 L234 H235 H236 P237 V243 N244 D245 Y248 D249 W250 L251 F252 Q253 L254 L255 L258 T259 V260 G261 D264
I270 A281 E284 S285 F286 L287 R288 I291 L296 I297 V300 R306 M307 L308 D312 P320 K321 D322 N323 V324 E325 L337 K338 G339 N345 S351 P355 R356 I357 R369 L370 W373 V393

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	67500	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	0.113	Depositor
Minimum map value	-0.074	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.019	Depositor
Map size (Å)	561.60004, 561.60004, 561.60004	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: MG, ANP, ADP

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	2.08	15/1945 (0.8%)	1.88	47/2634 (1.8%)
1	a	1.82	26/1945 (1.3%)	2.02	51/2634 (1.9%)
2	B	1.57	8/1952 (0.4%)	1.72	34/2642 (1.3%)
2	b	1.74	18/1952 (0.9%)	1.89	42/2642 (1.6%)
3	C	1.57	12/1934 (0.6%)	1.66	28/2618 (1.1%)
3	c	1.81	24/1934 (1.2%)	1.89	46/2618 (1.8%)
4	D	1.57	14/1910 (0.7%)	1.79	31/2586 (1.2%)
4	d	1.81	29/1910 (1.5%)	1.98	55/2586 (2.1%)
5	E	1.60	14/1886 (0.7%)	1.74	34/2541 (1.3%)
5	e	1.71	16/1886 (0.8%)	1.86	39/2541 (1.5%)
6	F	1.56	11/1823 (0.6%)	1.69	29/2463 (1.2%)
6	f	1.80	24/1800 (1.3%)	1.97	51/2433 (2.1%)
7	G	1.58	14/1932 (0.7%)	1.73	32/2609 (1.2%)
7	g	1.76	23/1932 (1.2%)	1.94	51/2609 (2.0%)
8	1	1.45	3/1541 (0.2%)	1.60	20/2087 (1.0%)
8	h	1.76	15/1541 (1.0%)	1.96	36/2087 (1.7%)
9	2	1.51	8/1750 (0.5%)	1.66	21/2373 (0.9%)
9	i	1.75	13/1750 (0.7%)	1.94	41/2373 (1.7%)
10	3	1.57	7/1611 (0.4%)	1.65	24/2174 (1.1%)
10	j	1.79	20/1611 (1.2%)	1.91	35/2174 (1.6%)
11	4	1.51	8/1589 (0.5%)	1.60	18/2142 (0.8%)
11	k	1.81	27/1589 (1.7%)	2.02	37/2142 (1.7%)
12	5	1.60	6/1681 (0.4%)	1.59	20/2274 (0.9%)
12	l	1.79	21/1681 (1.2%)	2.00	51/2274 (2.2%)
13	6	1.64	13/1795 (0.7%)	1.67	35/2420 (1.4%)
13	m	1.78	24/1795 (1.3%)	1.97	46/2420 (1.9%)
14	7	1.54	10/1821 (0.5%)	1.63	34/2470 (1.4%)
14	n	1.77	19/1846 (1.0%)	1.92	49/2503 (2.0%)
15	H	1.59	21/3014 (0.7%)	1.75	54/4058 (1.3%)
16	I	1.62	17/3061 (0.6%)	1.72	43/4121 (1.0%)
17	K	1.56	26/3121 (0.8%)	1.64	48/4213 (1.1%)
18	L	1.57	22/3128 (0.7%)	1.64	42/4204 (1.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	M	1.63	21/3023 (0.7%)	1.70	57/4070 (1.4%)
20	J	1.56	21/3073 (0.7%)	1.69	50/4129 (1.2%)
21	W	1.57	7/1557 (0.4%)	1.67	26/2111 (1.2%)
22	V	1.57	14/2309 (0.6%)	1.73	36/3115 (1.2%)
23	T	1.53	10/2235 (0.4%)	1.75	45/3017 (1.5%)
24	X	1.77	11/1058 (1.0%)	1.88	27/1432 (1.9%)
25	Y	1.79	5/438 (1.1%)	1.76	9/583 (1.5%)
26	Z	1.57	42/7122 (0.6%)	1.71	121/9645 (1.3%)
27	N	1.55	45/6994 (0.6%)	1.68	112/9455 (1.2%)
28	S	1.49	17/3966 (0.4%)	1.60	50/5355 (0.9%)
29	P	1.51	21/3663 (0.6%)	1.63	43/4940 (0.9%)
30	Q	1.52	15/3556 (0.4%)	1.65	56/4787 (1.2%)
31	R	1.60	20/3110 (0.6%)	1.85	77/4193 (1.8%)
32	U	1.45	12/2407 (0.5%)	1.56	20/3258 (0.6%)
33	O	1.60	16/3247 (0.5%)	1.70	53/4380 (1.2%)
All	All	1.63	805/110424 (0.7%)	1.75	2006/149135 (1.3%)

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	j	0	5
11	4	0	6
11	k	0	5
12	5	0	2
12	l	0	7
13	6	0	6
13	m	0	6
14	7	0	4
14	n	0	5
15	H	0	7
16	I	0	7
17	K	0	12
18	L	0	10
19	M	0	14
20	J	0	8
21	W	0	1
22	V	0	3
23	T	0	12
24	X	0	2
25	Y	0	2
26	Z	0	13
27	N	0	13
28	S	0	7
29	P	0	8
30	Q	0	9
31	R	0	16
32	U	0	2
33	O	0	6
All	All	0	308

All (805) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	242	GLN	CA-C	56.92	3.00	1.52
22	V	186	GLN	CA-CB	18.71	1.95	1.53
1	A	242	GLN	N-CA	-16.19	1.14	1.46
12	5	212	GLY	C-O	-14.51	1.00	1.23
14	7	229	GLY	C-O	-14.48	1.00	1.23
30	Q	434	TYR	C-O	-12.12	1.00	1.23
29	P	440	HIS	C-O	-12.10	1.00	1.23
4	D	240	GLU	C-O	-12.09	1.00	1.23
27	N	925	ASP	C-O	-12.09	1.00	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	89	GLN	C-O	-12.08	1.00	1.23
7	G	244	ASN	C-O	-12.07	1.00	1.23
19	M	434	ALA	C-OXT	-12.07	1.00	1.23
9	2	226	GLU	C-O	-12.06	1.00	1.23
16	I	437	LEU	C-O	-12.06	1.00	1.23
30	Q	434	TYR	C-OXT	-12.06	1.00	1.23
19	M	434	ALA	C-O	-12.06	1.00	1.23
3	C	244	THR	C-O	-12.05	1.00	1.23
6	F	233	ILE	C-O	-12.05	1.00	1.23
33	O	393	VAL	C-O	-12.05	1.00	1.23
24	X	133	SER	C-O	-12.05	1.00	1.23
12	5	212	GLY	C-OXT	-12.05	1.00	1.23
28	S	492	LYS	C-O	-12.05	1.00	1.23
30	Q	409	TYR	CB-CG	-12.05	1.33	1.51
17	K	428	LYS	C-O	-12.04	1.00	1.23
18	L	436	LYS	C-O	-12.04	1.00	1.23
6	F	233	ILE	C-OXT	-12.04	1.00	1.23
17	K	428	LYS	C-OXT	-12.04	1.00	1.23
27	N	15	GLU	CG-CD	-12.03	1.33	1.51
2	B	250	LEU	C-OXT	-12.03	1.00	1.23
33	O	393	VAL	C-OXT	-12.03	1.00	1.23
25	Y	89	GLN	C-OXT	-12.02	1.00	1.23
2	B	250	LEU	C-O	-12.02	1.00	1.23
13	6	222	ASP	C-OXT	-12.02	1.00	1.23
10	3	204	ASP	C-OXT	-12.01	1.00	1.23
16	I	437	LEU	C-OXT	-12.01	1.00	1.23
10	3	204	ASP	C-O	-12.00	1.00	1.23
13	6	222	ASP	C-O	-12.00	1.00	1.23
6	F	4	ASN	CA-CB	-10.37	1.26	1.53
31	R	70	TYR	CA-CB	9.77	1.75	1.53
22	V	187	ALA	N-CA	-9.69	1.26	1.46
1	a	111	ARG	NE-CZ	8.90	1.44	1.33
3	c	128	ARG	NE-CZ	8.90	1.44	1.33
17	K	207	ARG	C-N	8.67	1.48	1.33
6	f	161	GLY	CA-C	-8.51	1.38	1.51
3	c	211	GLU	CG-CD	8.50	1.64	1.51
27	N	873	ARG	CZ-NH2	8.48	1.44	1.33
23	T	60	ARG	CZ-NH1	8.43	1.44	1.33
31	R	186	TYR	CG-CD2	8.37	1.50	1.39
8	1	185	ARG	CZ-NH2	8.28	1.43	1.33
5	e	48	SER	CA-CB	8.27	1.65	1.52
4	d	164	ARG	NE-CZ	8.06	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	165	ARG	CZ-NH1	7.96	1.43	1.33
33	O	115	ARG	NE-CZ	7.91	1.43	1.33
4	d	95	ARG	CZ-NH1	7.90	1.43	1.33
27	N	474	SER	CA-CB	7.86	1.64	1.52
29	P	26	SER	CA-CB	7.84	1.64	1.52
17	K	252	ARG	NE-CZ	7.81	1.43	1.33
10	j	97	ARG	CD-NE	7.77	1.59	1.46
6	F	2	ARG	NE-CZ	7.76	1.43	1.33
32	U	129	GLY	N-CA	-7.76	1.34	1.46
10	3	202	ARG	CD-NE	7.71	1.59	1.46
5	e	2	ARG	NE-CZ	7.68	1.43	1.33
6	f	56	SER	CA-CB	7.67	1.64	1.52
1	A	122	ARG	NE-CZ	7.65	1.43	1.33
1	a	5	ARG	CZ-NH1	7.64	1.43	1.33
12	l	167	ARG	CZ-NH1	7.58	1.43	1.33
19	M	404	ARG	CD-NE	7.54	1.59	1.46
12	l	167	ARG	CD-NE	7.49	1.59	1.46
19	M	290	ARG	CD-NE	7.46	1.59	1.46
19	M	73	ARG	CZ-NH2	7.44	1.42	1.33
7	g	111	ARG	CZ-NH2	7.41	1.42	1.33
20	J	249	GLU	CD-OE2	7.39	1.33	1.25
13	m	213	ARG	CZ-NH2	7.36	1.42	1.33
28	S	175	SER	CA-CB	7.35	1.64	1.52
4	d	195	ARG	CZ-NH1	7.30	1.42	1.33
3	c	97	TYR	CB-CG	7.29	1.62	1.51
29	P	232	ARG	NE-CZ	7.28	1.42	1.33
3	c	57	GLU	CG-CD	7.26	1.62	1.51
1	a	62	TYR	CG-CD2	7.22	1.48	1.39
1	a	188	GLU	CD-OE1	7.22	1.33	1.25
4	d	109	ARG	NE-CZ	7.21	1.42	1.33
5	E	122	GLU	CD-OE2	7.21	1.33	1.25
11	k	149	ARG	CZ-NH1	7.20	1.42	1.33
31	R	246	TYR	CE1-CZ	7.20	1.48	1.38
3	c	30	HIS	CB-CG	7.20	1.63	1.50
8	h	29	ARG	CZ-NH1	7.20	1.42	1.33
2	b	236	ARG	CZ-NH1	7.18	1.42	1.33
27	N	786	ARG	CZ-NH1	7.17	1.42	1.33
15	H	194	SER	CA-CB	7.17	1.63	1.52
4	d	125	ARG	CD-NE	7.16	1.58	1.46
4	d	195	ARG	NE-CZ	7.15	1.42	1.33
29	P	263	HIS	CB-CG	7.15	1.62	1.50
20	J	151	GLY	CA-C	-7.13	1.40	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	90	ARG	CD-NE	7.13	1.58	1.46
30	Q	409	TYR	CD1-CE1	-7.11	1.28	1.39
14	n	137	TYR	CE1-CZ	7.09	1.47	1.38
28	S	160	ARG	CZ-NH2	7.08	1.42	1.33
1	a	233	GLU	CD-OE2	7.03	1.33	1.25
21	W	41	ARG	NE-CZ	7.02	1.42	1.33
31	R	70	TYR	CG-CD1	-7.02	1.30	1.39
11	k	93	ARG	NE-CZ	7.02	1.42	1.33
17	K	399	ARG	NE-CZ	7.02	1.42	1.33
3	c	49	ARG	CZ-NH2	7.00	1.42	1.33
14	7	143	ALA	CA-CB	-6.99	1.37	1.52
13	m	221	ARG	NE-CZ	6.97	1.42	1.33
15	H	90	ARG	CZ-NH2	6.95	1.42	1.33
33	O	81	TYR	CE2-CZ	6.94	1.47	1.38
25	Y	86	ARG	NE-CZ	6.93	1.42	1.33
29	P	351	ARG	CZ-NH2	6.93	1.42	1.33
1	A	241	GLU	CB-CG	6.92	1.65	1.52
17	K	121	ARG	CZ-NH2	6.91	1.42	1.33
28	S	266	SER	CA-CB	6.91	1.63	1.52
7	g	71	GLY	N-CA	-6.90	1.35	1.46
1	a	87	ARG	CZ-NH2	6.88	1.42	1.33
17	K	298	GLU	CD-OE1	6.84	1.33	1.25
26	Z	477	TYR	CZ-OH	6.84	1.49	1.37
22	V	20	ARG	CZ-NH1	6.83	1.42	1.33
26	Z	553	ARG	NE-CZ	6.83	1.42	1.33
24	X	92	SER	CB-OG	6.83	1.51	1.42
20	J	225	GLU	CD-OE1	6.82	1.33	1.25
2	b	156	TYR	CE1-CZ	6.81	1.47	1.38
4	D	164	ARG	CD-NE	6.80	1.58	1.46
13	6	221	ARG	CZ-NH2	6.79	1.41	1.33
26	Z	774	ARG	NE-CZ	6.78	1.41	1.33
3	c	209	ARG	CD-NE	6.78	1.57	1.46
6	f	100	ARG	CZ-NH2	6.77	1.41	1.33
14	n	182	ARG	CZ-NH1	6.77	1.41	1.33
26	Z	798	ARG	CZ-NH1	6.74	1.41	1.33
4	d	170	ARG	CZ-NH2	6.74	1.41	1.33
26	Z	757	SER	CA-CB	6.73	1.63	1.52
30	Q	13	ARG	CZ-NH1	6.71	1.41	1.33
11	4	70	ARG	NE-CZ	6.71	1.41	1.33
15	H	377	PHE	CB-CG	-6.69	1.40	1.51
24	X	96	ARG	NE-CZ	6.69	1.41	1.33
15	H	435	ARG	NE-CZ	6.68	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	186	ARG	CZ-NH2	6.67	1.41	1.33
27	N	210	SER	CA-CB	6.67	1.62	1.52
13	m	133	ARG	NE-CZ	6.63	1.41	1.33
7	g	70	ILE	C-N	6.62	1.45	1.33
11	k	190	ARG	CD-NE	6.62	1.57	1.46
13	6	28	ARG	CZ-NH2	6.62	1.41	1.33
4	d	179	ARG	CZ-NH1	6.62	1.41	1.33
3	C	143	TYR	CG-CD1	6.62	1.47	1.39
16	I	340	ARG	CD-NE	6.62	1.57	1.46
14	7	138	SER	CA-CB	6.61	1.62	1.52
26	Z	458	SER	CA-CB	6.60	1.62	1.52
8	h	185	ARG	NE-CZ	6.60	1.41	1.33
5	E	153	SER	C-N	6.58	1.44	1.33
27	N	921	ARG	NE-CZ	6.56	1.41	1.33
14	n	187	ARG	CZ-NH1	6.56	1.41	1.33
5	E	2	ARG	NE-CZ	6.55	1.41	1.33
33	O	89	SER	CA-CB	6.54	1.62	1.52
14	n	161	ARG	CZ-NH1	6.52	1.41	1.33
26	Z	263	ALA	N-CA	-6.52	1.33	1.46
4	D	88	ARG	NE-CZ	6.51	1.41	1.33
17	K	350	ARG	N-CA	-6.51	1.33	1.46
11	k	8	ARG	CZ-NH1	6.50	1.41	1.33
27	N	88	ARG	CZ-NH1	6.50	1.41	1.33
3	c	197	SER	CA-CB	6.50	1.62	1.52
12	l	159	ARG	CD-NE	6.49	1.57	1.46
2	b	240	SER	CA-CB	6.48	1.62	1.52
10	j	110	GLY	N-CA	-6.47	1.36	1.46
26	Z	136	ARG	CZ-NH1	6.46	1.41	1.33
4	d	154	TYR	CE2-CZ	-6.46	1.30	1.38
20	J	63	ARG	CZ-NH2	6.43	1.41	1.33
9	i	188	ARG	CZ-NH1	6.42	1.41	1.33
22	V	302	SER	CA-CB	6.42	1.62	1.52
18	L	392	ARG	CZ-NH1	6.41	1.41	1.33
27	N	447	SER	CA-CB	6.39	1.62	1.52
17	K	374	ARG	NE-CZ	6.38	1.41	1.33
1	a	20	GLU	CB-CG	6.38	1.64	1.52
15	H	78	PRO	N-CD	6.38	1.56	1.47
23	T	20	TYR	CZ-OH	6.38	1.48	1.37
19	M	429	SER	CA-CB	6.38	1.62	1.52
33	O	355	PRO	CA-C	-6.36	1.40	1.52
8	1	150	GLU	CD-OE2	6.35	1.32	1.25
12	l	7	ARG	NE-CZ	6.35	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	H	420	ARG	CZ-NH2	6.34	1.41	1.33
13	m	85	SER	CA-CB	6.34	1.62	1.52
5	e	168	SER	CA-CB	6.34	1.62	1.52
10	j	78	GLU	CG-CD	6.34	1.61	1.51
4	d	36	GLY	N-CA	-6.33	1.36	1.46
11	k	67	TYR	CG-CD1	6.33	1.47	1.39
26	Z	138	ARG	CZ-NH1	6.33	1.41	1.33
6	F	67	GLU	CD-OE1	6.32	1.32	1.25
26	Z	773	ARG	CZ-NH1	6.32	1.41	1.33
26	Z	287	ARG	CZ-NH2	6.32	1.41	1.33
3	C	8	ARG	CZ-NH2	6.31	1.41	1.33
4	d	88	ARG	CZ-NH2	6.31	1.41	1.33
15	H	420	ARG	NE-CZ	6.31	1.41	1.33
2	B	90	ARG	CZ-NH2	6.30	1.41	1.33
8	h	70	TYR	CG-CD1	6.28	1.47	1.39
3	C	17	ARG	CZ-NH2	6.28	1.41	1.33
4	D	179	ARG	CZ-NH2	6.27	1.41	1.33
7	g	165	ARG	CD-NE	6.26	1.57	1.46
12	l	124	GLY	CA-C	-6.26	1.41	1.51
6	f	163	ARG	CZ-NH1	6.26	1.41	1.33
26	Z	909	ARG	CZ-NH1	6.25	1.41	1.33
23	T	132	HIS	CB-CG	6.25	1.61	1.50
14	n	103	ARG	NE-CZ	6.24	1.41	1.33
31	R	324	ARG	CZ-NH1	6.24	1.41	1.33
8	h	130	GLY	CA-C	-6.23	1.41	1.51
3	c	3	ARG	CZ-NH2	6.22	1.41	1.33
15	H	158	GLY	N-CA	-6.22	1.36	1.46
11	k	149	ARG	CD-NE	6.22	1.57	1.46
13	6	130	SER	CA-CB	6.21	1.62	1.52
27	N	504	TYR	CZ-OH	6.21	1.48	1.37
5	E	124	ARG	CZ-NH1	6.21	1.41	1.33
12	l	73	ARG	CZ-NH1	6.20	1.41	1.33
1	a	101	TYR	CG-CD2	6.20	1.47	1.39
6	f	203	GLU	CG-CD	6.19	1.61	1.51
4	d	179	ARG	CD-NE	6.18	1.56	1.46
22	V	186	GLN	C-N	-6.18	1.19	1.34
7	g	15	GLY	N-CA	-6.17	1.36	1.46
11	k	21	VAL	CA-CB	-6.17	1.41	1.54
6	f	173	ARG	NE-CZ	6.17	1.41	1.33
6	f	164	SER	CA-CB	6.16	1.62	1.52
13	m	137	ARG	CZ-NH2	6.16	1.41	1.33
12	l	108	GLU	CB-CG	6.16	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	72	GLY	CA-C	-6.15	1.42	1.51
33	O	58	ARG	CD-NE	6.15	1.56	1.46
11	k	95	ARG	CZ-NH2	6.14	1.41	1.33
11	k	93	ARG	CD-NE	6.14	1.56	1.46
17	K	309	SER	CA-CB	6.13	1.62	1.52
27	N	604	ARG	CZ-NH1	6.13	1.41	1.33
5	e	151	GLU	CG-CD	6.13	1.61	1.51
11	k	70	ARG	CZ-NH2	6.13	1.41	1.33
10	j	138	SER	CA-CB	6.11	1.62	1.52
20	J	116	ARG	CZ-NH2	6.11	1.41	1.33
14	7	161	ARG	CZ-NH2	6.11	1.41	1.33
10	j	27	ARG	CZ-NH2	6.10	1.41	1.33
29	P	20	GLU	CD-OE1	6.10	1.32	1.25
1	A	62	TYR	CE1-CZ	6.10	1.46	1.38
7	g	87	ARG	NE-CZ	6.09	1.41	1.33
4	D	224	SER	CA-CB	6.09	1.62	1.52
2	B	99	ARG	NE-CZ	6.08	1.41	1.33
6	f	88	ARG	CZ-NH1	6.07	1.41	1.33
7	G	128	PHE	CG-CD1	6.07	1.47	1.38
31	R	176	ARG	CZ-NH1	6.06	1.41	1.33
10	j	98	ARG	CZ-NH1	6.05	1.41	1.33
28	S	160	ARG	NE-CZ	6.05	1.41	1.33
11	k	135	TYR	CE2-CZ	6.05	1.46	1.38
27	N	873	ARG	NE-CZ	6.05	1.41	1.33
8	h	68	SER	N-CA	-6.04	1.34	1.46
1	a	68	ARG	CZ-NH1	6.04	1.41	1.33
32	U	233	PHE	CG-CD1	6.04	1.47	1.38
7	g	4	TYR	CB-CG	-6.03	1.42	1.51
12	l	114	TYR	CE1-CZ	6.03	1.46	1.38
1	a	215	GLU	CG-CD	6.03	1.60	1.51
10	j	42	ILE	N-CA	-6.03	1.34	1.46
3	c	212	PHE	CG-CD2	6.03	1.47	1.38
4	d	109	ARG	CZ-NH1	6.03	1.40	1.33
8	h	36	ARG	NE-CZ	6.03	1.40	1.33
29	P	34	SER	CA-CB	6.02	1.61	1.52
4	D	181	GLU	CD-OE2	6.01	1.32	1.25
15	H	273	ARG	CZ-NH2	6.01	1.40	1.33
30	Q	409	TYR	CG-CD1	-6.01	1.31	1.39
31	R	393	PRO	CA-C	-6.01	1.40	1.52
1	a	140	GLU	CB-CG	6.01	1.63	1.52
6	f	136	TYR	CG-CD2	6.01	1.47	1.39
10	3	176	ARG	NE-CZ	6.00	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	L	53	HIS	CB-CG	6.00	1.60	1.50
9	i	123	TYR	CE1-CZ	5.99	1.46	1.38
26	Z	837	TYR	CB-CG	-5.99	1.42	1.51
30	Q	12	ARG	CD-NE	5.99	1.56	1.46
3	C	4	ARG	CZ-NH2	5.98	1.40	1.33
11	4	48	GLY	N-CA	-5.98	1.37	1.46
27	N	137	PHE	CG-CD1	5.98	1.47	1.38
3	c	91	ARG	NE-CZ	5.97	1.40	1.33
16	I	372	SER	CA-CB	5.97	1.61	1.52
22	V	135	ARG	CD-NE	5.97	1.56	1.46
12	l	203	GLU	CD-OE2	-5.97	1.19	1.25
13	m	188	PHE	CG-CD1	5.97	1.47	1.38
18	L	345	ARG	CD-NE	5.97	1.56	1.46
18	L	194	ARG	NE-CZ	5.96	1.40	1.33
10	j	86	PHE	N-CA	-5.96	1.34	1.46
24	X	54	GLU	CA-CB	5.96	1.67	1.53
2	B	246	ARG	NE-CZ	5.95	1.40	1.33
24	X	11	ARG	CD-NE	5.95	1.56	1.46
7	g	186	ARG	CZ-NH1	5.95	1.40	1.33
23	T	224	ARG	NE-CZ	5.95	1.40	1.33
14	n	54	SER	CB-OG	5.94	1.50	1.42
16	I	300	ARG	CZ-NH1	5.94	1.40	1.33
29	P	373	GLU	CG-CD	5.94	1.60	1.51
31	R	43	ARG	CZ-NH1	5.94	1.40	1.33
9	i	61	SER	CB-OG	5.94	1.50	1.42
4	D	156	SER	CA-CB	5.93	1.61	1.52
17	K	60	LEU	CA-CB	5.93	1.67	1.53
11	4	190	ARG	CZ-NH1	5.92	1.40	1.33
1	A	15	ARG	CZ-NH1	5.91	1.40	1.33
26	Z	34	GLU	CG-CD	5.90	1.60	1.51
6	f	50	ARG	CD-NE	5.90	1.56	1.46
9	2	20	SER	CA-CB	5.90	1.61	1.52
14	n	103	ARG	CD-NE	5.90	1.56	1.46
1	a	157	TYR	CB-CG	5.89	1.60	1.51
20	J	142	VAL	CB-CG1	5.89	1.65	1.52
12	l	72	GLU	CD-OE1	5.89	1.32	1.25
9	i	8	PHE	CG-CD2	5.89	1.47	1.38
28	S	211	ARG	CZ-NH1	5.89	1.40	1.33
27	N	599	TYR	CZ-OH	5.88	1.47	1.37
4	d	95	ARG	CZ-NH2	5.88	1.40	1.33
5	e	158	ARG	NE-CZ	5.87	1.40	1.33
3	C	156	TYR	CB-CG	-5.87	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	N	795	GLU	CD-OE2	5.87	1.32	1.25
22	V	187	ALA	C-N	-5.87	1.20	1.34
18	L	77	ARG	NE-CZ	5.86	1.40	1.33
28	S	211	ARG	NE-CZ	5.86	1.40	1.33
2	b	69	PRO	N-CD	-5.86	1.39	1.47
6	f	95	SER	CA-CB	5.86	1.61	1.52
27	N	398	ARG	CZ-NH1	5.86	1.40	1.33
27	N	653	ARG	NE-CZ	5.85	1.40	1.33
13	m	98	TYR	CE1-CZ	5.84	1.46	1.38
16	I	101	GLY	CA-C	-5.84	1.42	1.51
31	R	99	TYR	CE1-CZ	-5.84	1.30	1.38
5	e	169	GLU	CB-CG	5.84	1.63	1.52
2	b	207	ASP	CA-CB	5.83	1.66	1.53
17	K	73	ARG	CD-NE	5.83	1.56	1.46
31	R	312	TYR	CZ-OH	5.83	1.47	1.37
7	G	87	ARG	CZ-NH2	5.83	1.40	1.33
21	W	17	ARG	NE-CZ	5.83	1.40	1.33
28	S	491	GLU	CG-CD	5.83	1.60	1.51
8	h	174	ARG	CD-NE	5.82	1.56	1.46
2	b	48	GLU	CB-CG	5.82	1.63	1.52
27	N	15	GLU	CB-CG	-5.82	1.41	1.52
16	I	408	ARG	NE-CZ	5.82	1.40	1.33
19	M	42	ARG	NE-CZ	5.82	1.40	1.33
22	V	194	ARG	CZ-NH1	5.81	1.40	1.33
5	e	1	ASP	N-CA	5.81	1.57	1.46
19	M	196	ALA	CA-C	-5.81	1.37	1.52
18	L	259	SER	CA-CB	5.81	1.61	1.52
26	Z	928	ARG	NE-CZ	5.81	1.40	1.33
4	d	152	GLY	N-CA	-5.80	1.37	1.46
27	N	117	TYR	CE2-CZ	5.80	1.46	1.38
12	5	144	TYR	CG-CD2	5.80	1.46	1.39
5	E	114	ARG	NE-CZ	5.79	1.40	1.33
4	d	125	ARG	CZ-NH1	5.79	1.40	1.33
12	l	167	ARG	CZ-NH2	5.79	1.40	1.33
4	D	56	ARG	NE-CZ	5.79	1.40	1.33
3	c	159	TRP	CD2-CE3	-5.78	1.31	1.40
10	j	202	ARG	NE-CZ	5.78	1.40	1.33
9	2	129	SER	CA-CB	5.78	1.61	1.52
21	W	182	TYR	CG-CD1	5.78	1.46	1.39
26	Z	705	GLU	CB-CG	5.78	1.63	1.52
2	b	226	GLY	N-CA	-5.77	1.37	1.46
13	m	137	ARG	CD-NE	5.76	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	185	ILE	CA-CB	5.76	1.68	1.54
1	a	191	GLU	CD-OE2	5.76	1.31	1.25
2	b	7	PHE	CG-CD1	5.75	1.47	1.38
28	S	457	PRO	CA-C	-5.75	1.41	1.52
15	H	434	ARG	CZ-NH2	5.74	1.40	1.33
6	F	32	SER	CA-CB	5.74	1.61	1.52
30	Q	12	ARG	CZ-NH1	5.74	1.40	1.33
22	V	187	ALA	CA-CB	5.74	1.64	1.52
26	Z	295	ARG	NE-CZ	5.74	1.40	1.33
2	b	246	ARG	CZ-NH2	5.73	1.40	1.33
14	n	31	GLY	CA-C	-5.73	1.42	1.51
18	L	434	TYR	CE1-CZ	5.73	1.46	1.38
27	N	908	ARG	CZ-NH1	5.73	1.40	1.33
6	f	17	ARG	NE-CZ	5.73	1.40	1.33
32	U	34	VAL	N-CA	-5.73	1.34	1.46
18	L	434	TYR	CZ-OH	5.72	1.47	1.37
5	e	84	ALA	CA-CB	5.72	1.64	1.52
27	N	813	ARG	CD-NE	5.72	1.56	1.46
17	K	207	ARG	CZ-NH2	5.72	1.40	1.33
26	Z	74	SER	CA-CB	5.71	1.61	1.52
5	e	64	ARG	CZ-NH2	5.71	1.40	1.33
27	N	15	GLU	CA-CB	-5.71	1.41	1.53
1	a	71	GLY	N-CA	-5.71	1.37	1.46
12	l	7	ARG	CD-NE	5.70	1.56	1.46
3	c	97	TYR	CG-CD1	5.70	1.46	1.39
13	6	144	SER	CA-CB	5.70	1.61	1.52
31	R	102	LEU	CA-C	-5.70	1.38	1.52
7	G	81	GLY	CA-C	-5.70	1.42	1.51
7	g	128	PHE	CG-CD1	5.69	1.47	1.38
28	S	452	TYR	CE1-CZ	5.68	1.46	1.38
1	A	126	ARG	CZ-NH2	5.68	1.40	1.33
2	B	182	GLU	CG-CD	5.68	1.60	1.51
11	k	67	TYR	CE1-CZ	5.68	1.46	1.38
20	J	212	ARG	CZ-NH1	5.67	1.40	1.33
5	e	45	ARG	CZ-NH1	5.67	1.40	1.33
2	B	198	GLU	CD-OE2	5.67	1.31	1.25
6	f	98	PHE	CG-CD2	5.67	1.47	1.38
12	l	19	ARG	CZ-NH1	5.66	1.40	1.33
9	i	207	ARG	NE-CZ	5.66	1.40	1.33
14	n	175	GLU	CB-CG	5.66	1.62	1.52
4	d	46	ARG	CZ-NH2	5.66	1.40	1.33
9	i	100	VAL	CB-CG2	5.65	1.64	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	187	TYR	CB-CG	-5.65	1.43	1.51
6	F	127	TYR	CE2-CZ	5.65	1.45	1.38
6	f	94	SER	CA-CB	5.65	1.61	1.52
13	6	185	ARG	CZ-NH2	5.65	1.40	1.33
26	Z	417	SER	CA-CB	5.65	1.61	1.52
11	4	135	TYR	CE2-CZ	5.64	1.45	1.38
9	i	193	PRO	N-CD	-5.64	1.40	1.47
1	a	37	ARG	CZ-NH2	5.63	1.40	1.33
9	i	72	ARG	CZ-NH2	5.63	1.40	1.33
28	S	197	SER	CA-CB	5.63	1.61	1.52
12	l	106	ARG	NE-CZ	5.63	1.40	1.33
29	P	367	GLU	CD-OE1	5.62	1.31	1.25
17	K	396	ARG	CD-NE	5.62	1.56	1.46
1	a	15	ARG	CZ-NH2	5.62	1.40	1.33
2	b	138	GLY	N-CA	-5.62	1.37	1.46
3	c	150	SER	CA-CB	5.62	1.61	1.52
1	A	11	SER	CA-CB	5.62	1.61	1.52
20	J	71	TYR	CB-CG	-5.62	1.43	1.51
26	Z	439	TYR	CG-CD1	5.62	1.46	1.39
28	S	360	PHE	CE2-CZ	5.62	1.48	1.37
1	A	2	GLY	N-CA	5.62	1.54	1.46
10	j	187	TYR	CG-CD2	5.61	1.46	1.39
23	T	150	ARG	CZ-NH1	5.61	1.40	1.33
1	a	96	ARG	CZ-NH1	5.61	1.40	1.33
12	l	106	ARG	CZ-NH2	5.61	1.40	1.33
14	7	128	ARG	CZ-NH1	5.61	1.40	1.33
11	4	23	ARG	NE-CZ	5.61	1.40	1.33
3	c	136	TYR	CZ-OH	5.61	1.47	1.37
30	Q	268	SER	CA-CB	5.60	1.61	1.52
3	c	51	VAL	N-CA	-5.60	1.35	1.46
6	F	57	SER	CB-OG	5.60	1.49	1.42
19	M	245	LYS	CA-CB	5.59	1.66	1.53
9	i	196	ARG	CZ-NH2	5.59	1.40	1.33
13	m	221	ARG	CZ-NH2	5.58	1.40	1.33
27	N	515	ARG	CZ-NH2	5.58	1.40	1.33
29	P	115	ARG	NE-CZ	5.58	1.40	1.33
18	L	357	ARG	CZ-NH2	5.58	1.40	1.33
9	i	38	SER	CB-OG	-5.58	1.34	1.42
9	i	180	ILE	N-CA	-5.58	1.35	1.46
11	k	23	ARG	CZ-NH1	5.58	1.40	1.33
9	2	72	ARG	CZ-NH2	5.57	1.40	1.33
33	O	70	TYR	CA-CB	5.57	1.66	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	4	ARG	CZ-NH2	5.57	1.40	1.33
20	J	212	ARG	NE-CZ	5.57	1.40	1.33
15	H	88	ARG	CZ-NH1	5.57	1.40	1.33
16	I	111	GLU	CD-OE2	5.56	1.31	1.25
3	c	5	TYR	CG-CD2	5.56	1.46	1.39
18	L	77	ARG	CZ-NH1	5.56	1.40	1.33
7	G	112	LEU	C-N	5.55	1.43	1.33
7	G	141	GLY	CA-C	-5.54	1.43	1.51
26	Z	287	ARG	CZ-NH1	5.54	1.40	1.33
18	L	69	ARG	CD-NE	5.54	1.55	1.46
27	N	684	SER	CB-OG	5.54	1.49	1.42
7	g	135	GLY	CA-C	-5.53	1.43	1.51
15	H	432	ARG	CZ-NH1	5.53	1.40	1.33
19	M	42	ARG	CZ-NH2	5.53	1.40	1.33
6	f	38	ARG	NE-CZ	5.53	1.40	1.33
23	T	109	TYR	CZ-OH	5.53	1.47	1.37
23	T	186	ARG	CD-NE	5.53	1.55	1.46
31	R	130	GLN	CA-CB	5.53	1.66	1.53
15	H	346	ARG	CD-NE	5.53	1.55	1.46
20	J	112	ARG	NE-CZ	5.53	1.40	1.33
24	X	85	ARG	NE-CZ	5.53	1.40	1.33
19	M	409	SER	CA-CB	5.52	1.61	1.52
28	S	430	GLY	CA-C	-5.52	1.43	1.51
19	M	339	ARG	CZ-NH1	5.52	1.40	1.33
31	R	99	TYR	CB-CG	-5.51	1.43	1.51
8	h	126	ILE	CA-CB	-5.51	1.42	1.54
32	U	108	GLU	CG-CD	5.51	1.60	1.51
2	b	83	ARG	CD-NE	5.51	1.55	1.46
11	k	12	SER	CA-CB	5.50	1.61	1.52
27	N	394	ARG	CD-NE	5.50	1.55	1.46
26	Z	149	TRP	CZ2-CH2	5.50	1.47	1.37
14	n	41	ARG	NE-CZ	5.50	1.40	1.33
13	m	171	PRO	CA-C	-5.50	1.41	1.52
4	d	125	ARG	CZ-NH2	5.50	1.40	1.33
7	g	22	TYR	CE2-CZ	5.49	1.45	1.38
1	a	97	TYR	CG-CD1	5.49	1.46	1.39
2	b	178	ARG	CZ-NH1	5.49	1.40	1.33
6	f	211	SER	CA-CB	5.49	1.61	1.52
22	V	194	ARG	NE-CZ	5.49	1.40	1.33
7	G	134	PHE	N-CA	-5.49	1.35	1.46
20	J	313	LYS	CA-CB	5.49	1.66	1.53
32	U	158	PRO	CA-C	-5.49	1.41	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	Q	332	ARG	CZ-NH1	5.48	1.40	1.33
7	g	205	GLU	CD-OE1	5.48	1.31	1.25
17	K	396	ARG	CZ-NH1	5.48	1.40	1.33
4	d	46	ARG	NE-CZ	5.48	1.40	1.33
10	3	84	GLU	CD-OE2	5.48	1.31	1.25
33	O	356	ARG	CD-NE	5.48	1.55	1.46
4	D	93	SER	CB-OG	5.47	1.49	1.42
32	U	165	GLU	CB-CG	5.47	1.62	1.52
14	7	161	ARG	CD-NE	5.47	1.55	1.46
17	K	259	ARG	NE-CZ	5.47	1.40	1.33
20	J	152	GLY	N-CA	-5.47	1.37	1.46
12	l	64	ARG	CZ-NH1	5.46	1.40	1.33
32	U	158	PRO	N-CD	-5.46	1.40	1.47
22	V	28	TYR	CD1-CE1	5.46	1.47	1.39
13	6	103	PHE	CG-CD1	5.46	1.47	1.38
27	N	653	ARG	CZ-NH2	5.46	1.40	1.33
13	m	106	TYR	CZ-OH	5.46	1.47	1.37
21	W	124	GLU	CG-CD	5.45	1.60	1.51
19	M	50	ARG	CZ-NH1	5.45	1.40	1.33
18	L	392	ARG	CZ-NH2	5.45	1.40	1.33
27	N	809	ARG	CZ-NH2	5.45	1.40	1.33
29	P	298	SER	CA-CB	5.45	1.61	1.52
6	f	5	TYR	CE2-CZ	5.44	1.45	1.38
4	d	46	ARG	CZ-NH1	5.44	1.40	1.33
11	k	58	GLU	CB-CG	5.44	1.62	1.52
3	C	5	TYR	CD2-CE2	5.44	1.47	1.39
5	e	82	GLU	N-CA	-5.44	1.35	1.46
12	5	135	PHE	CG-CD1	5.44	1.47	1.38
14	7	88	GLU	CD-OE2	5.44	1.31	1.25
20	J	43	ARG	CZ-NH1	5.44	1.40	1.33
19	M	213	ARG	CZ-NH1	5.44	1.40	1.33
27	N	396	SER	CA-CB	5.44	1.61	1.52
27	N	889	ARG	CZ-NH2	5.44	1.40	1.33
21	W	21	PHE	CB-CG	5.43	1.60	1.51
4	D	118	TYR	CG-CD1	5.43	1.46	1.39
3	C	145	TYR	CG-CD1	5.43	1.46	1.39
10	3	102	TYR	CG-CD2	5.43	1.46	1.39
15	H	242	PRO	N-CA	-5.43	1.38	1.47
1	a	122	ARG	CZ-NH2	5.42	1.40	1.33
7	g	99	TYR	CB-CG	-5.42	1.43	1.51
26	Z	969	GLU	CD-OE1	5.42	1.31	1.25
4	d	172	PHE	CG-CD2	5.42	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	199	GLU	CB-CG	5.42	1.62	1.52
23	T	81	TYR	CE1-CZ	5.42	1.45	1.38
19	M	221	TYR	CE1-CZ	5.42	1.45	1.38
18	L	85	GLU	CD-OE1	5.42	1.31	1.25
14	n	76	TYR	CG-CD1	5.41	1.46	1.39
15	H	324	GLY	C-N	5.41	1.42	1.33
3	c	143	TYR	CE1-CZ	5.41	1.45	1.38
9	2	167	LEU	C-N	5.41	1.42	1.33
33	O	369	ARG	CZ-NH1	5.41	1.40	1.33
33	O	135	ARG	CZ-NH2	5.40	1.40	1.33
4	d	163	GLY	CA-C	-5.40	1.43	1.51
33	O	172	TYR	CE2-CZ	5.40	1.45	1.38
6	F	173	ARG	NE-CZ	5.40	1.40	1.33
33	O	291	ILE	CB-CG1	-5.40	1.39	1.54
11	k	36	ARG	CZ-NH1	5.39	1.40	1.33
16	I	436	TYR	CG-CD2	5.39	1.46	1.39
10	j	202	ARG	CZ-NH2	5.39	1.40	1.33
15	H	62	ARG	CZ-NH1	5.39	1.40	1.33
10	j	196	LYS	N-CA	-5.38	1.35	1.46
10	j	67	ARG	CZ-NH2	5.38	1.40	1.33
9	2	88	PHE	CB-CG	5.38	1.60	1.51
28	S	170	TYR	CZ-OH	5.38	1.47	1.37
26	Z	454	GLY	CA-C	5.38	1.60	1.51
8	h	102	TYR	CG-CD1	5.38	1.46	1.39
12	5	40	PHE	CE2-CZ	5.37	1.47	1.37
8	h	1	THR	N-CA	5.37	1.57	1.46
5	E	239	GLU	CD-OE2	-5.37	1.19	1.25
8	h	42	TRP	CG-CD1	-5.37	1.29	1.36
20	J	329	ARG	CZ-NH2	5.37	1.40	1.33
20	J	333	ARG	CZ-NH1	5.36	1.40	1.33
26	Z	149	TRP	CE3-CZ3	5.36	1.47	1.38
1	a	190	TRP	CZ2-CH2	5.36	1.47	1.37
2	b	246	ARG	NE-CZ	5.36	1.40	1.33
27	N	604	ARG	CG-CD	5.36	1.65	1.51
5	e	78	ARG	CZ-NH2	5.35	1.40	1.33
27	N	798	LYS	N-CA	-5.35	1.35	1.46
12	l	25	TRP	CD2-CE3	-5.35	1.32	1.40
13	m	157	LYS	N-CA	-5.35	1.35	1.46
20	J	249	GLU	CB-CG	5.35	1.62	1.52
26	Z	136	ARG	NE-CZ	5.35	1.40	1.33
5	e	123	GLU	CG-CD	-5.35	1.44	1.51
6	f	50	ARG	CZ-NH2	5.35	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	1	THR	N-CA	5.35	1.57	1.46
15	H	285	GLY	CA-C	-5.35	1.43	1.51
17	K	236	ARG	NE-CZ	5.35	1.40	1.33
26	Z	826	ARG	NE-CZ	5.35	1.40	1.33
13	m	105	TYR	CE1-CZ	5.34	1.45	1.38
32	U	162	GLU	CD-OE2	5.34	1.31	1.25
8	1	29	ARG	CZ-NH2	5.34	1.40	1.33
18	L	341	GLY	CA-C	-5.33	1.43	1.51
1	a	111	ARG	CD-NE	5.33	1.55	1.46
3	c	158	GLY	CA-C	-5.33	1.43	1.51
5	E	78	ARG	CD-NE	5.33	1.55	1.46
3	c	140	ASP	N-CA	-5.33	1.35	1.46
10	j	95	TYR	CB-CG	-5.33	1.43	1.51
14	7	35	ARG	CZ-NH2	5.33	1.40	1.33
33	O	166	ARG	CZ-NH2	5.33	1.40	1.33
32	U	121	LEU	N-CA	-5.32	1.35	1.46
10	j	115	SER	CA-CB	5.32	1.60	1.52
29	P	149	GLU	CD-OE1	5.32	1.31	1.25
32	U	254	ARG	CZ-NH2	5.32	1.40	1.33
27	N	202	PHE	CG-CD1	5.32	1.46	1.38
1	A	64	PHE	CG-CD1	5.32	1.46	1.38
11	k	50	ALA	C-N	5.31	1.42	1.33
20	J	311	ASP	CB-CG	5.31	1.62	1.51
16	I	205	PRO	N-CA	-5.31	1.38	1.47
24	X	113	GLU	CD-OE2	-5.31	1.19	1.25
27	N	296	CYS	CB-SG	5.31	1.91	1.82
30	Q	378	SER	CA-CB	5.31	1.60	1.52
18	L	205	GLU	CD-OE1	5.30	1.31	1.25
18	L	315	PHE	CG-CD1	5.30	1.46	1.38
13	m	28	ARG	CZ-NH1	5.30	1.40	1.33
14	7	41	ARG	CD-NE	5.30	1.55	1.46
17	K	380	GLY	CA-C	-5.30	1.43	1.51
13	6	38	ARG	CZ-NH2	5.29	1.40	1.33
11	k	187	ASP	C-N	5.29	1.42	1.33
13	6	161	GLU	CB-CG	5.29	1.62	1.52
18	L	314	GLY	CA-C	5.29	1.60	1.51
11	k	86	GLN	N-CA	-5.29	1.35	1.46
1	A	122	ARG	CZ-NH1	5.29	1.40	1.33
3	c	17	ARG	CZ-NH2	5.28	1.40	1.33
6	F	125	ARG	CZ-NH2	5.28	1.40	1.33
24	X	81	SER	N-CA	-5.28	1.35	1.46
2	b	104	TYR	CB-CG	-5.28	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	20	VAL	CB-CG1	5.28	1.64	1.52
14	n	219	TRP	CB-CG	5.28	1.59	1.50
7	g	82	ARG	CD-NE	5.28	1.55	1.46
17	K	424	PHE	CG-CD2	5.28	1.46	1.38
26	Z	19	SER	CA-CB	5.27	1.60	1.52
12	l	127	PHE	CG-CD2	5.27	1.46	1.38
17	K	255	ARG	CD-NE	5.27	1.55	1.46
26	Z	242	PHE	CG-CD1	5.27	1.46	1.38
30	Q	110	SER	CA-CB	5.27	1.60	1.52
14	n	213	GLN	CA-CB	5.27	1.65	1.53
29	P	221	TYR	CG-CD1	5.27	1.46	1.39
22	V	76	THR	C-N	5.27	1.42	1.33
8	h	134	ILE	CA-C	-5.26	1.39	1.52
1	a	224	PHE	CE2-CZ	5.26	1.47	1.37
27	N	232	LEU	N-CA	-5.26	1.35	1.46
14	n	27	LEU	C-N	5.26	1.42	1.33
23	T	266	TYR	CG-CD1	5.26	1.46	1.39
1	a	146	TYR	CE2-CZ	5.25	1.45	1.38
12	l	156	LEU	C-N	5.25	1.42	1.33
6	f	166	GLY	CA-C	-5.25	1.43	1.51
26	Z	604	GLY	N-CA	-5.25	1.38	1.46
3	c	66	TYR	CB-CG	-5.25	1.43	1.51
7	G	22	TYR	CG-CD2	5.25	1.46	1.39
15	H	283	TYR	CE2-CZ	5.25	1.45	1.38
11	k	93	ARG	CZ-NH1	5.24	1.39	1.33
15	H	373	ARG	CZ-NH1	5.24	1.39	1.33
4	D	117	ARG	NE-CZ	5.24	1.39	1.33
13	6	91	ARG	NE-CZ	5.24	1.39	1.33
25	Y	20	LYS	N-CA	-5.24	1.35	1.46
28	S	170	TYR	CG-CD1	5.24	1.46	1.39
30	Q	322	GLU	CG-CD	5.24	1.59	1.51
8	h	193	TYR	CE1-CZ	5.23	1.45	1.38
17	K	226	VAL	CB-CG2	-5.23	1.41	1.52
19	M	132	VAL	C-N	5.23	1.42	1.33
32	U	2	SER	N-CA	-5.23	1.35	1.46
8	h	84	GLU	CD-OE2	5.23	1.31	1.25
1	a	126	ARG	CD-NE	5.23	1.55	1.46
7	g	111	ARG	NE-CZ	5.23	1.39	1.33
7	g	186	ARG	NE-CZ	5.22	1.39	1.33
11	k	105	GLY	C-N	5.22	1.42	1.33
31	R	106	ASN	CA-C	-5.22	1.39	1.52
3	C	190	GLU	CD-OE1	5.21	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	223	TYR	CE1-CZ	5.21	1.45	1.38
13	m	117	ASP	N-CA	-5.21	1.35	1.46
16	I	343	ARG	CD-NE	5.21	1.55	1.46
7	g	82	ARG	NE-CZ	5.21	1.39	1.33
14	n	156	ARG	NE-CZ	5.21	1.39	1.33
26	Z	269	TYR	N-CA	-5.21	1.35	1.46
29	P	355	GLU	N-CA	-5.21	1.35	1.46
15	H	273	ARG	CD-NE	5.20	1.55	1.46
7	G	111	ARG	NE-CZ	5.20	1.39	1.33
13	m	39	TYR	CE2-CZ	5.20	1.45	1.38
13	m	72	VAL	CB-CG2	5.20	1.63	1.52
14	n	85	GLU	CG-CD	5.20	1.59	1.51
28	S	228	GLU	CD-OE1	-5.20	1.20	1.25
2	b	89	SER	CA-CB	5.20	1.60	1.52
11	k	8	ARG	CZ-NH2	5.20	1.39	1.33
26	Z	832	ARG	NE-CZ	5.20	1.39	1.33
7	G	126	ARG	CD-NE	5.19	1.55	1.46
17	K	121	ARG	CZ-NH1	5.19	1.39	1.33
25	Y	86	ARG	CD-NE	5.19	1.55	1.46
9	i	24	PRO	N-CD	-5.19	1.40	1.47
13	m	101	ARG	NE-CZ	5.19	1.39	1.33
13	m	33	TYR	CZ-OH	5.19	1.46	1.37
24	X	11	ARG	CZ-NH2	5.19	1.39	1.33
27	N	155	GLY	N-CA	5.19	1.53	1.46
5	e	114	ARG	CD-NE	5.18	1.55	1.46
24	X	22	ARG	NE-CZ	5.18	1.39	1.33
4	d	95	ARG	CD-NE	5.18	1.55	1.46
6	f	224	TYR	CZ-OH	5.18	1.46	1.37
3	c	4	ARG	CZ-NH1	5.18	1.39	1.33
5	e	61	GLU	CD-OE1	5.17	1.31	1.25
11	4	36	ARG	CZ-NH2	5.17	1.39	1.33
22	V	232	GLU	N-CA	-5.17	1.36	1.46
29	P	220	TYR	CE1-CZ	5.17	1.45	1.38
31	R	138	GLY	CA-C	-5.17	1.43	1.51
26	Z	919	GLU	CD-OE1	5.17	1.31	1.25
17	K	45	SER	CA-CB	5.16	1.60	1.52
20	J	120	TYR	CE2-CZ	5.16	1.45	1.38
20	J	270	ARG	NE-CZ	5.16	1.39	1.33
10	j	49	PHE	CE1-CZ	5.16	1.47	1.37
10	j	158	GLU	CG-CD	5.16	1.59	1.51
27	N	502	PHE	CB-CG	-5.16	1.42	1.51
29	P	145	GLU	CG-CD	5.16	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	15	ARG	NE-CZ	5.15	1.39	1.33
24	X	85	ARG	CZ-NH1	5.15	1.39	1.33
26	Z	64	TYR	CG-CD1	5.15	1.45	1.39
11	k	139	TYR	CB-CG	-5.15	1.44	1.51
1	A	230	GLU	CD-OE2	5.14	1.31	1.25
4	d	146	TYR	CE2-CZ	5.14	1.45	1.38
7	g	136	GLY	N-CA	-5.14	1.38	1.46
5	E	45	ARG	CZ-NH1	5.14	1.39	1.33
17	K	207	ARG	CD-NE	5.14	1.55	1.46
7	g	226	PHE	CG-CD2	5.14	1.46	1.38
6	F	94	SER	CA-CB	5.14	1.60	1.52
4	d	117	ARG	NE-CZ	5.13	1.39	1.33
10	j	176	ARG	NE-CZ	5.13	1.39	1.33
14	n	126	PHE	CG-CD2	5.13	1.46	1.38
28	S	245	GLY	CA-C	-5.13	1.43	1.51
11	k	96	ARG	CZ-NH1	5.13	1.39	1.33
13	m	34	SER	CB-OG	5.13	1.49	1.42
14	7	41	ARG	CZ-NH2	5.13	1.39	1.33
17	K	290	ARG	NE-CZ	5.13	1.39	1.33
27	N	549	TYR	CG-CD2	5.13	1.45	1.39
32	U	47	ARG	CZ-NH2	5.13	1.39	1.33
29	P	123	ARG	CZ-NH1	5.13	1.39	1.33
13	6	133	ARG	CZ-NH2	5.12	1.39	1.33
18	L	303	ARG	NE-CZ	5.12	1.39	1.33
5	E	53	SER	CA-CB	5.12	1.60	1.52
7	G	165	ARG	CD-NE	5.12	1.55	1.46
16	I	429	GLU	CG-CD	-5.12	1.44	1.51
4	d	187	GLU	CD-OE2	5.12	1.31	1.25
31	R	69	GLU	CA-C	-5.12	1.39	1.52
12	l	191	HIS	C-N	5.12	1.45	1.34
11	4	130	TYR	C-N	5.12	1.42	1.33
16	I	139	GLU	CD-OE1	5.12	1.31	1.25
4	D	109	ARG	CD-NE	5.11	1.55	1.46
9	2	170	GLY	N-CA	-5.11	1.38	1.46
21	W	56	GLY	C-O	5.11	1.31	1.23
2	b	15	SER	CA-CB	5.11	1.60	1.52
4	d	56	ARG	CZ-NH1	5.11	1.39	1.33
6	f	15	THR	C-N	5.11	1.42	1.33
7	g	76	GLY	CA-C	-5.11	1.43	1.51
11	k	171	ARG	CZ-NH1	5.11	1.39	1.33
14	n	174	GLU	CG-CD	5.11	1.59	1.51
27	N	563	GLY	CA-C	-5.10	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	42	ARG	CZ-NH1	5.10	1.39	1.33
13	m	185	ARG	CZ-NH1	5.10	1.39	1.33
29	P	295	SER	CA-CB	5.10	1.60	1.52
26	Z	893	PHE	CE1-CZ	5.10	1.47	1.37
27	N	600	THR	N-CA	-5.10	1.36	1.46
6	f	173	ARG	CD-NE	5.10	1.55	1.46
12	l	203	GLU	CD-OE1	-5.09	1.20	1.25
7	G	214	TRP	NE1-CE2	5.09	1.44	1.37
13	6	161	GLU	CG-CD	5.09	1.59	1.51
4	D	48	SER	CA-CB	5.09	1.60	1.52
27	N	511	GLY	CA-C	-5.09	1.43	1.51
29	P	364	ARG	NE-CZ	5.09	1.39	1.33
31	R	422	ARG	CZ-NH1	5.09	1.39	1.33
29	P	232	ARG	CD-NE	5.09	1.55	1.46
3	C	120	GLY	CA-C	-5.09	1.43	1.51
19	M	172	VAL	CB-CG1	5.08	1.63	1.52
26	Z	616	LEU	CA-C	-5.08	1.39	1.52
13	m	108	HIS	CA-C	-5.08	1.39	1.52
3	C	5	TYR	CG-CD1	5.08	1.45	1.39
31	R	141	TYR	CE2-CZ	5.08	1.45	1.38
5	E	124	ARG	CD-NE	5.08	1.55	1.46
17	K	336	ARG	CZ-NH2	5.08	1.39	1.33
16	I	155	SER	CA-CB	5.08	1.60	1.52
31	R	54	ILE	N-CA	-5.08	1.36	1.46
18	L	345	ARG	CZ-NH2	5.07	1.39	1.33
19	M	67	GLU	C-O	5.07	1.32	1.23
1	a	62	TYR	CG-CD1	5.07	1.45	1.39
11	k	156	GLU	CD-OE1	5.07	1.31	1.25
13	m	213	ARG	NE-CZ	5.07	1.39	1.33
12	5	88	TYR	CG-CD1	5.06	1.45	1.39
19	M	225	GLY	CA-C	-5.06	1.43	1.51
1	A	37	ARG	CZ-NH2	5.06	1.39	1.33
2	b	104	TYR	CE2-CZ	5.05	1.45	1.38
16	I	422	ARG	CD-NE	5.05	1.55	1.46
1	A	13	GLU	CB-CG	5.05	1.61	1.52
3	c	216	ARG	NE-CZ	5.05	1.39	1.33
26	Z	623	ARG	CZ-NH2	5.05	1.39	1.33
18	L	386	PHE	CG-CD1	5.05	1.46	1.38
26	Z	444	GLU	CB-CG	5.05	1.61	1.52
27	N	813	ARG	NE-CZ	5.05	1.39	1.33
7	g	87	ARG	CG-CD	5.05	1.64	1.51
11	k	182	LYS	CA-CB	5.05	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	M	433	TYR	CG-CD1	5.05	1.45	1.39
13	m	38	ARG	CD-NE	5.05	1.55	1.46
23	T	233	VAL	CA-CB	-5.05	1.44	1.54
27	N	908	ARG	NE-CZ	5.05	1.39	1.33
4	d	30	CYS	CB-SG	5.04	1.90	1.82
33	O	81	TYR	CB-CG	-5.04	1.44	1.51
2	b	90	ARG	NE-CZ	5.04	1.39	1.33
11	4	149	ARG	CZ-NH2	5.04	1.39	1.33
26	Z	813	PHE	CG-CD1	5.04	1.46	1.38
30	Q	51	ARG	CZ-NH1	5.04	1.39	1.33
5	E	157	TYR	CE1-CZ	5.03	1.45	1.38
33	O	187	SER	CA-CB	5.03	1.60	1.52
3	C	123	GLN	CA-CB	5.03	1.65	1.53
6	f	78	PRO	N-CD	-5.03	1.40	1.47
9	i	174	ASP	CA-CB	5.03	1.65	1.53
26	Z	730	ALA	CA-C	-5.03	1.39	1.52
5	E	117	GLU	CD-OE2	5.02	1.31	1.25
18	L	191	ARG	NE-CZ	5.02	1.39	1.33
29	P	168	TYR	CZ-OH	5.02	1.46	1.37
31	R	43	ARG	CZ-NH2	5.02	1.39	1.33
10	j	84	GLU	CD-OE2	5.02	1.31	1.25
9	2	19	ARG	CZ-NH1	5.02	1.39	1.33
20	J	35	ARG	NE-CZ	5.02	1.39	1.33
20	J	373	ARG	CZ-NH2	5.02	1.39	1.33
8	h	29	ARG	CD-NE	5.02	1.54	1.46
27	N	768	ILE	N-CA	-5.02	1.36	1.46
30	Q	146	TYR	CD1-CE1	5.02	1.46	1.39
7	G	15	GLY	CA-C	-5.02	1.43	1.51
4	d	83	LEU	N-CA	-5.01	1.36	1.46
7	g	22	TYR	CZ-OH	5.01	1.46	1.37
16	I	346	ARG	CD-NE	5.01	1.54	1.46
5	E	26	GLY	CA-C	-5.01	1.43	1.51
21	W	57	ALA	CA-C	-5.01	1.40	1.52
26	Z	415	MET	C-N	5.01	1.45	1.34
27	N	162	ARG	CD-NE	5.01	1.54	1.46
16	I	356	SER	CA-CB	5.00	1.60	1.52
27	N	912	GLU	N-CA	-5.00	1.36	1.46
6	f	178	PHE	CE2-CZ	5.00	1.46	1.37
1	A	82	ARG	CZ-NH2	5.00	1.39	1.33
26	Z	545	SER	CA-CB	5.00	1.60	1.52

All (2006) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	70	TYR	CB-CG-CD2	26.43	136.86	121.00
1	A	241	GLU	C-N-CA	-26.18	56.24	121.70
22	V	186	GLN	N-CA-CB	-25.12	65.38	110.60
4	D	127	PHE	CB-CG-CD2	-20.55	106.41	120.80
6	f	106	ARG	NE-CZ-NH1	19.24	129.92	120.30
1	a	21	TYR	CB-CG-CD2	-18.92	109.65	121.00
22	V	20	ARG	NE-CZ-NH1	17.33	128.97	120.30
4	D	127	PHE	CB-CG-CD1	16.51	132.35	120.80
4	d	109	ARG	NE-CZ-NH1	-16.35	112.12	120.30
22	V	61	TYR	CB-CG-CD1	-16.11	111.33	121.00
27	N	222	TYR	CB-CG-CD1	-15.88	111.47	121.00
1	a	146	TYR	CB-CG-CD2	-15.62	111.63	121.00
14	n	30	TYR	CB-CG-CD2	-15.56	111.67	121.00
26	Z	272	TYR	CB-CG-CD1	15.31	130.19	121.00
8	h	124	TYR	CB-CG-CD2	-15.26	111.85	121.00
32	U	100	ARG	NE-CZ-NH2	-15.26	112.67	120.30
22	V	187	ALA	N-CA-CB	-15.25	88.75	110.10
27	N	859	ASN	CB-CA-C	-15.14	80.12	110.40
2	b	156	TYR	CB-CG-CD2	-15.10	111.94	121.00
26	Z	826	ARG	NE-CZ-NH2	-15.07	112.77	120.30
4	d	109	ARG	NE-CZ-NH2	14.98	127.79	120.30
8	1	193	TYR	CB-CG-CD2	-14.98	112.01	121.00
1	a	225	PHE	CB-CG-CD2	-14.36	110.75	120.80
27	N	861	TYR	N-CA-CB	-14.14	85.15	110.60
11	k	83	PHE	CB-CG-CD1	14.05	130.63	120.80
33	O	288	ARG	NE-CZ-NH1	14.04	127.32	120.30
7	g	186	ARG	NE-CZ-NH2	13.91	127.26	120.30
13	m	213	ARG	NE-CZ-NH1	13.71	127.16	120.30
27	N	117	TYR	CB-CG-CD2	-13.70	112.78	121.00
27	N	866	TYR	CB-CG-CD2	-13.66	112.80	121.00
9	2	123	TYR	CB-CG-CD1	-13.56	112.86	121.00
3	c	91	ARG	NE-CZ-NH2	-13.56	113.52	120.30
31	R	63	TYR	CB-CG-CD1	-13.56	112.87	121.00
15	H	289	ARG	NE-CZ-NH1	13.38	126.99	120.30
1	a	225	PHE	CB-CG-CD1	13.34	130.14	120.80
9	i	90	TYR	CB-CG-CD1	-13.33	113.00	121.00
27	N	873	ARG	NE-CZ-NH1	13.32	126.96	120.30
6	f	93	TYR	CB-CG-CD1	13.26	128.96	121.00
20	J	257	ARG	NE-CZ-NH1	13.24	126.92	120.30
32	U	100	ARG	NE-CZ-NH1	13.16	126.88	120.30
15	H	434	ARG	NE-CZ-NH1	13.14	126.87	120.30
30	Q	238	TYR	CB-CG-CD1	-13.05	113.17	121.00
33	O	69	PHE	CB-CG-CD1	13.02	129.91	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Z	272	TYR	CB-CG-CD2	-12.89	113.27	121.00
9	2	72	ARG	NE-CZ-NH2	-12.85	113.87	120.30
2	B	5	TYR	CB-CG-CD2	-12.85	113.29	121.00
8	1	193	TYR	CB-CG-CD1	12.82	128.69	121.00
8	h	124	TYR	CB-CG-CD1	12.78	128.67	121.00
27	N	859	ASN	N-CA-CB	12.75	133.55	110.60
18	L	127	TYR	CB-CG-CD1	-12.69	113.39	121.00
9	i	190	TYR	CB-CG-CD2	-12.69	113.39	121.00
27	N	896	PHE	CB-CG-CD2	12.60	129.62	120.80
2	b	75	TYR	CB-CG-CD1	-12.57	113.46	121.00
27	N	653	ARG	NE-CZ-NH2	-12.55	114.02	120.30
28	S	345	TYR	CB-CG-CD2	-12.55	113.47	121.00
2	B	90	ARG	NE-CZ-NH1	12.54	126.57	120.30
1	A	241	GLU	O-C-N	12.52	142.73	122.70
5	E	95	TYR	CB-CG-CD2	-12.51	113.50	121.00
20	J	228	ARG	NE-CZ-NH1	12.48	126.54	120.30
25	Y	84	TYR	CB-CG-CD2	-12.46	113.52	121.00
1	A	241	GLU	CA-C-N	-12.43	89.86	117.20
27	N	222	TYR	CB-CG-CD2	12.39	128.43	121.00
7	G	156	TYR	CB-CG-CD2	-12.38	113.58	121.00
10	j	66	PHE	CB-CG-CD2	-12.35	112.16	120.80
10	j	45	TYR	CB-CG-CD1	-12.27	113.64	121.00
23	T	266	TYR	CB-CG-CD2	-12.27	113.64	121.00
1	A	37	ARG	NE-CZ-NH2	12.26	126.43	120.30
1	A	235	ARG	NE-CZ-NH1	12.19	126.39	120.30
7	G	22	TYR	CB-CG-CD2	-12.17	113.70	121.00
29	P	179	PHE	CB-CG-CD2	-12.14	112.30	120.80
4	d	20	TYR	CB-CG-CD2	-12.08	113.75	121.00
10	j	66	PHE	CB-CG-CD1	12.08	129.25	120.80
4	d	56	ARG	NE-CZ-NH1	12.06	126.33	120.30
1	A	242	GLN	CB-CA-C	11.95	134.30	110.40
9	2	72	ARG	NE-CZ-NH1	11.93	126.27	120.30
4	D	170	ARG	NE-CZ-NH1	11.92	126.26	120.30
12	l	19	ARG	NE-CZ-NH1	11.91	126.26	120.30
27	N	417	ARG	NE-CZ-NH1	-11.91	114.34	120.30
2	B	178	ARG	NE-CZ-NH2	-11.90	114.35	120.30
8	h	70	TYR	CB-CG-CD1	-11.86	113.88	121.00
4	D	56	ARG	NE-CZ-NH1	11.81	126.20	120.30
11	k	8	ARG	NE-CZ-NH2	-11.79	114.40	120.30
18	L	329	ARG	NE-CZ-NH2	-11.72	114.44	120.30
33	O	106	PHE	CB-CG-CD1	11.70	128.99	120.80
29	P	267	PHE	CB-CG-CD1	11.68	128.98	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	4	ARG	NE-CZ-NH1	11.62	126.11	120.30
18	L	361	PHE	CB-CG-CD1	11.59	128.91	120.80
6	F	125	ARG	NE-CZ-NH1	11.59	126.09	120.30
8	h	82	PHE	CB-CG-CD1	11.58	128.91	120.80
12	5	167	ARG	NE-CZ-NH1	11.56	126.08	120.30
12	l	113	TYR	CB-CG-CD1	-11.54	114.07	121.00
31	R	70	TYR	CB-CG-CD1	-11.55	114.07	121.00
32	U	24	ARG	NE-CZ-NH2	-11.54	114.53	120.30
4	d	127	PHE	CB-CG-CD1	-11.54	112.72	120.80
1	a	23	PHE	CB-CG-CD1	-11.50	112.75	120.80
26	Z	339	PHE	CB-CG-CD1	11.50	128.85	120.80
17	K	236	ARG	NE-CZ-NH2	-11.40	114.60	120.30
1	a	95	PHE	CB-CG-CD1	11.40	128.78	120.80
19	M	213	ARG	NE-CZ-NH1	11.39	126.00	120.30
15	H	307	PHE	CB-CG-CD2	-11.38	112.84	120.80
20	J	228	ARG	NE-CZ-NH2	-11.37	114.61	120.30
6	f	106	ARG	NE-CZ-NH2	-11.37	114.62	120.30
17	K	350	ARG	NE-CZ-NH2	-11.34	114.63	120.30
18	L	127	TYR	CB-CG-CD2	11.27	127.76	121.00
4	D	139	ARG	NE-CZ-NH1	11.27	125.93	120.30
2	b	156	TYR	CB-CG-CD1	11.20	127.72	121.00
30	Q	409	TYR	CB-CG-CD1	-11.19	114.28	121.00
11	k	190	ARG	NE-CZ-NH1	11.17	125.88	120.30
11	k	83	PHE	CB-CG-CD2	-11.14	113.00	120.80
33	O	288	ARG	NE-CZ-NH2	-11.13	114.74	120.30
1	a	15	ARG	NE-CZ-NH2	-11.07	114.77	120.30
20	J	116	ARG	NE-CZ-NH2	-11.05	114.77	120.30
14	7	137	TYR	CB-CG-CD2	-11.03	114.38	121.00
7	g	74	TYR	CB-CG-CD2	10.99	127.60	121.00
12	l	114	TYR	CB-CG-CD2	-10.98	114.41	121.00
29	P	220	TYR	CB-CG-CD2	-10.94	114.43	121.00
30	Q	75	ARG	NE-CZ-NH2	-10.91	114.84	120.30
16	I	85	PHE	CB-CG-CD1	10.90	128.43	120.80
5	E	45	ARG	NE-CZ-NH2	10.88	125.74	120.30
29	P	193	TYR	CB-CG-CD2	-10.88	114.47	121.00
7	G	156	TYR	CB-CG-CD1	10.85	127.51	121.00
27	N	866	TYR	CB-CG-CD1	10.79	127.47	121.00
6	F	58	TYR	CB-CG-CD1	10.79	127.47	121.00
28	S	360	PHE	CB-CG-CD1	-10.76	113.27	120.80
13	m	77	PHE	CB-CG-CD1	10.70	128.29	120.80
30	Q	321	TYR	CB-CG-CD2	-10.69	114.58	121.00
3	C	4	ARG	NE-CZ-NH1	10.69	125.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	164	ARG	NE-CZ-NH1	-10.67	114.96	120.30
31	R	70	TYR	CG-CD1-CE1	10.66	129.83	121.30
12	l	90	TYR	CB-CG-CD2	-10.65	114.61	121.00
7	G	165	ARG	NE-CZ-NH2	-10.61	114.99	120.30
3	c	23	TYR	CB-CG-CD2	-10.60	114.64	121.00
27	N	117	TYR	CB-CG-CD1	10.60	127.36	121.00
7	G	22	TYR	CB-CG-CD1	10.58	127.35	121.00
3	c	116	ASP	CB-CG-OD2	-10.57	108.78	118.30
1	A	62	TYR	CB-CG-CD1	-10.57	114.66	121.00
6	F	125	ARG	NE-CZ-NH2	-10.56	115.02	120.30
6	f	93	TYR	CB-CG-CD2	-10.53	114.68	121.00
9	i	69	TYR	CB-CG-CD2	10.51	127.31	121.00
5	E	114	ARG	NE-CZ-NH1	10.50	125.55	120.30
22	V	186	GLN	CB-CA-C	10.49	131.38	110.40
29	P	115	ARG	NE-CZ-NH2	-10.48	115.06	120.30
9	i	88	PHE	CB-CG-CD1	-10.47	113.47	120.80
18	L	386	PHE	CB-CG-CD1	10.46	128.12	120.80
27	N	873	ARG	NE-CZ-NH2	-10.46	115.07	120.30
33	O	252	PHE	CB-CG-CD2	-10.45	113.48	120.80
17	K	49	PHE	CB-CG-CD2	-10.45	113.48	120.80
3	c	91	ARG	NE-CZ-NH1	10.44	125.52	120.30
11	k	8	ARG	NE-CZ-NH1	10.43	125.52	120.30
29	P	193	TYR	CB-CG-CD1	10.42	127.25	121.00
29	P	395	ARG	NE-CZ-NH2	-10.42	115.09	120.30
11	k	73	TYR	CB-CG-CD2	-10.37	114.78	121.00
5	E	1	ASP	CB-CG-OD2	-10.36	108.98	118.30
33	O	190	TYR	CB-CG-CD2	-10.36	114.79	121.00
16	I	362	LEU	CB-CG-CD1	10.35	128.59	111.00
15	H	90	ARG	NE-CZ-NH2	-10.34	115.13	120.30
14	7	128	ARG	NE-CZ-NH1	10.31	125.46	120.30
2	B	234	ARG	NE-CZ-NH2	-10.29	115.16	120.30
2	b	128	ARG	NE-CZ-NH2	-10.27	115.16	120.30
20	J	200	ARG	NE-CZ-NH1	10.27	125.43	120.30
16	I	128	TYR	CB-CG-CD1	-10.18	114.89	121.00
1	a	95	PHE	CB-CG-CD2	-10.17	113.68	120.80
12	l	104	TYR	CB-CG-CD2	-10.16	114.90	121.00
10	3	73	TYR	CB-CG-CD2	10.16	127.10	121.00
6	F	1	PHE	CB-CG-CD1	10.15	127.91	120.80
30	Q	51	ARG	NE-CZ-NH1	10.11	125.36	120.30
12	l	152	ASP	CB-CG-OD1	-10.09	109.22	118.30
11	k	117	TYR	CB-CG-CD1	-10.09	114.95	121.00
28	S	64	ARG	NE-CZ-NH1	10.06	125.33	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	125	MET	CG-SD-CE	-10.03	84.15	100.20
11	k	67	TYR	CB-CG-CD1	-10.03	114.98	121.00
1	a	21	TYR	CB-CG-CD1	10.01	127.01	121.00
6	f	17	ARG	NE-CZ-NH1	9.99	125.30	120.30
2	B	4	ARG	NE-CZ-NH2	9.99	125.29	120.30
4	d	95	ARG	NE-CZ-NH1	9.98	125.29	120.30
7	g	95	PHE	CB-CG-CD2	-9.94	113.84	120.80
13	m	185	ARG	NE-CZ-NH1	9.93	125.27	120.30
19	M	73	ARG	NE-CZ-NH2	9.93	125.26	120.30
3	c	142	ARG	NE-CZ-NH2	-9.92	115.34	120.30
29	P	47	ARG	NE-CZ-NH2	9.88	125.24	120.30
4	D	16	PHE	CB-CG-CD1	9.87	127.71	120.80
11	k	59	TYR	CB-CG-CD2	-9.85	115.09	121.00
13	m	217	TYR	CB-CG-CD2	9.85	126.91	121.00
12	l	69	ARG	NE-CZ-NH2	-9.83	115.38	120.30
12	5	104	TYR	CB-CG-CD1	9.83	126.90	121.00
15	H	346	ARG	NE-CZ-NH2	-9.83	115.39	120.30
12	l	104	TYR	CB-CG-CD1	9.83	126.90	121.00
20	J	333	ARG	NE-CZ-NH1	-9.82	115.39	120.30
27	N	88	ARG	NE-CZ-NH1	9.81	125.21	120.30
8	h	82	PHE	CB-CG-CD2	-9.81	113.93	120.80
19	M	357	ARG	NE-CZ-NH1	9.81	125.20	120.30
31	R	70	TYR	CD1-CG-CD2	-9.80	107.11	117.90
29	P	267	PHE	CB-CG-CD2	-9.80	113.94	120.80
30	Q	335	PHE	CB-CG-CD2	-9.78	113.95	120.80
8	h	70	TYR	CB-CG-CD2	9.77	126.86	121.00
20	J	200	ARG	NE-CZ-NH2	-9.74	115.43	120.30
9	i	90	TYR	CG-CD2-CE2	-9.72	113.52	121.30
31	R	31	PHE	CB-CG-CD1	9.72	127.61	120.80
23	T	97	SER	N-CA-CB	9.71	125.07	110.50
31	R	179	PHE	CB-CG-CD2	-9.71	114.01	120.80
16	I	85	PHE	CB-CG-CD2	-9.70	114.01	120.80
26	Z	574	TYR	CB-CG-CD1	9.69	126.82	121.00
15	H	78	PRO	CA-N-CD	-9.69	97.94	111.50
17	K	294	ARG	NE-CZ-NH2	-9.66	115.47	120.30
19	M	404	ARG	NE-CZ-NH1	9.65	125.12	120.30
11	k	23	ARG	NE-CZ-NH2	9.64	125.12	120.30
19	M	433	TYR	CB-CG-CD2	-9.61	115.24	121.00
7	G	165	ARG	NE-CZ-NH1	9.60	125.10	120.30
3	c	49	ARG	NE-CZ-NH1	9.57	125.09	120.30
31	R	335	ARG	NE-CZ-NH2	-9.52	115.54	120.30
14	n	129	TYR	CB-CG-CD2	9.50	126.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	187	ALA	N-CA-C	9.49	136.63	111.00
23	T	266	TYR	CB-CG-CD1	9.49	126.70	121.00
3	c	145	TYR	CB-CG-CD2	9.48	126.69	121.00
26	Z	574	TYR	CB-CG-CD2	-9.46	115.32	121.00
29	P	232	ARG	NE-CZ-NH2	-9.45	115.57	120.30
11	k	117	TYR	CB-CG-CD2	9.44	126.66	121.00
5	e	145	TYR	CB-CG-CD1	-9.43	115.34	121.00
18	L	194	ARG	NE-CZ-NH2	-9.42	115.59	120.30
6	F	221	PHE	CB-CG-CD2	-9.41	114.21	120.80
33	O	135	ARG	NE-CZ-NH1	9.39	125.00	120.30
27	N	786	ARG	NE-CZ-NH1	-9.37	115.61	120.30
26	Z	623	ARG	NE-CZ-NH1	9.35	124.97	120.30
29	P	234	TYR	CB-CG-CD1	-9.34	115.40	121.00
27	N	202	PHE	CB-CG-CD1	9.32	127.32	120.80
26	Z	339	PHE	CB-CG-CD2	-9.31	114.28	120.80
29	P	351	ARG	NE-CZ-NH1	9.29	124.94	120.30
27	N	463	TYR	CB-CG-CD1	-9.27	115.44	121.00
22	V	230	TYR	CB-CG-CD2	-9.26	115.44	121.00
6	f	221	PHE	CB-CG-CD2	-9.24	114.33	120.80
9	i	123	TYR	CB-CG-CD2	-9.23	115.46	121.00
14	n	188	ASP	CB-CG-OD2	-9.23	109.99	118.30
27	N	593	PHE	CB-CG-CD1	-9.22	114.35	120.80
18	L	117	TYR	CB-CG-CD2	-9.21	115.47	121.00
3	c	17	ARG	NE-CZ-NH1	9.20	124.90	120.30
27	N	894	ARG	NE-CZ-NH1	9.19	124.90	120.30
1	a	153	TYR	CB-CG-CD2	-9.15	115.51	121.00
11	k	73	TYR	CB-CG-CD1	9.13	126.48	121.00
8	h	142	PHE	CB-CG-CD1	-9.12	114.41	120.80
4	d	146	TYR	CB-CG-CD2	-9.12	115.53	121.00
20	J	292	MET	N-CA-CB	9.11	127.00	110.60
6	F	2	ARG	NE-CZ-NH1	9.11	124.85	120.30
33	O	62	TYR	CB-CG-CD1	9.10	126.46	121.00
2	B	246	ARG	NE-CZ-NH2	-9.09	115.75	120.30
20	J	70	SER	N-CA-CB	9.08	124.12	110.50
5	e	94	TYR	CB-CG-CD1	9.07	126.44	121.00
8	h	174	ARG	NE-CZ-NH1	9.07	124.84	120.30
3	C	113	ARG	NE-CZ-NH1	9.05	124.82	120.30
20	J	71	TYR	CB-CG-CD2	-9.04	115.58	121.00
5	e	18	TYR	CB-CG-CD2	-9.01	115.59	121.00
18	L	386	PHE	CB-CG-CD2	-9.01	114.49	120.80
4	d	16	PHE	CB-CG-CD1	-8.97	114.52	120.80
14	n	76	TYR	CB-CG-CD1	8.97	126.38	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	H	222	ARG	NE-CZ-NH2	-8.97	115.82	120.30
23	T	186	ARG	NE-CZ-NH2	-8.97	115.82	120.30
3	C	145	TYR	CB-CG-CD2	-8.96	115.62	121.00
31	R	63	TYR	CB-CG-CD2	8.95	126.37	121.00
27	N	896	PHE	CB-CG-CD1	-8.92	114.56	120.80
28	S	452	TYR	CB-CG-CD2	-8.92	115.65	121.00
23	T	199	PHE	CB-CG-CD2	8.91	127.04	120.80
32	U	67	PHE	CB-CG-CD2	8.91	127.03	120.80
27	N	161	TYR	CB-CG-CD2	-8.90	115.66	121.00
19	M	203	ARG	NE-CZ-NH2	-8.90	115.85	120.30
15	H	62	ARG	NE-CZ-NH2	-8.89	115.86	120.30
29	P	103	TYR	CB-CG-CD1	-8.88	115.67	121.00
23	T	81	TYR	CB-CG-CD2	8.88	126.33	121.00
15	H	88	ARG	NE-CZ-NH1	8.88	124.74	120.30
2	B	97	TYR	CB-CG-CD2	-8.87	115.68	121.00
15	H	307	PHE	CB-CG-CD1	8.88	127.01	120.80
28	S	298	ARG	NE-CZ-NH1	8.87	124.73	120.30
14	n	129	TYR	CB-CG-CD1	-8.86	115.68	121.00
23	T	234	TYR	CB-CG-CD2	-8.86	115.68	121.00
19	M	339	ARG	NE-CZ-NH1	8.84	124.72	120.30
12	l	73	ARG	NE-CZ-NH2	-8.83	115.89	120.30
25	Y	41	ASP	CB-CG-OD2	8.83	126.25	118.30
29	P	179	PHE	CB-CG-CD1	8.82	126.98	120.80
9	2	186	TYR	CB-CG-CD2	-8.80	115.72	121.00
21	W	41	ARG	NE-CZ-NH2	-8.80	115.90	120.30
5	e	145	TYR	CB-CG-CD2	8.79	126.28	121.00
10	3	176	ARG	NE-CZ-NH2	-8.80	115.90	120.30
7	g	110	ASP	CB-CG-OD1	8.79	126.21	118.30
5	e	159	TYR	CG-CD1-CE1	-8.79	114.27	121.30
9	i	75	ARG	NE-CZ-NH1	8.79	124.69	120.30
25	Y	84	TYR	CB-CG-CD1	8.78	126.27	121.00
24	X	45	PHE	CB-CG-CD1	8.77	126.94	120.80
32	U	67	PHE	CB-CG-CD1	-8.76	114.67	120.80
6	F	1	PHE	CB-CG-CD2	-8.75	114.67	120.80
21	W	60	ARG	NE-CZ-NH1	-8.75	115.93	120.30
6	F	86	TYR	CB-CG-CD2	-8.74	115.75	121.00
26	Z	840	ARG	NE-CZ-NH2	-8.74	115.93	120.30
15	H	397	SER	N-CA-CB	8.73	123.60	110.50
7	g	165	ARG	NE-CZ-NH1	8.73	124.67	120.30
4	D	179	ARG	NE-CZ-NH1	8.73	124.67	120.30
1	a	68	ARG	NE-CZ-NH2	8.73	124.67	120.30
31	R	252	TYR	CB-CG-CD2	-8.72	115.77	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	H	457	PHE	CB-CG-CD2	-8.72	114.70	120.80
26	Z	826	ARG	NE-CZ-NH1	8.71	124.66	120.30
7	g	22	TYR	CB-CG-CD2	-8.70	115.78	121.00
26	Z	358	TYR	CB-CG-CD1	8.69	126.21	121.00
8	h	142	PHE	CB-CG-CD2	8.68	126.88	120.80
27	N	211	PHE	CB-CG-CD1	8.68	126.87	120.80
14	7	195	PHE	CB-CG-CD1	8.67	126.87	120.80
22	V	251	TYR	CB-CG-CD2	8.67	126.20	121.00
1	A	242	GLN	CA-C-O	-8.66	101.90	120.10
18	L	342	ARG	NE-CZ-NH1	8.66	124.63	120.30
24	X	91	PHE	CB-CG-CD2	-8.66	114.73	120.80
13	m	160	TYR	CB-CG-CD1	-8.66	115.80	121.00
26	Z	264	PHE	CB-CG-CD2	8.64	126.85	120.80
16	I	282	ASP	CB-CG-OD1	-8.63	110.53	118.30
10	j	45	TYR	CB-CG-CD2	8.62	126.17	121.00
1	A	222	ASP	CB-CG-OD2	-8.62	110.54	118.30
29	P	37	ASP	CB-CG-OD2	8.60	126.04	118.30
17	K	426	PHE	CB-CG-CD2	-8.60	114.78	120.80
27	N	348	PHE	CB-CG-CD1	8.60	126.82	120.80
4	d	9	PHE	CB-CG-CD1	8.59	126.81	120.80
22	V	108	TYR	CB-CG-CD2	-8.58	115.85	121.00
1	a	146	TYR	CB-CG-CD1	8.57	126.14	121.00
13	6	38	ARG	NE-CZ-NH2	8.57	124.59	120.30
5	e	148	PHE	CB-CG-CD1	8.57	126.80	120.80
16	I	114	ASP	CB-CG-OD1	8.54	125.99	118.30
27	N	11	ALA	N-CA-CB	-8.54	98.14	110.10
27	N	211	PHE	CB-CG-CD2	-8.54	114.82	120.80
26	Z	837	TYR	CB-CG-CD1	8.52	126.11	121.00
4	d	170	ARG	NE-CZ-NH1	8.52	124.56	120.30
4	d	9	PHE	CB-CG-CD2	-8.51	114.84	120.80
28	S	475	TYR	CB-CG-CD2	8.49	126.09	121.00
31	R	222	ARG	NE-CZ-NH1	8.49	124.55	120.30
21	W	179	ARG	NE-CZ-NH2	-8.49	116.06	120.30
8	h	36	ARG	NE-CZ-NH2	-8.48	116.06	120.30
1	a	101	TYR	CG-CD2-CE2	-8.48	114.52	121.30
22	V	230	TYR	CB-CG-CD1	8.47	126.08	121.00
16	I	300	ARG	NE-CZ-NH1	8.44	124.52	120.30
27	N	921	ARG	NE-CZ-NH2	-8.43	116.08	120.30
32	U	179	ARG	NE-CZ-NH2	-8.42	116.09	120.30
1	a	111	ARG	NE-CZ-NH2	-8.42	116.09	120.30
12	5	104	TYR	CB-CG-CD2	-8.41	115.95	121.00
16	I	136	VAL	CG1-CB-CG2	8.41	124.35	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	5	TYR	CB-CG-CD2	-8.39	115.97	121.00
12	l	73	ARG	NE-CZ-NH1	8.39	124.49	120.30
3	C	130	PHE	CB-CG-CD1	8.38	126.67	120.80
1	a	87	ARG	NE-CZ-NH2	-8.38	116.11	120.30
15	H	434	ARG	NE-CZ-NH2	-8.38	116.11	120.30
20	J	311	ASP	C-N-CA	8.38	142.64	121.70
13	m	174	TYR	CB-CG-CD2	-8.35	115.99	121.00
19	M	386	PHE	CB-CG-CD1	8.35	126.64	120.80
26	Z	193	PHE	CB-CG-CD1	8.35	126.64	120.80
26	Z	774	ARG	NE-CZ-NH2	-8.34	116.13	120.30
20	J	147	TYR	CB-CG-CD2	-8.34	116.00	121.00
17	K	411	TYR	CB-CG-CD2	-8.33	116.00	121.00
7	G	111	ARG	NE-CZ-NH1	8.33	124.46	120.30
12	5	137	TYR	CB-CG-CD1	8.33	126.00	121.00
22	V	95	LEU	CB-CG-CD2	8.32	125.15	111.00
8	1	19	ARG	NE-CZ-NH1	8.31	124.46	120.30
33	O	69	PHE	CB-CG-CD2	-8.31	114.98	120.80
4	D	117	ARG	NE-CZ-NH2	8.31	124.45	120.30
31	R	43	ARG	NE-CZ-NH1	8.29	124.45	120.30
10	3	73	TYR	CB-CG-CD1	-8.29	116.03	121.00
26	Z	408	TYR	CB-CG-CD2	-8.29	116.03	121.00
1	A	111	ARG	NE-CZ-NH1	-8.28	116.16	120.30
32	U	24	ARG	NE-CZ-NH1	8.28	124.44	120.30
17	K	73	ARG	NE-CZ-NH2	-8.28	116.16	120.30
26	Z	165	TYR	CB-CG-CD1	8.27	125.96	121.00
14	7	126	PHE	CB-CG-CD2	-8.26	115.02	120.80
17	K	424	PHE	CB-CG-CD1	8.26	126.58	120.80
28	S	298	ARG	NE-CZ-NH2	-8.25	116.18	120.30
30	Q	387	TYR	CB-CG-CD1	-8.24	116.05	121.00
1	a	149	ASP	CB-CG-OD2	-8.23	110.89	118.30
13	6	174	TYR	CB-CG-CD1	8.23	125.94	121.00
12	l	54	PHE	CB-CG-CD2	8.23	126.56	120.80
31	R	31	PHE	CB-CG-CD2	-8.22	115.05	120.80
7	G	111	ARG	NE-CZ-NH2	-8.21	116.19	120.30
28	S	345	TYR	CB-CG-CD1	8.21	125.92	121.00
31	R	222	ARG	NE-CZ-NH2	-8.21	116.20	120.30
15	H	331	ARG	NE-CZ-NH1	8.20	124.40	120.30
22	V	196	TYR	CB-CG-CD1	8.19	125.91	121.00
4	D	118	TYR	CB-CG-CD1	8.18	125.91	121.00
5	E	159	TYR	CB-CG-CD1	-8.18	116.09	121.00
17	K	290	ARG	NE-CZ-NH2	-8.18	116.21	120.30
12	5	90	TYR	CB-CG-CD2	8.18	125.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	213	ARG	NE-CZ-NH2	-8.16	116.22	120.30
6	F	58	TYR	CB-CG-CD2	-8.14	116.12	121.00
13	m	117	ASP	CB-CG-OD2	-8.13	110.98	118.30
27	N	202	PHE	CB-CG-CD2	-8.13	115.11	120.80
12	l	159	ARG	NE-CZ-NH2	-8.11	116.24	120.30
5	E	114	ARG	NE-CZ-NH2	-8.10	116.25	120.30
4	D	139	ARG	NE-CZ-NH2	-8.09	116.25	120.30
13	6	75	TYR	CB-CG-CD2	8.08	125.85	121.00
30	Q	409	TYR	CD1-CG-CD2	8.08	126.78	117.90
20	J	270	ARG	NE-CZ-NH1	-8.07	116.26	120.30
10	j	124	ASP	CB-CG-OD1	8.07	125.56	118.30
13	m	77	PHE	CB-CG-CD2	-8.06	115.16	120.80
26	Z	302	SER	N-CA-CB	8.06	122.59	110.50
26	Z	136	ARG	NE-CZ-NH2	-8.04	116.28	120.30
7	g	4	TYR	CG-CD2-CE2	8.04	127.73	121.30
30	Q	67	THR	C-N-CA	8.04	141.79	121.70
7	G	89	ARG	NE-CZ-NH1	8.03	124.32	120.30
11	4	107	TYR	CB-CG-CD2	-8.03	116.18	121.00
23	T	210	PHE	CB-CG-CD2	-8.03	115.18	120.80
14	7	95	TYR	CB-CG-CD1	-8.02	116.19	121.00
15	H	333	MET	CG-SD-CE	-8.01	87.38	100.20
15	H	208	TYR	CB-CG-CD2	8.00	125.80	121.00
7	g	82	ARG	NE-CZ-NH1	7.99	124.30	120.30
26	Z	751	ASP	CB-CG-OD2	7.99	125.49	118.30
23	T	51	TYR	CB-CG-CD2	-7.99	116.21	121.00
2	b	235	PHE	CB-CG-CD1	-7.99	115.21	120.80
31	R	363	PHE	CB-CG-CD2	-7.98	115.22	120.80
31	R	357	PHE	CB-CG-CD2	-7.97	115.22	120.80
33	O	291	ILE	CB-CA-C	-7.97	95.66	111.60
4	d	20	TYR	CB-CG-CD1	7.96	125.78	121.00
4	d	164	ARG	NE-CZ-NH2	7.95	124.28	120.30
30	Q	409	TYR	CG-CD1-CE1	-7.91	114.97	121.30
5	E	7	PHE	CB-CG-CD2	-7.91	115.26	120.80
4	d	110	TYR	CB-CG-CD2	-7.89	116.26	121.00
6	f	146	PHE	CB-CG-CD2	-7.89	115.27	120.80
3	c	82	ASP	CB-CG-OD2	-7.89	111.20	118.30
4	D	172	PHE	CB-CG-CD2	-7.89	115.28	120.80
24	X	51	ARG	NE-CZ-NH1	7.89	124.25	120.30
1	A	62	TYR	CB-CG-CD2	7.89	125.73	121.00
18	L	88	TYR	CB-CG-CD2	-7.89	116.27	121.00
4	D	16	PHE	CB-CG-CD2	-7.87	115.29	120.80
21	W	109	ARG	NE-CZ-NH2	7.86	124.23	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	160	ARG	NE-CZ-NH1	7.85	124.22	120.30
20	J	312	ARG	N-CA-CB	7.84	124.72	110.60
5	e	14	PHE	CB-CG-CD1	7.84	126.29	120.80
15	H	454	TYR	CB-CG-CD2	7.83	125.70	121.00
8	h	87	TYR	CB-CG-CD2	-7.83	116.30	121.00
1	a	222	ASP	CB-CG-OD2	-7.83	111.25	118.30
13	m	5	TYR	CB-CG-CD2	-7.83	116.31	121.00
6	f	88	ARG	NE-CZ-NH2	7.82	124.21	120.30
29	P	220	TYR	CB-CG-CD1	7.82	125.69	121.00
13	m	33	TYR	CB-CG-CD2	7.81	125.69	121.00
2	b	23	TYR	CB-CG-CD2	-7.80	116.32	121.00
4	d	106	TYR	CB-CG-CD2	-7.80	116.32	121.00
27	N	463	TYR	CB-CG-CD2	7.78	125.67	121.00
30	Q	410	ASP	CB-CG-OD2	-7.77	111.31	118.30
20	J	310	ILE	O-C-N	-7.77	110.27	122.70
27	N	45	ASP	CB-CG-OD2	-7.75	111.32	118.30
10	j	79	ARG	NE-CZ-NH1	7.75	124.18	120.30
18	L	290	ARG	NE-CZ-NH1	7.74	124.17	120.30
26	Z	849	ARG	NE-CZ-NH2	-7.74	116.43	120.30
6	f	81	ARG	NE-CZ-NH1	-7.74	116.43	120.30
5	E	18	TYR	CB-CG-CD1	7.73	125.64	121.00
2	b	204	PHE	CB-CG-CD2	-7.73	115.39	120.80
1	a	153	TYR	CB-CG-CD1	7.72	125.64	121.00
15	H	400	ARG	NE-CZ-NH2	7.71	124.16	120.30
6	f	81	ARG	CD-NE-CZ	7.71	134.39	123.60
3	c	181	ASP	CB-CG-OD1	7.70	125.23	118.30
15	H	438	ALA	N-CA-CB	7.69	120.87	110.10
7	g	74	TYR	CB-CG-CD1	-7.69	116.39	121.00
15	H	331	ARG	NE-CZ-NH2	-7.69	116.46	120.30
14	7	41	ARG	NE-CZ-NH1	7.67	124.14	120.30
1	A	10	PHE	CB-CG-CD1	7.66	126.16	120.80
14	7	91	TYR	CB-CG-CD2	-7.66	116.41	121.00
4	d	73	PHE	CB-CG-CD1	-7.64	115.45	120.80
20	J	312	ARG	NE-CZ-NH1	7.64	124.12	120.30
13	6	217	TYR	CB-CG-CD2	-7.64	116.42	121.00
31	R	110	ILE	N-CA-CB	7.64	128.37	110.80
1	a	111	ARG	NE-CZ-NH1	7.62	124.11	120.30
4	D	117	ARG	NE-CZ-NH1	-7.62	116.49	120.30
4	d	56	ARG	NE-CZ-NH2	-7.62	116.49	120.30
29	P	357	TYR	CB-CG-CD1	7.62	125.57	121.00
2	b	122	THR	N-CA-CB	7.61	124.76	110.30
3	c	143	TYR	CB-CG-CD1	-7.61	116.43	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	L	345	ARG	NE-CZ-NH1	7.61	124.10	120.30
27	N	657	MET	CG-SD-CE	-7.60	88.03	100.20
9	i	203	TYR	CG-CD1-CE1	7.60	127.38	121.30
7	g	243	ILE	CA-CB-CG1	7.60	125.44	111.00
7	g	185	ALA	N-CA-CB	7.59	120.72	110.10
5	E	78	ARG	NE-CZ-NH1	7.58	124.09	120.30
15	H	208	TYR	CB-CG-CD1	-7.58	116.45	121.00
27	N	98	VAL	CA-CB-CG1	-7.57	99.54	110.90
29	P	397	ALA	N-CA-CB	7.57	120.70	110.10
13	m	217	TYR	CB-CG-CD1	-7.57	116.46	121.00
26	Z	551	LEU	CB-CA-C	-7.57	95.83	110.20
24	X	96	ARG	NE-CZ-NH2	-7.56	116.52	120.30
2	b	148	TYR	CB-CG-CD2	7.55	125.53	121.00
1	a	23	PHE	CB-CG-CD2	7.55	126.08	120.80
14	n	91	TYR	CB-CG-CD2	-7.55	116.47	121.00
2	B	220	ASP	CB-CG-OD2	-7.55	111.51	118.30
22	V	187	ALA	CB-CA-C	-7.55	98.78	110.10
1	A	222	ASP	N-CA-CB	7.54	124.18	110.60
7	G	214	TRP	CB-CG-CD1	7.53	136.79	127.00
4	d	46	ARG	NE-CZ-NH1	7.52	124.06	120.30
30	Q	70	ALA	N-CA-CB	7.51	120.62	110.10
11	k	95	ARG	NE-CZ-NH1	7.51	124.05	120.30
27	N	195	THR	CA-CB-CG2	-7.50	101.89	112.40
28	S	45	THR	CA-CB-CG2	-7.50	101.90	112.40
10	j	43	PHE	CB-CG-CD2	-7.50	115.55	120.80
10	3	45	TYR	CB-CG-CD2	-7.50	116.50	121.00
31	R	334	ARG	NE-CZ-NH2	-7.50	116.55	120.30
11	4	70	ARG	NE-CZ-NH2	-7.50	116.55	120.30
19	M	290	ARG	NE-CZ-NH1	7.49	124.05	120.30
13	6	106	TYR	CB-CG-CD2	-7.49	116.51	121.00
1	a	55	LEU	CB-CA-C	-7.49	95.97	110.20
16	I	280	PHE	CB-CG-CD2	7.48	126.04	120.80
8	1	19	ARG	NE-CZ-NH2	-7.48	116.56	120.30
14	7	95	TYR	CB-CG-CD2	7.48	125.49	121.00
3	c	23	TYR	CG-CD2-CE2	-7.48	115.32	121.30
6	F	127	TYR	CB-CG-CD1	-7.48	116.51	121.00
15	H	341	ASP	CB-CG-OD2	-7.48	111.57	118.30
13	6	145	LEU	CB-CG-CD1	7.47	123.71	111.00
29	P	13	TYR	CB-CG-CD2	-7.47	116.52	121.00
3	C	12	PHE	CB-CG-CD1	7.47	126.03	120.80
30	Q	153	ASP	CB-CG-OD2	-7.47	111.58	118.30
24	X	97	TYR	CB-CG-CD1	-7.46	116.52	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	251	TYR	CB-CG-CD1	-7.46	116.53	121.00
27	N	809	ARG	NE-CZ-NH1	7.46	124.03	120.30
13	6	2	PHE	CB-CG-CD2	-7.44	115.59	120.80
1	a	21	TYR	CG-CD2-CE2	-7.43	115.35	121.30
26	Z	751	ASP	CB-CG-OD1	-7.43	111.61	118.30
26	Z	712	ASP	CB-CG-OD2	-7.42	111.62	118.30
31	R	43	ARG	NE-CZ-NH2	-7.42	116.59	120.30
23	T	82	PHE	CB-CG-CD1	7.41	125.99	120.80
16	I	408	ARG	NE-CZ-NH2	-7.41	116.60	120.30
7	g	18	PHE	CB-CG-CD1	-7.41	115.61	120.80
9	2	88	PHE	CB-CG-CD1	-7.40	115.62	120.80
11	k	121	TYR	CB-CG-CD2	-7.39	116.56	121.00
32	U	233	PHE	CB-CG-CD2	7.39	125.97	120.80
14	7	152	ASN	N-CA-CB	7.39	123.90	110.60
16	I	135	PHE	CB-CG-CD2	7.39	125.97	120.80
4	d	117	ARG	NE-CZ-NH2	-7.39	116.61	120.30
27	N	439	VAL	CA-CB-CG2	-7.39	99.82	110.90
13	6	21	ALA	N-CA-CB	7.39	120.44	110.10
27	N	809	ARG	NE-CZ-NH2	-7.39	116.61	120.30
30	Q	12	ARG	NE-CZ-NH2	-7.38	116.61	120.30
9	2	97	TYR	CB-CG-CD1	-7.37	116.58	121.00
19	M	203	ARG	NE-CZ-NH1	7.37	123.99	120.30
8	h	45	ARG	NE-CZ-NH2	-7.37	116.62	120.30
1	A	209	PHE	CB-CG-CD1	7.35	125.95	120.80
11	4	130	TYR	CD1-CE1-CZ	7.35	126.42	119.80
3	c	201	ASP	CB-CG-OD2	-7.35	111.69	118.30
26	Z	165	TYR	CB-CG-CD2	-7.35	116.59	121.00
30	Q	386	PHE	CB-CG-CD2	-7.35	115.66	120.80
21	W	41	ARG	NE-CZ-NH1	7.34	123.97	120.30
20	J	96	VAL	CG1-CB-CG2	7.33	122.64	110.90
29	P	123	ARG	NE-CZ-NH1	-7.33	116.64	120.30
1	A	10	PHE	CB-CG-CD2	-7.32	115.67	120.80
1	A	215	GLU	N-CA-CB	7.32	123.78	110.60
29	P	356	TYR	CB-CG-CD2	-7.32	116.61	121.00
14	n	195	PHE	CB-CG-CD2	-7.31	115.68	120.80
26	Z	623	ARG	NE-CZ-NH2	-7.31	116.64	120.30
26	Z	60	ASP	CB-CG-OD2	-7.31	111.72	118.30
11	k	70	ARG	NE-CZ-NH2	-7.30	116.65	120.30
19	M	166	ARG	NE-CZ-NH1	7.30	123.95	120.30
28	S	461	PHE	CB-CA-C	-7.29	95.81	110.40
15	H	90	ARG	NE-CZ-NH1	7.29	123.95	120.30
6	f	81	ARG	NE-CZ-NH2	-7.29	116.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	253	PHE	CB-CG-CD1	7.28	125.90	120.80
13	m	102	PHE	CB-CG-CD2	7.28	125.90	120.80
2	b	4	ARG	NE-CZ-NH2	-7.28	116.66	120.30
33	O	49	PHE	CB-CG-CD2	7.27	125.89	120.80
27	N	502	PHE	CB-CG-CD1	-7.26	115.72	120.80
2	B	178	ARG	NE-CZ-NH1	7.26	123.93	120.30
16	I	182	SER	N-CA-CB	7.26	121.38	110.50
32	U	72	TYR	CB-CG-CD1	7.26	125.35	121.00
14	n	36	PHE	CB-CG-CD1	-7.25	115.72	120.80
2	B	83	ARG	NE-CZ-NH2	-7.25	116.68	120.30
26	Z	459	ALA	CB-CA-C	-7.25	99.23	110.10
1	a	224	PHE	CB-CG-CD2	-7.24	115.73	120.80
27	N	906	ARG	NE-CZ-NH2	-7.24	116.68	120.30
30	Q	291	TYR	CB-CG-CD2	-7.24	116.66	121.00
14	n	16	TYR	CB-CG-CD1	-7.24	116.66	121.00
17	K	340	PHE	CB-CG-CD1	-7.23	115.74	120.80
17	K	350	ARG	NE-CZ-NH1	7.22	123.91	120.30
5	E	157	TYR	CB-CG-CD2	-7.22	116.67	121.00
27	N	907	ASP	CB-CG-OD2	-7.21	111.81	118.30
26	Z	561	ASP	CB-CG-OD1	-7.20	111.82	118.30
4	d	118	TYR	CB-CG-CD2	-7.20	116.68	121.00
17	K	204	ASP	CB-CG-OD1	-7.20	111.82	118.30
3	C	91	ARG	NE-CZ-NH1	7.19	123.90	120.30
21	W	78	ASP	CB-CG-OD2	-7.19	111.83	118.30
11	k	96	ARG	NE-CZ-NH2	7.18	123.89	120.30
1	A	5	ARG	NE-CZ-NH1	7.18	123.89	120.30
27	N	62	ALA	CB-CA-C	-7.18	99.33	110.10
7	g	153	TYR	CB-CG-CD1	-7.17	116.69	121.00
3	c	89	THR	N-CA-CB	7.17	123.93	110.30
6	f	221	PHE	CB-CG-CD1	7.17	125.82	120.80
22	V	87	PHE	CB-CG-CD2	-7.17	115.78	120.80
31	R	312	TYR	CB-CG-CD2	-7.16	116.70	121.00
14	7	186	TYR	CB-CG-CD1	7.16	125.30	121.00
6	f	224	TYR	CG-CD2-CE2	-7.15	115.58	121.30
12	l	121	ARG	NE-CZ-NH2	7.15	123.87	120.30
27	N	502	PHE	CB-CG-CD2	7.14	125.80	120.80
3	C	136	TYR	CB-CG-CD1	-7.14	116.72	121.00
11	k	152	MET	CG-SD-CE	-7.13	88.80	100.20
32	U	72	TYR	CB-CG-CD2	-7.12	116.73	121.00
26	Z	761	PHE	CB-CG-CD2	-7.12	115.82	120.80
16	I	128	TYR	CB-CG-CD2	7.11	125.27	121.00
4	D	56	ARG	NE-CZ-NH2	-7.11	116.75	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	38	ARG	NE-CZ-NH2	-7.11	116.75	120.30
12	5	90	TYR	CB-CG-CD1	-7.10	116.74	121.00
31	R	186	TYR	CG-CD2-CE2	-7.10	115.62	121.30
1	a	87	ARG	NE-CZ-NH1	7.10	123.85	120.30
22	V	185	ILE	CG1-CB-CG2	-7.10	95.77	111.40
14	n	6	VAL	CG1-CB-CG2	7.10	122.26	110.90
9	i	17	ASP	CB-CG-OD1	7.10	124.69	118.30
13	m	160	TYR	CD1-CE1-CZ	-7.09	113.42	119.80
23	T	144	TYR	CB-CG-CD2	7.09	125.25	121.00
1	A	224	PHE	CB-CG-CD1	7.09	125.76	120.80
9	i	196	ARG	NE-CZ-NH2	-7.08	116.76	120.30
24	X	122	TYR	CB-CG-CD1	7.08	125.25	121.00
12	5	65	LEU	CB-CG-CD2	7.07	123.02	111.00
30	Q	251	THR	CA-CB-CG2	-7.07	102.51	112.40
17	K	270	PHE	CB-CG-CD2	-7.07	115.85	120.80
9	i	82	MET	CG-SD-CE	-7.06	88.90	100.20
16	I	256	TYR	CB-CG-CD1	-7.06	116.77	121.00
31	R	343	GLU	N-CA-CB	7.05	123.28	110.60
10	j	177	ASP	CB-CG-OD1	-7.04	111.96	118.30
29	P	73	ASP	CB-CG-OD1	7.02	124.62	118.30
29	P	357	TYR	CB-CG-CD2	-7.02	116.79	121.00
30	Q	321	TYR	CB-CG-CD1	7.02	125.21	121.00
27	N	653	ARG	NE-CZ-NH1	7.02	123.81	120.30
3	C	209	ARG	NE-CZ-NH1	7.01	123.80	120.30
22	V	20	ARG	NE-CZ-NH2	-7.01	116.80	120.30
4	d	136	PHE	CB-CG-CD2	-7.00	115.90	120.80
2	B	204	PHE	CB-CG-CD1	7.00	125.70	120.80
1	a	224	PHE	CG-CD2-CE2	-7.00	113.10	120.80
17	K	259	ARG	NE-CZ-NH2	-7.00	116.80	120.30
15	H	225	VAL	CA-CB-CG2	-7.00	100.41	110.90
28	S	160	ARG	NE-CZ-NH2	-6.99	116.80	120.30
26	Z	773	ARG	NE-CZ-NH1	6.99	123.80	120.30
1	a	155	VAL	CA-CB-CG2	6.99	121.38	110.90
26	Z	142	ASP	CB-CG-OD2	6.99	124.59	118.30
30	Q	335	PHE	CB-CG-CD1	6.98	125.69	120.80
24	X	87	PHE	CB-CG-CD1	6.98	125.68	120.80
30	Q	67	THR	N-CA-CB	6.97	123.55	110.30
21	W	78	ASP	CB-CG-OD1	6.97	124.58	118.30
30	Q	110	SER	C-N-CA	6.97	139.13	121.70
31	R	24	TYR	CB-CG-CD2	6.97	125.18	121.00
24	X	51	ARG	NE-CZ-NH2	-6.97	116.82	120.30
18	L	53	HIS	CA-CB-CG	6.96	125.44	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	X	110	PRO	N-CA-CB	6.96	111.65	103.30
3	c	8	ARG	NE-CZ-NH1	6.96	123.78	120.30
8	h	102	TYR	CB-CG-CD1	-6.96	116.83	121.00
4	d	117	ARG	NE-CZ-NH1	6.95	123.78	120.30
13	m	133	ARG	NE-CZ-NH1	6.95	123.77	120.30
14	7	195	PHE	CB-CG-CD2	-6.95	115.94	120.80
6	f	232	TYR	CB-CG-CD2	-6.95	116.83	121.00
31	R	68	GLU	O-C-N	6.94	133.81	122.70
23	T	224	ARG	NE-CZ-NH2	-6.94	116.83	120.30
2	b	73	ALA	N-CA-CB	6.93	119.81	110.10
28	S	150	LYS	N-CA-CB	6.93	123.08	110.60
11	4	67	TYR	CB-CG-CD2	-6.93	116.84	121.00
19	M	187	ASP	CB-CG-OD2	-6.93	112.07	118.30
9	i	161	ALA	N-CA-CB	6.92	119.79	110.10
22	V	61	TYR	CG-CD1-CE1	-6.92	115.77	121.30
9	i	174	ASP	CB-CG-OD1	-6.92	112.08	118.30
13	6	105	TYR	CG-CD1-CE1	-6.91	115.77	121.30
3	c	142	ARG	NE-CZ-NH1	6.91	123.75	120.30
6	f	80	ALA	N-CA-CB	6.91	119.77	110.10
24	X	85	ARG	NE-CZ-NH1	-6.90	116.85	120.30
4	D	188	GLU	OE1-CD-OE2	6.90	131.58	123.30
5	e	124	ARG	NE-CZ-NH2	6.89	123.75	120.30
19	M	265	ASP	CB-CG-OD2	-6.88	112.11	118.30
8	h	39	ASP	CB-CG-OD1	-6.88	112.11	118.30
11	k	135	TYR	CG-CD2-CE2	-6.88	115.79	121.30
8	h	61	TYR	CB-CG-CD2	-6.88	116.87	121.00
30	Q	409	TYR	N-CA-CB	-6.88	98.22	110.60
18	L	108	VAL	CA-CB-CG2	-6.88	100.59	110.90
14	n	185	TYR	CB-CG-CD2	6.87	125.12	121.00
8	h	174	ARG	NE-CZ-NH2	-6.87	116.86	120.30
14	7	129	TYR	CB-CG-CD2	6.87	125.12	121.00
26	Z	548	ASP	CB-CG-OD2	-6.87	112.12	118.30
13	6	98	TYR	CB-CG-CD2	-6.86	116.88	121.00
7	g	61	VAL	CA-CB-CG2	6.86	121.19	110.90
19	M	331	ASP	CB-CG-OD2	-6.85	112.13	118.30
3	c	23	TYR	CG-CD1-CE1	-6.85	115.82	121.30
7	g	134	PHE	CB-CG-CD2	-6.85	116.01	120.80
29	P	356	TYR	CB-CG-CD1	6.85	125.11	121.00
4	D	137	ASP	CB-CG-OD2	-6.85	112.14	118.30
10	j	95	TYR	CG-CD1-CE1	-6.84	115.83	121.30
15	H	266	ARG	NE-CZ-NH2	-6.84	116.88	120.30
5	e	52	GLU	OE1-CD-OE2	6.84	131.51	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	228	TYR	CZ-CE2-CD2	-6.84	113.64	119.80
4	D	47	ARG	NE-CZ-NH1	6.84	123.72	120.30
13	m	5	TYR	CB-CG-CD1	6.84	125.10	121.00
3	C	203	SER	N-CA-CB	6.84	120.75	110.50
12	l	95	LEU	CB-CG-CD1	6.83	122.62	111.00
27	N	266	SER	N-CA-CB	6.83	120.75	110.50
13	6	221	ARG	NE-CZ-NH1	6.83	123.72	120.30
27	N	890	PHE	CB-CG-CD1	-6.83	116.02	120.80
13	m	98	TYR	CB-CG-CD1	6.82	125.09	121.00
24	X	17	TYR	CZ-CE2-CD2	6.82	125.94	119.80
26	Z	193	PHE	CB-CG-CD2	-6.82	116.02	120.80
10	j	35	VAL	CA-CB-CG1	-6.82	100.67	110.90
19	M	243	PHE	CB-CG-CD2	6.82	125.57	120.80
14	n	201	ASP	N-CA-CB	6.81	122.86	110.60
30	Q	209	TYR	CB-CG-CD2	6.81	125.09	121.00
17	K	333	ARG	NE-CZ-NH2	-6.81	116.89	120.30
13	m	156	PHE	CD1-CE1-CZ	-6.81	111.93	120.10
33	O	135	ARG	NE-CZ-NH2	-6.81	116.89	120.30
31	R	134	TRP	CE3-CZ3-CH2	6.80	128.69	121.20
26	Z	295	ARG	NE-CZ-NH1	6.80	123.70	120.30
19	M	299	ARG	NE-CZ-NH2	-6.79	116.91	120.30
7	g	238	PHE	CB-CG-CD2	-6.79	116.05	120.80
13	6	41	PRO	N-CA-CB	6.78	111.44	103.30
24	X	16	GLU	N-CA-CB	6.78	122.81	110.60
1	a	101	TYR	CZ-CE2-CD2	6.78	125.90	119.80
8	h	46	SER	N-CA-CB	6.78	120.66	110.50
6	f	201	ARG	NE-CZ-NH2	-6.76	116.92	120.30
12	l	137	TYR	CB-CG-CD2	-6.76	116.94	121.00
11	k	193	ASP	CB-CG-OD1	-6.76	112.21	118.30
11	4	32	ASP	CB-CG-OD2	-6.76	112.22	118.30
13	6	174	TYR	CB-CG-CD2	-6.76	116.95	121.00
14	n	93	PHE	CB-CG-CD2	-6.75	116.07	120.80
3	c	49	ARG	NE-CZ-NH2	-6.75	116.92	120.30
14	n	188	ASP	CB-CG-OD1	6.75	124.38	118.30
27	N	11	ALA	CB-CA-C	6.74	120.21	110.10
2	b	148	TYR	CB-CG-CD1	-6.74	116.95	121.00
12	l	146	TRP	CE2-CD2-CG	-6.74	101.91	107.30
30	Q	238	TYR	CG-CD2-CE2	-6.74	115.91	121.30
18	L	157	ARG	NE-CZ-NH1	6.74	123.67	120.30
2	B	128	ARG	NE-CZ-NH1	-6.73	116.93	120.30
30	Q	306	TYR	CB-CG-CD2	-6.73	116.96	121.00
16	I	422	ARG	NE-CZ-NH2	-6.73	116.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	j	103	PHE	CB-CG-CD1	6.72	125.51	120.80
9	2	196	ARG	NE-CZ-NH2	-6.72	116.94	120.30
33	O	29	PHE	N-CA-CB	6.72	122.70	110.60
9	i	8	PHE	CB-CG-CD1	-6.72	116.10	120.80
15	H	222	ARG	NE-CZ-NH1	6.71	123.66	120.30
30	Q	127	ARG	NE-CZ-NH1	-6.71	116.95	120.30
27	N	904	VAL	CA-CB-CG2	-6.70	100.85	110.90
6	f	122	TYR	CB-CG-CD1	-6.70	116.98	121.00
10	3	198	TYR	CB-CG-CD1	-6.70	116.98	121.00
9	i	18	THR	CA-CB-CG2	-6.69	103.03	112.40
23	T	138	ASP	CB-CG-OD2	-6.69	112.28	118.30
7	g	197	TYR	CD1-CE1-CZ	6.69	125.82	119.80
27	N	889	ARG	NE-CZ-NH2	-6.68	116.96	120.30
20	J	212	ARG	NE-CZ-NH2	-6.68	116.96	120.30
14	7	91	TYR	CB-CG-CD1	6.68	125.01	121.00
24	X	129	LEU	CB-CG-CD2	6.67	122.34	111.00
11	4	95	ARG	NE-CZ-NH1	6.67	123.64	120.30
13	m	98	TYR	CB-CG-CD2	-6.67	117.00	121.00
33	O	215	TYR	CB-CG-CD1	6.67	125.00	121.00
17	K	374	ARG	NE-CZ-NH1	6.66	123.63	120.30
7	g	4	TYR	CB-CG-CD1	6.66	125.00	121.00
5	E	128	ARG	NE-CZ-NH2	-6.66	116.97	120.30
27	N	217	MET	CG-SD-CE	-6.66	89.55	100.20
6	f	88	ARG	NH1-CZ-NH2	-6.66	112.08	119.40
12	l	146	TRP	CB-CG-CD2	-6.66	117.95	126.60
5	E	161	ALA	N-CA-CB	6.65	119.41	110.10
26	Z	795	THR	N-CA-CB	6.65	122.93	110.30
30	Q	153	ASP	CB-CG-OD1	6.65	124.28	118.30
13	m	133	ARG	NE-CZ-NH2	-6.65	116.98	120.30
13	m	67	ARG	NE-CZ-NH2	6.64	123.62	120.30
24	X	97	TYR	CB-CG-CD2	6.64	124.98	121.00
23	T	15	PHE	CB-CG-CD2	-6.64	116.15	120.80
2	b	87	ASP	CB-CG-OD1	6.63	124.27	118.30
10	3	182	TRP	NE1-CE2-CD2	6.63	113.93	107.30
3	C	186	ASP	CB-CG-OD1	-6.62	112.34	118.30
23	T	161	TRP	CB-CG-CD2	-6.62	117.99	126.60
8	h	133	PHE	CB-CG-CD1	6.62	125.43	120.80
23	T	81	TYR	CB-CG-CD1	-6.62	117.03	121.00
27	N	770	LYS	N-CA-CB	6.62	122.51	110.60
23	T	130	ASP	CB-CG-OD1	6.62	124.25	118.30
10	3	85	THR	CA-CB-CG2	-6.61	103.14	112.40
14	7	161	ARG	NE-CZ-NH2	-6.61	116.99	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	O	369	ARG	NE-CZ-NH1	6.61	123.61	120.30
31	R	252	TYR	CB-CG-CD1	6.61	124.96	121.00
5	e	19	SER	N-CA-CB	6.60	120.41	110.50
7	g	137	VAL	CG1-CB-CG2	6.60	121.46	110.90
13	6	156	PHE	CB-CG-CD2	6.60	125.42	120.80
1	A	99	TYR	CB-CG-CD2	-6.60	117.04	121.00
8	1	102	TYR	CB-CG-CD1	-6.60	117.04	121.00
27	N	604	ARG	NE-CZ-NH1	6.60	123.60	120.30
31	R	68	GLU	C-N-CA	6.59	138.19	121.70
5	E	2	ARG	NE-CZ-NH2	-6.59	117.00	120.30
31	R	21	VAL	CA-CB-CG2	-6.59	101.02	110.90
31	R	321	TYR	CB-CG-CD1	-6.59	117.05	121.00
14	n	129	TYR	CG-CD1-CE1	-6.58	116.03	121.30
1	a	209	PHE	CB-CG-CD1	6.57	125.40	120.80
33	O	284	GLU	CB-CG-CD	-6.57	96.47	114.20
13	6	76	HIS	CA-CB-CG	-6.57	102.44	113.60
18	L	70	TYR	CB-CG-CD1	-6.57	117.06	121.00
1	A	242	GLN	N-CA-C	-6.56	93.28	111.00
10	j	72	LEU	CB-CG-CD2	6.56	122.16	111.00
31	R	153	THR	CA-CB-CG2	-6.56	103.21	112.40
1	a	62	TYR	CG-CD2-CE2	-6.55	116.06	121.30
6	F	12	PHE	CB-CG-CD1	6.55	125.39	120.80
18	L	361	PHE	CB-CG-CD2	-6.55	116.21	120.80
12	l	159	ARG	NE-CZ-NH1	6.55	123.58	120.30
24	X	45	PHE	CB-CG-CD2	-6.55	116.22	120.80
31	R	307	TYR	CB-CG-CD1	6.55	124.93	121.00
26	Z	869	ASP	CB-CG-OD2	6.54	124.19	118.30
12	5	40	PHE	CB-CG-CD1	6.54	125.38	120.80
16	I	153	THR	N-CA-CB	6.54	122.73	110.30
23	T	247	ASP	CB-CG-OD1	-6.54	112.41	118.30
6	f	86	TYR	CB-CG-CD1	-6.54	117.08	121.00
6	F	127	TYR	CZ-CE2-CD2	-6.54	113.92	119.80
18	L	401	PHE	CB-CG-CD1	6.53	125.37	120.80
14	n	4	PRO	N-CA-CB	6.53	111.14	103.30
7	G	110	ASP	CB-CG-OD2	-6.53	112.42	118.30
18	L	400	PHE	CB-CG-CD2	-6.53	116.23	120.80
27	N	203	ARG	NE-CZ-NH1	6.53	123.56	120.30
14	7	137	TYR	CB-CG-CD1	6.52	124.91	121.00
15	H	389	PHE	CB-CG-CD1	6.52	125.36	120.80
1	A	196	PHE	CB-CG-CD2	-6.52	116.24	120.80
8	1	91	ASP	CB-CG-OD2	-6.52	112.44	118.30
24	X	22	ARG	NE-CZ-NH2	-6.52	117.04	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	Z	338	HIS	N-CA-CB	6.51	122.32	110.60
5	e	1	ASP	CB-CG-OD1	-6.51	112.44	118.30
2	b	90	ARG	NE-CZ-NH1	6.51	123.55	120.30
12	l	113	TYR	CG-CD1-CE1	-6.51	116.09	121.30
31	R	70	TYR	CA-C-O	-6.51	106.43	120.10
23	T	14	ALA	CB-CA-C	-6.50	100.35	110.10
31	R	141	TYR	CB-CG-CD1	6.50	124.90	121.00
21	W	122	ARG	NE-CZ-NH1	6.50	123.55	120.30
26	Z	843	ASP	CB-CG-OD1	6.50	124.15	118.30
6	f	88	ARG	NE-CZ-NH1	6.50	123.55	120.30
7	g	4	TYR	CD1-CE1-CZ	6.49	125.64	119.80
7	G	142	ALA	CB-CA-C	-6.49	100.36	110.10
26	Z	264	PHE	CB-CG-CD1	-6.49	116.25	120.80
11	k	23	ARG	CB-CA-C	-6.49	97.42	110.40
6	f	5	TYR	CZ-CE2-CD2	-6.49	113.96	119.80
7	g	22	TYR	CB-CG-CD1	6.48	124.89	121.00
17	K	73	ARG	NE-CZ-NH1	6.48	123.54	120.30
26	Z	408	TYR	CG-CD2-CE2	-6.47	116.12	121.30
22	V	269	ARG	NE-CZ-NH2	-6.47	117.06	120.30
27	N	788	TYR	CZ-CE2-CD2	-6.47	113.98	119.80
27	N	415	PHE	CB-CG-CD2	-6.46	116.27	120.80
12	5	212	GLY	CA-C-O	-6.46	108.97	120.60
19	M	221	TYR	CB-CG-CD1	-6.46	117.12	121.00
30	Q	34	ASP	CB-CG-OD2	-6.46	112.49	118.30
31	R	345	TYR	CB-CG-CD2	6.46	124.87	121.00
5	e	18	TYR	CG-CD1-CE1	-6.46	116.14	121.30
26	Z	561	ASP	CB-CG-OD2	6.45	124.11	118.30
14	7	229	GLY	CA-C-O	-6.45	108.99	120.60
16	I	378	GLU	N-CA-CB	6.45	122.21	110.60
12	5	78	ALA	CB-CA-C	-6.45	100.43	110.10
23	T	118	ASN	CA-CB-CG	-6.44	99.23	113.40
21	W	157	PHE	CB-CG-CD2	-6.44	116.29	120.80
26	Z	98	ASP	CB-CG-OD2	-6.44	112.50	118.30
26	Z	441	TYR	CB-CG-CD1	6.44	124.86	121.00
1	A	37	ARG	NE-CZ-NH1	-6.43	117.08	120.30
12	l	155	TYR	CB-CG-CD2	-6.43	117.14	121.00
3	C	221	ASP	CB-CG-OD2	-6.42	112.52	118.30
4	D	118	TYR	CB-CG-CD2	-6.42	117.15	121.00
19	M	291	PHE	CB-CG-CD1	-6.42	116.31	120.80
6	f	81	ARG	NH1-CZ-NH2	6.41	126.46	119.40
19	M	349	PHE	CB-CG-CD1	6.41	125.29	120.80
11	k	159	ASP	CB-CG-OD2	6.41	124.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	M	129	LEU	CB-CG-CD2	-6.41	100.10	111.00
29	P	367	GLU	OE1-CD-OE2	-6.41	115.61	123.30
1	A	50	VAL	CA-CB-CG1	-6.41	101.29	110.90
20	J	147	TYR	CB-CG-CD1	6.41	124.84	121.00
2	B	89	SER	N-CA-CB	6.41	120.11	110.50
9	i	69	TYR	CZ-CE2-CD2	-6.41	114.04	119.80
26	Z	280	ASP	CB-CG-OD2	-6.40	112.54	118.30
12	l	181	THR	CA-CB-CG2	-6.40	103.44	112.40
4	d	73	PHE	CB-CG-CD2	6.39	125.28	120.80
1	A	25	ALA	N-CA-CB	6.39	119.05	110.10
24	X	17	TYR	CG-CD2-CE2	-6.39	116.18	121.30
13	6	105	TYR	CB-CG-CD2	-6.39	117.16	121.00
26	Z	441	TYR	CB-CG-CD2	-6.39	117.17	121.00
16	I	180	SER	N-CA-CB	6.39	120.08	110.50
17	K	118	TYR	CB-CG-CD2	-6.39	117.17	121.00
5	E	162	LYS	N-CA-CB	6.38	122.09	110.60
5	e	75	ALA	CB-CA-C	-6.38	100.53	110.10
20	J	316	PHE	CB-CG-CD1	-6.38	116.33	120.80
13	m	106	TYR	CB-CG-CD1	6.38	124.83	121.00
4	d	157	TRP	CB-CG-CD2	-6.37	118.31	126.60
5	e	148	PHE	CB-CG-CD2	-6.37	116.34	120.80
9	i	114	HIS	CA-CB-CG	-6.37	102.77	113.60
14	7	24	ALA	N-CA-CB	6.37	119.02	110.10
4	d	139	ARG	NE-CZ-NH2	-6.37	117.12	120.30
5	e	130	PHE	CB-CG-CD1	-6.37	116.34	120.80
10	3	146	PHE	CB-CA-C	-6.37	97.67	110.40
4	d	52	LEU	N-CA-CB	6.36	123.13	110.40
4	d	139	ARG	NE-CZ-NH1	6.36	123.48	120.30
17	K	318	THR	CA-CB-CG2	-6.36	103.50	112.40
5	e	110	ASP	CB-CG-OD1	6.35	124.02	118.30
21	W	113	PHE	CB-CG-CD2	-6.35	116.35	120.80
12	5	40	PHE	CB-CG-CD2	-6.35	116.36	120.80
15	H	242	PRO	N-CA-CB	6.34	110.91	103.30
5	E	18	TYR	CB-CG-CD2	-6.34	117.19	121.00
20	J	310	ILE	CB-CA-C	-6.34	98.93	111.60
10	j	95	TYR	CB-CG-CD2	-6.33	117.20	121.00
20	J	235	VAL	CA-CB-CG2	-6.32	101.41	110.90
26	Z	295	ARG	NE-CZ-NH2	-6.32	117.14	120.30
25	Y	41	ASP	CB-CG-OD1	-6.32	112.61	118.30
26	Z	405	ASN	N-CA-CB	6.32	121.97	110.60
12	l	7	ARG	NE-CZ-NH2	-6.31	117.14	120.30
11	4	98	TYR	CB-CG-CD2	-6.31	117.22	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	K	289	ASP	CB-CG-OD1	-6.31	112.62	118.30
20	J	350	MET	N-CA-CB	6.31	121.96	110.60
4	d	127	PHE	CG-CD1-CE1	-6.30	113.87	120.80
6	f	131	LEU	CB-CA-C	-6.30	98.23	110.20
15	H	283	TYR	CB-CG-CD2	-6.30	117.22	121.00
19	M	213	ARG	NE-CZ-NH2	-6.30	117.15	120.30
13	m	200	ASP	CB-CG-OD1	-6.30	112.63	118.30
7	g	95	PHE	CB-CG-CD1	6.29	125.21	120.80
18	L	69	ARG	NE-CZ-NH2	-6.29	117.15	120.30
3	C	58	GLN	CB-CA-C	-6.29	97.82	110.40
27	N	15	GLU	CB-CA-C	-6.29	97.82	110.40
9	i	34	LEU	N-CA-CB	6.29	122.98	110.40
17	K	234	PHE	CB-CG-CD2	-6.29	116.40	120.80
12	l	179	HIS	N-CA-CB	6.28	121.91	110.60
1	A	196	PHE	CB-CG-CD1	6.28	125.20	120.80
6	f	121	SER	N-CA-CB	6.28	119.92	110.50
19	M	226	THR	CA-CB-CG2	-6.28	103.61	112.40
27	N	161	TYR	CB-CG-CD1	6.28	124.77	121.00
12	5	207	PHE	CB-CG-CD1	6.28	125.19	120.80
33	O	370	LEU	CB-CG-CD2	6.28	121.67	111.00
19	M	433	TYR	CB-CG-CD1	6.28	124.77	121.00
8	h	61	TYR	CB-CG-CD1	6.27	124.76	121.00
23	T	220	PHE	CB-CG-CD2	-6.27	116.41	120.80
16	I	319	ARG	NE-CZ-NH2	-6.27	117.16	120.30
20	J	282	PHE	CB-CG-CD2	-6.27	116.41	120.80
11	k	23	ARG	NH1-CZ-NH2	-6.26	112.51	119.40
31	R	68	GLU	CA-C-N	-6.26	103.42	117.20
1	a	166	GLN	CG-CD-OE1	-6.26	109.08	121.60
2	b	142	PHE	CB-CG-CD2	-6.26	116.42	120.80
12	l	36	GLU	N-CA-CB	6.26	121.86	110.60
22	V	170	PRO	N-CD-CG	6.26	112.58	103.20
2	b	75	TYR	CG-CD2-CE2	-6.25	116.30	121.30
18	L	290	ARG	NE-CZ-NH2	-6.25	117.17	120.30
17	K	428	LYS	N-CA-CB	6.25	121.85	110.60
4	d	112	ALA	CB-CA-C	-6.24	100.73	110.10
28	S	292	TYR	CB-CG-CD1	6.24	124.74	121.00
33	O	291	ILE	N-CA-CB	6.23	125.14	110.80
30	Q	286	TYR	CB-CG-CD1	6.23	124.74	121.00
7	G	153	TYR	CB-CG-CD1	-6.22	117.27	121.00
27	N	675	VAL	CA-CB-CG2	-6.22	101.56	110.90
10	j	199	LEU	CB-CA-C	-6.22	98.38	110.20
15	H	320	ASP	CB-CG-OD1	6.22	123.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	110	ILE	O-C-N	-6.22	112.75	122.70
2	B	234	ARG	NE-CZ-NH1	6.21	123.41	120.30
24	X	10	PHE	CB-CG-CD1	-6.21	116.45	120.80
32	U	101	ALA	CB-CA-C	-6.21	100.78	110.10
4	d	54	ASP	CB-CG-OD1	6.21	123.89	118.30
2	B	90	ARG	NE-CZ-NH2	-6.21	117.19	120.30
6	f	175	LEU	CB-CA-C	-6.21	98.41	110.20
3	c	145	TYR	CB-CG-CD1	-6.20	117.28	121.00
4	d	224	SER	N-CA-CB	6.20	119.80	110.50
7	g	186	ARG	NH1-CZ-NH2	-6.20	112.58	119.40
6	F	4	ASN	CA-CB-CG	-6.20	99.76	113.40
26	Z	622	HIS	N-CA-CB	6.20	121.76	110.60
28	S	170	TYR	CB-CG-CD2	6.20	124.72	121.00
10	3	135	PHE	CB-CG-CD1	-6.20	116.46	120.80
27	N	333	SER	N-CA-CB	6.20	119.80	110.50
30	Q	112	ASP	CB-CG-OD2	-6.19	112.73	118.30
10	3	161	ASP	CB-CG-OD1	-6.19	112.73	118.30
7	g	156	TYR	CB-CG-CD2	-6.18	117.29	121.00
2	b	104	TYR	CZ-CE2-CD2	-6.18	114.24	119.80
12	5	187	TYR	CB-CG-CD2	-6.18	117.29	121.00
33	O	15	ARG	NE-CZ-NH1	-6.18	117.21	120.30
24	X	87	PHE	CB-CG-CD2	-6.18	116.47	120.80
1	a	130	VAL	CG1-CB-CG2	6.18	120.78	110.90
1	A	99	TYR	CB-CG-CD1	6.18	124.71	121.00
14	7	11	VAL	N-CA-C	-6.18	94.32	111.00
26	Z	323	TYR	CD1-CE1-CZ	6.17	125.35	119.80
27	N	787	MET	CG-SD-CE	-6.17	90.33	100.20
26	Z	11	THR	CA-CB-CG2	-6.17	103.77	112.40
12	l	55	TRP	CG-CD2-CE3	-6.16	128.35	133.90
20	J	244	ILE	N-CA-C	-6.16	94.36	111.00
2	b	12	PHE	C-N-CA	6.16	137.10	121.70
10	j	102	TYR	CG-CD1-CE1	-6.16	116.37	121.30
27	N	788	TYR	N-CA-CB	6.16	121.69	110.60
32	U	33	CYS	N-CA-C	-6.16	94.37	111.00
15	H	457	PHE	CB-CG-CD1	6.16	125.11	120.80
10	3	202	ARG	NE-CZ-NH2	-6.15	117.22	120.30
16	I	114	ASP	CB-CG-OD2	-6.15	112.77	118.30
17	K	411	TYR	CB-CG-CD1	6.15	124.69	121.00
33	O	9	THR	CA-CB-CG2	-6.15	103.79	112.40
27	N	210	SER	N-CA-CB	6.15	119.72	110.50
10	j	197	ARG	NE-CZ-NH1	6.14	123.37	120.30
11	k	138	PHE	CB-CG-CD1	6.14	125.10	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	249	ALA	CB-CA-C	-6.14	100.90	110.10
30	Q	286	TYR	CB-CG-CD2	-6.14	117.32	121.00
6	F	232	TYR	CB-CG-CD1	6.13	124.68	121.00
10	3	21	ALA	N-CA-CB	6.13	118.69	110.10
2	b	82	TYR	CG-CD2-CE2	-6.13	116.39	121.30
4	d	34	VAL	CG1-CB-CG2	6.13	120.71	110.90
16	I	165	ASP	N-CA-CB	6.13	121.64	110.60
18	L	117	TYR	CZ-CE2-CD2	-6.13	114.28	119.80
27	N	396	SER	N-CA-CB	6.13	119.69	110.50
31	R	58	GLU	O-C-N	-6.13	112.90	122.70
2	b	179	TRP	CG-CD2-CE3	-6.12	128.39	133.90
22	V	21	ASP	CB-CG-OD1	6.12	123.81	118.30
7	g	99	TYR	CG-CD2-CE2	-6.12	116.40	121.30
30	Q	339	TYR	CB-CG-CD2	-6.12	117.33	121.00
1	a	154	TYR	CB-CG-CD1	6.12	124.67	121.00
20	J	42	ARG	NE-CZ-NH1	-6.12	117.24	120.30
9	i	90	TYR	CZ-CE2-CD2	6.12	125.30	119.80
23	T	109	TYR	CB-CG-CD1	-6.12	117.33	121.00
28	S	174	ARG	NE-CZ-NH2	-6.12	117.24	120.30
21	W	114	VAL	CG1-CB-CG2	-6.11	101.13	110.90
31	R	331	ARG	NE-CZ-NH2	-6.11	117.25	120.30
6	f	66	ASP	CB-CG-OD1	-6.11	112.80	118.30
20	J	282	PHE	CB-CG-CD1	6.11	125.07	120.80
22	V	61	TYR	CB-CG-CD2	6.11	124.66	121.00
5	e	55	SER	N-CA-CB	6.10	119.65	110.50
13	m	156	PHE	CG-CD1-CE1	6.10	127.51	120.80
14	n	189	ALA	O-C-N	6.10	132.47	122.70
17	K	348	GLU	N-CA-CB	6.10	121.58	110.60
4	D	164	ARG	NE-CZ-NH2	-6.10	117.25	120.30
13	m	22	VAL	CA-CB-CG2	6.09	120.04	110.90
33	O	98	TYR	CB-CG-CD2	-6.09	117.34	121.00
8	h	34	LEU	CB-CG-CD2	6.09	121.35	111.00
1	A	157	TYR	CB-CG-CD1	-6.09	117.35	121.00
26	Z	6	ASP	CB-CG-OD2	6.09	123.78	118.30
7	g	177	ASP	N-CA-CB	6.08	121.55	110.60
26	Z	280	ASP	CB-CG-OD1	6.08	123.78	118.30
12	l	69	ARG	NE-CZ-NH1	6.08	123.34	120.30
27	N	137	PHE	CB-CG-CD2	6.08	125.05	120.80
31	R	422	ARG	NE-CZ-NH1	6.08	123.34	120.30
33	O	248	TYR	CZ-CE2-CD2	6.07	125.26	119.80
20	J	397	ALA	CB-CA-C	-6.07	101.00	110.10
13	m	131	TYR	CZ-CE2-CD2	-6.07	114.34	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	I	436	TYR	CB-CG-CD1	6.07	124.64	121.00
30	Q	309	ARG	NE-CZ-NH2	-6.07	117.27	120.30
30	Q	146	TYR	CB-CG-CD1	-6.06	117.36	121.00
1	a	159	ALA	N-CA-CB	6.06	118.58	110.10
16	I	256	TYR	CB-CG-CD2	6.06	124.63	121.00
7	g	225	LYS	CB-CA-C	-6.05	98.29	110.40
21	W	17	ARG	NE-CZ-NH2	6.05	123.33	120.30
26	Z	754	LYS	CA-CB-CG	6.05	126.72	113.40
28	S	367	TYR	CB-CG-CD1	6.05	124.63	121.00
31	R	70	TYR	CA-CB-CG	6.05	124.89	113.40
3	c	128	ARG	CD-NE-CZ	6.04	132.06	123.60
14	n	30	TYR	CG-CD2-CE2	-6.04	116.46	121.30
8	1	90	LYS	CB-CA-C	-6.04	98.32	110.40
26	Z	774	ARG	NE-CZ-NH1	6.04	123.32	120.30
31	R	24	TYR	CB-CG-CD1	-6.04	117.38	121.00
14	n	224	ASP	CB-CG-OD2	6.03	123.73	118.30
1	A	101	TYR	CZ-CE2-CD2	6.03	125.23	119.80
16	I	135	PHE	CB-CG-CD1	-6.03	116.58	120.80
27	N	673	PRO	CA-N-CD	6.03	120.14	111.70
26	Z	846	PHE	CB-CG-CD2	-6.03	116.58	120.80
28	S	286	TYR	CB-CG-CD2	6.03	124.61	121.00
6	f	58	TYR	CB-CG-CD2	6.02	124.61	121.00
14	n	161	ARG	NE-CZ-NH1	6.02	123.31	120.30
12	l	88	TYR	CB-CG-CD1	-6.02	117.39	121.00
20	J	144	ASP	CB-CG-OD2	6.02	123.71	118.30
26	Z	811	SER	N-CA-CB	6.02	119.53	110.50
14	n	91	TYR	CB-CG-CD1	6.01	124.61	121.00
13	6	116	GLU	O-C-N	-6.01	113.08	122.70
26	Z	385	PHE	CB-CG-CD2	-6.01	116.59	120.80
27	N	788	TYR	CB-CG-CD1	-6.01	117.39	121.00
14	n	129	TYR	CG-CD2-CE2	6.01	126.11	121.30
19	M	371	ASP	CB-CG-OD2	-6.01	112.89	118.30
9	2	88	PHE	CB-CG-CD2	6.01	125.01	120.80
20	J	235	VAL	CB-CA-C	-6.01	99.98	111.40
12	l	90	TYR	CG-CD1-CE1	-6.00	116.50	121.30
30	Q	165	PHE	CB-CG-CD1	-6.00	116.60	120.80
26	Z	299	ASP	CB-CG-OD1	-6.00	112.90	118.30
4	d	95	ARG	NH1-CZ-NH2	-6.00	112.80	119.40
18	L	313	ASP	CB-CG-OD1	-6.00	112.90	118.30
28	S	55	ARG	NE-CZ-NH1	6.00	123.30	120.30
33	O	62	TYR	CB-CG-CD2	-6.00	117.40	121.00
9	2	186	TYR	CB-CG-CD1	6.00	124.60	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	O	250	TRP	CG-CD2-CE3	-5.99	128.51	133.90
14	n	130	VAL	CA-CB-CG2	5.99	119.88	110.90
6	f	122	TYR	CG-CD2-CE2	-5.98	116.52	121.30
26	Z	419	VAL	CA-CB-CG2	-5.98	101.93	110.90
8	1	111	TYR	CB-CG-CD2	5.98	124.59	121.00
19	M	345	ARG	NE-CZ-NH2	-5.98	117.31	120.30
7	g	243	ILE	CA-CB-CG2	-5.97	98.95	110.90
14	n	186	TYR	CB-CG-CD2	-5.97	117.42	121.00
8	1	185	ARG	NE-CZ-NH1	5.97	123.29	120.30
26	Z	427	GLN	O-C-N	5.97	132.25	122.70
14	n	37	ASN	CB-CA-C	-5.97	98.46	110.40
14	n	41	ARG	NE-CZ-NH2	-5.97	117.31	120.30
2	B	222	LEU	CB-CG-CD1	5.97	121.15	111.00
12	l	54	PHE	CB-CG-CD1	-5.96	116.62	120.80
9	i	200	GLN	N-CA-CB	5.96	121.33	110.60
20	J	297	LEU	CB-CG-CD1	5.96	121.13	111.00
7	g	99	TYR	CD1-CG-CD2	5.96	124.45	117.90
14	7	89	PRO	CA-N-CD	5.95	120.03	111.70
11	4	73	TYR	CB-CG-CD1	-5.95	117.43	121.00
13	6	7	ASP	CB-CA-C	-5.94	98.51	110.40
1	A	209	PHE	CB-CG-CD2	-5.94	116.64	120.80
19	M	53	HIS	CA-CB-CG	5.94	123.70	113.60
28	S	273	PHE	CB-CG-CD2	5.94	124.96	120.80
1	a	154	TYR	CB-CG-CD2	-5.94	117.44	121.00
1	a	209	PHE	CB-CG-CD2	-5.94	116.64	120.80
15	H	96	PRO	N-CA-CB	5.94	110.42	103.30
27	N	328	PHE	CB-CG-CD1	5.94	124.96	120.80
1	a	204	ALA	CB-CA-C	-5.93	101.20	110.10
2	b	128	ARG	NE-CZ-NH1	5.93	123.27	120.30
2	B	4	ARG	NH1-CZ-NH2	-5.93	112.87	119.40
15	H	156	VAL	N-CA-C	-5.93	94.98	111.00
4	D	164	ARG	NE-CZ-NH1	5.93	123.27	120.30
7	G	107	ALA	CB-CA-C	-5.93	101.21	110.10
23	T	52	LEU	CB-CG-CD1	5.93	121.07	111.00
3	C	5	TYR	CB-CG-CD1	5.92	124.55	121.00
31	R	134	TRP	CB-CG-CD2	-5.92	118.90	126.60
2	B	36	GLY	N-CA-C	-5.92	98.30	113.10
3	c	130	PHE	CB-CG-CD1	5.92	124.94	120.80
5	e	76	ASP	CB-CG-OD1	5.92	123.63	118.30
19	M	366	ARG	NE-CZ-NH2	-5.92	117.34	120.30
28	S	64	ARG	NE-CZ-NH2	-5.92	117.34	120.30
7	G	197	TYR	CB-CG-CD1	5.91	124.55	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	185	ALA	N-CA-CB	5.91	118.38	110.10
14	n	128	ARG	NE-CZ-NH1	5.91	123.25	120.30
4	d	168	THR	N-CA-CB	-5.91	99.08	110.30
4	D	103	THR	N-CA-CB	5.91	121.52	110.30
33	O	166	ARG	NE-CZ-NH1	5.91	123.25	120.30
5	e	85	ARG	NE-CZ-NH2	-5.90	117.35	120.30
26	Z	857	LEU	C-N-CA	5.90	134.68	122.30
8	h	102	TYR	CB-CG-CD2	5.89	124.54	121.00
1	a	13	GLU	CB-CA-C	-5.89	98.62	110.40
16	I	232	LEU	CB-CG-CD2	5.89	121.02	111.00
22	V	186	GLN	CA-CB-CG	5.89	126.36	113.40
26	Z	142	ASP	CB-CG-OD1	-5.89	113.00	118.30
28	S	82	TYR	CB-CG-CD1	-5.89	117.47	121.00
6	f	58	TYR	CB-CG-CD1	-5.88	117.47	121.00
9	i	140	SER	N-CA-CB	-5.88	101.67	110.50
19	M	323	VAL	N-CA-C	-5.88	95.12	111.00
31	R	238	PHE	CB-CG-CD2	5.88	124.92	120.80
2	b	178	ARG	NE-CZ-NH2	-5.88	117.36	120.30
3	c	134	PHE	N-CA-CB	5.88	121.18	110.60
7	g	4	TYR	CG-CD1-CE1	-5.88	116.60	121.30
5	e	179	TRP	CB-CG-CD2	-5.87	118.97	126.60
12	l	137	TYR	CZ-CE2-CD2	-5.87	114.52	119.80
8	1	142	PHE	CB-CG-CD2	-5.87	116.69	120.80
9	2	196	ARG	NE-CZ-NH1	5.87	123.23	120.30
13	m	117	ASP	CB-CG-OD1	5.87	123.58	118.30
2	b	246	ARG	NE-CZ-NH1	5.87	123.23	120.30
9	i	188	ARG	N-CA-CB	5.87	121.16	110.60
2	b	235	PHE	CB-CG-CD2	5.86	124.90	120.80
2	B	46	ALA	N-CA-CB	5.86	118.31	110.10
10	3	113	SER	N-CA-CB	5.86	119.30	110.50
26	Z	557	GLU	OE1-CD-OE2	-5.86	116.26	123.30
27	N	325	PHE	CB-CG-CD1	5.86	124.90	120.80
3	C	201	ASP	CB-CG-OD2	-5.86	113.03	118.30
22	V	108	TYR	CG-CD1-CE1	-5.86	116.61	121.30
30	Q	84	TYR	CG-CD1-CE1	-5.86	116.61	121.30
18	L	132	ARG	NE-CZ-NH2	-5.86	117.37	120.30
13	6	176	SER	N-CA-CB	5.86	119.28	110.50
23	T	199	PHE	CB-CG-CD1	-5.86	116.70	120.80
5	e	94	TYR	CB-CG-CD2	-5.85	117.49	121.00
13	m	176	SER	N-CA-CB	5.85	119.28	110.50
14	7	161	ARG	NE-CZ-NH1	5.85	123.23	120.30
30	Q	132	PHE	CB-CG-CD1	-5.85	116.70	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	I	419	ALA	N-CA-CB	5.85	118.29	110.10
11	k	116	LEU	N-CA-CB	5.85	122.09	110.40
26	Z	98	ASP	CB-CG-OD1	5.84	123.56	118.30
6	f	228	ALA	N-CA-CB	5.84	118.28	110.10
26	Z	869	ASP	CB-CG-OD1	-5.84	113.04	118.30
16	I	130	VAL	CA-CB-CG1	-5.84	102.14	110.90
3	c	225	TYR	CB-CG-CD2	-5.84	117.50	121.00
28	S	457	PRO	CA-N-CD	5.84	119.87	111.70
4	d	14	HIS	N-CA-CB	5.83	121.10	110.60
26	Z	851	ALA	CB-CA-C	-5.83	101.35	110.10
30	Q	124	PHE	CB-CG-CD1	5.83	124.88	120.80
26	Z	165	TYR	CD1-CE1-CZ	5.83	125.05	119.80
8	h	185	ARG	NE-CZ-NH2	-5.83	117.39	120.30
5	e	224	ASP	CB-CG-OD2	-5.83	113.06	118.30
9	i	88	PHE	CB-CG-CD2	5.83	124.88	120.80
18	L	119	VAL	CA-CB-CG2	5.83	119.64	110.90
13	m	217	TYR	CG-CD1-CE1	5.82	125.96	121.30
19	M	115	LYS	N-CA-CB	5.82	121.08	110.60
16	I	83	LYS	N-CA-CB	5.82	121.07	110.60
23	T	184	ALA	CB-CA-C	-5.82	101.37	110.10
2	b	138	GLY	CA-C-O	5.81	131.06	120.60
3	c	136	TYR	N-CA-CB	5.81	121.06	110.60
5	e	156	PHE	CB-CG-CD2	-5.81	116.73	120.80
20	J	120	TYR	CB-CG-CD1	-5.80	117.52	121.00
6	f	167	ALA	N-CA-CB	5.80	118.22	110.10
1	A	5	ARG	NE-CZ-NH2	-5.80	117.40	120.30
26	Z	956	LEU	N-CA-C	-5.80	95.33	111.00
8	1	185	ARG	CD-NE-CZ	-5.80	115.48	123.60
32	U	22	TYR	CB-CG-CD1	-5.80	117.52	121.00
1	a	174	GLU	CB-CA-C	-5.80	98.81	110.40
5	e	235	LEU	CB-CA-C	-5.80	99.19	110.20
7	G	11	PHE	CB-CG-CD2	5.80	124.86	120.80
13	m	125	PHE	CB-CG-CD2	5.79	124.86	120.80
15	H	454	TYR	CG-CD2-CE2	5.79	125.94	121.30
20	J	382	PHE	CB-CG-CD2	-5.79	116.75	120.80
19	M	299	ARG	NE-CZ-NH1	5.79	123.19	120.30
2	b	220	ASP	CB-CG-OD2	5.79	123.51	118.30
2	B	212	ALA	N-CA-CB	5.79	118.20	110.10
26	Z	893	PHE	CG-CD1-CE1	-5.79	114.43	120.80
29	P	303	PHE	CB-CG-CD2	-5.79	116.75	120.80
31	R	33	LEU	CB-CG-CD1	5.79	120.84	111.00
31	R	99	TYR	CA-CB-CG	-5.79	102.41	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	101	TYR	CG-CD2-CE2	5.78	125.93	121.30
9	i	101	ALA	CB-CA-C	-5.78	101.42	110.10
26	Z	195	PHE	CB-CG-CD2	5.78	124.85	120.80
32	U	16	LEU	CB-CG-CD1	5.78	120.83	111.00
16	I	65	ILE	CA-CB-CG1	5.78	121.98	111.00
2	b	90	ARG	O-C-N	-5.78	113.46	122.70
20	J	63	ARG	NE-CZ-NH1	5.78	123.19	120.30
1	A	242	GLN	CA-CB-CG	5.77	126.10	113.40
7	g	99	TYR	CB-CG-CD1	-5.77	117.54	121.00
10	3	23	ALA	CB-CA-C	-5.77	101.45	110.10
31	R	334	ARG	NE-CZ-NH1	5.77	123.19	120.30
5	e	39	VAL	CA-CB-CG2	-5.77	102.25	110.90
7	g	108	PHE	CB-CG-CD1	-5.77	116.76	120.80
4	D	109	ARG	NE-CZ-NH1	5.77	123.18	120.30
19	M	345	ARG	NE-CZ-NH1	5.77	123.18	120.30
27	N	314	LEU	CB-CG-CD1	5.77	120.80	111.00
31	R	99	TYR	CZ-CE2-CD2	5.77	124.99	119.80
12	l	7	ARG	NE-CZ-NH1	5.76	123.18	120.30
2	B	173	THR	CA-CB-CG2	-5.76	104.33	112.40
33	O	178	TYR	CB-CG-CD2	-5.76	117.54	121.00
29	P	47	ARG	NH1-CZ-NH2	-5.76	113.06	119.40
21	W	25	ARG	NE-CZ-NH2	-5.76	117.42	120.30
2	b	181	ASP	CB-CG-OD2	-5.75	113.12	118.30
28	S	126	LYS	N-CA-CB	5.75	120.95	110.60
4	D	126	PRO	CA-N-CD	5.75	119.75	111.70
14	7	35	ARG	NE-CZ-NH1	-5.75	117.43	120.30
3	C	156	TYR	CB-CG-CD2	-5.74	117.55	121.00
31	R	99	TYR	CG-CD2-CE2	-5.74	116.71	121.30
11	k	80	VAL	CA-CB-CG2	-5.74	102.29	110.90
15	H	341	ASP	CB-CG-OD1	5.74	123.47	118.30
24	X	87	PHE	N-CA-C	-5.74	95.50	111.00
10	j	185	VAL	CG1-CB-CG2	5.74	120.08	110.90
17	K	415	VAL	CB-CA-C	-5.74	100.50	111.40
17	K	213	GLY	N-CA-C	-5.74	98.76	113.10
22	V	108	TYR	CD1-CE1-CZ	5.74	124.96	119.80
4	d	101	PRO	C-N-CA	5.73	136.03	121.70
13	m	67	ARG	NE-CZ-NH1	-5.73	117.43	120.30
13	6	144	SER	CB-CA-C	-5.73	99.21	110.10
28	S	64	ARG	N-CA-CB	5.73	120.92	110.60
28	S	481	TYR	CA-C-O	-5.73	108.06	120.10
10	j	67	ARG	NE-CZ-NH2	-5.73	117.44	120.30
28	S	273	PHE	CB-CG-CD1	-5.72	116.79	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	221	LYS	N-CA-CB	5.72	120.90	110.60
1	A	153	TYR	CB-CG-CD1	-5.72	117.57	121.00
28	S	55	ARG	NE-CZ-NH2	-5.72	117.44	120.30
4	d	238	LYS	N-CA-CB	5.72	120.89	110.60
7	G	126	ARG	NE-CZ-NH2	5.72	123.16	120.30
26	Z	358	TYR	CB-CG-CD2	-5.72	117.57	121.00
10	j	161	ASP	CB-CG-OD1	5.71	123.44	118.30
27	N	534	ASP	CB-CG-OD2	-5.71	113.16	118.30
31	R	304	TYR	CB-CG-CD1	-5.71	117.57	121.00
3	c	160	LYS	CB-CA-C	-5.71	98.99	110.40
8	1	56	ALA	CB-CA-C	-5.71	101.54	110.10
2	b	99	ARG	NE-CZ-NH2	-5.70	117.45	120.30
7	G	45	ALA	N-CA-CB	5.70	118.08	110.10
23	T	82	PHE	CB-CG-CD2	-5.70	116.81	120.80
10	j	141	ALA	CB-CA-C	-5.70	101.55	110.10
9	i	78	SER	N-CA-CB	5.70	119.05	110.50
10	3	49	PHE	N-CA-CB	5.70	120.85	110.60
19	M	422	VAL	CA-CB-CG2	-5.70	102.36	110.90
7	G	11	PHE	CB-CG-CD1	-5.69	116.81	120.80
8	1	168	SER	N-CA-CB	5.69	119.04	110.50
7	g	16	ARG	NE-CZ-NH2	-5.69	117.45	120.30
16	I	170	VAL	CA-CB-CG2	-5.69	102.36	110.90
2	b	92	VAL	CA-CB-CG1	5.69	119.43	110.90
7	g	87	ARG	NE-CZ-NH2	-5.69	117.45	120.30
30	Q	399	VAL	CG1-CB-CG2	5.69	120.00	110.90
12	l	97	MET	CG-SD-CE	-5.69	91.10	100.20
14	n	30	TYR	CG-CD1-CE1	-5.68	116.75	121.30
1	A	29	THR	C-N-CA	5.68	135.91	121.70
27	N	812	ALA	N-CA-CB	5.68	118.06	110.10
29	P	319	GLU	OE1-CD-OE2	5.68	130.12	123.30
2	b	90	ARG	NE-CZ-NH2	-5.68	117.46	120.30
12	l	145	LYS	CA-CB-CG	5.68	125.90	113.40
14	n	30	TYR	CD1-CG-CD2	5.68	124.15	117.90
1	a	58	THR	CA-CB-CG2	-5.68	104.45	112.40
5	E	152	PRO	CA-N-CD	5.68	119.65	111.70
26	Z	581	VAL	CA-CB-CG2	-5.68	102.38	110.90
29	P	6	PRO	N-CA-CB	5.68	110.11	103.30
29	P	168	TYR	CB-CG-CD1	-5.68	117.59	121.00
5	E	45	ARG	NE-CZ-NH1	-5.68	117.46	120.30
30	Q	261	VAL	CA-CB-CG2	-5.68	102.38	110.90
25	Y	83	ARG	NE-CZ-NH1	5.67	123.14	120.30
26	Z	269	TYR	CB-CG-CD2	-5.67	117.60	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	N	674	GLN	CB-CA-C	-5.67	99.05	110.40
27	N	526	TYR	CB-CG-CD2	5.67	124.40	121.00
13	6	218	GLU	N-CA-CB	5.67	120.81	110.60
31	R	134	TRP	CB-CG-CD1	5.67	134.37	127.00
7	g	199	ALA	O-C-N	-5.67	113.63	122.70
26	Z	49	LEU	CB-CG-CD2	5.67	120.63	111.00
23	T	51	TYR	CA-CB-CG	-5.66	102.64	113.40
27	N	921	ARG	NE-CZ-NH1	5.66	123.13	120.30
2	b	20	GLN	N-CA-CB	5.66	120.79	110.60
9	i	131	SER	N-CA-CB	5.66	118.99	110.50
19	M	291	PHE	CB-CG-CD2	5.66	124.76	120.80
21	W	17	ARG	O-C-N	5.66	131.76	122.70
26	Z	296	SER	N-CA-CB	5.66	118.99	110.50
26	Z	516	THR	CA-CB-CG2	-5.66	104.47	112.40
33	O	190	TYR	CG-CD2-CE2	-5.66	116.77	121.30
12	l	148	LEU	CB-CG-CD2	-5.66	101.38	111.00
11	k	117	TYR	CD1-CE1-CZ	5.66	124.89	119.80
26	Z	903	MET	CA-CB-CG	5.66	122.91	113.30
11	k	139	TYR	CG-CD2-CE2	-5.65	116.78	121.30
26	Z	496	ALA	N-CA-CB	5.65	118.01	110.10
27	N	231	ASN	O-C-N	-5.65	113.66	122.70
15	H	62	ARG	NE-CZ-NH1	5.65	123.13	120.30
26	Z	838	TYR	CB-CG-CD1	5.65	124.39	121.00
33	O	29	PHE	CB-CG-CD1	5.65	124.75	120.80
10	3	182	TRP	CE2-CD2-CE3	5.64	125.47	118.70
22	V	87	PHE	CB-CG-CD1	5.64	124.75	120.80
10	j	75	LEU	O-C-N	-5.64	113.68	122.70
13	6	57	PHE	CB-CG-CD2	-5.64	116.85	120.80
19	M	434	ALA	CB-CA-C	-5.64	101.64	110.10
8	h	193	TYR	CG-CD1-CE1	-5.64	116.79	121.30
15	H	443	PHE	CB-CG-CD1	-5.64	116.86	120.80
3	c	101	TYR	CZ-CE2-CD2	-5.63	114.73	119.80
7	g	221	ASN	N-CA-CB	5.63	120.74	110.60
5	E	122	GLU	CG-CD-OE1	5.63	129.57	118.30
27	N	88	ARG	NE-CZ-NH2	-5.63	117.48	120.30
3	c	192	ALA	N-CA-CB	5.63	117.98	110.10
6	f	178	PHE	CB-CG-CD1	5.63	124.74	120.80
27	N	300	ASN	N-CA-CB	5.63	120.74	110.60
31	R	207	ARG	NE-CZ-NH2	-5.63	117.48	120.30
1	a	224	PHE	CZ-CE2-CD2	5.63	126.86	120.10
12	l	121	ARG	NE-CZ-NH1	-5.63	117.49	120.30
7	g	165	ARG	NE-CZ-NH2	-5.62	117.49	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	197	TYR	CG-CD2-CE2	-5.62	116.80	121.30
11	k	89	ALA	N-CA-CB	5.62	117.97	110.10
8	h	35	THR	CA-CB-CG2	-5.62	104.53	112.40
11	k	135	TYR	CB-CG-CD2	-5.62	117.63	121.00
13	6	108	HIS	N-CA-C	-5.62	95.83	111.00
20	J	311	ASP	CA-CB-CG	5.62	125.76	113.40
2	b	121	ALA	CB-CA-C	-5.62	101.67	110.10
4	d	176	ASN	CB-CA-C	-5.62	99.17	110.40
7	g	177	ASP	CB-CG-OD2	-5.62	113.25	118.30
3	C	49	ARG	NE-CZ-NH1	5.62	123.11	120.30
11	4	44	MET	CG-SD-CE	-5.61	91.22	100.20
8	h	185	ARG	N-CA-CB	5.61	120.70	110.60
27	N	422	TYR	CB-CG-CD2	-5.61	117.63	121.00
3	c	121	TYR	CB-CA-C	-5.61	99.18	110.40
4	d	170	ARG	NH1-CZ-NH2	-5.61	113.23	119.40
5	e	125	LEU	CB-CG-CD1	-5.61	101.47	111.00
14	n	95	TYR	CB-CG-CD1	-5.61	117.64	121.00
26	Z	426	TYR	CA-CB-CG	-5.61	102.75	113.40
4	d	223	SER	N-CA-CB	5.60	118.91	110.50
5	e	114	ARG	NE-CZ-NH2	-5.60	117.50	120.30
8	h	143	ARG	NE-CZ-NH2	5.60	123.10	120.30
13	m	96	LEU	CB-CG-CD2	5.60	120.52	111.00
16	I	161	GLN	CG-CD-OE1	-5.60	110.40	121.60
30	Q	86	MET	CG-SD-CE	5.60	109.16	100.20
4	d	125	ARG	NE-CZ-NH2	-5.60	117.50	120.30
19	M	372	ASP	CB-CG-OD2	-5.60	113.26	118.30
11	k	153	THR	N-CA-CB	5.59	120.93	110.30
3	C	206	THR	CA-CB-CG2	-5.59	104.57	112.40
7	G	126	ARG	NE-CZ-NH1	5.59	123.10	120.30
25	Y	72	ASP	CB-CG-OD2	-5.59	113.26	118.30
14	7	156	ARG	NE-CZ-NH1	5.59	123.09	120.30
2	b	142	PHE	CG-CD1-CE1	-5.59	114.66	120.80
5	e	95	TYR	CB-CA-C	-5.59	99.23	110.40
13	6	147	MET	CG-SD-CE	-5.59	91.26	100.20
9	i	21	THR	CA-CB-CG2	-5.58	104.58	112.40
13	6	34	SER	N-CA-CB	5.58	118.88	110.50
14	n	187	ARG	NE-CZ-NH2	5.58	123.09	120.30
29	P	117	SER	N-CA-CB	5.58	118.87	110.50
14	n	66	LEU	N-CA-CB	5.58	121.56	110.40
22	V	185	ILE	CA-CB-CG2	5.58	122.06	110.90
6	f	119	THR	CA-CB-CG2	-5.58	104.59	112.40
7	G	32	THR	CA-CB-CG2	-5.58	104.59	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	157	TYR	CG-CD1-CE1	-5.58	116.84	121.30
9	i	200	GLN	CB-CA-C	-5.58	99.25	110.40
1	A	17	TYR	CB-CG-CD2	5.58	124.34	121.00
14	7	35	ARG	NE-CZ-NH2	5.58	123.09	120.30
17	K	412	ALA	C-N-CA	5.58	135.64	121.70
26	Z	535	VAL	CA-CB-CG2	-5.58	102.54	110.90
1	A	101	TYR	CG-CD2-CE2	-5.57	116.84	121.30
18	L	243	PHE	CB-CG-CD1	5.57	124.70	120.80
29	P	340	ASP	CB-CG-OD2	5.57	123.32	118.30
13	m	6	GLY	N-CA-C	-5.57	99.17	113.10
6	F	100	ARG	NE-CZ-NH2	-5.57	117.51	120.30
28	S	129	GLU	CB-CA-C	-5.57	99.26	110.40
8	h	193	TYR	CZ-CE2-CD2	-5.57	114.79	119.80
13	m	221	ARG	NE-CZ-NH2	-5.57	117.52	120.30
31	R	70	TYR	N-CA-CB	5.57	120.62	110.60
17	K	294	ARG	N-CA-CB	5.57	120.62	110.60
13	m	92	ASN	CB-CA-C	-5.57	99.27	110.40
29	P	405	PRO	CA-N-CD	5.56	119.49	111.70
19	M	425	ARG	NE-CZ-NH2	-5.56	117.52	120.30
29	P	325	ASP	CB-CG-OD2	-5.56	113.29	118.30
7	g	111	ARG	NE-CZ-NH2	-5.56	117.52	120.30
29	P	373	GLU	OE1-CD-OE2	5.56	129.97	123.30
33	O	248	TYR	CB-CG-CD1	5.56	124.34	121.00
19	M	318	ASP	CB-CG-OD1	5.56	123.30	118.30
4	d	222	LEU	CB-CA-C	-5.55	99.65	110.20
6	F	201	ARG	NE-CZ-NH2	-5.55	117.52	120.30
15	H	299	ARG	NE-CZ-NH2	-5.55	117.52	120.30
10	j	197	ARG	NE-CZ-NH2	-5.55	117.52	120.30
10	3	49	PHE	CB-CG-CD2	5.55	124.69	120.80
26	Z	402	ASP	CB-CG-OD2	5.55	123.30	118.30
18	L	404	ARG	NE-CZ-NH1	-5.55	117.52	120.30
20	J	381	ASP	CB-CG-OD2	-5.55	113.30	118.30
14	7	129	TYR	CB-CG-CD1	-5.55	117.67	121.00
26	Z	281	ALA	CB-CA-C	-5.55	101.78	110.10
5	e	85	ARG	NE-CZ-NH1	5.55	123.07	120.30
12	5	113	TYR	CB-CG-CD1	-5.55	117.67	121.00
19	M	380	ALA	N-CA-CB	5.55	117.87	110.10
33	O	171	PHE	CB-CG-CD2	-5.54	116.92	120.80
6	f	39	SER	N-CA-CB	5.54	118.81	110.50
11	4	73	TYR	N-CA-C	-5.54	96.04	111.00
27	N	93	GLU	N-CA-CB	5.54	120.57	110.60
10	j	153	TYR	CB-CG-CD1	-5.54	117.68	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	141	ALA	CB-CA-C	-5.54	101.79	110.10
17	K	88	ARG	NE-CZ-NH1	5.54	123.07	120.30
2	b	247	LEU	CB-CA-C	-5.53	99.69	110.20
15	H	283	TYR	CG-CD2-CE2	-5.53	116.87	121.30
26	Z	750	GLU	N-CA-CB	5.53	120.56	110.60
8	1	142	PHE	CB-CG-CD1	5.53	124.67	120.80
26	Z	770	GLU	N-CA-CB	5.53	120.55	110.60
26	Z	551	LEU	N-CA-CB	5.53	121.45	110.40
30	Q	77	PHE	CB-CA-C	-5.53	99.34	110.40
5	e	89	VAL	CG1-CB-CG2	5.53	119.74	110.90
9	2	75	ARG	NE-CZ-NH1	-5.53	117.54	120.30
13	6	67	ARG	NE-CZ-NH2	-5.53	117.54	120.30
5	E	223	TYR	CB-CG-CD2	-5.52	117.69	121.00
13	6	33	TYR	CB-CG-CD1	-5.52	117.69	121.00
28	S	217	PHE	CB-CG-CD1	-5.52	116.93	120.80
26	Z	375	ASP	CB-CG-OD2	-5.52	113.33	118.30
2	B	142	PHE	N-CA-CB	-5.52	100.67	110.60
23	T	173	GLU	N-CA-CB	5.52	120.53	110.60
12	l	54	PHE	CG-CD1-CE1	5.52	126.87	120.80
14	n	195	PHE	CB-CG-CD1	5.52	124.66	120.80
2	B	101	TYR	CB-CG-CD1	-5.52	117.69	121.00
2	b	69	PRO	N-CD-CG	5.51	111.47	103.20
6	f	137	ASP	CB-CG-OD1	5.51	123.26	118.30
22	V	61	TYR	CD1-CG-CD2	5.51	123.97	117.90
16	I	340	ARG	NE-CZ-NH1	5.51	123.06	120.30
26	Z	488	ALA	CB-CA-C	-5.51	101.83	110.10
2	B	54	PRO	CA-N-CD	5.51	119.41	111.70
15	H	279	LEU	CA-C-O	5.51	131.67	120.10
18	L	243	PHE	CB-CG-CD2	-5.51	116.94	120.80
27	N	398	ARG	NE-CZ-NH2	5.51	123.06	120.30
3	C	161	ALA	CB-CA-C	-5.51	101.84	110.10
8	h	8	PHE	CB-CG-CD1	-5.51	116.94	120.80
13	6	125	PHE	CB-CG-CD1	5.51	124.66	120.80
27	N	282	TYR	CG-CD1-CE1	5.50	125.70	121.30
30	Q	112	ASP	CB-CG-OD1	5.50	123.25	118.30
31	R	345	TYR	CB-CG-CD1	-5.50	117.70	121.00
10	j	135	PHE	N-CA-CB	5.50	120.50	110.60
5	e	14	PHE	CB-CG-CD2	-5.50	116.95	120.80
15	H	374	LYS	N-CA-CB	5.50	120.50	110.60
19	M	270	ALA	CB-CA-C	-5.49	101.86	110.10
33	O	215	TYR	CB-CG-CD2	-5.49	117.71	121.00
26	Z	802	ASP	CB-CG-OD2	5.49	123.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	S	442	PHE	CB-CG-CD1	-5.49	116.96	120.80
6	F	56	SER	N-CA-CB	5.48	118.72	110.50
8	1	137	TYR	CB-CG-CD2	-5.48	117.71	121.00
26	Z	582	ASP	CB-CG-OD2	-5.48	113.37	118.30
19	M	32	THR	CA-CB-CG2	-5.48	104.73	112.40
32	U	44	SER	N-CA-CB	5.48	118.72	110.50
11	k	72	ASP	CB-CG-OD2	-5.48	113.37	118.30
17	K	315	ILE	N-CA-C	-5.48	96.21	111.00
10	j	103	PHE	CB-CG-CD2	-5.48	116.97	120.80
30	Q	306	TYR	CB-CG-CD1	5.48	124.28	121.00
7	g	61	VAL	CA-CB-CG1	-5.47	102.69	110.90
23	T	20	TYR	CG-CD2-CE2	-5.47	116.92	121.30
9	i	196	ARG	NE-CZ-NH1	5.47	123.04	120.30
14	7	10	SER	N-CA-CB	5.47	118.71	110.50
23	T	138	ASP	CB-CG-OD1	5.47	123.22	118.30
28	S	45	THR	N-CA-C	-5.47	96.22	111.00
19	M	404	ARG	NH1-CZ-NH2	-5.47	113.38	119.40
32	U	114	THR	O-C-N	5.47	131.45	122.70
27	N	651	PHE	CB-CG-CD2	-5.47	116.97	120.80
27	N	907	ASP	CB-CG-OD1	5.47	123.22	118.30
6	f	9	THR	CA-CB-OG1	5.46	120.47	109.00
27	N	526	TYR	CB-CG-CD1	-5.46	117.72	121.00
6	F	93	TYR	CB-CG-CD1	5.46	124.28	121.00
33	O	252	PHE	CB-CG-CD1	5.46	124.62	120.80
29	P	364	ARG	NE-CZ-NH1	-5.46	117.57	120.30
10	j	96	GLU	N-CA-CB	5.46	120.42	110.60
2	b	142	PHE	CD1-CE1-CZ	5.45	126.64	120.10
17	K	212	TYR	CB-CG-CD2	-5.45	117.73	121.00
27	N	124	TYR	CA-CB-CG	-5.45	103.04	113.40
10	j	148	MET	N-CA-CB	5.45	120.41	110.60
14	7	104	ARG	NE-CZ-NH2	5.45	123.03	120.30
6	f	178	PHE	CG-CD1-CE1	5.45	126.80	120.80
32	U	253	ASP	CB-CG-OD1	-5.45	113.39	118.30
14	7	24	ALA	CB-CA-C	-5.45	101.93	110.10
19	M	425	ARG	NE-CZ-NH1	5.45	123.03	120.30
31	R	246	TYR	CG-CD2-CE2	5.45	125.66	121.30
6	F	221	PHE	CB-CG-CD1	5.44	124.61	120.80
4	d	157	TRP	CD1-CG-CD2	5.44	110.65	106.30
7	g	99	TYR	C-N-CA	5.44	135.29	121.70
30	Q	76	GLU	N-CA-C	5.44	125.68	111.00
3	C	145	TYR	CB-CG-CD1	5.44	124.26	121.00
12	l	155	TYR	CG-CD1-CE1	-5.43	116.95	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	177	VAL	N-CA-C	-5.43	96.33	111.00
11	4	84	VAL	CA-CB-CG2	-5.43	102.75	110.90
23	T	20	TYR	CB-CG-CD2	-5.43	117.74	121.00
28	S	101	LYS	N-CA-CB	5.43	120.38	110.60
4	d	216	ASP	CB-CG-OD1	-5.43	113.41	118.30
7	g	227	VAL	CA-CB-CG2	-5.43	102.75	110.90
27	N	188	TYR	CB-CG-CD2	-5.43	117.74	121.00
31	R	65	TYR	CD1-CE1-CZ	5.43	124.69	119.80
3	c	5	TYR	CB-CG-CD1	-5.43	117.74	121.00
31	R	181	TYR	CZ-CE2-CD2	5.43	124.69	119.80
21	W	122	ARG	NE-CZ-NH2	-5.43	117.59	120.30
30	Q	68	MET	CA-CB-CG	5.43	122.53	113.30
22	V	196	TYR	CG-CD1-CE1	5.42	125.64	121.30
26	Z	287	ARG	NE-CZ-NH2	-5.42	117.59	120.30
10	3	182	TRP	CE2-CD2-CG	-5.42	102.96	107.30
10	3	187	TYR	CB-CG-CD2	5.42	124.25	121.00
23	T	21	ALA	N-CA-CB	5.42	117.69	110.10
9	i	36	ARG	CB-CA-C	-5.42	99.56	110.40
20	J	69	GLY	C-N-CA	5.42	135.25	121.70
6	f	5	TYR	CB-CG-CD1	5.42	124.25	121.00
26	Z	759	ARG	NE-CZ-NH2	-5.42	117.59	120.30
27	N	795	GLU	CB-CA-C	-5.42	99.57	110.40
33	O	373	TRP	CB-CG-CD2	-5.42	119.56	126.60
7	G	85	VAL	CA-CB-CG2	-5.42	102.78	110.90
23	T	202	LEU	CB-CG-CD2	5.42	120.20	111.00
14	n	226	LYS	N-CA-CB	5.41	120.34	110.60
33	O	110	ASP	CB-CG-OD1	-5.41	113.43	118.30
33	O	150	LEU	N-CA-CB	5.41	121.23	110.40
14	n	116	VAL	CA-CB-CG1	-5.41	102.79	110.90
21	W	146	GLU	N-CA-CB	5.41	120.33	110.60
4	d	118	TYR	CB-CG-CD1	5.41	124.24	121.00
14	7	194	ASN	N-CA-CB	5.41	120.33	110.60
18	L	272	GLU	N-CA-CB	5.41	120.33	110.60
3	c	123	GLN	CA-CB-CG	5.40	125.28	113.40
4	d	127	PHE	CD1-CG-CD2	5.40	125.32	118.30
6	F	148	PRO	CA-N-CD	5.40	119.26	111.70
27	N	463	TYR	CD1-CE1-CZ	-5.40	114.94	119.80
4	d	29	THR	N-CA-CB	5.40	120.56	110.30
11	k	10	GLN	CB-CA-C	-5.40	99.60	110.40
6	f	152	VAL	CA-CB-CG1	-5.40	102.80	110.90
21	W	181	LEU	O-C-N	-5.40	114.06	122.70
20	J	382	PHE	CB-CG-CD1	5.40	124.58	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	56	ALA	N-CA-CB	5.39	117.65	110.10
7	g	116	VAL	CA-CB-CG1	5.39	118.99	110.90
4	D	216	ASP	CB-CG-OD1	-5.39	113.45	118.30
5	E	95	TYR	CB-CG-CD1	5.39	124.24	121.00
2	b	158	PRO	N-CA-CB	5.39	109.77	103.30
5	E	2	ARG	CD-NE-CZ	5.39	131.15	123.60
21	W	160	ALA	CB-CA-C	-5.39	102.02	110.10
1	a	80	ASP	CB-CG-OD2	-5.39	113.45	118.30
27	N	233	ASN	CB-CA-C	5.39	121.18	110.40
6	f	23	TYR	CB-CG-CD1	5.39	124.23	121.00
2	B	200	VAL	N-CA-C	-5.39	96.46	111.00
10	j	43	PHE	CB-CG-CD1	5.38	124.57	120.80
2	B	90	ARG	N-CA-CB	5.38	120.29	110.60
26	Z	263	ALA	CB-CA-C	-5.38	102.02	110.10
12	l	50	ALA	CB-CA-C	-5.38	102.03	110.10
6	f	178	PHE	CD1-CE1-CZ	-5.38	113.64	120.10
15	H	367	ARG	NE-CZ-NH1	-5.38	117.61	120.30
28	S	77	THR	C-N-CA	5.38	135.15	121.70
31	R	99	TYR	CB-CG-CD2	-5.38	117.77	121.00
18	L	361	PHE	CD1-CE1-CZ	5.38	126.55	120.10
10	j	14	MET	CG-SD-CE	-5.38	91.60	100.20
19	M	266	ALA	CB-CA-C	-5.38	102.03	110.10
24	X	89	LEU	CB-CG-CD1	5.38	120.14	111.00
11	k	67	TYR	CD1-CE1-CZ	-5.38	114.96	119.80
26	Z	106	TRP	CB-CG-CD2	-5.37	119.61	126.60
31	R	343	GLU	CB-CA-C	-5.37	99.65	110.40
20	J	367	MET	CG-SD-CE	-5.37	91.61	100.20
12	l	113	TYR	CD1-CE1-CZ	5.37	124.63	119.80
15	H	310	GLU	CB-CA-C	5.37	121.14	110.40
10	3	98	ARG	NE-CZ-NH2	5.37	122.98	120.30
13	m	184	VAL	CA-CB-CG2	-5.37	102.85	110.90
12	5	142	SER	N-CA-CB	5.37	118.55	110.50
31	R	291	SER	CB-CA-C	5.37	120.30	110.10
7	g	197	TYR	CG-CD1-CE1	-5.36	117.01	121.30
10	3	45	TYR	CG-CD2-CE2	-5.36	117.01	121.30
31	R	349	SER	N-CA-CB	5.36	118.54	110.50
31	R	204	TRP	CG-CD2-CE3	-5.36	129.07	133.90
29	P	6	PRO	CA-N-CD	-5.36	104.00	111.50
19	M	320	ARG	NE-CZ-NH1	5.36	122.98	120.30
8	h	45	ARG	NE-CZ-NH1	5.36	122.98	120.30
31	R	125	GLU	N-CA-CB	5.36	120.24	110.60
20	J	116	ARG	NE-CZ-NH1	5.36	122.98	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	144	TYR	CZ-CE2-CD2	5.35	124.62	119.80
12	5	88	TYR	CG-CD2-CE2	-5.35	117.02	121.30
7	g	99	TYR	CG-CD1-CE1	-5.35	117.02	121.30
9	i	118	SER	N-CA-CB	5.35	118.53	110.50
23	T	265	ASP	CB-CG-OD1	5.35	123.12	118.30
17	K	423	LYS	CD-CE-NZ	-5.35	99.39	111.70
27	N	282	TYR	CB-CG-CD1	5.35	124.21	121.00
6	F	185	PRO	CA-N-CD	5.35	119.19	111.70
27	N	334	VAL	CG1-CB-CG2	-5.35	102.34	110.90
4	D	213	VAL	CA-CB-CG1	5.35	118.92	110.90
24	X	62	ASP	CB-CG-OD1	5.35	123.11	118.30
31	R	30	ALA	N-CA-CB	5.35	117.59	110.10
26	Z	210	TYR	CB-CG-CD1	-5.35	117.79	121.00
13	6	33	TYR	CB-CG-CD2	5.34	124.21	121.00
24	X	95	GLU	OE1-CD-OE2	5.34	129.71	123.30
2	B	7	PHE	CB-CG-CD1	5.34	124.54	120.80
17	K	161	MET	CG-SD-CE	-5.34	91.65	100.20
6	f	50	ARG	NE-CZ-NH2	5.34	122.97	120.30
6	f	219	THR	N-CA-C	-5.34	96.58	111.00
9	i	196	ARG	N-CA-CB	5.34	120.22	110.60
7	G	214	TRP	CB-CG-CD2	-5.34	119.66	126.60
27	N	921	ARG	CD-NE-CZ	5.34	131.08	123.60
18	L	431	THR	C-N-CA	5.34	135.05	121.70
22	V	197	TYR	CB-CG-CD1	-5.34	117.80	121.00
23	T	177	PHE	CD1-CE1-CZ	5.33	126.50	120.10
4	d	117	ARG	CD-NE-CZ	5.33	131.06	123.60
13	m	75	TYR	CG-CD2-CE2	-5.33	117.03	121.30
3	C	49	ARG	NE-CZ-NH2	-5.33	117.63	120.30
11	4	130	TYR	CG-CD1-CE1	-5.33	117.03	121.30
26	Z	96	TYR	CB-CG-CD1	-5.33	117.80	121.00
27	N	237	LEU	CB-CG-CD2	5.33	120.06	111.00
7	g	99	TYR	CB-CG-CD2	-5.33	117.80	121.00
26	Z	408	TYR	CZ-CE2-CD2	5.33	124.60	119.80
3	c	148	TYR	CB-CG-CD2	-5.33	117.80	121.00
4	d	66	ASP	CB-CG-OD1	-5.33	113.50	118.30
27	N	775	CYS	CA-CB-SG	-5.33	104.41	114.00
14	n	60	MET	CG-SD-CE	-5.33	91.68	100.20
19	M	386	PHE	CG-CD1-CE1	5.33	126.66	120.80
22	V	273	ARG	NE-CZ-NH1	5.33	122.96	120.30
4	D	46	ARG	CB-CA-C	-5.32	99.75	110.40
26	Z	439	TYR	CZ-CE2-CD2	-5.32	115.01	119.80
9	i	97	TYR	CB-CG-CD1	-5.32	117.81	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	118	ASP	CB-CG-OD1	5.32	123.09	118.30
5	E	128	ARG	NH1-CZ-NH2	5.32	125.25	119.40
27	N	396	SER	CB-CA-C	-5.32	100.00	110.10
9	2	104	ASP	CB-CG-OD1	5.32	123.08	118.30
15	H	257	THR	CA-CB-CG2	-5.32	104.96	112.40
27	N	883	SER	O-C-N	-5.32	114.20	122.70
31	R	417	TYR	CB-CG-CD2	-5.32	117.81	121.00
26	Z	397	ASP	CB-CG-OD2	5.31	123.08	118.30
32	U	145	ASP	CB-CG-OD1	5.31	123.08	118.30
33	O	215	TYR	CZ-CE2-CD2	-5.31	115.02	119.80
6	f	118	ASN	CB-CA-C	-5.31	99.78	110.40
20	J	229	MET	N-CA-CB	5.31	120.16	110.60
7	g	197	TYR	CG-CD2-CE2	5.31	125.55	121.30
9	i	198	GLU	N-CA-CB	5.31	120.16	110.60
13	m	149	PHE	CB-CG-CD1	5.31	124.52	120.80
17	K	340	PHE	CB-CG-CD2	5.31	124.52	120.80
19	M	372	ASP	CB-CG-OD1	5.31	123.08	118.30
33	O	307	MET	CG-SD-CE	-5.31	91.70	100.20
4	d	118	TYR	CG-CD2-CE2	-5.31	117.05	121.30
14	n	30	TYR	CB-CG-CD1	5.31	124.19	121.00
1	A	137	VAL	N-CA-C	-5.31	96.67	111.00
20	J	344	ARG	NE-CZ-NH2	5.31	122.95	120.30
30	Q	238	TYR	CD1-CG-CD2	5.31	123.74	117.90
30	Q	276	ASP	CB-CG-OD2	-5.31	113.52	118.30
6	f	170	TYR	CG-CD2-CE2	5.31	125.55	121.30
14	n	219	TRP	CE2-CD2-CE3	5.31	125.07	118.70
30	Q	241	GLU	O-C-N	-5.31	114.21	122.70
28	S	116	ALA	CB-CA-C	-5.30	102.14	110.10
13	6	222	ASP	CA-C-O	-5.30	108.97	120.10
2	B	250	LEU	CA-C-O	-5.30	108.97	120.10
5	E	115	PHE	CB-CG-CD2	5.30	124.51	120.80
5	E	76	ASP	CB-CG-OD2	-5.30	113.53	118.30
3	c	159	TRP	CG-CD2-CE3	-5.30	129.13	133.90
7	G	244	ASN	CA-C-O	-5.30	108.98	120.10
19	M	265	ASP	CB-CG-OD1	5.30	123.07	118.30
23	T	71	GLN	N-CA-CB	5.29	120.13	110.60
1	a	157	TYR	O-C-N	5.29	131.17	122.70
4	d	127	PHE	CG-CD2-CE2	-5.29	114.98	120.80
11	k	17	SER	N-CA-CB	5.29	118.44	110.50
4	D	240	GLU	CA-C-O	-5.29	108.98	120.10
27	N	925	ASP	CA-C-O	-5.29	108.98	120.10
33	O	337	LEU	N-CA-C	-5.29	96.70	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	233	ILE	CA-C-O	-5.29	108.99	120.10
24	X	133	SER	CA-C-O	-5.29	108.99	120.10
12	5	207	PHE	CB-CG-CD2	-5.29	117.10	120.80
30	Q	434	TYR	CA-C-O	-5.29	108.99	120.10
3	C	244	THR	CA-C-O	-5.29	109.00	120.10
7	G	145	TYR	CB-CG-CD2	-5.29	117.83	121.00
18	L	436	LYS	CA-C-O	-5.29	109.00	120.10
22	V	42	ARG	NE-CZ-NH2	-5.29	117.66	120.30
25	Y	89	GLN	CA-C-O	-5.29	109.00	120.10
18	L	434	TYR	CD1-CE1-CZ	-5.28	115.05	119.80
26	Z	918	ASP	CB-CA-C	-5.28	99.83	110.40
29	P	13	TYR	CA-CB-CG	5.28	123.44	113.40
31	R	107	GLU	O-C-N	-5.28	114.25	122.70
3	C	161	ALA	N-CA-CB	5.28	117.49	110.10
10	3	25	ASP	CB-CG-OD2	-5.28	113.55	118.30
17	K	428	LYS	CA-C-O	-5.28	109.01	120.10
33	O	393	VAL	CA-C-O	-5.28	109.01	120.10
8	h	57	ASP	CB-CG-OD1	5.28	123.05	118.30
26	Z	849	ARG	NE-CZ-NH1	5.28	122.94	120.30
3	c	223	GLU	N-CA-CB	5.28	120.09	110.60
10	3	204	ASP	CA-C-O	-5.28	109.02	120.10
28	S	263	ASP	CB-CG-OD2	-5.28	113.55	118.30
5	e	124	ARG	N-CA-CB	5.27	120.09	110.60
19	M	434	ALA	CA-C-O	-5.27	109.03	120.10
30	Q	291	TYR	CG-CD2-CE2	-5.27	117.08	121.30
27	N	518	ALA	N-CA-CB	5.27	117.48	110.10
28	S	492	LYS	CA-C-O	-5.27	109.03	120.10
5	e	110	ASP	CB-CG-OD2	-5.27	113.56	118.30
13	m	68	PHE	CB-CG-CD2	-5.27	117.11	120.80
16	I	437	LEU	CA-C-O	-5.27	109.04	120.10
26	Z	582	ASP	CB-CG-OD1	5.27	123.04	118.30
23	T	51	TYR	CB-CG-CD1	5.27	124.16	121.00
26	Z	745	LEU	CB-CG-CD1	5.27	119.95	111.00
28	S	425	ARG	NE-CZ-NH2	-5.27	117.67	120.30
12	l	88	TYR	CG-CD1-CE1	-5.27	117.09	121.30
8	h	191	ASP	CB-CG-OD1	-5.26	113.56	118.30
12	l	54	PHE	CD1-CE1-CZ	-5.26	113.78	120.10
13	m	33	TYR	CB-CG-CD1	-5.26	117.84	121.00
13	m	167	LYS	CB-CA-C	-5.26	99.87	110.40
7	G	207	ASP	CB-CG-OD1	-5.26	113.56	118.30
8	h	124	TYR	CG-CD1-CE1	5.26	125.51	121.30
18	L	56	ALA	CB-CA-C	-5.26	102.21	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	123	GLU	N-CA-CB	5.26	120.07	110.60
13	6	186	ASP	CB-CG-OD1	-5.26	113.57	118.30
29	P	440	HIS	CA-C-O	-5.26	109.06	120.10
32	U	55	PRO	CA-N-CD	5.26	119.06	111.70
27	N	877	GLN	OE1-CD-NE2	5.25	133.99	121.90
15	H	300	THR	CA-CB-CG2	-5.25	105.05	112.40
16	I	291	ARG	NE-CZ-NH1	5.25	122.93	120.30
17	K	427	TYR	CB-CG-CD1	-5.25	117.85	121.00
31	R	96	GLN	N-CA-CB	5.25	120.06	110.60
20	J	18	GLY	CA-C-O	-5.25	111.15	120.60
1	A	224	PHE	CB-CG-CD2	-5.25	117.12	120.80
14	n	76	TYR	CG-CD2-CE2	5.25	125.50	121.30
9	2	226	GLU	CA-C-O	-5.25	109.08	120.10
27	N	144	CYS	O-C-N	5.25	131.10	122.70
3	c	18	LEU	CB-CG-CD1	-5.25	102.08	111.00
8	h	191	ASP	CB-CG-OD2	5.25	123.02	118.30
21	W	155	ASP	CB-CG-OD1	5.25	123.02	118.30
27	N	436	ASP	N-CA-CB	5.25	120.04	110.60
28	S	196	ARG	NE-CZ-NH1	5.25	122.92	120.30
30	Q	15	VAL	CG1-CB-CG2	-5.25	102.50	110.90
10	j	131	GLU	OE1-CD-OE2	5.24	129.59	123.30
14	7	138	SER	N-CA-C	-5.24	96.84	111.00
17	K	135	MET	CG-SD-CE	-5.24	91.81	100.20
19	M	340	SER	N-CA-CB	5.24	118.37	110.50
27	N	89	PHE	CZ-CE2-CD2	-5.24	113.81	120.10
33	O	248	TYR	CB-CG-CD2	-5.24	117.86	121.00
33	O	141	ASN	CB-CA-C	5.24	120.88	110.40
4	D	88	ARG	NE-CZ-NH2	-5.24	117.68	120.30
9	2	104	ASP	CB-CG-OD2	-5.24	113.59	118.30
17	K	194	GLN	C-N-CA	5.24	134.79	121.70
5	E	130	PHE	CB-CG-CD1	-5.23	117.14	120.80
15	H	261	ARG	NE-CZ-NH2	-5.23	117.68	120.30
8	h	124	TYR	CD1-CE1-CZ	-5.23	115.09	119.80
14	7	186	TYR	CB-CG-CD2	-5.23	117.86	121.00
23	T	16	GLU	N-CA-CB	5.23	120.02	110.60
9	2	42	TRP	CE2-CD2-CE3	5.23	124.98	118.70
12	5	126	ILE	N-CA-C	-5.23	96.88	111.00
17	K	273	GLU	OE1-CD-OE2	5.23	129.58	123.30
31	R	69	GLU	N-CA-CB	5.23	120.01	110.60
5	E	75	ALA	CB-CA-C	-5.23	102.26	110.10
9	2	157	ASP	CB-CG-OD1	-5.22	113.60	118.30
22	V	225	LEU	CB-CG-CD2	5.22	119.88	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	157	TYR	N-CA-CB	5.22	120.00	110.60
4	D	144	LYS	N-CA-CB	5.22	120.00	110.60
18	L	392	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	b	83	ARG	NE-CZ-NH1	5.22	122.91	120.30
17	K	385	ALA	N-CA-CB	5.22	117.41	110.10
18	L	331	ASP	CB-CG-OD2	-5.22	113.60	118.30
11	4	93	ARG	NE-CZ-NH2	5.22	122.91	120.30
6	F	100	ARG	NE-CZ-NH1	5.22	122.91	120.30
19	M	73	ARG	NE-CZ-NH1	-5.22	117.69	120.30
33	O	55	THR	CA-CB-CG2	-5.22	105.10	112.40
5	e	209	ALA	N-CA-CB	5.21	117.40	110.10
3	C	244	THR	CA-CB-CG2	-5.21	105.10	112.40
16	I	408	ARG	NE-CZ-NH1	5.21	122.91	120.30
18	L	331	ASP	CB-CG-OD1	5.21	122.99	118.30
12	l	25	TRP	CB-CG-CD2	-5.21	119.83	126.60
8	1	192	GLU	OE1-CD-OE2	-5.21	117.05	123.30
12	l	72	GLU	N-CA-CB	5.21	119.98	110.60
5	e	159	TYR	CB-CG-CD2	-5.21	117.88	121.00
5	E	133	ALA	N-CA-CB	5.21	117.39	110.10
14	7	200	ILE	N-CA-C	-5.21	96.94	111.00
33	O	191	THR	CA-CB-CG2	-5.21	105.11	112.40
12	l	64	ARG	NE-CZ-NH2	5.21	122.90	120.30
19	M	187	ASP	CB-CG-OD1	5.21	122.98	118.30
27	N	347	SER	N-CA-CB	5.21	118.31	110.50
17	K	49	PHE	CG-CD1-CE1	-5.20	115.08	120.80
19	M	283	LEU	CB-CG-CD2	5.20	119.85	111.00
12	l	201	LYS	N-CA-CB	5.20	119.96	110.60
31	R	327	ASP	CB-CG-OD2	-5.20	113.62	118.30
6	F	86	TYR	CB-CG-CD1	5.20	124.12	121.00
9	2	205	PHE	CB-CG-CD2	-5.20	117.16	120.80
9	i	166	ASP	CB-CG-OD1	-5.20	113.62	118.30
7	G	104	PRO	CA-N-CD	5.20	118.97	111.70
7	G	126	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
20	J	94	TYR	CB-CG-CD2	-5.19	117.88	121.00
3	c	121	TYR	CB-CG-CD1	-5.19	117.89	121.00
29	P	123	ARG	NE-CZ-NH2	5.19	122.90	120.30
33	O	255	LEU	CB-CG-CD2	5.19	119.83	111.00
12	l	21	THR	CA-CB-CG2	-5.19	105.13	112.40
6	F	200	LEU	CB-CG-CD2	5.19	119.82	111.00
21	W	144	PHE	CB-CG-CD2	-5.19	117.17	120.80
3	c	70	ASP	CB-CG-OD1	5.19	122.97	118.30
11	k	117	TYR	CZ-CE2-CD2	5.19	124.47	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	186	ASP	CB-CG-OD2	5.19	122.97	118.30
23	T	177	PHE	CG-CD1-CE1	-5.19	115.09	120.80
3	c	244	THR	CA-CB-CG2	-5.18	105.14	112.40
7	g	145	TYR	CB-CG-CD2	-5.18	117.89	121.00
8	1	81	VAL	CA-CB-CG1	5.18	118.67	110.90
14	7	132	LEU	N-CA-CB	-5.18	100.03	110.40
23	T	72	THR	CA-CB-CG2	-5.18	105.14	112.40
28	S	487	THR	CA-CB-CG2	-5.18	105.15	112.40
31	R	243	LEU	CB-CG-CD1	5.18	119.80	111.00
14	n	187	ARG	CD-NE-CZ	5.18	130.85	123.60
3	C	195	THR	N-CA-CB	5.18	120.14	110.30
21	W	69	PHE	CG-CD1-CE1	5.18	126.50	120.80
1	A	157	TYR	CB-CG-CD2	5.17	124.11	121.00
5	E	127	SER	N-CA-C	-5.17	97.03	111.00
28	S	141	LEU	O-C-N	-5.17	114.42	122.70
3	c	216	ARG	NE-CZ-NH2	-5.17	117.71	120.30
14	n	37	ASN	CA-CB-CG	-5.17	102.02	113.40
13	6	145	LEU	CB-CA-C	-5.17	100.37	110.20
16	I	239	GLN	N-CA-CB	5.17	119.91	110.60
28	S	444	GLU	CG-CD-OE1	5.17	128.65	118.30
30	Q	313	ASP	CB-CG-OD2	-5.17	113.65	118.30
33	O	281	ALA	N-CA-CB	5.17	117.34	110.10
24	X	19	GLU	OE1-CD-OE2	5.17	129.50	123.30
13	m	58	ALA	N-CA-CB	5.17	117.34	110.10
14	n	93	PHE	CG-CD1-CE1	-5.17	115.11	120.80
1	A	15	ARG	NE-CZ-NH1	5.17	122.88	120.30
31	R	175	ALA	CB-CA-C	-5.17	102.35	110.10
11	4	36	ARG	NE-CZ-NH1	5.17	122.88	120.30
31	R	231	LEU	CB-CG-CD2	5.17	119.78	111.00
28	S	453	ASP	CB-CG-OD1	-5.16	113.65	118.30
30	Q	238	TYR	CD1-CE1-CZ	-5.16	115.15	119.80
18	L	91	THR	C-N-CA	5.16	134.60	121.70
28	S	253	PHE	CG-CD1-CE1	5.16	126.48	120.80
8	h	124	TYR	CG-CD2-CE2	-5.16	117.17	121.30
26	Z	487	SER	N-CA-CB	5.16	118.24	110.50
16	I	403	ALA	CB-CA-C	-5.16	102.37	110.10
31	R	109	LYS	C-N-CA	5.15	134.58	121.70
10	j	153	TYR	CG-CD2-CE2	-5.15	117.18	121.30
26	Z	272	TYR	CD1-CE1-CZ	5.15	124.44	119.80
28	S	233	LEU	CB-CG-CD2	5.15	119.75	111.00
4	d	118	TYR	CZ-CE2-CD2	5.15	124.43	119.80
1	a	41	CYS	CB-CA-C	5.14	120.69	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	20	PHE	CZ-CE2-CD2	-5.14	113.93	120.10
14	n	87	LEU	N-CA-CB	5.14	120.69	110.40
26	Z	843	ASP	CB-CG-OD2	-5.14	113.67	118.30
27	N	70	TYR	N-CA-CB	5.14	119.86	110.60
1	a	123	ALA	CB-CA-C	-5.14	102.39	110.10
1	a	183	ASP	N-CA-CB	5.14	119.86	110.60
3	c	23	TYR	CZ-CE2-CD2	5.14	124.43	119.80
27	N	124	TYR	CZ-CE2-CD2	-5.14	115.17	119.80
28	S	449	LEU	CB-CG-CD2	5.14	119.74	111.00
3	c	82	ASP	N-CA-CB	5.14	119.86	110.60
3	C	106	PRO	CA-N-CD	5.14	118.90	111.70
11	k	120	ASP	CB-CG-OD1	-5.14	113.67	118.30
27	N	59	GLU	CB-CA-C	-5.14	100.12	110.40
5	E	94	TYR	CB-CG-CD2	-5.14	117.92	121.00
2	b	71	ILE	N-CA-CB	5.13	122.61	110.80
13	m	194	ARG	NE-CZ-NH2	-5.13	117.73	120.30
12	5	137	TYR	CB-CG-CD2	-5.13	117.92	121.00
14	n	17	ASP	CB-CG-OD2	-5.13	113.68	118.30
17	K	225	ALA	N-CA-CB	5.13	117.29	110.10
23	T	99	SER	N-CA-CB	5.13	118.20	110.50
6	F	126	PRO	CA-N-CD	5.13	118.88	111.70
18	L	348	GLU	N-CA-CB	5.13	119.84	110.60
27	N	146	LYS	O-C-N	5.13	130.91	122.70
6	f	53	ASP	N-CA-CB	5.13	119.83	110.60
16	I	166	PRO	CA-N-CD	5.13	118.88	111.70
20	J	168	VAL	CA-CB-CG2	-5.13	103.21	110.90
27	N	322	ASP	CB-CG-OD1	5.13	122.92	118.30
7	G	95	PHE	CB-CG-CD1	-5.12	117.21	120.80
25	Y	29	LEU	CB-CG-CD2	5.12	119.71	111.00
17	K	422	ASP	CB-CG-OD1	-5.12	113.69	118.30
7	G	214	TRP	CG-CD1-NE1	5.12	115.22	110.10
17	K	79	LEU	O-C-N	5.12	130.89	122.70
1	a	126	ARG	NE-CZ-NH1	5.12	122.86	120.30
15	H	308	PHE	CB-CG-CD1	5.12	124.38	120.80
26	Z	970	TYR	CD1-CE1-CZ	-5.12	115.19	119.80
30	Q	264	TYR	CB-CG-CD2	-5.12	117.93	121.00
12	l	90	TYR	CB-CG-CD1	5.12	124.07	121.00
9	2	164	TRP	CB-CG-CD2	-5.12	119.95	126.60
15	H	272	ILE	N-CA-C	-5.12	97.19	111.00
15	H	445	LYS	N-CA-CB	5.12	119.81	110.60
26	Z	794	ASP	CB-CG-OD2	-5.12	113.70	118.30
7	g	115	TYR	CD1-CE1-CZ	-5.11	115.20	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	57	PHE	CB-CG-CD1	5.11	124.38	120.80
19	M	186	LEU	C-N-CA	5.11	134.48	121.70
33	O	104	ALA	N-CA-CB	5.11	117.26	110.10
3	c	100	THR	N-CA-CB	5.11	120.01	110.30
3	c	159	TRP	CZ3-CH2-CZ2	-5.11	115.47	121.60
11	4	188	GLY	N-CA-C	-5.11	100.32	113.10
18	L	161	ARG	NE-CZ-NH2	-5.11	117.75	120.30
30	Q	8	LEU	CB-CG-CD2	5.11	119.69	111.00
28	S	484	ASP	CB-CG-OD1	5.11	122.90	118.30
19	M	221	TYR	CB-CG-CD2	5.11	124.06	121.00
24	X	42	GLU	CA-CB-CG	5.11	124.63	113.40
15	H	162	ARG	NE-CZ-NH1	-5.10	117.75	120.30
10	j	75	LEU	CA-C-O	5.10	130.82	120.10
22	V	143	PRO	N-CA-CB	5.10	109.42	103.30
6	F	2	ARG	NE-CZ-NH2	-5.10	117.75	120.30
6	f	154	GLU	N-CA-CB	5.10	119.78	110.60
27	N	876	PRO	CA-N-CD	5.10	118.84	111.70
3	c	183	MET	CB-CA-C	-5.10	100.20	110.40
9	i	190	TYR	CB-CG-CD1	5.10	124.06	121.00
8	1	124	TYR	CA-CB-CG	5.10	123.08	113.40
27	N	49	LEU	N-CA-CB	5.10	120.59	110.40
26	Z	569	ALA	N-CA-CB	5.09	117.23	110.10
1	A	104	PRO	CA-N-CD	5.09	118.83	111.70
14	7	28	GLY	N-CA-C	-5.09	100.37	113.10
32	U	7	LYS	N-CA-CB	5.09	119.77	110.60
33	O	230	PHE	N-CA-CB	5.09	119.76	110.60
23	T	157	TYR	CB-CG-CD2	5.09	124.05	121.00
26	Z	562	TRP	N-CA-CB	5.09	119.76	110.60
14	n	219	TRP	CD2-CE2-CZ2	-5.09	116.19	122.30
14	7	126	PHE	CB-CG-CD1	5.09	124.36	120.80
17	K	236	ARG	NH1-CZ-NH2	5.09	125.00	119.40
9	2	202	SER	N-CA-CB	5.09	118.13	110.50
23	T	157	TYR	CZ-CE2-CD2	-5.09	115.22	119.80
27	N	767	ALA	CB-CA-C	-5.09	102.47	110.10
10	j	94	LEU	CB-CG-CD2	5.08	119.64	111.00
21	W	69	PHE	CB-CG-CD1	5.08	124.36	120.80
21	W	130	LYS	N-CA-CB	5.08	119.75	110.60
20	J	120	TYR	N-CA-CB	5.08	119.75	110.60
26	Z	616	LEU	CB-CG-CD1	-5.08	102.36	111.00
29	P	59	LEU	CA-CB-CG	5.08	126.98	115.30
24	X	122	TYR	CB-CG-CD2	-5.08	117.95	121.00
6	f	101	LYS	CB-CA-C	-5.08	100.25	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	140	ASP	CB-CG-OD1	-5.08	113.73	118.30
7	g	238	PHE	CG-CD2-CE2	-5.07	115.22	120.80
19	M	371	ASP	CB-CG-OD1	5.07	122.87	118.30
13	6	129	GLY	CA-C-O	-5.07	111.47	120.60
17	K	399	ARG	NE-CZ-NH1	5.07	122.84	120.30
10	j	188	ILE	CB-CA-C	-5.07	101.46	111.60
15	H	306	ILE	N-CA-CB	5.07	122.46	110.80
21	W	175	THR	CA-CB-CG2	-5.07	105.30	112.40
7	G	154	TRP	CG-CD2-CE3	-5.07	129.34	133.90
15	H	186	PRO	CA-N-CD	5.07	118.80	111.70
15	H	308	PHE	CB-CG-CD2	-5.07	117.25	120.80
27	N	160	GLY	N-CA-C	5.07	125.77	113.10
33	O	189	TYR	CB-CG-CD1	-5.07	117.96	121.00
15	H	373	ARG	NE-CZ-NH1	-5.07	117.77	120.30
27	N	295	THR	N-CA-CB	5.07	119.92	110.30
1	A	9	ILE	CA-CB-CG1	5.06	120.62	111.00
8	1	169	SER	CB-CA-C	-5.06	100.48	110.10
11	4	36	ARG	NE-CZ-NH2	-5.06	117.77	120.30
23	T	216	GLU	OE1-CD-OE2	5.06	129.38	123.30
2	B	5	TYR	CG-CD2-CE2	-5.06	117.25	121.30
22	V	186	GLN	C-N-CA	-5.06	109.05	121.70
2	B	214	ILE	N-CA-C	-5.06	97.34	111.00
5	E	128	ARG	NE-CZ-NH1	-5.06	117.77	120.30
21	W	20	ASP	CB-CG-OD2	5.06	122.85	118.30
12	l	146	TRP	CD2-CE2-CZ2	-5.06	116.23	122.30
1	A	35	ALA	N-CA-CB	5.06	117.18	110.10
9	2	123	TYR	CB-CG-CD2	5.06	124.03	121.00
20	J	18	GLY	O-C-N	5.06	130.79	122.70
20	J	126	LEU	N-CA-CB	5.06	120.51	110.40
26	Z	109	PRO	CA-N-CD	5.06	118.78	111.70
29	P	266	TYR	CB-CG-CD2	-5.06	117.97	121.00
1	a	13	GLU	N-CA-CB	5.05	119.70	110.60
6	F	81	ARG	NE-CZ-NH2	-5.05	117.77	120.30
33	O	138	LEU	N-CA-CB	5.05	120.51	110.40
33	O	245	ASP	CB-CG-OD2	-5.05	113.75	118.30
1	A	64	PHE	N-CA-CB	5.05	119.69	110.60
28	S	399	TYR	CB-CG-CD2	-5.05	117.97	121.00
5	e	179	TRP	CB-CG-CD1	5.05	133.56	127.00
9	i	3	ILE	N-CA-C	-5.05	97.36	111.00
26	Z	818	CYS	N-CA-CB	5.05	119.69	110.60
8	h	67	THR	CA-CB-CG2	-5.05	105.34	112.40
9	i	70	THR	CA-CB-CG2	-5.05	105.33	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	15	ARG	NE-CZ-NH2	5.05	122.82	120.30
2	B	5	TYR	CB-CG-CD1	5.05	124.03	121.00
16	I	376	ASN	O-C-N	5.05	130.77	122.70
13	m	96	LEU	CB-CA-C	-5.04	100.61	110.20
26	Z	551	LEU	CB-CG-CD1	-5.04	102.42	111.00
7	g	110	ASP	CB-CG-OD2	-5.04	113.76	118.30
12	l	5	ALA	N-CA-CB	5.04	117.16	110.10
3	C	51	VAL	CA-CB-CG1	-5.04	103.33	110.90
6	f	208	ASP	CB-CG-OD1	-5.04	113.76	118.30
26	Z	465	GLY	C-N-CA	5.04	134.30	121.70
31	R	141	TYR	CA-CB-CG	-5.04	103.82	113.40
9	i	90	TYR	CB-CG-CD2	5.04	124.02	121.00
31	R	233	ASP	CB-CG-OD1	-5.04	113.76	118.30
11	k	149	ARG	NE-CZ-NH1	5.04	122.82	120.30
16	I	173	MET	N-CA-C	-5.04	97.40	111.00
31	R	141	TYR	CG-CD1-CE1	5.04	125.33	121.30
5	E	41	GLY	N-CA-C	-5.03	100.52	113.10
16	I	103	PRO	N-CD-CG	5.03	110.75	103.20
31	R	99	TYR	N-CA-CB	5.03	119.66	110.60
9	i	71	SER	C-N-CA	5.03	134.28	121.70
26	Z	471	LEU	CB-CG-CD2	-5.03	102.45	111.00
18	L	117	TYR	CG-CD1-CE1	-5.03	117.28	121.30
20	J	287	ASN	CB-CA-C	-5.03	100.34	110.40
33	O	264	ASP	CB-CA-C	5.03	120.46	110.40
16	I	60	LEU	N-CA-CB	5.03	120.45	110.40
17	K	196	ASP	CB-CG-OD1	-5.03	113.78	118.30
31	R	338	TYR	CB-CG-CD2	-5.03	117.98	121.00
33	O	87	LYS	N-CA-CB	5.03	119.65	110.60
33	O	286	PHE	CB-CG-CD2	-5.03	117.28	120.80
12	l	8	PHE	CA-C-O	5.03	130.65	120.10
4	D	223	SER	N-CA-CB	5.03	118.04	110.50
17	K	349	ARG	NE-CZ-NH1	-5.03	117.79	120.30
6	f	224	TYR	CD1-CE1-CZ	-5.02	115.28	119.80
9	2	206	PRO	CA-N-CD	5.02	118.73	111.70
23	T	116	GLN	N-CA-CB	5.02	119.64	110.60
14	n	221	PHE	CZ-CE2-CD2	5.02	126.13	120.10
14	n	137	TYR	CB-CG-CD1	-5.02	117.99	121.00
5	E	145	TYR	CB-CG-CD1	-5.02	117.99	121.00
13	6	137	ARG	NE-CZ-NH1	-5.02	117.79	120.30
2	b	120	GLU	N-CA-CB	5.02	119.63	110.60
3	c	181	ASP	CB-CG-OD2	-5.02	113.78	118.30
10	3	113	SER	CB-CA-C	-5.02	100.57	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	M	357	ARG	NE-CZ-NH2	-5.02	117.79	120.30
21	W	33	VAL	CA-CB-CG2	-5.02	103.37	110.90
29	P	115	ARG	CA-CB-CG	5.02	124.44	113.40
5	e	75	ALA	N-CA-CB	5.02	117.12	110.10
3	C	17	ARG	CD-NE-CZ	5.02	130.62	123.60
18	L	434	TYR	CB-CG-CD2	5.02	124.01	121.00
26	Z	773	ARG	NE-CZ-NH2	-5.02	117.79	120.30
16	I	239	GLN	CB-CG-CD	-5.01	98.56	111.60
19	M	415	PHE	CB-CG-CD2	-5.01	117.29	120.80
4	d	16	PHE	CB-CG-CD2	5.01	124.31	120.80
4	d	152	GLY	O-C-N	-5.01	114.68	122.70
5	e	57	GLU	O-C-N	-5.01	114.68	122.70
9	i	19	ARG	NE-CZ-NH1	5.01	122.81	120.30
10	j	204	ASP	CA-CB-CG	-5.01	102.38	113.40
1	A	93	ALA	CB-CA-C	-5.01	102.58	110.10
1	A	235	ARG	NE-CZ-NH2	-5.01	117.79	120.30
5	E	124	ARG	CB-CA-C	-5.01	100.38	110.40
25	Y	28	SER	N-CA-CB	5.01	118.02	110.50
28	S	404	LEU	N-CA-CB	-5.01	100.38	110.40
1	a	174	GLU	N-CA-CB	5.01	119.61	110.60
11	4	43	LEU	CB-CA-C	-5.01	100.69	110.20
20	J	249	GLU	N-CA-CB	5.01	119.61	110.60
2	B	233	PRO	CA-N-CD	5.00	118.71	111.70
11	4	183	ILE	CA-CB-CG2	-5.00	100.89	110.90
26	Z	603	VAL	CA-CB-CG2	-5.00	103.39	110.90
3	c	168	THR	CA-CB-CG2	5.00	119.41	112.40
14	n	2	GLN	CG-CD-NE2	-5.00	104.69	116.70
1	A	141	LEU	CB-CG-CD1	-5.00	102.49	111.00
26	Z	845	LEU	CB-CG-CD1	5.00	119.51	111.00
27	N	98	VAL	CG1-CB-CG2	5.00	118.91	110.90
26	Z	633	GLU	O-C-N	5.00	130.70	122.70

There are no chirality outliers.

All (308) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	185	ARG	Sidechain
8	1	45	ARG	Sidechain
9	2	186	TYR	Sidechain
9	2	75	ARG	Sidechain
9	2	90	TYR	Sidechain
9	2	97	TYR	Sidechain

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Mol	Chain	Res	Type	Group
10	3	102	TYR	Sidechain
10	3	45	TYR	Sidechain
10	3	73	TYR	Sidechain
10	3	98	ARG	Sidechain
11	4	107	TYR	Sidechain
11	4	135	TYR	Sidechain
11	4	171	ARG	Sidechain
11	4	73	TYR	Sidechain
11	4	85	ARG	Sidechain
11	4	95	ARG	Sidechain
12	5	113	TYR	Sidechain
12	5	137	TYR	Sidechain
13	6	105	TYR	Sidechain
13	6	106	TYR	Sidechain
13	6	194	ARG	Sidechain
13	6	28	ARG	Sidechain
13	6	33	TYR	Sidechain
13	6	98	TYR	Sidechain
14	7	137	TYR	Sidechain
14	7	186	TYR	Sidechain
14	7	193	ARG	Sidechain
14	7	95	TYR	Sidechain
1	A	101	TYR	Sidechain
1	A	154	TYR	Sidechain
1	A	195	GLU	Peptide
1	A	21	TYR	Sidechain
1	A	214	LEU	Peptide
1	A	37	ARG	Sidechain
1	A	82	ARG	Sidechain
1	A	96	ARG	Sidechain
2	B	101	TYR	Sidechain
2	B	16	GLY	Mainchain
2	B	235	PHE	Sidechain
2	B	4	ARG	Sidechain
2	B	83	ARG	Sidechain
2	B	97	TYR	Sidechain
3	C	145	TYR	Sidechain
3	C	19	TYR	Sidechain
3	C	4	ARG	Sidechain
3	C	66	TYR	Sidechain
4	D	127	PHE	Sidechain
4	D	39	CYS	Peptide

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Mol	Chain	Res	Type	Group
5	E	128	ARG	Sidechain,Peptide
5	E	2	ARG	Sidechain
5	E	64	ARG	Sidechain
6	F	127	TYR	Sidechain
6	F	156	TYR	Sidechain
6	F	170	TYR	Sidechain
6	F	232	TYR	Sidechain
6	F	93	TYR	Sidechain
7	G	145	TYR	Sidechain
7	G	165	ARG	Sidechain
7	G	186	ARG	Sidechain
7	G	99	TYR	Sidechain
15	H	145	TYR	Sidechain
15	H	292	ARG	Sidechain
15	H	319	PHE	Sidechain
15	H	357	ARG	Sidechain
15	H	373	ARG	Sidechain
15	H	443	PHE	Sidechain
15	H	457	PHE	Sidechain
16	I	100	ARG	Peptide
16	I	128	TYR	Sidechain
16	I	182	SER	Peptide
16	I	223	GLY	Peptide
16	I	246	ARG	Sidechain
16	I	346	ARG	Sidechain
16	I	64	ARG	Sidechain
20	J	153	LEU	Peptide
20	J	214	SER	Peptide
20	J	22	TYR	Sidechain
20	J	222	TYR	Sidechain
20	J	228	ARG	Sidechain
20	J	310	ILE	Mainchain
20	J	71	TYR	Peptide
20	J	94	TYR	Sidechain
17	K	103	ILE	Peptide
17	K	121	ARG	Sidechain
17	K	176	GLY	Peptide
17	K	198	TYR	Sidechain
17	K	207	ARG	Sidechain
17	K	215	PRO	Peptide
17	K	246	TYR	Sidechain
17	K	329	LEU	Peptide

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Mol	Chain	Res	Type	Group
17	K	333	ARG	Peptide
17	K	396	ARG	Sidechain
17	K	411	TYR	Sidechain
17	K	427	TYR	Sidechain
18	L	168	TYR	Sidechain
18	L	191	ARG	Sidechain
18	L	194	ARG	Sidechain
18	L	207	PHE	Sidechain
18	L	255	TYR	Sidechain
18	L	261	ARG	Sidechain
18	L	269	TYR	Sidechain
18	L	290	ARG	Sidechain
18	L	291	PHE	Sidechain
18	L	77	ARG	Sidechain
19	M	229	THR	Mainchain
19	M	243	PHE	Sidechain
19	M	255	TYR	Sidechain
19	M	267	PHE	Sidechain
19	M	320	ARG	Sidechain,Peptide
19	M	327	THR	Peptide
19	M	354	GLU	Mainchain
19	M	366	ARG	Sidechain
19	M	381	ARG	Sidechain
19	M	432	PHE	Sidechain
19	M	45	ARG	Sidechain
19	M	50	ARG	Sidechain
19	M	73	ARG	Sidechain
27	N	188	TYR	Sidechain
27	N	282	TYR	Sidechain
27	N	340	HIS	Sidechain
27	N	415	PHE	Sidechain
27	N	559	TYR	Sidechain
27	N	599	TYR	Sidechain
27	N	604	ARG	Sidechain
27	N	651	PHE	Sidechain
27	N	786	ARG	Sidechain
27	N	809	ARG	Sidechain
27	N	894	ARG	Sidechain
27	N	906	ARG	Sidechain
27	N	921	ARG	Sidechain
33	O	248	TYR	Sidechain
33	O	288	ARG	Sidechain

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Mol	Chain	Res	Type	Group
33	O	369	ARG	Sidechain
33	O	60	ARG	Sidechain
33	O	62	TYR	Sidechain
33	O	81	TYR	Sidechain
29	P	103	TYR	Sidechain
29	P	110	LEU	Peptide
29	P	13	TYR	Sidechain
29	P	168	TYR	Sidechain
29	P	234	TYR	Sidechain
29	P	336	HIS	Sidechain
29	P	386	GLN	Peptide
29	P	79	LEU	Mainchain
30	Q	124	PHE	Peptide
30	Q	161	LEU	Peptide
30	Q	165	PHE	Sidechain
30	Q	209	TYR	Sidechain
30	Q	286	TYR	Sidechain
30	Q	383	ASP	Peptide
30	Q	400	TYR	Sidechain
30	Q	403	PRO	Peptide
30	Q	67	THR	Peptide
31	R	120	LEU	Peptide
31	R	123	ASP	Peptide
31	R	141	TYR	Sidechain
31	R	214	TYR	Sidechain
31	R	222	ARG	Sidechain
31	R	246	TYR	Sidechain
31	R	328	PHE	Sidechain
31	R	331	ARG	Sidechain
31	R	335	ARG	Sidechain
31	R	345	TYR	Sidechain
31	R	417	TYR	Sidechain
31	R	62	TYR	Sidechain
31	R	63	TYR	Sidechain
31	R	65	TYR	Sidechain
31	R	70	TYR	Sidechain
31	R	99	TYR	Sidechain
28	S	111	ARG	Sidechain
28	S	119	TYR	Sidechain
28	S	271	ARG	Sidechain
28	S	272	TYR	Sidechain
28	S	332	PHE	Sidechain

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Mol	Chain	Res	Type	Group
28	S	346	TYR	Sidechain
28	S	384	ARG	Sidechain
23	T	144	TYR	Sidechain
23	T	197	TYR	Sidechain
23	T	199	PHE	Sidechain
23	T	20	TYR	Sidechain
23	T	220	PHE	Sidechain
23	T	251	HIS	Peptide
23	T	266	TYR	Sidechain
23	T	51	TYR	Sidechain
23	T	72	THR	Peptide
23	T	91	SER	Peptide
23	T	96	LEU	Mainchain,Peptide
32	U	210	TYR	Sidechain
32	U	24	ARG	Sidechain
22	V	135	ARG	Sidechain
22	V	203	TYR	Sidechain
22	V	42	ARG	Sidechain
21	W	41	ARG	Sidechain
24	X	27	ILE	Peptide
24	X	96	ARG	Sidechain
25	Y	35	PHE	Sidechain
25	Y	86	ARG	Sidechain
26	Z	269	TYR	Sidechain
26	Z	408	TYR	Sidechain
26	Z	439	TYR	Sidechain
26	Z	477	TYR	Sidechain
26	Z	553	ARG	Sidechain
26	Z	564	ARG	Sidechain
26	Z	574	TYR	Sidechain
26	Z	608	TYR	Sidechain
26	Z	759	ARG	Sidechain
26	Z	773	ARG	Sidechain
26	Z	838	TYR	Sidechain
26	Z	840	ARG	Sidechain
26	Z	849	ARG	Sidechain
1	a	101	TYR	Sidechain
1	a	111	ARG	Sidechain
1	a	119	TYR	Sidechain
1	a	146	TYR	Sidechain
1	a	225	PHE	Sidechain
1	a	3	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	a	62	TYR	Sidechain
1	a	68	ARG	Sidechain
1	a	97	TYR	Sidechain
1	a	99	TYR	Sidechain
2	b	128	ARG	Sidechain
2	b	130	PHE	Sidechain
2	b	145	PHE	Sidechain
2	b	174	PHE	Sidechain
2	b	236	ARG	Sidechain
2	b	5	TYR	Sidechain
2	b	83	ARG	Sidechain
2	b	97	TYR	Sidechain
2	b	99	ARG	Sidechain
3	c	101	TYR	Sidechain
3	c	136	TYR	Sidechain
3	c	17	ARG	Sidechain
3	c	207	TYR	Sidechain
3	c	212	PHE	Sidechain
3	c	225	TYR	Sidechain
3	c	23	TYR	Sidechain
3	c	49	ARG	Sidechain
3	c	5	TYR	Sidechain
3	c	91	ARG	Sidechain
4	d	106	TYR	Sidechain
4	d	139	ARG	Sidechain
4	d	146	TYR	Sidechain
4	d	164	ARG	Sidechain
4	d	177	TYR	Sidechain
4	d	20	TYR	Sidechain
4	d	47	ARG	Sidechain
4	d	9	PHE	Sidechain
4	d	95	ARG	Sidechain
5	e	127	SER	Peptide
5	e	128	ARG	Sidechain
5	e	139	HIS	Sidechain
5	e	145	TYR	Sidechain
5	e	159	TYR	Sidechain
5	e	18	TYR	Sidechain
5	e	85	ARG	Sidechain
6	f	125	ARG	Sidechain
6	f	136	TYR	Sidechain
6	f	163	ARG	Sidechain

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Mol	Chain	Res	Type	Group
6	f	17	ARG	Sidechain
6	f	58	TYR	Sidechain
7	g	115	TYR	Sidechain
7	g	126	ARG	Sidechain
7	g	143	HIS	Sidechain
7	g	153	TYR	Sidechain
7	g	165	ARG	Sidechain
7	g	18	PHE	Sidechain
7	g	4	TYR	Sidechain
7	g	74	TYR	Sidechain
7	g	82	ARG	Sidechain
8	h	135	TYR	Sidechain
8	h	137	TYR	Sidechain
8	h	29	ARG	Sidechain
8	h	38	HIS	Sidechain
8	h	61	TYR	Sidechain
9	i	196	ARG	Sidechain
9	i	205	PHE	Sidechain
9	i	207	ARG	Sidechain
10	j	135	PHE	Sidechain
10	j	176	ARG	Sidechain
10	j	45	TYR	Sidechain
10	j	97	ARG	Sidechain
10	j	98	ARG	Sidechain
11	k	135	TYR	Sidechain
11	k	67	TYR	Sidechain
11	k	85	ARG	Sidechain
11	k	96	ARG	Sidechain
11	k	98	TYR	Sidechain
12	l	137	TYR	Sidechain
12	l	155	TYR	Sidechain
12	l	167	ARG	Sidechain
12	l	170	TYR	Sidechain
12	l	178	TYR	Sidechain
12	l	187	TYR	Sidechain
12	l	69	ARG	Sidechain
13	m	101	ARG	Sidechain
13	m	123	TYR	Sidechain
13	m	39	TYR	Sidechain
13	m	75	TYR	Sidechain
13	m	79	HIS	Sidechain
13	m	98	TYR	Sidechain

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Mol	Chain	Res	Type	Group
14	n	129	TYR	Sidechain
14	n	193	ARG	Sidechain
14	n	208	PHE	Sidechain
14	n	41	ARG	Sidechain
14	n	93	PHE	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%)	226 (95%)	10 (4%)	3 (1%)	12 48
1	a	239/252 (95%)	230 (96%)	8 (3%)	1 (0%)	34 72
2	B	248/250 (99%)	238 (96%)	7 (3%)	3 (1%)	13 50
2	b	248/250 (99%)	236 (95%)	8 (3%)	4 (2%)	9 44
3	C	242/258 (94%)	234 (97%)	7 (3%)	1 (0%)	34 72
3	c	242/258 (94%)	230 (95%)	11 (4%)	1 (0%)	34 72
4	D	238/254 (94%)	222 (93%)	12 (5%)	4 (2%)	9 42
4	d	238/254 (94%)	227 (95%)	10 (4%)	1 (0%)	34 72
5	E	240/260 (92%)	225 (94%)	11 (5%)	4 (2%)	9 42
5	e	240/260 (92%)	233 (97%)	4 (2%)	3 (1%)	12 48
6	F	231/234 (99%)	219 (95%)	9 (4%)	3 (1%)	12 48
6	f	229/234 (98%)	224 (98%)	5 (2%)	0	100 100
7	G	241/288 (84%)	230 (95%)	7 (3%)	4 (2%)	9 42
7	g	241/288 (84%)	231 (96%)	8 (3%)	2 (1%)	19 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
8	1	194/215 (90%)	185 (95%)	8 (4%)	1 (0%)	29 69
8	h	194/215 (90%)	185 (95%)	9 (5%)	0	100 100
9	2	224/261 (86%)	211 (94%)	11 (5%)	2 (1%)	17 57
9	i	224/261 (86%)	207 (92%)	14 (6%)	3 (1%)	12 48
10	3	202/205 (98%)	190 (94%)	10 (5%)	2 (1%)	15 55
10	j	202/205 (98%)	190 (94%)	12 (6%)	0	100 100
11	4	193/198 (98%)	187 (97%)	5 (3%)	1 (0%)	29 69
11	k	193/198 (98%)	181 (94%)	12 (6%)	0	100 100
12	5	210/287 (73%)	203 (97%)	7 (3%)	0	100 100
12	l	210/287 (73%)	204 (97%)	5 (2%)	1 (0%)	29 69
13	6	220/241 (91%)	209 (95%)	11 (5%)	0	100 100
13	m	220/241 (91%)	207 (94%)	12 (6%)	1 (0%)	29 69
14	7	227/266 (85%)	210 (92%)	12 (5%)	5 (2%)	6 35
14	n	230/266 (86%)	215 (94%)	15 (6%)	0	100 100
15	H	376/467 (80%)	340 (90%)	25 (7%)	11 (3%)	4 29
16	I	383/437 (88%)	349 (91%)	28 (7%)	6 (2%)	9 44
17	K	387/428 (90%)	354 (92%)	23 (6%)	10 (3%)	5 31
18	L	386/437 (88%)	362 (94%)	19 (5%)	5 (1%)	12 48
19	M	377/434 (87%)	342 (91%)	25 (7%)	10 (3%)	5 31
20	J	384/405 (95%)	354 (92%)	21 (6%)	9 (2%)	6 34
21	W	195/268 (73%)	184 (94%)	8 (4%)	3 (2%)	10 46
22	V	287/306 (94%)	263 (92%)	17 (6%)	7 (2%)	6 33
23	T	264/274 (96%)	241 (91%)	17 (6%)	6 (2%)	6 34
24	X	125/156 (80%)	99 (79%)	23 (18%)	3 (2%)	6 33
25	Y	47/89 (53%)	39 (83%)	7 (15%)	1 (2%)	7 36
26	Z	902/993 (91%)	835 (93%)	52 (6%)	15 (2%)	9 42
27	N	886/945 (94%)	837 (94%)	42 (5%)	7 (1%)	19 60
28	S	473/523 (90%)	441 (93%)	21 (4%)	11 (2%)	6 34
29	P	438/445 (98%)	410 (94%)	19 (4%)	9 (2%)	7 36
30	Q	432/434 (100%)	388 (90%)	28 (6%)	16 (4%)	3 24
31	R	377/429 (88%)	358 (95%)	16 (4%)	3 (1%)	19 60

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
32	U	296/338 (88%)	283 (96%)	8 (3%)	5 (2%)	9 42
33	O	386/393 (98%)	377 (98%)	6 (2%)	3 (1%)	19 60
All	All	13700/15139 (90%)	12845 (94%)	665 (5%)	190 (1%)	15 46

All (190) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	215	GLU
2	B	93	ALA
5	E	114	ARG
11	4	25	ILE
15	H	77	ALA
15	H	145	TYR
15	H	206	VAL
16	I	115	ASP
17	K	104	ASP
17	K	334	LEU
17	K	398	ASN
17	K	416	LYS
17	K	418	ASP
17	K	419	ASN
18	L	432	ILE
19	M	172	VAL
19	M	177	THR
19	M	180	TYR
19	M	230	LEU
20	J	72	VAL
20	J	312	ARG
20	J	341	ILE
22	V	200	ASN
23	T	97	SER
23	T	173	GLU
24	X	29	VAL
26	Z	82	MET
26	Z	85	VAL
26	Z	728	LYS
27	N	856	PHE
27	N	862	SER
28	S	47	THR
28	S	101	LYS
28	S	150	LYS

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Mol	Chain	Res	Type
28	S	172	ASN
29	P	89	LEU
30	Q	44	ALA
30	Q	68	MET
30	Q	384	LYS
31	R	125	GLU
31	R	280	ILE
32	U	146	ASP
1	a	159	ALA
7	g	9	SER
2	B	94	HIS
4	D	30	CYS
5	E	120	SER
5	E	125	LEU
7	G	59	LYS
7	G	68	ARG
14	7	83	ALA
15	H	456	LYS
17	K	177	LEU
18	L	101	ILE
18	L	406	ASP
19	M	321	VAL
22	V	115	GLY
23	T	91	SER
23	T	99	SER
23	T	258	ASN
24	X	115	SER
26	Z	309	GLN
26	Z	339	PHE
27	N	359	ALA
28	S	153	GLU
28	S	303	ASN
29	P	111	ASP
29	P	126	THR
30	Q	46	VAL
30	Q	49	LYS
30	Q	51	ARG
30	Q	75	ARG
30	Q	170	ASP
30	Q	387	TYR
30	Q	406	ASP
32	U	6	GLU

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Mol	Chain	Res	Type
2	b	226	GLY
7	g	221	ASN
9	i	183	ASP
12	l	206	SER
13	m	19	ASP
1	A	159	ALA
1	A	181	LYS
4	D	205	ALA
5	E	116	GLY
6	F	4	ASN
9	2	91	GLN
9	2	166	ASP
14	7	27	LEU
14	7	81	ALA
16	I	337	ALA
17	K	171	TYR
17	K	342	SER
19	M	318	ASP
19	M	355	ASP
20	J	70	SER
20	J	82	LYS
20	J	249	GLU
20	J	335	MET
21	W	144	PHE
24	X	41	GLU
25	Y	31	GLU
26	Z	76	LYS
26	Z	376	SER
26	Z	611	THR
26	Z	887	GLY
26	Z	947	GLY
27	N	174	LEU
27	N	490	LEU
27	N	560	ALA
28	S	44	THR
29	P	88	GLN
29	P	132	VAL
29	P	328	ALA
29	P	397	ALA
30	Q	126	LYS
30	Q	309	ARG
32	U	5	HIS

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Mol	Chain	Res	Type
33	O	119	SER
2	b	97	TYR
3	c	219	ALA
4	d	102	VAL
5	e	125	LEU
3	C	220	ASN
4	D	48	SER
6	F	32	SER
7	G	67	ASP
10	3	181	GLY
15	H	179	SER
15	H	181	TYR
16	I	293	ASP
17	K	49	PHE
18	L	328	ASN
20	J	251	ASP
26	Z	896	LYS
26	Z	938	GLN
28	S	126	LYS
28	S	132	ALA
29	P	273	TYR
30	Q	124	PHE
30	Q	253	ASN
30	Q	286	TYR
32	U	184	GLY
33	O	243	VAL
5	e	45	ARG
9	i	171	SER
9	i	196	ARG
4	D	99	GLU
6	F	6	ASP
7	G	16	ARG
14	7	77	ASP
15	H	94	GLU
15	H	314	VAL
19	M	229	THR
19	M	432	PHE
20	J	376	HIS
21	W	149	GLN
21	W	190	ILE
22	V	184	ASN
22	V	262	THR

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Mol	Chain	Res	Type
23	T	235	PHE
26	Z	885	ALA
26	Z	930	GLY
28	S	83	PRO
28	S	97	THR
29	P	130	ILE
30	Q	47	ASP
31	R	106	ASN
32	U	179	ARG
2	b	2	THR
8	1	48	SER
14	7	10	SER
15	H	190	ARG
16	I	83	LYS
16	I	338	LEU
16	I	340	ARG
19	M	179	THR
27	N	415	PHE
5	e	129	PRO
18	L	350	PRO
22	V	185	ILE
33	O	320	PRO
15	H	203	LYS
2	b	31	GLY
10	3	183	GLY
22	V	143	PRO
26	Z	19	SER
2	B	228	PRO
22	V	112	PRO
15	H	75	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	206/210 (98%)	202 (98%)	4 (2%)	57 75

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	a	206/210 (98%)	199 (97%)	7 (3%)	37	60
2	B	209/209 (100%)	203 (97%)	6 (3%)	42	64
2	b	209/209 (100%)	205 (98%)	4 (2%)	57	75
3	C	203/216 (94%)	202 (100%)	1 (0%)	88	93
3	c	203/216 (94%)	199 (98%)	4 (2%)	55	74
4	D	212/226 (94%)	210 (99%)	2 (1%)	78	87
4	d	212/226 (94%)	207 (98%)	5 (2%)	49	69
5	E	198/215 (92%)	193 (98%)	5 (2%)	47	68
5	e	198/215 (92%)	193 (98%)	5 (2%)	47	68
6	F	192/193 (100%)	186 (97%)	6 (3%)	40	62
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%)	198 (98%)	3 (2%)	65	80
8	1	162/178 (91%)	160 (99%)	2 (1%)	71	83
8	h	162/178 (91%)	156 (96%)	6 (4%)	34	58
9	2	185/214 (86%)	183 (99%)	2 (1%)	73	84
9	i	185/214 (86%)	179 (97%)	6 (3%)	39	61
10	3	172/173 (99%)	171 (99%)	1 (1%)	86	92
10	j	172/173 (99%)	168 (98%)	4 (2%)	50	70
11	4	173/175 (99%)	172 (99%)	1 (1%)	86	92
11	k	173/175 (99%)	163 (94%)	10 (6%)	20	45
12	5	169/235 (72%)	164 (97%)	5 (3%)	41	63
12	l	169/235 (72%)	163 (96%)	6 (4%)	35	59
13	6	185/201 (92%)	184 (100%)	1 (0%)	88	93
13	m	185/201 (92%)	178 (96%)	7 (4%)	33	57
14	7	195/224 (87%)	193 (99%)	2 (1%)	76	86
14	n	198/224 (88%)	186 (94%)	12 (6%)	18	44
15	H	320/399 (80%)	312 (98%)	8 (2%)	47	68
16	I	342/385 (89%)	335 (98%)	7 (2%)	55	74
17	K	342/374 (91%)	335 (98%)	7 (2%)	55	74
18	L	332/377 (88%)	326 (98%)	6 (2%)	59	77

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	M	329/375 (88%)	323 (98%)	6 (2%)	59 77
20	J	336/352 (96%)	327 (97%)	9 (3%)	44 65
21	W	171/230 (74%)	170 (99%)	1 (1%)	86 92
22	V	253/268 (94%)	247 (98%)	6 (2%)	49 69
23	T	249/256 (97%)	241 (97%)	8 (3%)	39 61
24	X	116/144 (81%)	112 (97%)	4 (3%)	37 60
25	Y	50/81 (62%)	49 (98%)	1 (2%)	55 74
26	Z	773/850 (91%)	752 (97%)	21 (3%)	44 65
27	N	745/797 (94%)	734 (98%)	11 (2%)	65 80
28	S	447/489 (91%)	436 (98%)	11 (2%)	47 68
29	P	412/415 (99%)	405 (98%)	7 (2%)	60 78
30	Q	391/391 (100%)	383 (98%)	8 (2%)	55 74
31	R	333/379 (88%)	328 (98%)	5 (2%)	65 80
32	U	271/308 (88%)	271 (100%)	0	100 100
33	O	363/368 (99%)	354 (98%)	9 (2%)	47 68
All	All	11900/13054 (91%)	11635 (98%)	265 (2%)	54 71

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

Mol	Chain	Res	Type
1	a	10	PHE
1	a	117	GLN
1	a	124	TYR
1	a	130	VAL
1	a	144	SER
1	a	225	PHE
1	a	235	ARG
2	b	127	VAL
2	b	181	ASP
2	b	187	ASP
2	b	220	ASP
3	c	18	LEU
3	c	119	GLN
3	c	164	VAL
3	c	177	MET
4	d	9	PHE
4	d	12	ASP

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Mol	Chain	Res	Type
4	d	63	SER
4	d	68	HIS
4	d	124	VAL
5	e	35	LYS
5	e	59	ILE
5	e	158	ARG
5	e	169	GLU
5	e	186	LYS
6	f	46	VAL
6	f	53	ASP
6	f	71	LEU
6	f	73	LEU
6	f	116	GLN
6	f	137	ASP
6	f	178	PHE
7	g	172	LEU
7	g	181	GLU
7	g	214	TRP
8	h	31	THR
8	h	32	ASP
8	h	36	ARG
8	h	72	THR
8	h	159	LEU
8	h	187	ILE
9	i	25	ILE
9	i	80	LEU
9	i	123	TYR
9	i	186	TYR
9	i	214	LYS
9	i	215	GLU
10	j	84	GLU
10	j	92	SER
10	j	140	THR
10	j	159	PRO
11	k	4	ILE
11	k	28	LEU
11	k	40	PRO
11	k	53	THR
11	k	93	ARG
11	k	94	SER
11	k	101	ASN
11	k	126	VAL

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Mol	Chain	Res	Type
11	k	191	GLN
11	k	195	PHE
12	l	4	LEU
12	l	8	PHE
12	l	9	GLN
12	l	104	TYR
12	l	106	ARG
12	l	139	VAL
13	m	57	PHE
13	m	117	ASP
13	m	123	TYR
13	m	128	VAL
13	m	130	SER
13	m	134	GLU
13	m	213	ARG
14	n	3	GLN
14	n	6	VAL
14	n	30	TYR
14	n	56	ASP
14	n	63	ILE
14	n	66	LEU
14	n	125	GLN
14	n	162	GLU
14	n	181	MET
14	n	187	ARG
14	n	210	LYS
14	n	221	PHE
1	A	77	PRO
1	A	105	CYS
1	A	117	GLN
1	A	208	GLU
2	B	3	ASP
2	B	18	LEU
2	B	101	TYR
2	B	112	SER
2	B	128	ARG
2	B	132	VAL
3	C	206	THR
4	D	49	THR
4	D	102	VAL
5	E	128	ARG
5	E	178	GLU

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Mol	Chain	Res	Type
5	E	206	GLU
5	E	208	ASN
5	E	217	GLN
6	F	1	PHE
6	F	14	PRO
6	F	37	LEU
6	F	73	LEU
6	F	139	SER
6	F	219	THR
7	G	18	PHE
7	G	80	ASP
7	G	181	GLU
7	G	183	LEU
7	G	208	PHE
7	G	214	TRP
8	1	4	MET
8	1	124	TYR
9	2	183	ASP
9	2	222	ASP
10	3	155	PRO
11	4	130	TYR
12	5	95	LEU
12	5	104	TYR
12	5	137	TYR
12	5	141	ASP
12	5	177	LEU
13	6	169	LYS
14	7	122	ASN
14	7	154	LEU
15	H	78	PRO
15	H	82	TRP
15	H	174	VAL
15	H	254	THR
15	H	267	THR
15	H	327	ASN
15	H	421	SER
15	H	436	LYS
16	I	108	THR
16	I	177	PRO
16	I	207	LEU
16	I	219	VAL
16	I	292	TYR

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Mol	Chain	Res	Type
16	I	340	ARG
16	I	401	LEU
17	K	60	LEU
17	K	121	ARG
17	K	146	LEU
17	K	241	GLU
17	K	330	ARG
17	K	387	MET
17	K	426	PHE
18	L	53	HIS
18	L	131	VAL
18	L	243	PHE
18	L	333	LEU
18	L	361	PHE
18	L	415	LEU
19	M	127	VAL
19	M	245	LYS
19	M	249	PRO
19	M	301	VAL
19	M	337	LEU
19	M	344	ASP
20	J	21	PRO
20	J	22	TYR
20	J	122	LEU
20	J	133	LEU
20	J	172	GLU
20	J	299	ILE
20	J	302	PRO
20	J	350	MET
20	J	359	LYS
21	W	164	PRO
22	V	20	ARG
22	V	31	SER
22	V	32	ILE
22	V	72	PRO
22	V	147	VAL
22	V	192	LEU
23	T	79	GLU
23	T	82	PHE
23	T	89	TYR
23	T	150	ARG
23	T	170	ASN

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Mol	Chain	Res	Type
23	T	173	GLU
23	T	197	TYR
23	T	257	THR
24	X	11	ARG
24	X	39	GLU
24	X	42	GLU
24	X	124	LYS
25	Y	38	PHE
26	Z	1	MET
26	Z	6	ASP
26	Z	117	ASP
26	Z	185	ASP
26	Z	195	PHE
26	Z	242	PHE
26	Z	296	SER
26	Z	302	SER
26	Z	309	GLN
26	Z	339	PHE
26	Z	341	TYR
26	Z	525	MET
26	Z	767	TYR
26	Z	806	GLU
26	Z	815	MET
26	Z	845	LEU
26	Z	846	PHE
26	Z	898	HIS
26	Z	910	PRO
26	Z	936	VAL
26	Z	965	LEU
27	N	175	ASP
27	N	248	GLU
27	N	347	SER
27	N	360	GLN
27	N	398	ARG
27	N	434	SER
27	N	569	LYS
27	N	707	ASN
27	N	855	GLU
27	N	873	ARG
27	N	918	GLU
28	S	32	GLN
28	S	45	THR

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Mol	Chain	Res	Type
28	S	59	ASP
28	S	101	LYS
28	S	133	GLU
28	S	165	PRO
28	S	180	ASN
28	S	199	GLU
28	S	265	SER
28	S	403	SER
28	S	475	TYR
29	P	80	THR
29	P	127	GLU
29	P	129	LYS
29	P	279	ASP
29	P	309	MET
29	P	392	LYS
29	P	400	VAL
30	Q	8	LEU
30	Q	75	ARG
30	Q	92	LYS
30	Q	148	LYS
30	Q	240	PHE
30	Q	279	LYS
30	Q	286	TYR
30	Q	339	TYR
31	R	95	ASP
31	R	117	ILE
31	R	119	LYS
31	R	238	PHE
31	R	359	VAL
33	O	58	ARG
33	O	60	ARG
33	O	62	TYR
33	O	70	TYR
33	O	83	LEU
33	O	184	ASP
33	O	237	PRO
33	O	270	ILE
33	O	307	MET

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (102) such sidechains are listed below:

Mol	Chain	Res	Type
2	b	149	GLN
3	c	58	GLN
3	c	124	HIS
4	d	68	HIS
4	d	94	HIS
4	d	116	GLN
4	d	236	GLN
5	e	172	GLN
6	f	198	GLN
6	f	209	ASN
7	g	19	GLN
7	g	200	HIS
8	h	62	HIS
8	h	120	HIS
8	h	157	HIS
8	h	161	GLN
10	j	71	ASN
10	j	172	ASN
11	k	41	HIS
11	k	61	GLN
11	k	101	ASN
11	k	133	HIS
12	l	66	HIS
12	l	179	HIS
13	m	36	ASN
13	m	108	HIS
13	m	152	ASN
13	m	153	GLN
14	n	2	GLN
14	n	26	ASN
14	n	194	ASN
14	n	213	GLN
1	A	200	HIS
2	B	94	HIS
2	B	149	GLN
3	C	93	HIS
3	C	102	ASN
3	C	151	ASN
4	D	53	GLN
5	E	172	GLN
5	E	180	HIS
5	E	208	ASN
6	F	30	GLN

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Mol	Chain	Res	Type
6	F	142	HIS
7	G	178	HIS
7	G	240	GLN
8	1	28	ASN
8	1	89	ASN
8	1	92	ASN
9	2	30	ASN
9	2	85	GLN
9	2	165	ASN
9	2	172	ASN
9	2	194	ASN
10	3	47	HIS
11	4	55	GLN
11	4	191	GLN
12	5	66	HIS
12	5	176	ASN
13	6	152	ASN
13	6	153	GLN
14	7	74	ASN
14	7	131	ASN
15	H	51	GLN
15	H	265	ASN
15	H	356	ASN
17	K	308	GLN
17	K	388	GLN
18	L	273	HIS
18	L	328	ASN
19	M	72	ASN
19	M	149	ASN
22	V	40	HIS
22	V	279	HIS
23	T	170	ASN
26	Z	168	GLN
26	Z	276	ASN
26	Z	309	GLN
26	Z	327	GLN
26	Z	429	ASN
26	Z	760	HIS
26	Z	833	GLN
27	N	176	GLN
27	N	219	ASN
27	N	233	ASN

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Mol	Chain	Res	Type
28	S	39	ASN
28	S	177	ASN
29	P	48	GLN
29	P	113	ASN
29	P	263	HIS
29	P	337	HIS
29	P	394	ASN
30	Q	37	GLN
30	Q	213	GLN
31	R	143	GLN
31	R	399	GLN
32	U	21	HIS
32	U	71	ASN
32	U	142	GLN
32	U	262	GLN
33	O	116	ASN
33	O	326	HIS

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 12 ligands modelled in this entry, 6 are monoatomic - leaving 6 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
36	ADP	M	501	35	24,29,29	1.39	5 (20%)	29,45,45	2.07	9 (31%)
34	ANP	L	501	35	29,33,33	3.38	10 (34%)	31,52,52	2.57	10 (32%)
34	ANP	J	501	35	29,33,33	2.90	8 (27%)	31,52,52	2.66	10 (32%)
34	ANP	K	501	35	29,33,33	2.38	10 (34%)	31,52,52	2.63	10 (32%)
34	ANP	I	501	35	29,33,33	3.37	8 (27%)	31,52,52	2.90	12 (38%)
34	ANP	H	501	35	29,33,33	3.55	12 (41%)	31,52,52	2.57	12 (38%)

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
36	ADP	M	501	35	-	8/12/32/32	0/3/3/3
34	ANP	L	501	35	-	3/14/38/38	0/3/3/3
34	ANP	J	501	35	-	5/14/38/38	0/3/3/3
34	ANP	K	501	35	-	3/14/38/38	0/3/3/3
34	ANP	I	501	35	-	8/14/38/38	0/3/3/3
34	ANP	H	501	35	-	8/14/38/38	0/3/3/3

All (53) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	H	501	ANP	PB-O3A	15.84	1.79	1.59
34	I	501	ANP	PB-O3A	14.66	1.77	1.59
34	L	501	ANP	PB-O3A	14.12	1.76	1.59
34	J	501	ANP	PB-O3A	10.31	1.72	1.59
34	K	501	ANP	PB-O3A	7.27	1.68	1.59
34	J	501	ANP	PG-O1G	6.27	1.56	1.46
34	K	501	ANP	PG-O1G	6.14	1.55	1.46
34	I	501	ANP	PG-O1G	5.67	1.55	1.46
34	I	501	ANP	PB-N3B	5.28	1.77	1.63
34	H	501	ANP	PG-O3G	-4.98	1.43	1.56
34	L	501	ANP	PB-N3B	4.89	1.76	1.63
34	K	501	ANP	PG-N3B	4.70	1.75	1.63
34	L	501	ANP	O4'-C1'	4.54	1.47	1.41
34	J	501	ANP	PG-N3B	4.44	1.75	1.63
34	J	501	ANP	PB-N3B	4.42	1.74	1.63
34	J	501	ANP	PB-O1B	4.09	1.52	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	I	501	ANP	PB-O1B	4.06	1.52	1.46
34	L	501	ANP	C2'-C1'	-4.02	1.47	1.53
34	L	501	ANP	PB-O1B	3.93	1.52	1.46
34	H	501	ANP	C3'-C4'	3.64	1.62	1.53
34	H	501	ANP	PB-N3B	3.56	1.72	1.63
34	L	501	ANP	PG-O1G	3.37	1.51	1.46
36	M	501	ADP	C8-N7	-3.15	1.29	1.34
34	I	501	ANP	PG-N3B	2.90	1.70	1.63
34	K	501	ANP	PB-N3B	2.82	1.70	1.63
36	M	501	ADP	O4'-C1'	2.81	1.45	1.41
34	H	501	ANP	C8-N7	-2.78	1.29	1.34
34	H	501	ANP	C6-N6	2.77	1.44	1.34
34	J	501	ANP	PB-O2B	-2.70	1.49	1.56
34	H	501	ANP	PB-O1B	2.62	1.50	1.46
34	K	501	ANP	PB-O1B	2.56	1.50	1.46
34	L	501	ANP	PG-O3G	-2.55	1.49	1.56
34	I	501	ANP	C8-N7	-2.55	1.30	1.34
34	K	501	ANP	PG-O3G	-2.55	1.49	1.56
34	J	501	ANP	C2'-C1'	-2.48	1.50	1.53
34	L	501	ANP	PG-N3B	2.46	1.69	1.63
34	H	501	ANP	PG-O1G	2.41	1.50	1.46
34	L	501	ANP	C2-N3	2.40	1.36	1.32
34	L	501	ANP	PG-O2G	-2.38	1.50	1.56
34	H	501	ANP	C5'-C4'	2.35	1.58	1.51
36	M	501	ADP	C4-N3	-2.35	1.32	1.35
34	K	501	ANP	C2'-C1'	-2.27	1.50	1.53
34	H	501	ANP	PA-O2A	-2.24	1.44	1.55
34	H	501	ANP	C2'-C3'	-2.22	1.47	1.53
34	K	501	ANP	PB-O2B	-2.11	1.51	1.56
34	I	501	ANP	C6-N6	2.09	1.41	1.34
34	J	501	ANP	C6-N6	2.09	1.41	1.34
34	K	501	ANP	C2-N1	2.07	1.37	1.33
34	I	501	ANP	C4-N3	-2.06	1.32	1.35
36	M	501	ADP	C5-C4	-2.06	1.35	1.40
36	M	501	ADP	O3'-C3'	2.05	1.47	1.43
34	H	501	ANP	C2-N3	2.04	1.35	1.32
34	K	501	ANP	O4'-C1'	2.03	1.43	1.41

All (63) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	J	501	ANP	O1G-PG-N3B	-9.11	98.36	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	I	501	ANP	O1G-PG-N3B	-9.03	98.48	111.77
34	I	501	ANP	PB-O3A-PA	7.58	159.32	132.62
34	L	501	ANP	O1G-PG-N3B	-7.51	100.72	111.77
34	K	501	ANP	O1G-PG-N3B	-7.26	101.07	111.77
34	H	501	ANP	O1G-PG-N3B	-6.99	101.48	111.77
36	M	501	ADP	PA-O3A-PB	6.78	156.09	132.83
34	K	501	ANP	O1B-PB-N3B	-6.16	102.70	111.77
34	K	501	ANP	O2B-PB-O1B	6.01	122.53	109.92
34	L	501	ANP	O2B-PB-O1B	5.65	121.77	109.92
34	L	501	ANP	PB-O3A-PA	5.52	152.06	132.62
34	H	501	ANP	N6-C6-N1	5.51	130.01	118.57
34	J	501	ANP	PB-O3A-PA	5.39	151.61	132.62
34	H	501	ANP	PB-O3A-PA	5.30	151.27	132.62
34	L	501	ANP	N6-C6-N1	5.17	129.30	118.57
34	J	501	ANP	O1B-PB-N3B	-5.12	104.22	111.77
34	I	501	ANP	N6-C6-N1	5.06	129.07	118.57
34	K	501	ANP	PB-O3A-PA	4.94	150.00	132.62
34	J	501	ANP	O2B-PB-O1B	4.51	119.38	109.92
36	M	501	ADP	N6-C6-N1	4.13	127.16	118.57
34	H	501	ANP	O2B-PB-O1B	3.96	118.22	109.92
34	I	501	ANP	C1'-N9-C4	3.74	133.21	126.64
36	M	501	ADP	C4-C5-N7	-3.72	105.52	109.40
34	I	501	ANP	C5-C6-N1	-3.72	111.92	120.35
34	H	501	ANP	N3-C2-N1	3.53	134.20	128.68
34	L	501	ANP	C5-C6-N6	-3.40	115.19	120.35
34	I	501	ANP	O2B-PB-O1B	3.28	116.80	109.92
34	I	501	ANP	O2G-PG-O3G	3.28	116.38	107.64
34	I	501	ANP	O3A-PB-N3B	-3.24	97.60	106.59
34	H	501	ANP	C5-C6-N1	-3.15	113.21	120.35
34	J	501	ANP	N3-C2-N1	3.08	133.50	128.68
34	K	501	ANP	C5-C6-N1	-3.07	113.39	120.35
34	K	501	ANP	C5-C6-N6	2.98	124.88	120.35
34	H	501	ANP	O4'-C4'-C3'	-2.90	99.38	105.11
34	J	501	ANP	C5-C6-N1	-2.87	113.85	120.35
36	M	501	ADP	C2'-C3'-C4'	2.77	108.02	102.64
34	I	501	ANP	C4-C5-N7	-2.73	106.55	109.40
34	L	501	ANP	O1B-PB-N3B	-2.69	107.81	111.77
34	J	501	ANP	O4'-C1'-C2'	2.59	110.72	106.93
34	L	501	ANP	O2G-PG-O3G	2.56	114.45	107.64
36	M	501	ADP	O3'-C3'-C4'	-2.55	103.69	111.05
34	K	501	ANP	C4-C5-N7	-2.53	106.77	109.40
34	L	501	ANP	O4'-C4'-C3'	-2.45	100.26	105.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	H	501	ANP	C5-C6-N6	-2.45	116.62	120.35
34	H	501	ANP	O1B-PB-N3B	-2.43	108.19	111.77
34	H	501	ANP	C1'-N9-C4	2.42	130.90	126.64
34	J	501	ANP	N6-C6-N1	2.42	123.59	118.57
36	M	501	ADP	C5-C6-N6	-2.41	116.69	120.35
34	J	501	ANP	O2G-PG-O3G	2.40	114.03	107.64
34	K	501	ANP	O2B-PB-O3A	2.37	112.55	104.64
34	L	501	ANP	C5-C6-N1	-2.33	115.07	120.35
36	M	501	ADP	C2-N1-C6	-2.27	114.86	118.75
34	J	501	ANP	C1'-N9-C4	2.26	130.61	126.64
36	M	501	ADP	N3-C2-N1	2.26	132.21	128.68
34	H	501	ANP	C3'-C2'-C1'	-2.17	97.71	100.98
34	I	501	ANP	C2-N1-C6	2.15	122.43	118.75
34	I	501	ANP	O1B-PB-N3B	-2.11	108.66	111.77
34	H	501	ANP	O2'-C2'-C1'	-2.11	103.06	110.85
34	I	501	ANP	C3'-C2'-C1'	2.10	104.15	100.98
34	K	501	ANP	C3'-C2'-C1'	2.10	104.15	100.98
34	K	501	ANP	O3'-C3'-C2'	2.10	118.61	111.82
34	L	501	ANP	O2'-C2'-C1'	-2.01	103.42	110.85
36	M	501	ADP	C5-C6-N1	-2.00	115.81	120.35

There are no chirality outliers.

All (35) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	H	501	ANP	PB-N3B-PG-O1G
34	H	501	ANP	PG-N3B-PB-O1B
34	H	501	ANP	C5'-O5'-PA-O1A
34	I	501	ANP	PG-N3B-PB-O3A
34	I	501	ANP	PA-O3A-PB-O1B
34	I	501	ANP	PA-O3A-PB-O2B
34	I	501	ANP	C5'-O5'-PA-O3A
34	K	501	ANP	PB-N3B-PG-O1G
34	K	501	ANP	PG-N3B-PB-O1B
34	L	501	ANP	PB-N3B-PG-O1G
34	J	501	ANP	PB-N3B-PG-O1G
34	J	501	ANP	PG-N3B-PB-O1B
34	J	501	ANP	C5'-O5'-PA-O1A
34	J	501	ANP	C5'-O5'-PA-O3A
36	M	501	ADP	PA-O3A-PB-O3B
36	M	501	ADP	C5'-O5'-PA-O1A
34	I	501	ANP	C3'-C4'-C5'-O5'

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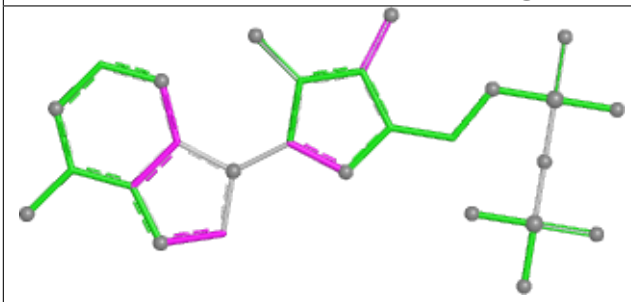
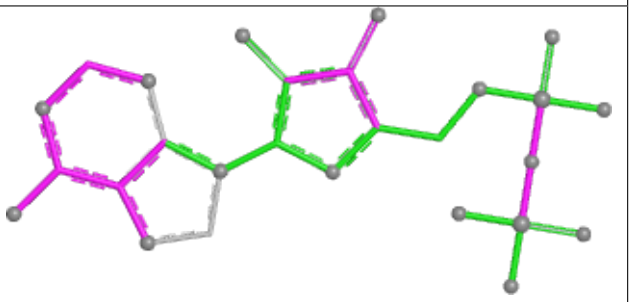
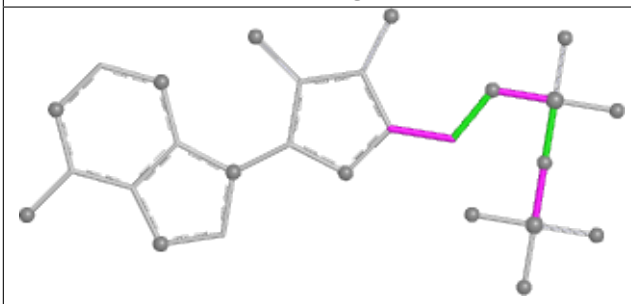
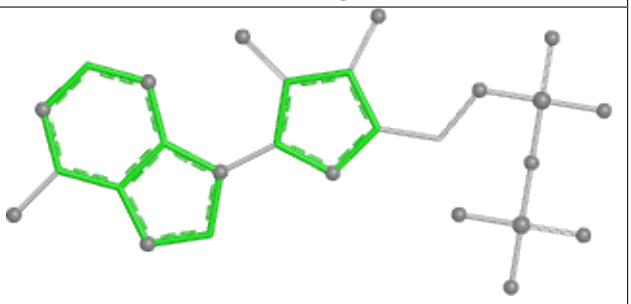
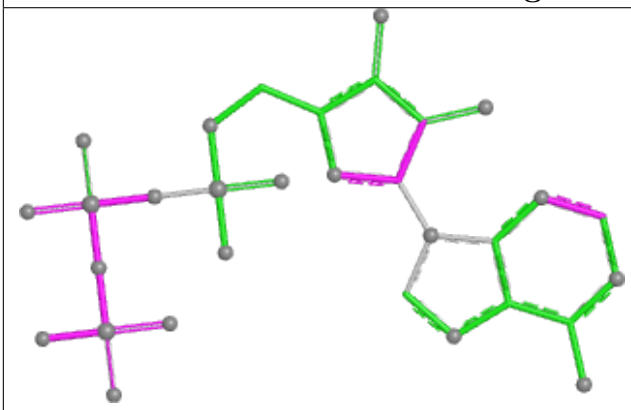
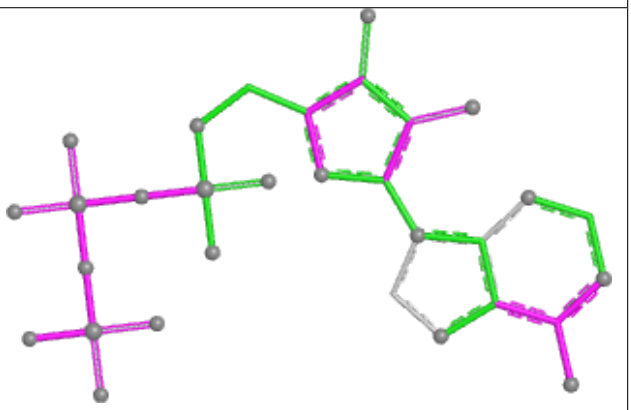
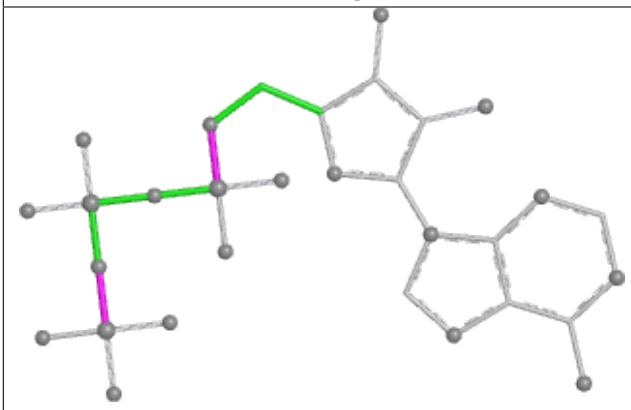
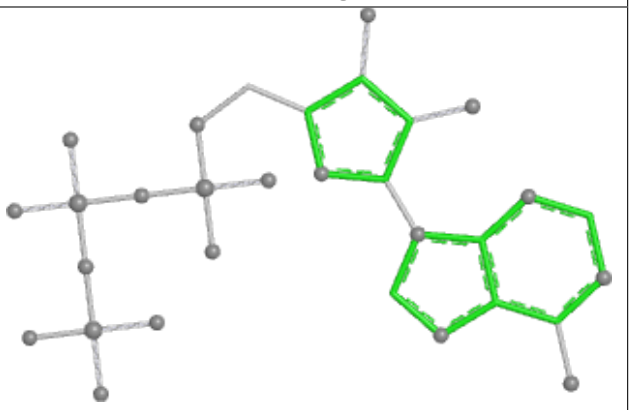
Mol	Chain	Res	Type	Atoms
34	I	501	ANP	O4'-C4'-C5'-O5'
34	I	501	ANP	PB-O3A-PA-O1A
36	M	501	ADP	PA-O3A-PB-O2B
34	H	501	ANP	C5'-O5'-PA-O3A
34	L	501	ANP	C5'-O5'-PA-O3A
34	K	501	ANP	O4'-C4'-C5'-O5'
34	H	501	ANP	C5'-O5'-PA-O2A
34	I	501	ANP	C5'-O5'-PA-O2A
34	L	501	ANP	C5'-O5'-PA-O2A
36	M	501	ADP	C5'-O5'-PA-O2A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

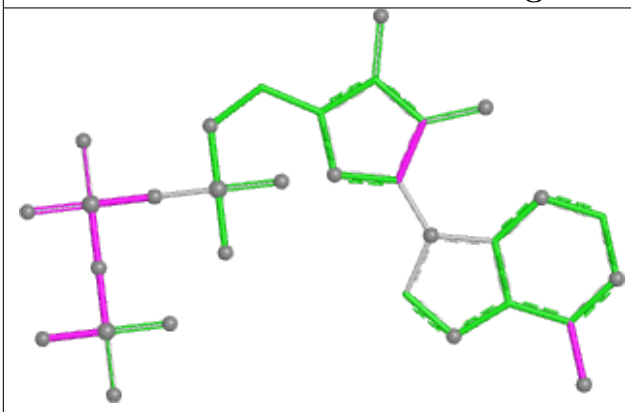
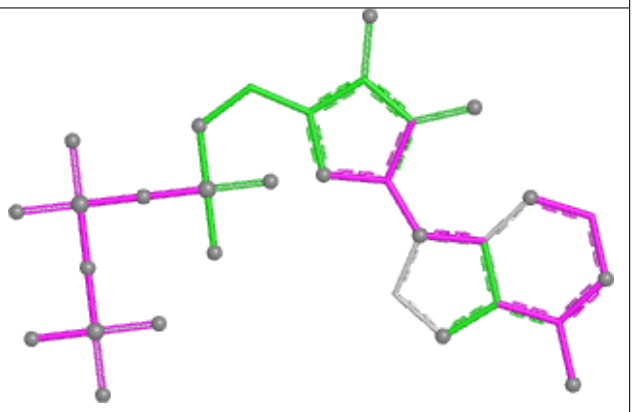
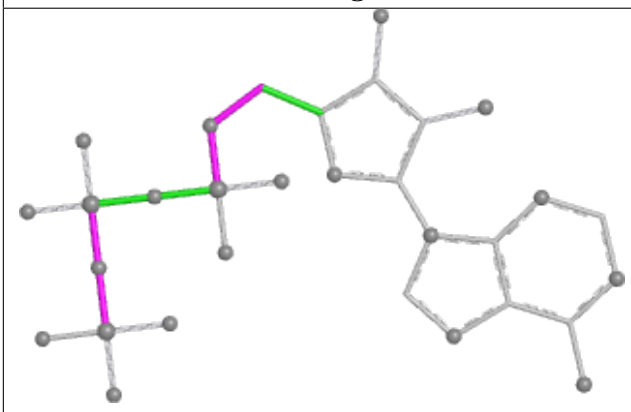
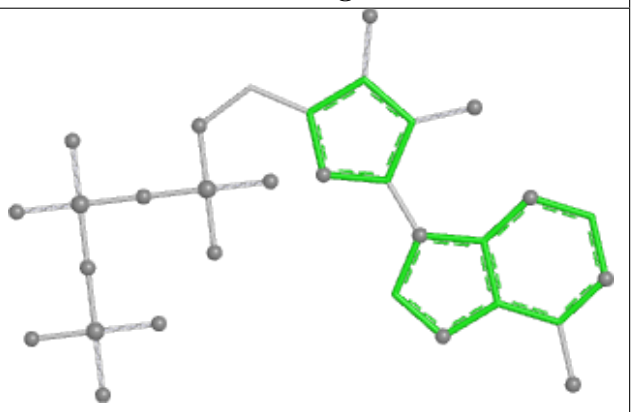
There are no ring outliers.

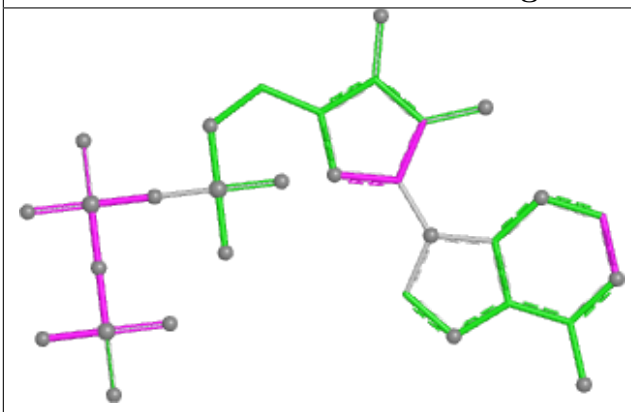
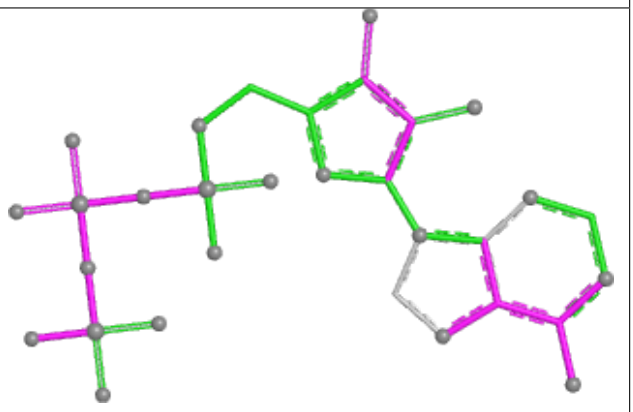
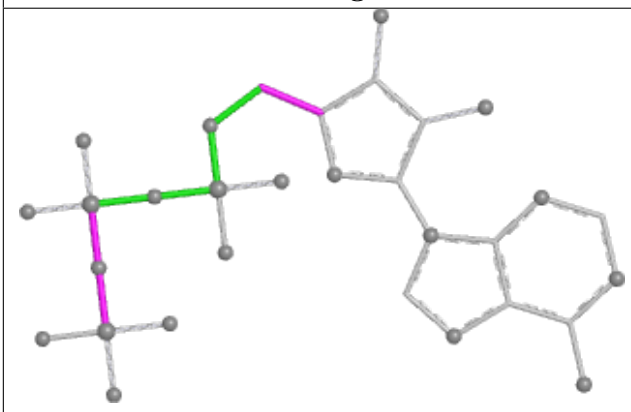
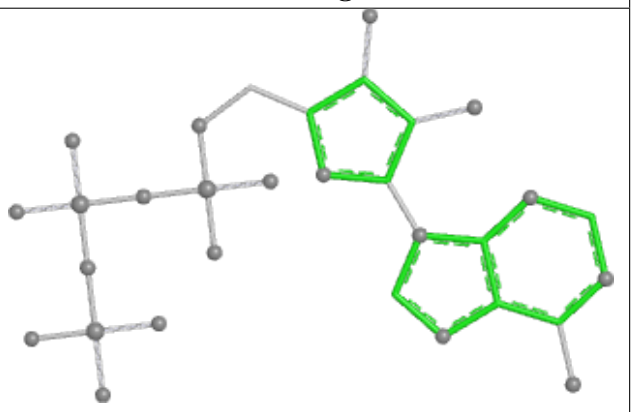
No monomer is involved in short contacts.

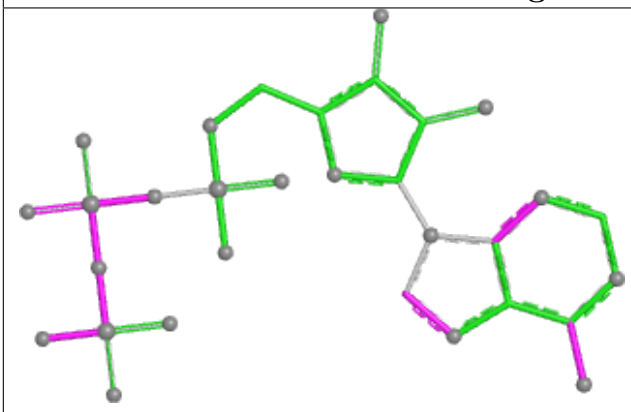
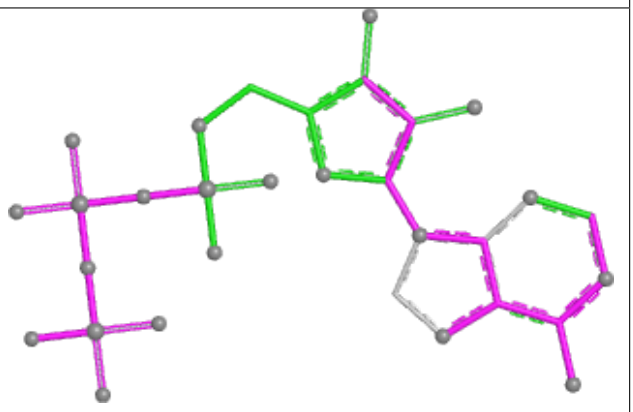
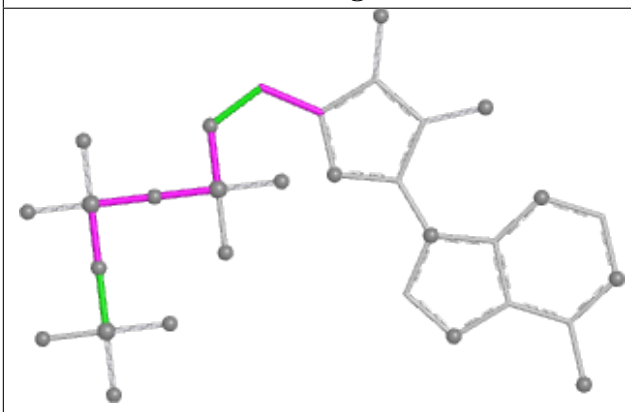
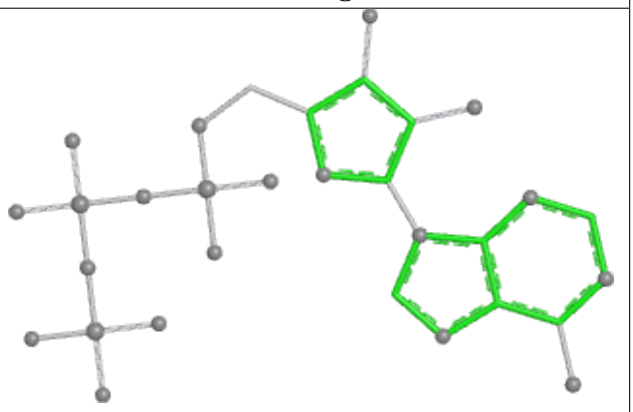
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

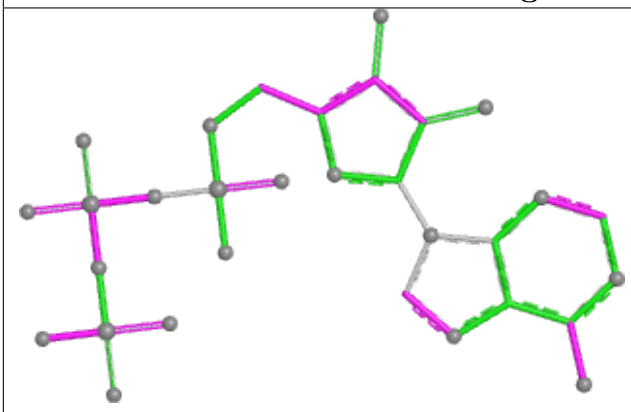
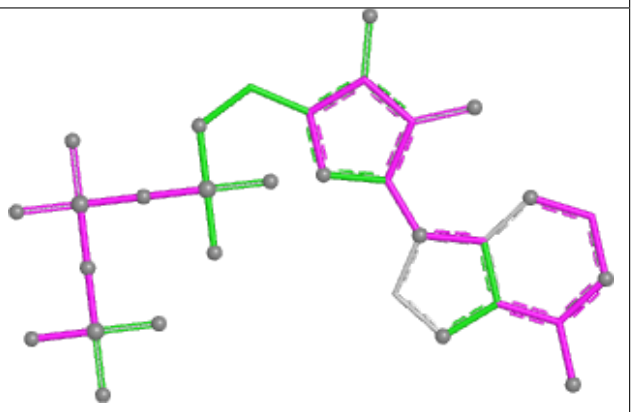
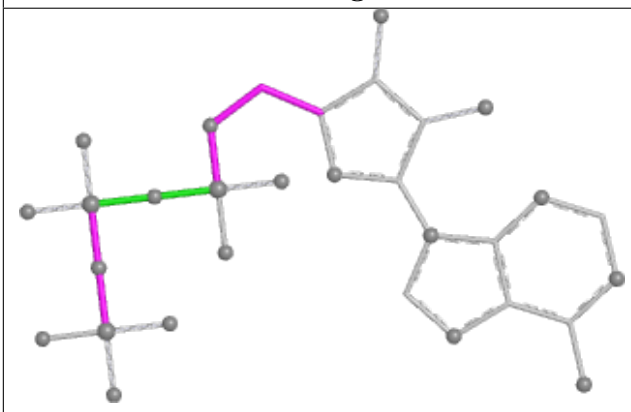
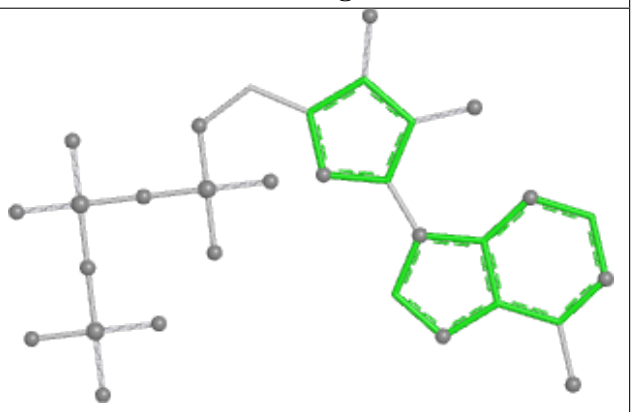
Ligand ADP M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANP L 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANP J 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANP K 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ANP I 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand ANP 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

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	V	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	V	186:GLN	C	187:ALA	N	1.19

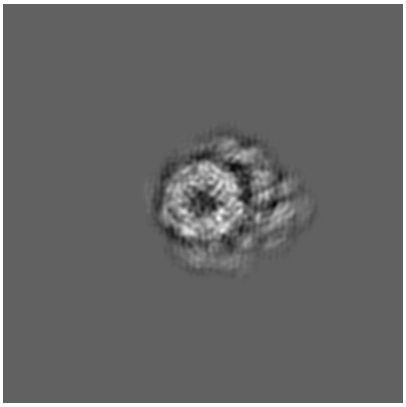
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3536. These allow visual inspection of the internal detail of the map and identification of artifacts.

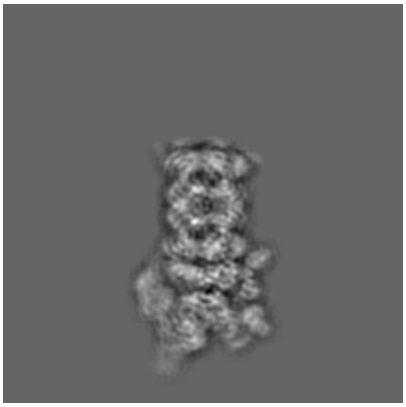
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

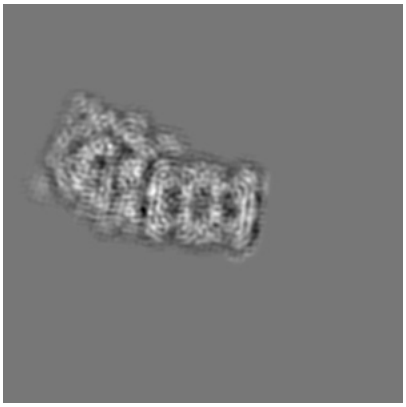
6.1.1 Primary map



X



Y

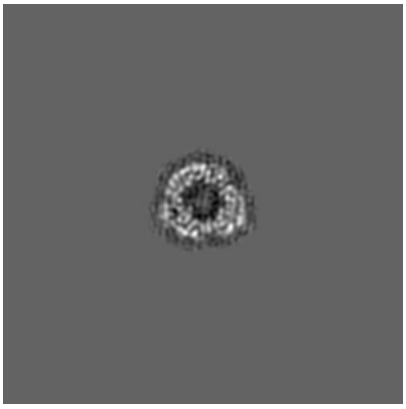


Z

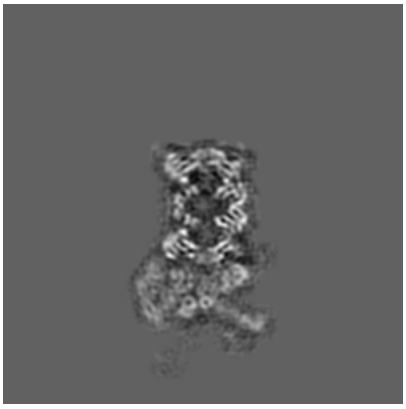
The images above show the map projected in three orthogonal directions.

6.2 Central slices

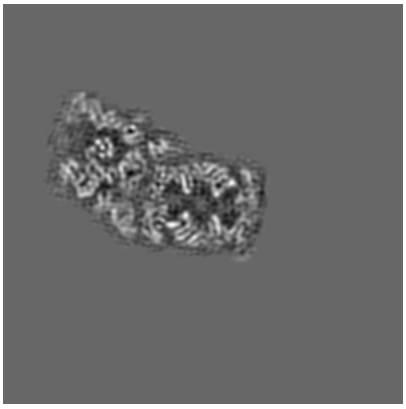
6.2.1 Primary map



X Index: 208



Y Index: 208

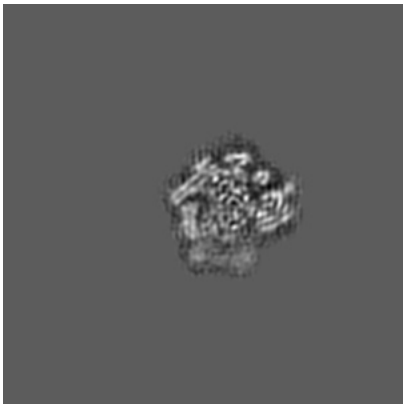


Z Index: 208

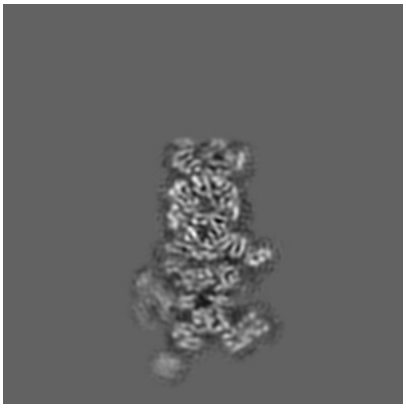
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 135



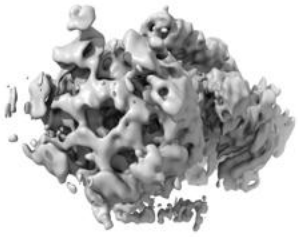
Y Index: 226

Z Index: 199

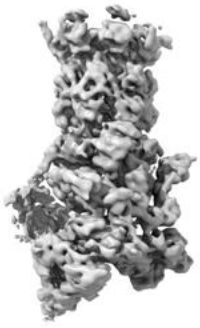
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

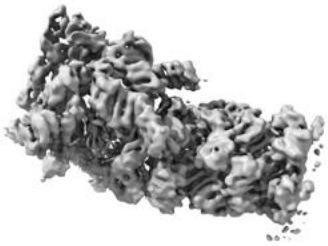
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

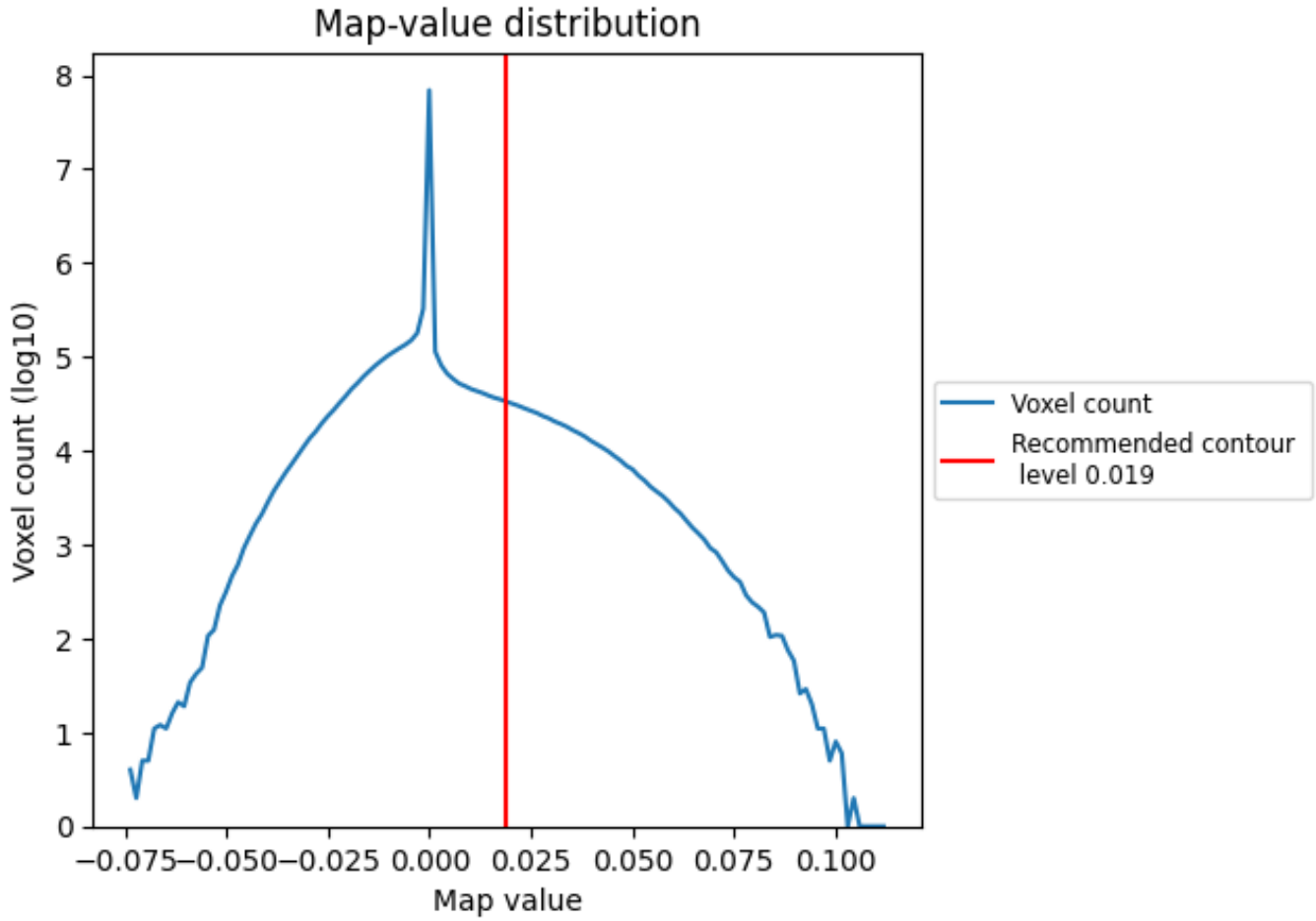
6.5 Mask visualisation (i)

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

7 Map analysis

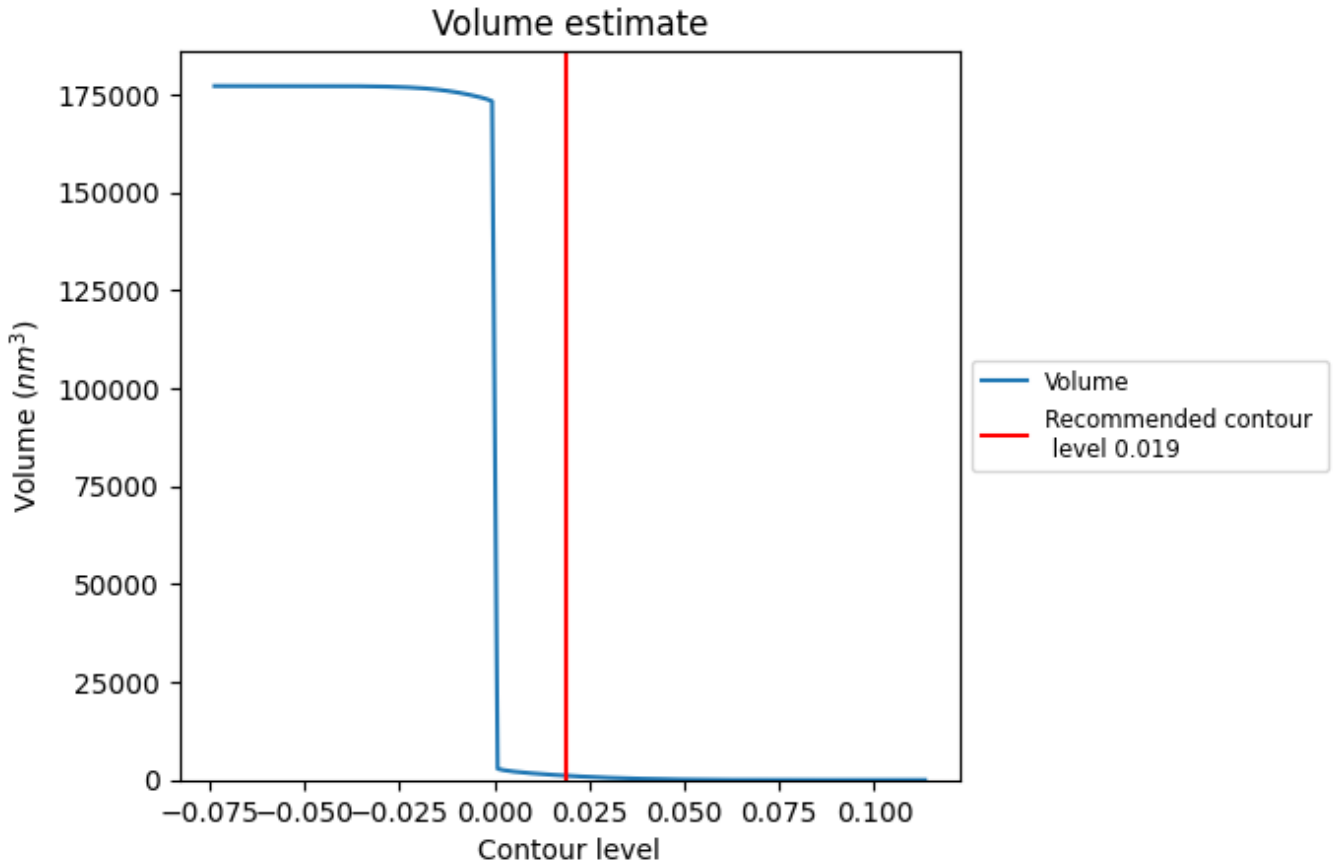
This section contains the results of statistical analysis of the map.

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.

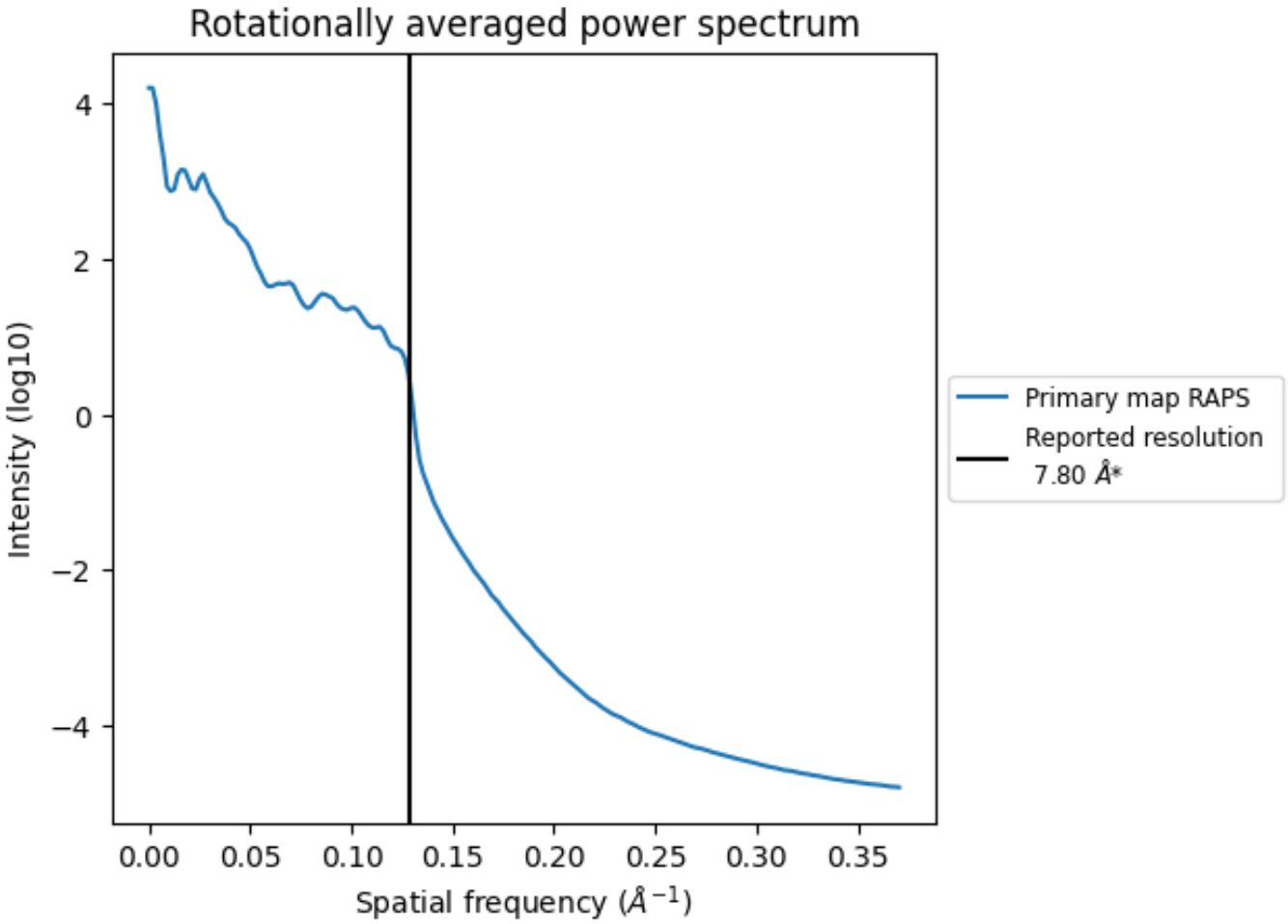
7.2 Volume estimate



The volume at the recommended contour level is 1087 nm^3; this corresponds to an approximate mass of 982 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 0.128 Å^{-1}

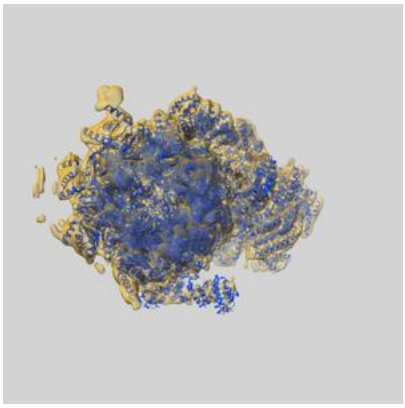
8 Fourier-Shell correlation

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

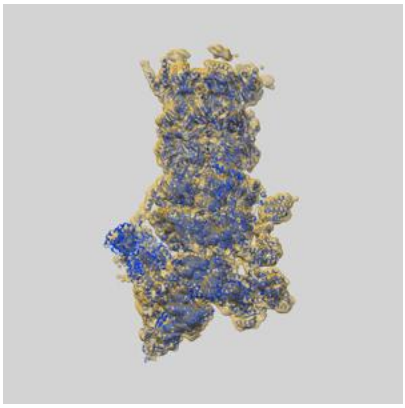
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3536 and PDB model 5MPB. Per-residue inclusion information can be found in section 3 on page 13.

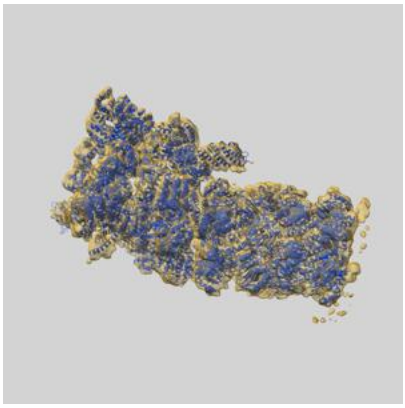
9.1 Map-model overlay



X



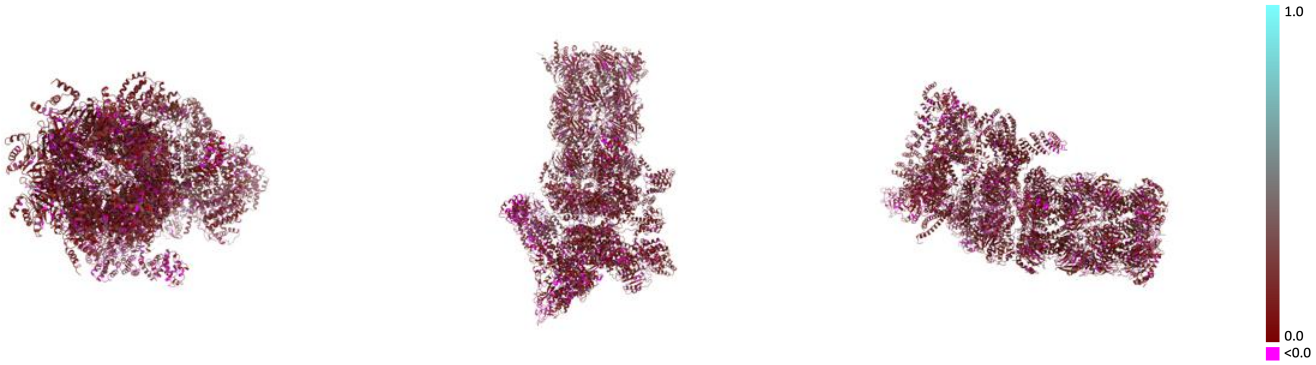
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.019 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.

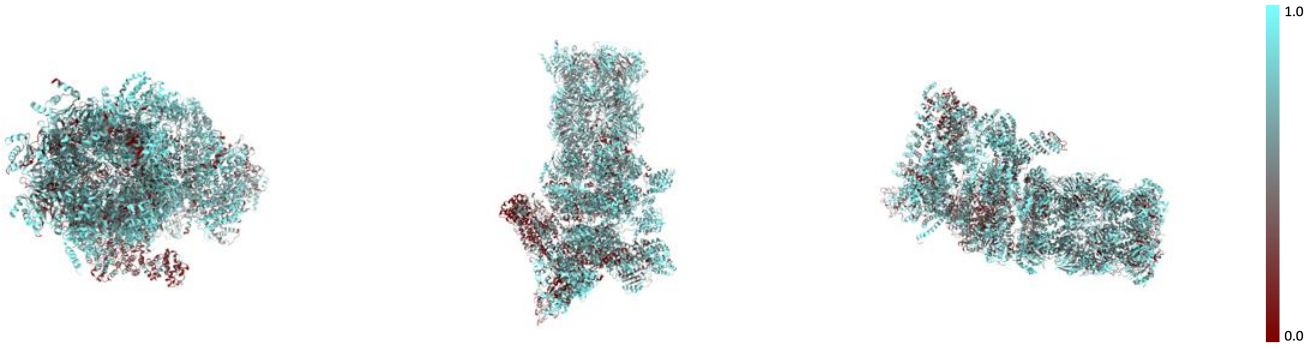
9.2 Q-score mapped to coordinate model (i)



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.

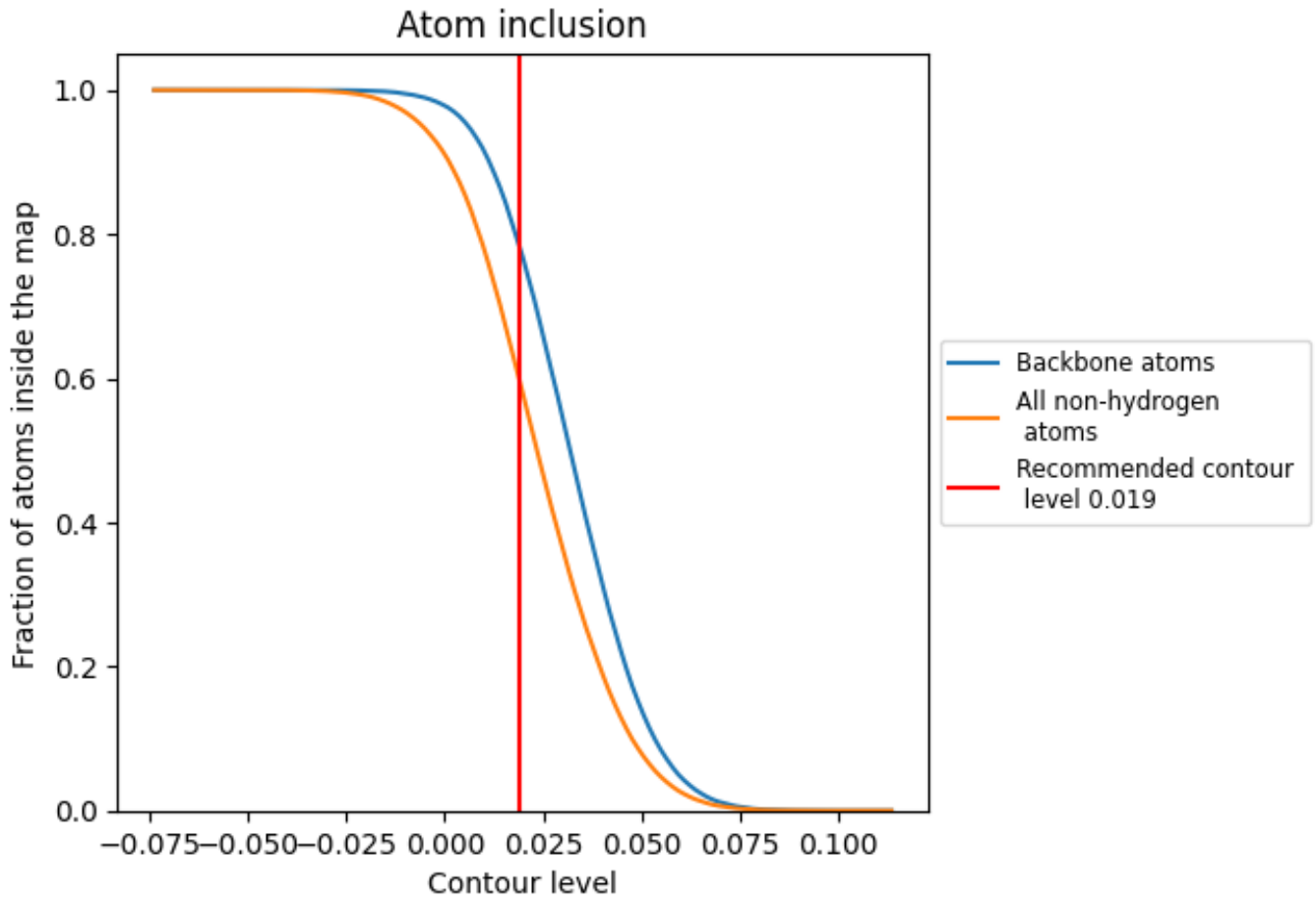
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.019).

9.4 Atom inclusion (i)



At the recommended contour level, 78% of all backbone atoms, 60% 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 (0.019) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5969	0.1320
1	0.6860	0.1420
2	0.6736	0.1490
3	0.6086	0.1400
4	0.6800	0.1450
5	0.7209	0.1460
6	0.6945	0.1410
7	0.6754	0.1420
A	0.6114	0.1320
B	0.5867	0.1420
C	0.6232	0.1430
D	0.6509	0.1410
E	0.6372	0.1460
F	0.6657	0.1450
G	0.6735	0.1440
H	0.5786	0.1290
I	0.4349	0.1190
J	0.5371	0.1260
K	0.5522	0.1250
L	0.5878	0.1350
M	0.5350	0.1290
N	0.5908	0.1320
O	0.6853	0.1470
P	0.7719	0.1510
Q	0.6964	0.1370
R	0.7156	0.1460
S	0.5747	0.1300
T	0.5037	0.1260
U	0.5899	0.1380
V	0.6055	0.1380
W	0.5939	0.1200
X	0.2577	0.0610
Y	0.4651	0.1010
Z	0.2845	0.0710
a	0.6221	0.1400

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Chain	Atom inclusion	Q-score
b	0.5666	0.1360
c	0.5883	0.1410
d	0.6471	0.1360
e	0.6197	0.1450
f	0.6481	0.1460
g	0.6536	0.1440
h	0.6745	0.1410
i	0.6275	0.1350
j	0.5932	0.1320
k	0.6852	0.1430
l	0.6911	0.1370
m	0.6702	0.1330
n	0.6417	0.1350