Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 12:56 am GMT

PDB ID	:	6FVW
EMDB ID	:	EMD-4322
Title	:	26S proteasome, s4 state
Authors	:	Eisele, M.R.; Reed, R.G.; Rudack, T.; Schweitzer, A.; Beck, F.; Nagy, I.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Tomko, R.J.; Sakata, E.
Deposited on	:	2018-03-05
Resolution	:	4.50 Å(reported)

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

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

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

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

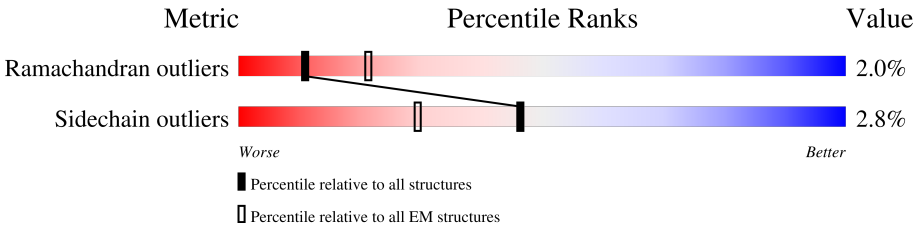
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 4.50 Å.

Percentile scores (ranging between 0-100) for global validation metrics of the entry are shown in the following graphic. The table shows the number of entries on which the scores are based.



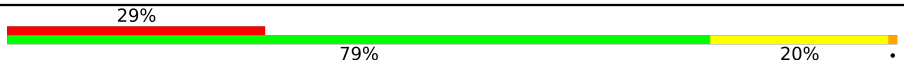
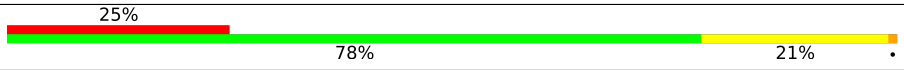
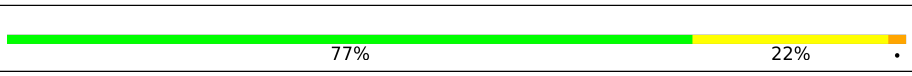
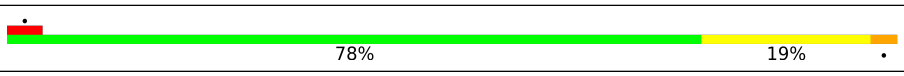
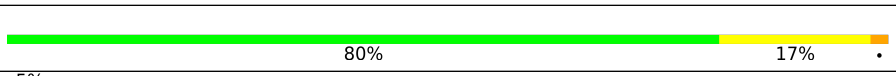
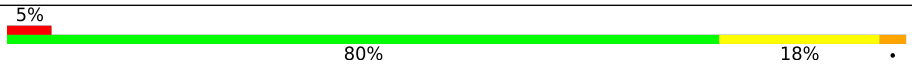
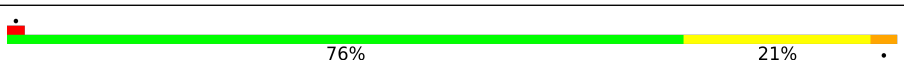
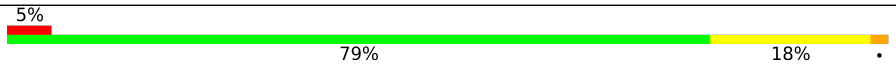
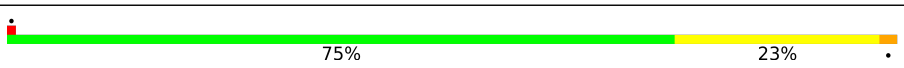
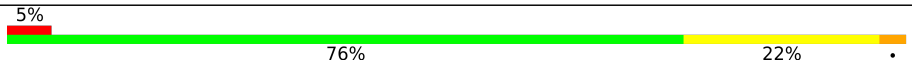
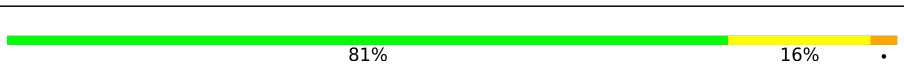
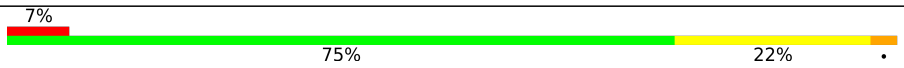
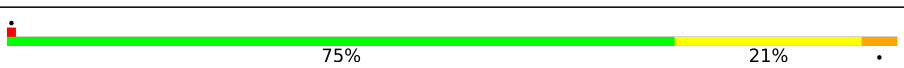
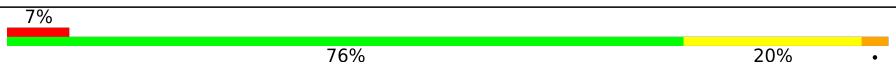
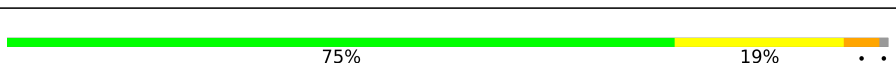
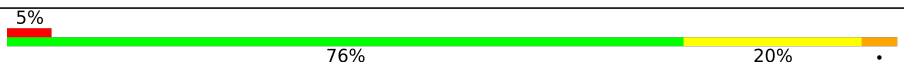
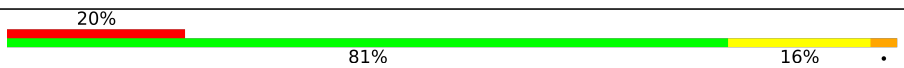
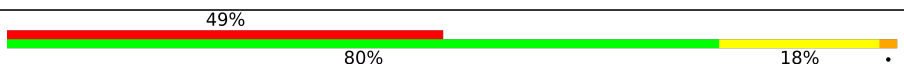
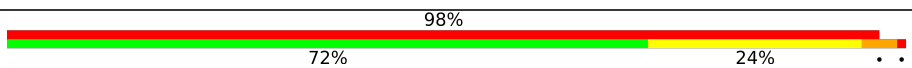
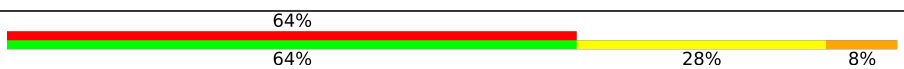
Metric	Whole archive (#Entries)	EM structures (#Entries)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

The table below summarises the geometric issues observed across the polymeric chains and their fit to the map. The red, orange, yellow and green segments of the bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions <=5% The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion < 40%). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	244	76% 22%
1	a	244	25% 80% 19%
2	B	247	81% 17%
2	b	247	26% 76% 21%
3	C	241	77% 22%
3	c	241	27% 76% 22%
4	D	252	5% 75% 21%
4	d	252	32% 73% 24%
5	E	245	80% 18%

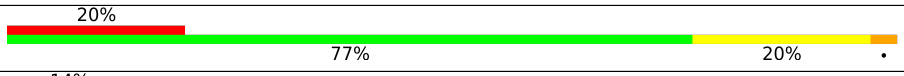
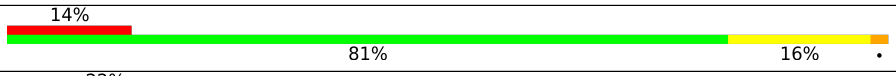
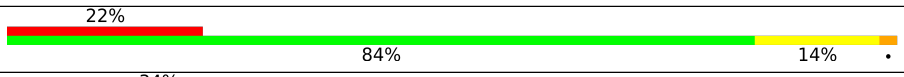
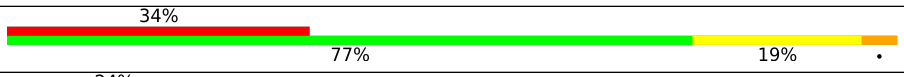
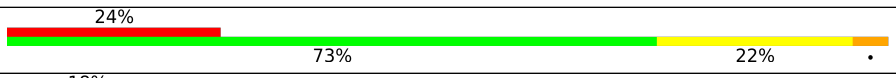
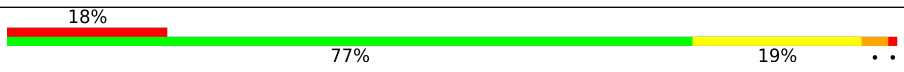
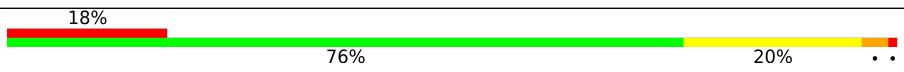
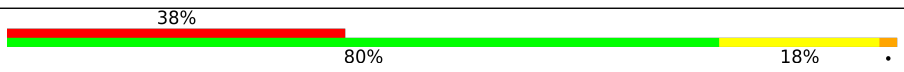
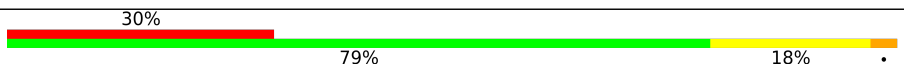
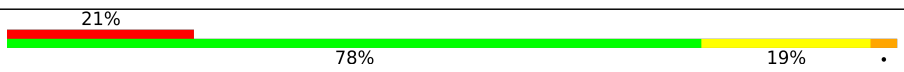
Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	e	245	
6	F	232	
6	f	232	
7	G	245	
7	g	245	
8	1	196	
8	h	196	
9	2	226	
9	i	226	
10	3	204	
10	j	204	
11	4	195	
11	k	195	
12	5	212	
12	l	212	
13	6	222	
13	m	222	
14	7	232	
14	n	232	
15	W	197	
16	V	289	
17	T	266	
18	X	127	
19	Y	89	
20	Z	970	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
21	N	922	
22	S	475	
23	P	440	
24	Q	434	
25	R	405	
26	U	304	
27	O	388	
28	H	426	
29	I	385	
30	K	384	
31	L	388	
32	M	421	
33	J	403	

2 Entry composition (i)

There are 37 unique types of molecules in this entry. The entry contains 110594 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	244	Total	C	N	O	S	0	0
			1924	1223	323	370	8		
1	A	244	Total	C	N	O	S	0	0
			1924	1223	323	370	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	247	Total	C	N	O	S	0	0
			1892	1206	312	371	3		
2	B	247	Total	C	N	O	S	0	0
			1892	1206	312	371	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	241	Total	C	N	O	S	0	0
			1884	1190	315	376	3		
3	C	241	Total	C	N	O	S	0	0
			1884	1190	315	376	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	252	Total	C	N	O	S	0	0
			1986	1237	351	394	4		
4	D	252	Total	C	N	O	S	0	0
			1986	1237	351	394	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	245	Total	C	N	O	S	0	0
			1889	1179	317	386	7		
5	E	245	Total	C	N	O	S	0	0
			1889	1179	317	386	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	f	232	Total	C	N	O	S	0	0
			1784	1120	311	349	4		
6	F	232	Total	C	N	O	S	0	0
			1784	1120	311	349	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	245	Total	C	N	O	S	0	0
			1905	1211	331	359	4		
7	G	245	Total	C	N	O	S	0	0
			1905	1211	331	359	4		

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

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

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

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

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

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

Continued on next page...

Continued from previous page...

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
30	K	384	Total	C	N	O	S	0	0
			3041	1911	533	587	10		

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

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

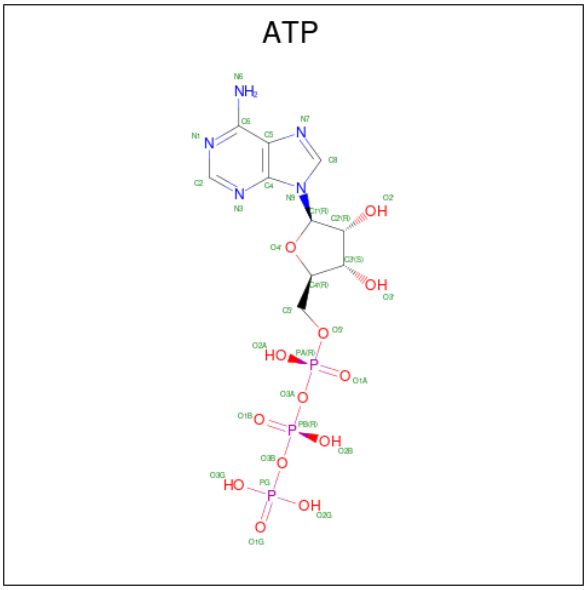
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
33	J	403	Total	C	N	O	S	0	0
			3156	1986	563	590	17		

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



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

Continued on next page...

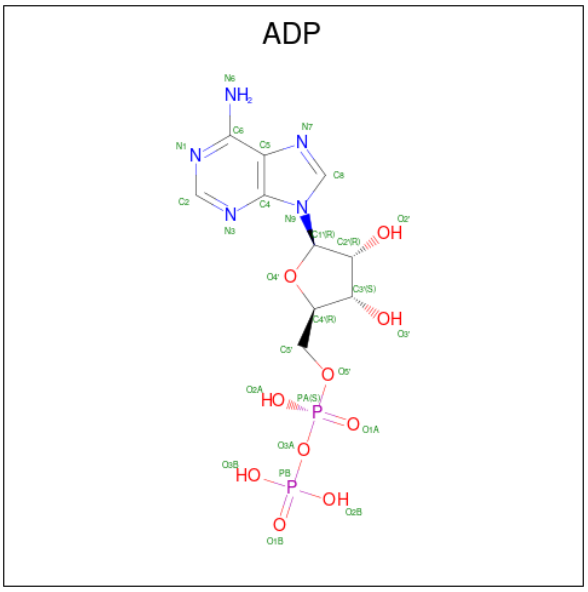
Continued from previous page...

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

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

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

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



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

- Molecule 37 is water.

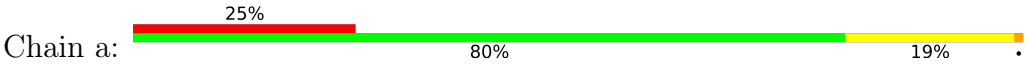
Mol	Chain	Residues	Atoms		AltConf
37	H	3	Total	O	0
			3	3	
37	I	3	Total	O	0
			3	3	
37	K	4	Total	O	0
			4	4	
37	L	4	Total	O	0
			4	4	
37	M	3	Total	O	0
			3	3	
37	J	3	Total	O	0
			3	3	

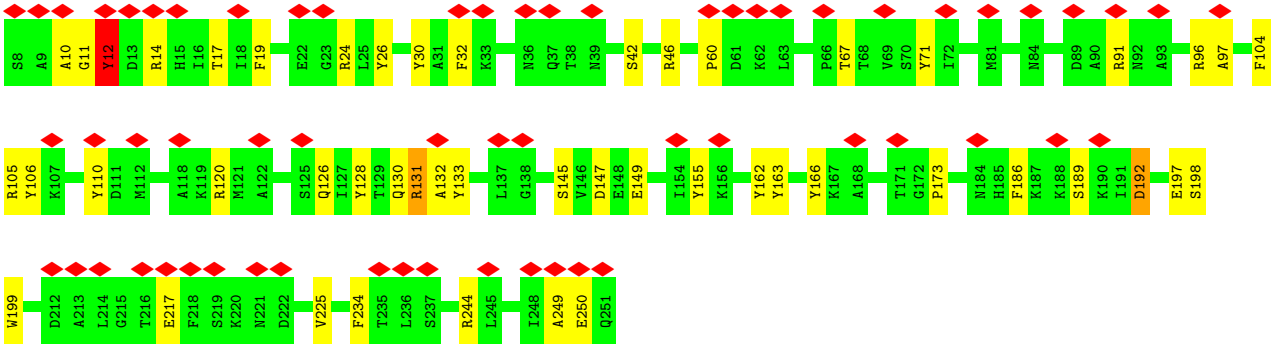
3 Residue-property plots (i)

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

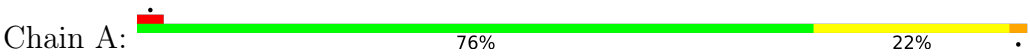
Chain a:

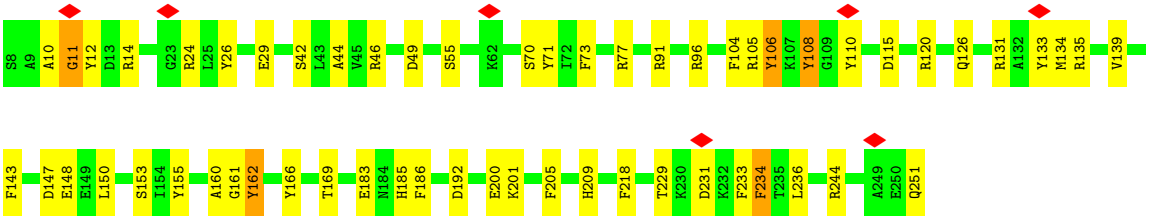




• Molecule 1: Proteasome subunit alpha type-1

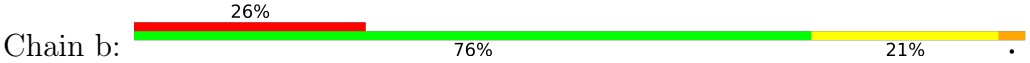
Chain A:

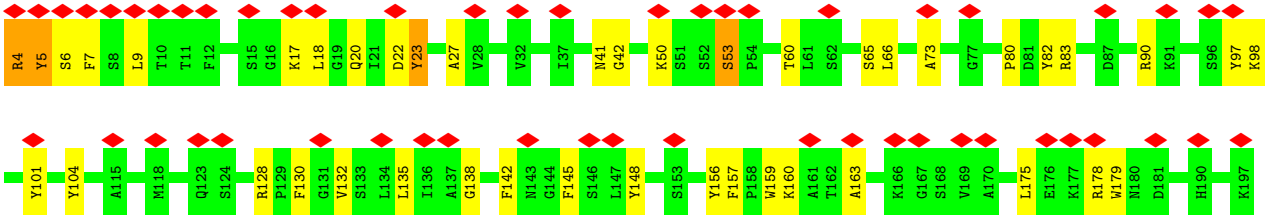


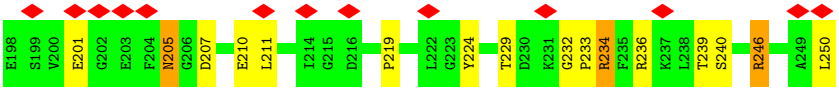


• Molecule 2: Proteasome subunit alpha type-2

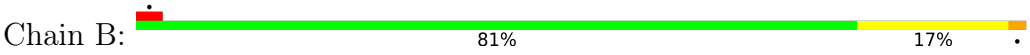
Chain b:

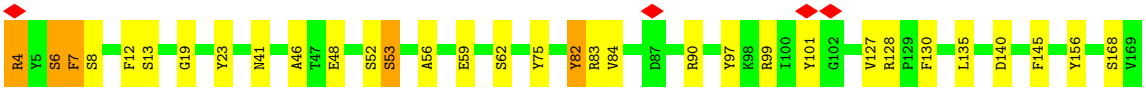




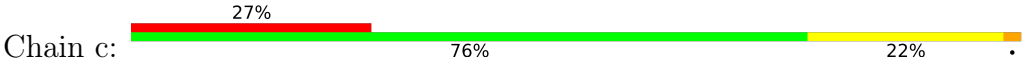


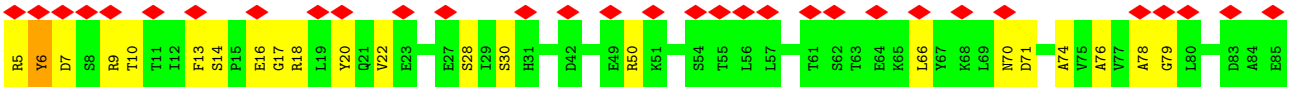
• Molecule 2: Proteasome subunit alpha type-2

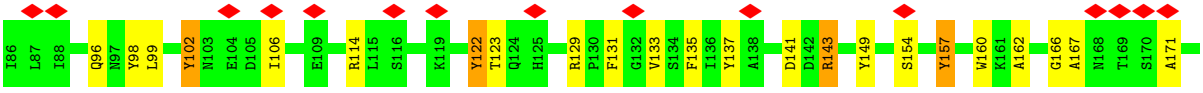


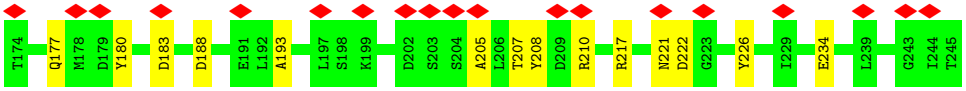


• Molecule 3: Proteasome subunit alpha type-3

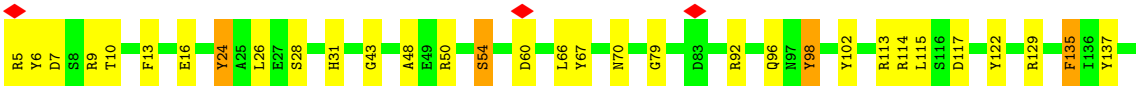


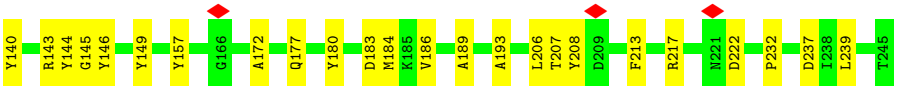




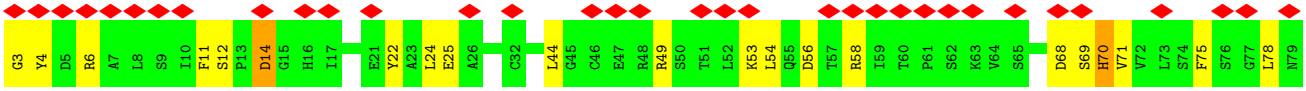


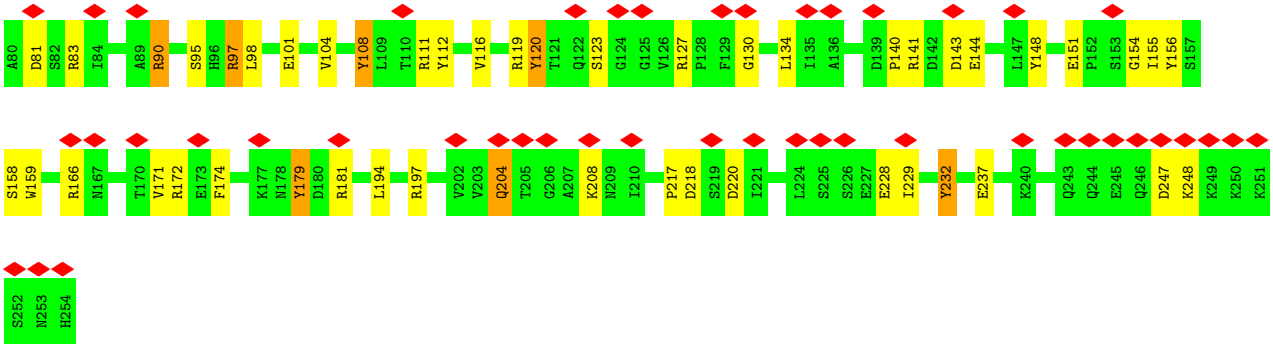
• Molecule 3: Proteasome subunit alpha type-3



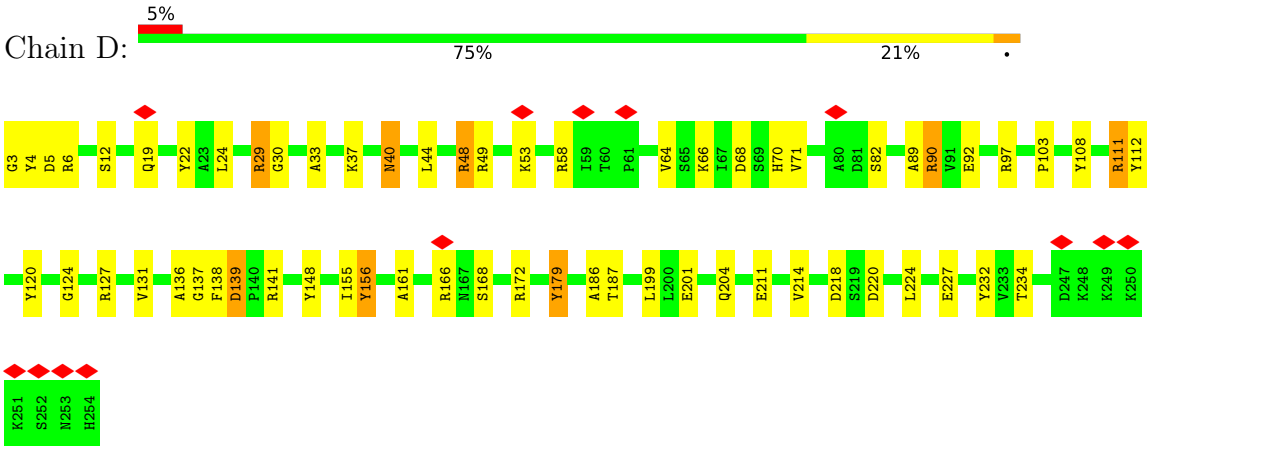


• Molecule 4: Proteasome subunit alpha type-4

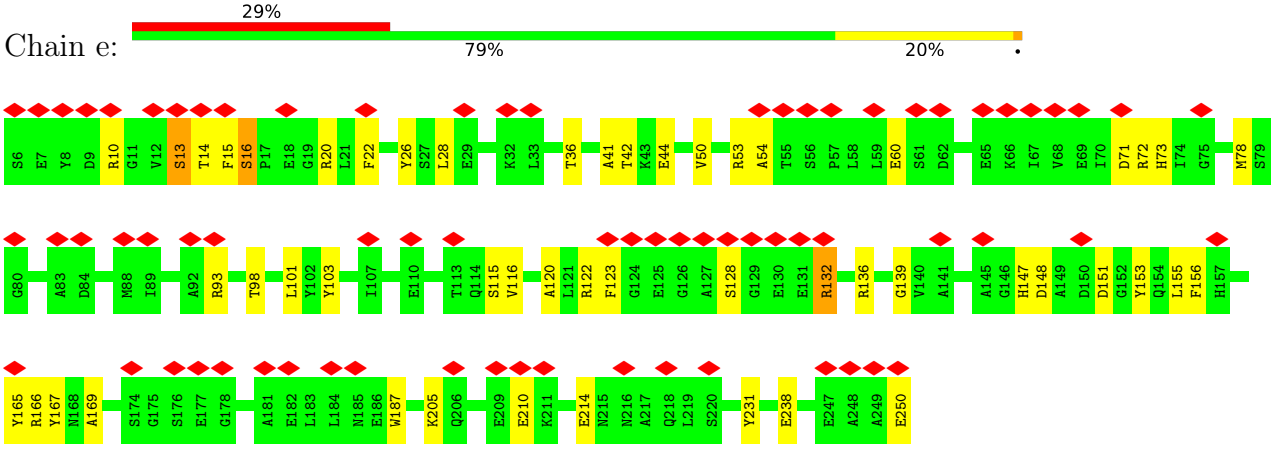




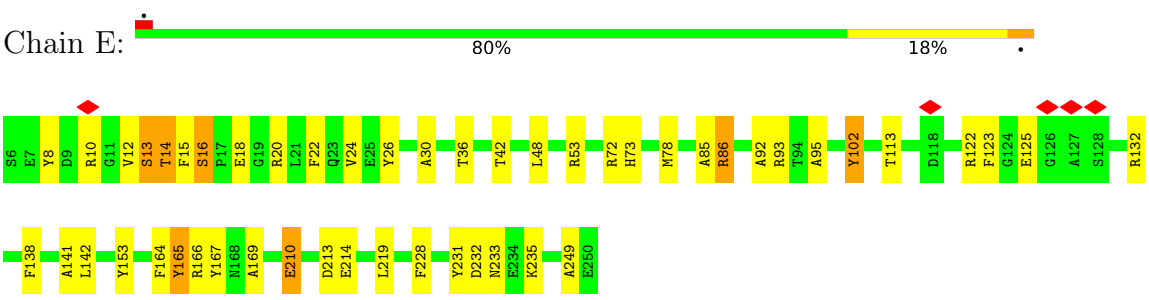
• Molecule 4: Proteasome subunit alpha type-4



• Molecule 5: Proteasome subunit alpha type-5

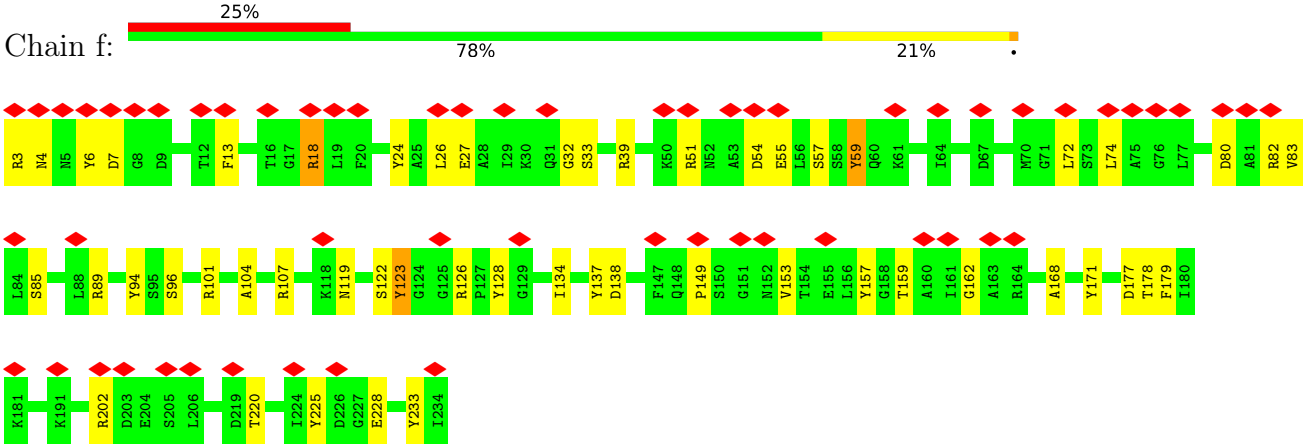


• Molecule 5: Proteasome subunit alpha type-5



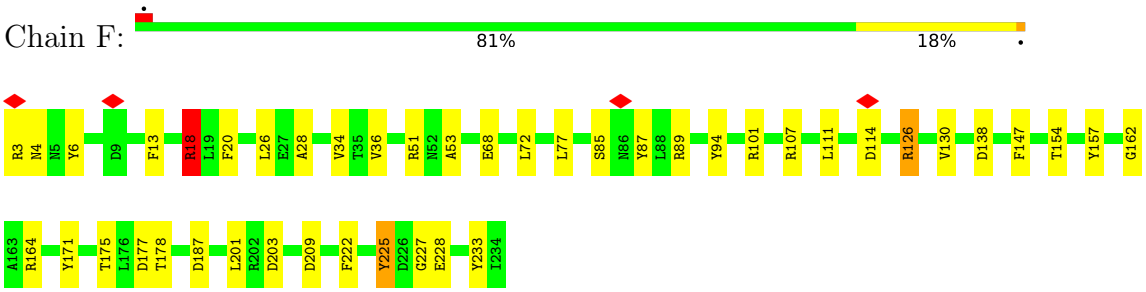
• Molecule 6: Proteasome subunit alpha type-6

Chain f:



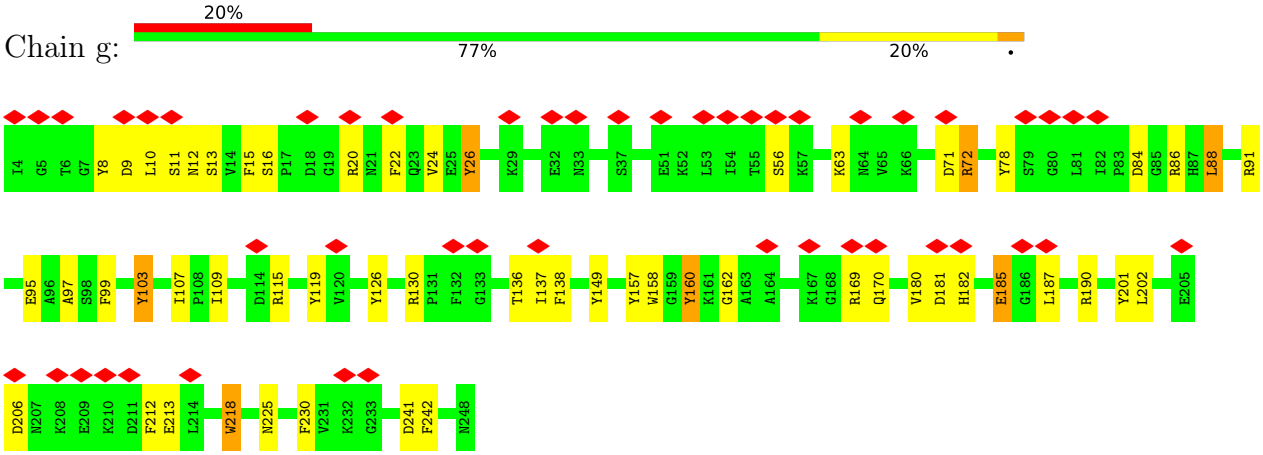
• Molecule 6: Proteasome subunit alpha type-6

Chain F:



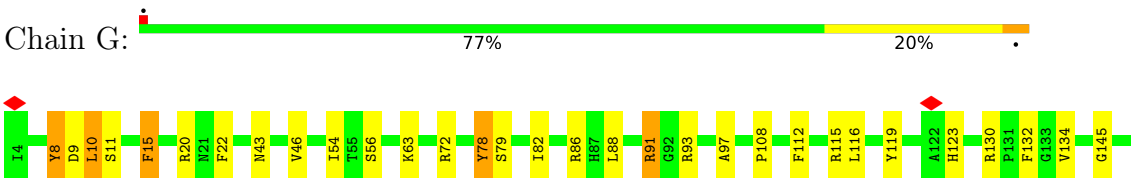
• Molecule 7: Probable proteasome subunit alpha type-7

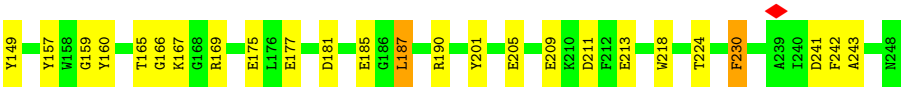
Chain g:



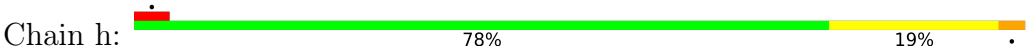
• Molecule 7: Probable proteasome subunit alpha type-7

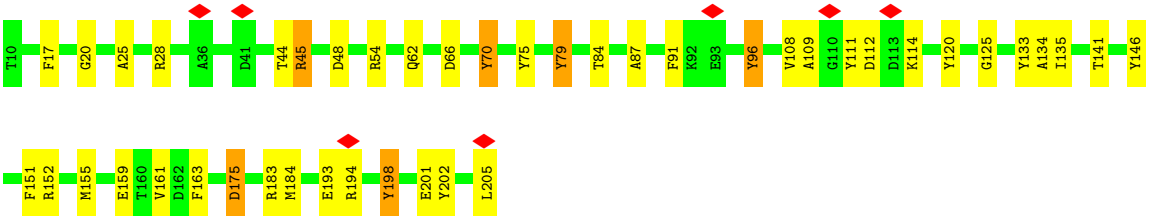
Chain G:



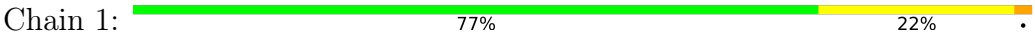


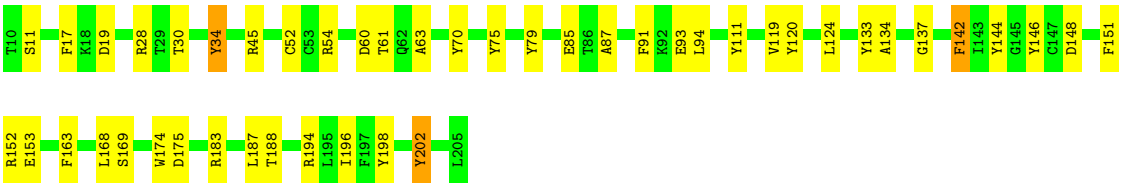
• Molecule 8: Proteasome subunit beta type-1



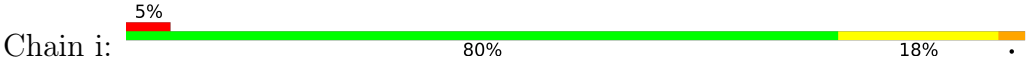


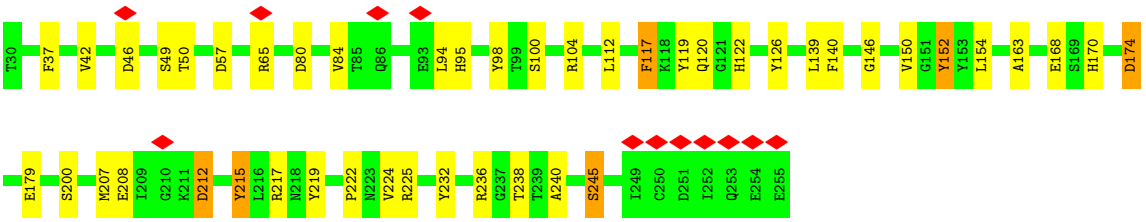
• Molecule 8: Proteasome subunit beta type-1



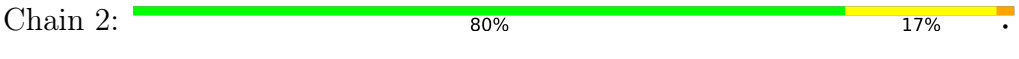


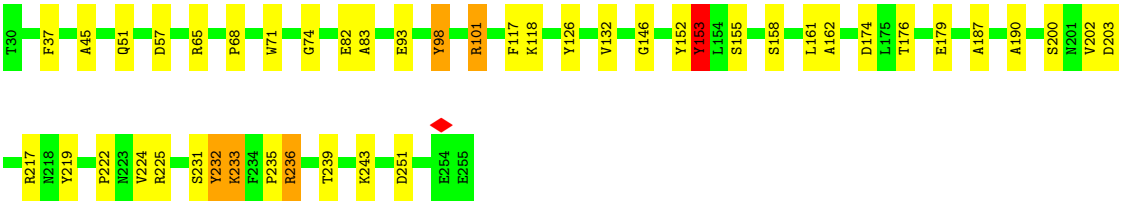
• Molecule 9: Proteasome subunit beta type-2



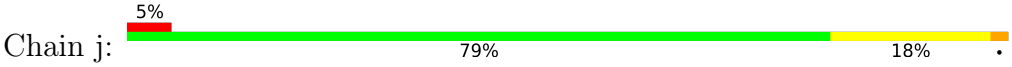


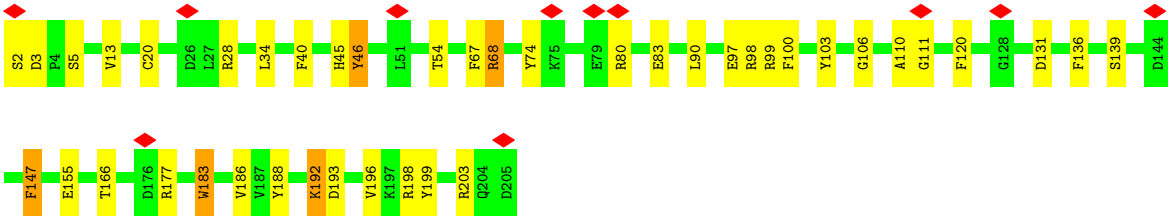
• Molecule 9: Proteasome subunit beta type-2



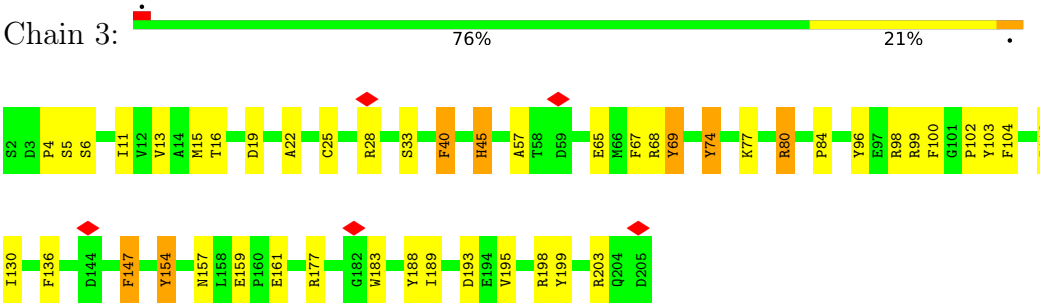


• Molecule 10: Proteasome subunit beta type-3

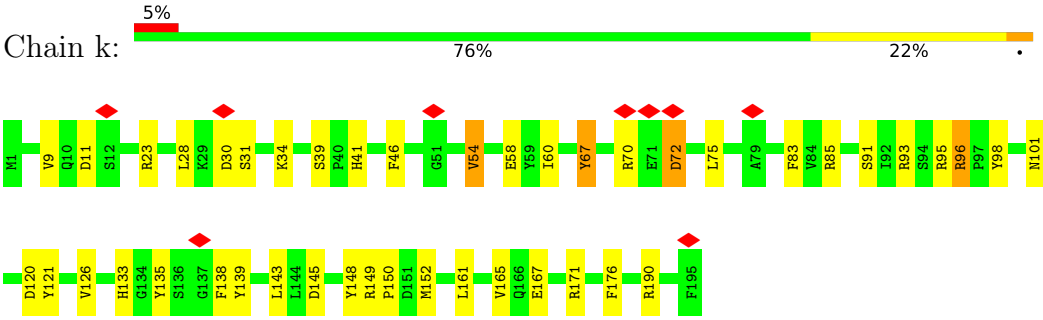




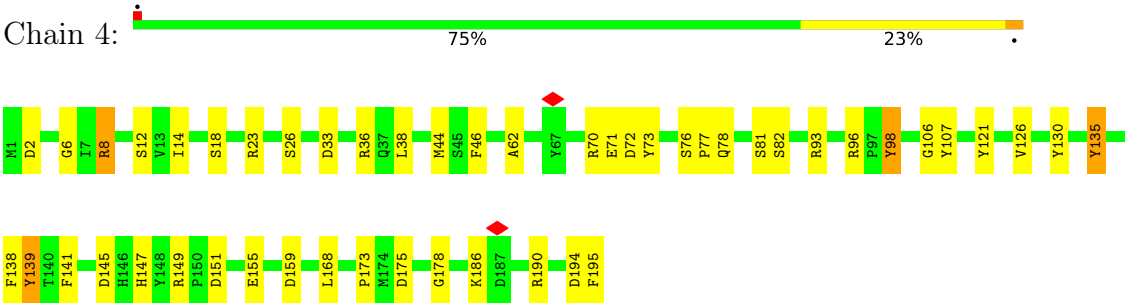
• Molecule 10: Proteasome subunit beta type-3



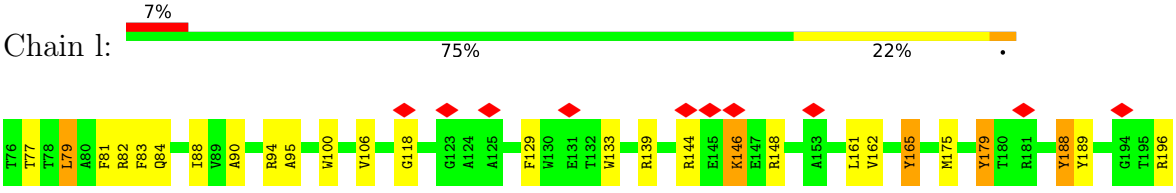
• Molecule 11: Proteasome subunit beta type-4

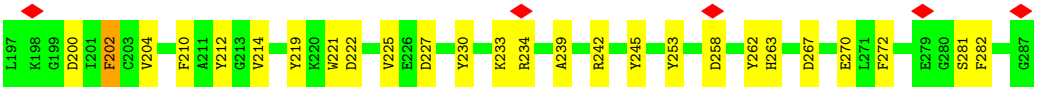


• Molecule 11: Proteasome subunit beta type-4



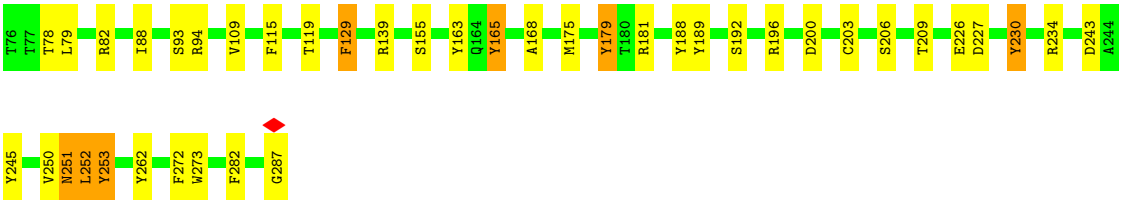
• Molecule 12: Proteasome subunit beta type-5





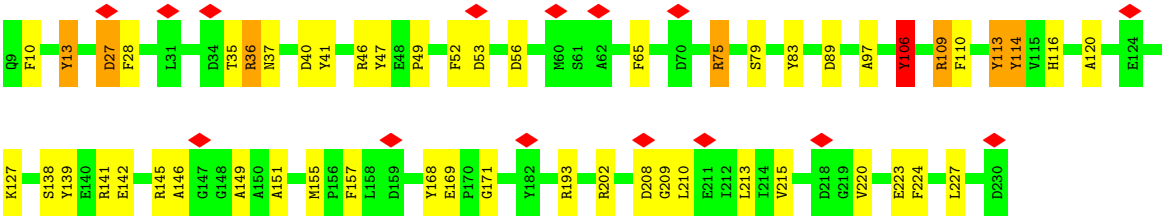
• Molecule 12: Proteasome subunit beta type-5

Chain 5:



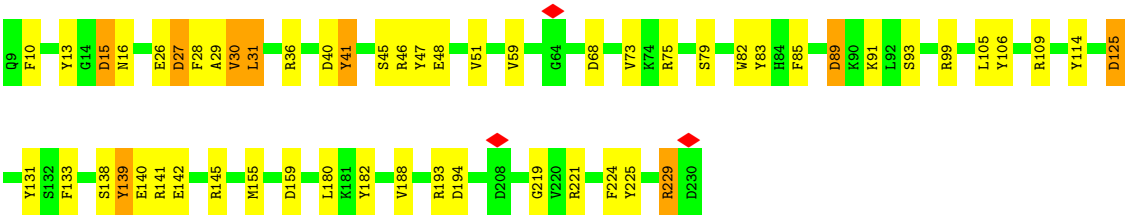
• Molecule 13: Proteasome subunit beta type-6

Chain m:



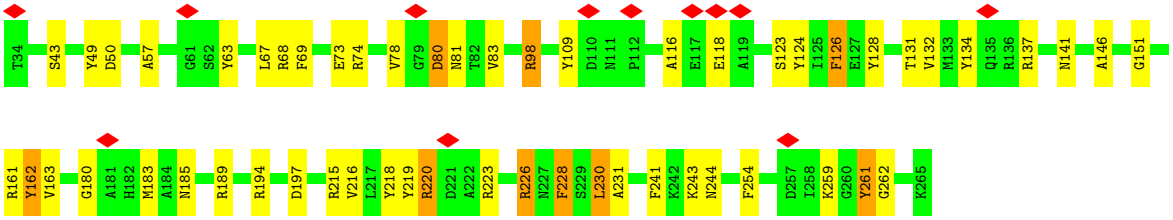
• Molecule 13: Proteasome subunit beta type-6

Chain 6:



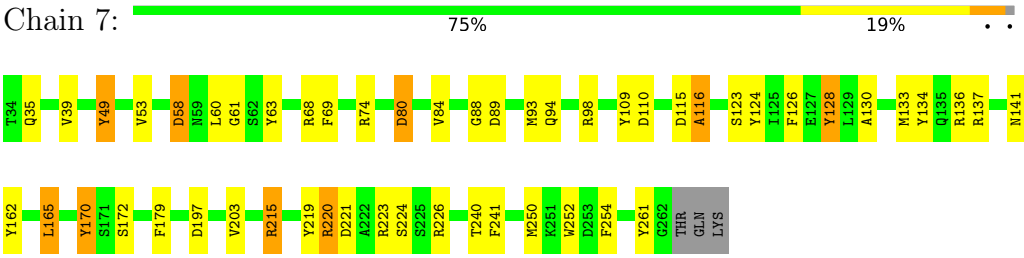
• Molecule 14: Proteasome subunit beta type-7

Chain n:



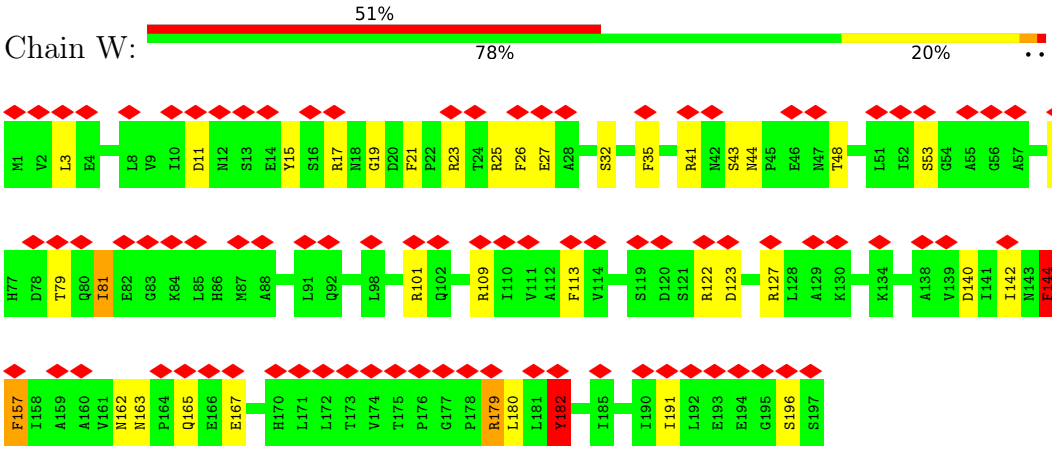
• Molecule 14: Proteasome subunit beta type-7

Chain 7:



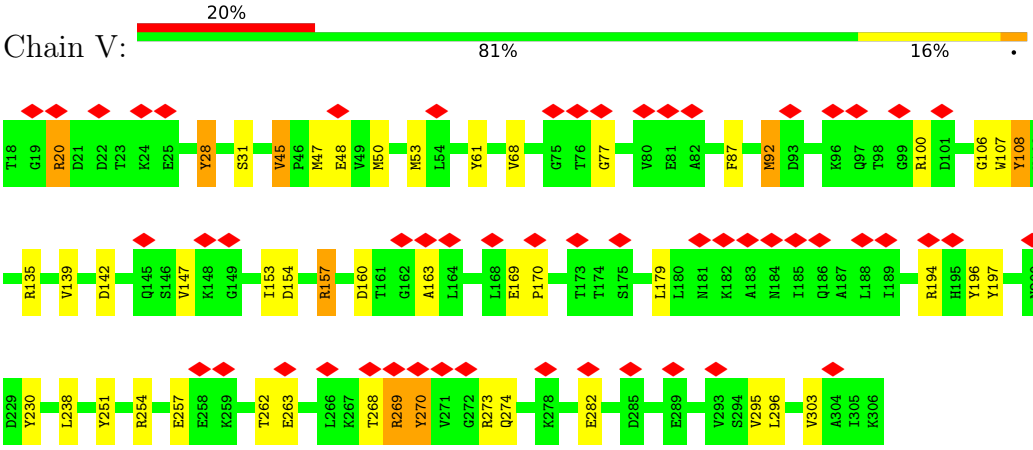
• Molecule 15: 26S proteasome regulatory subunit RPN10

Chain W:



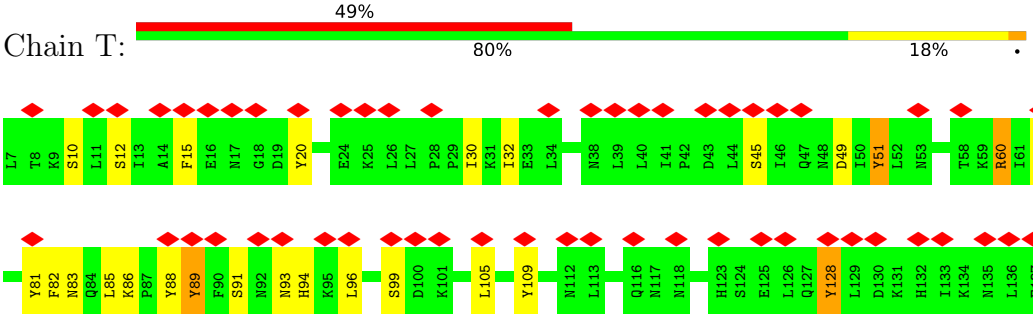
• Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

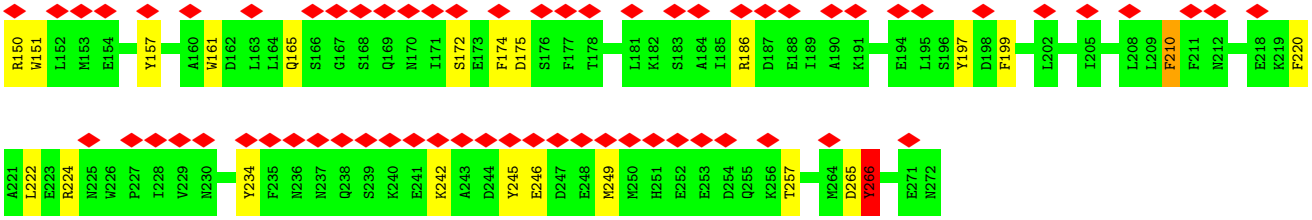
Chain V:



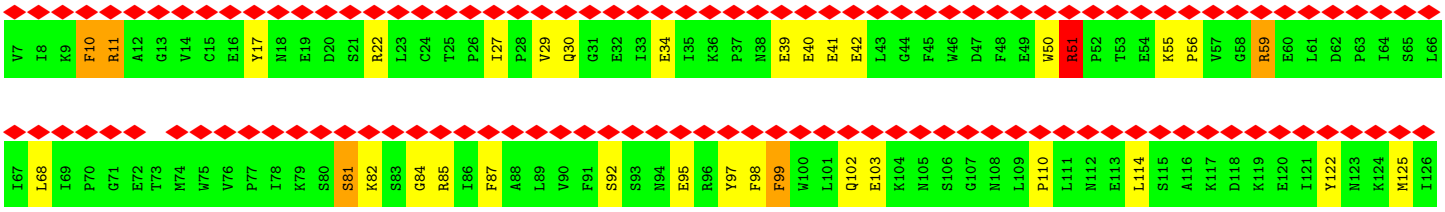
• Molecule 17: 26S proteasome regulatory subunit RPN12

Chain T:

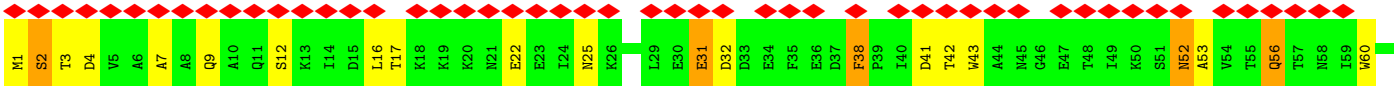


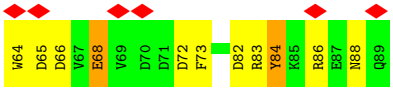


• Molecule 18: 26S proteasome regulatory subunit RPN13

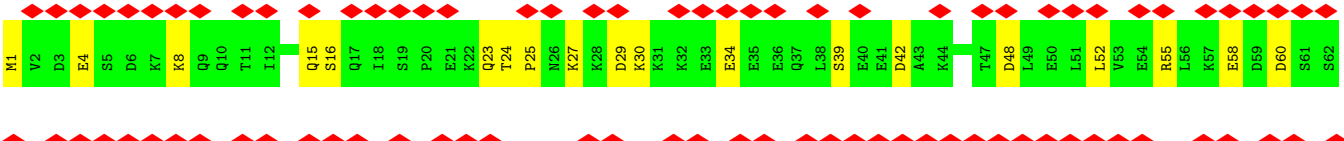


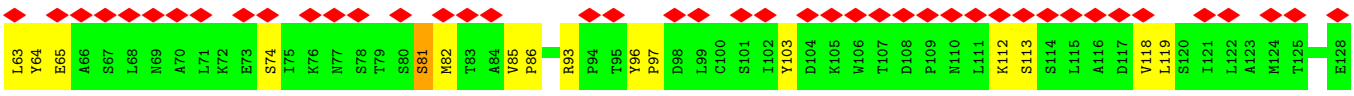
• Molecule 19: 26S proteasome complex subunit SEM1

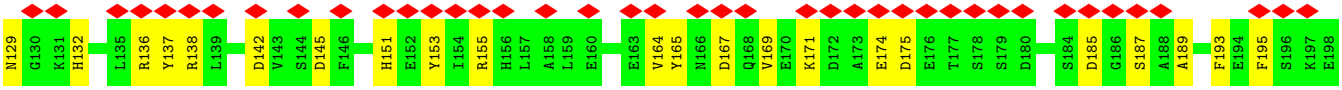


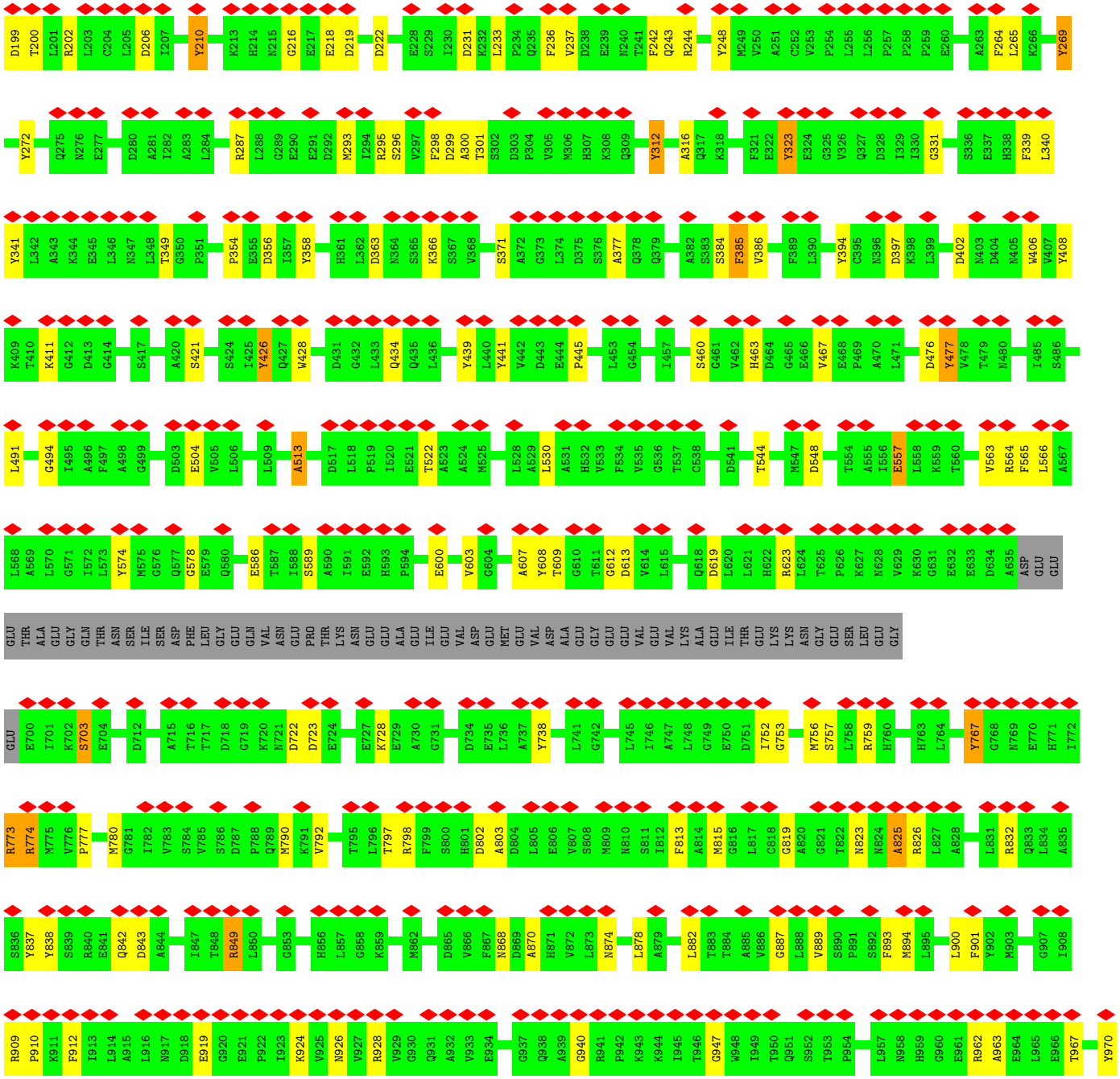


• Molecule 20: 26S proteasome regulatory subunit RPN1

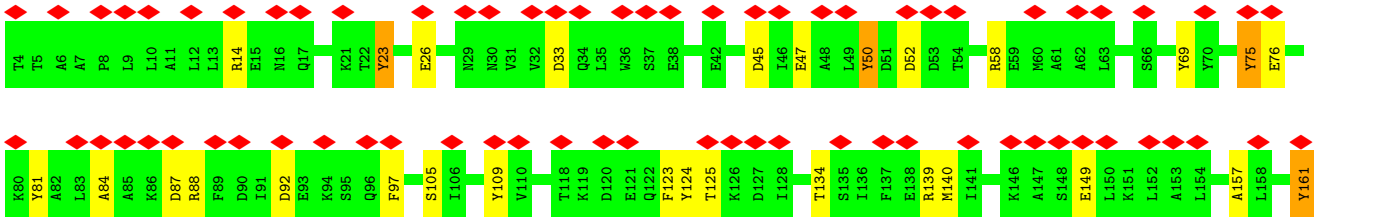


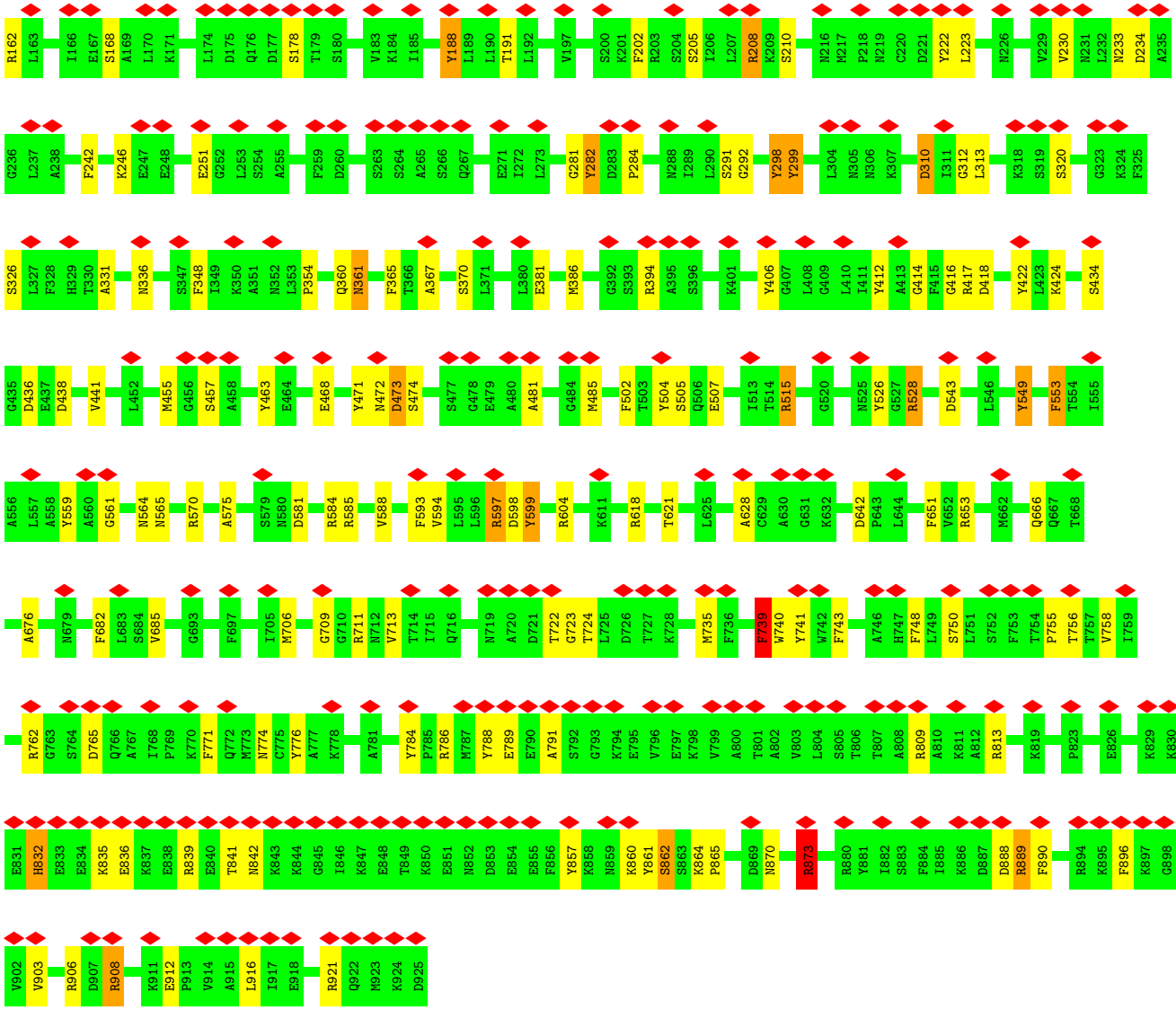






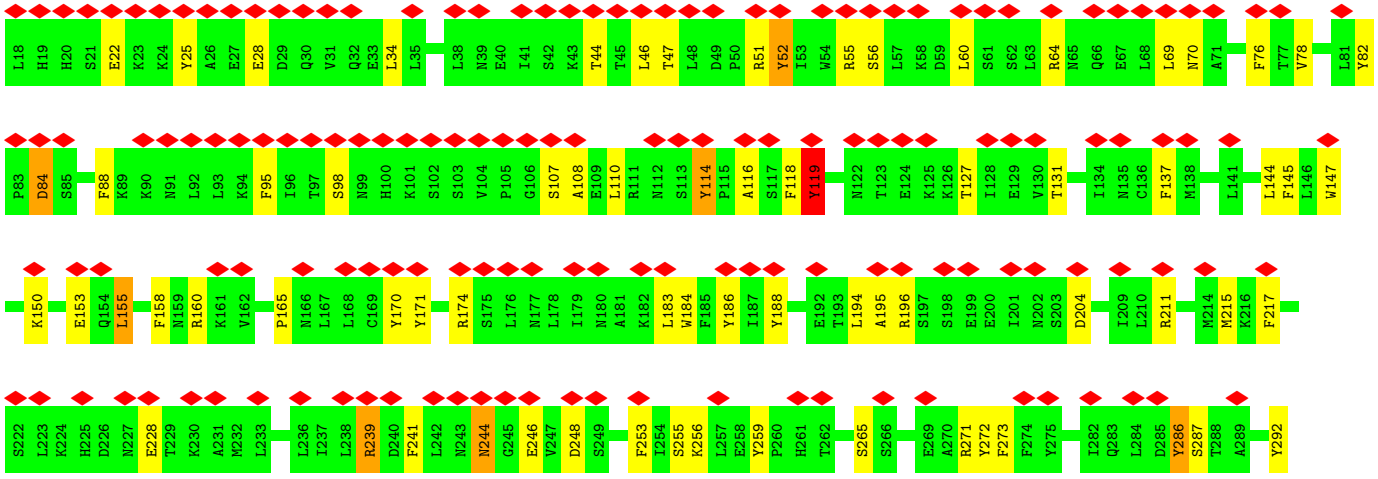
• Molecule 21: 26S proteasome regulatory subunit RPN2

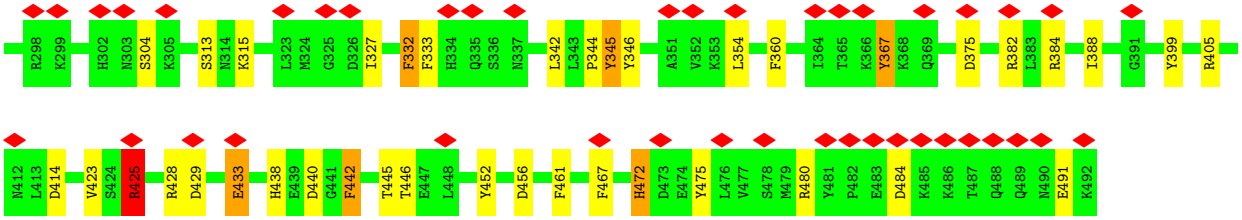




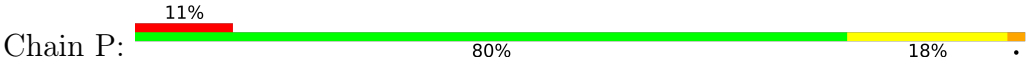
• Molecule 22: 26S proteasome regulatory subunit RPN3

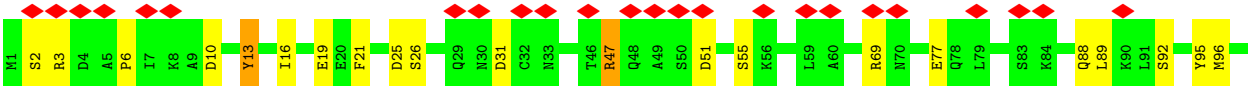
Chain S:

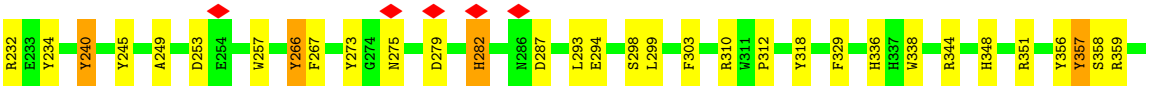


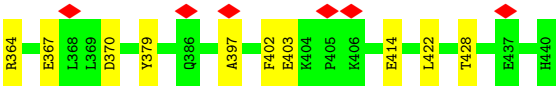


• Molecule 23: 26S proteasome regulatory subunit RPN5

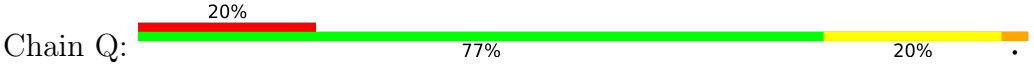


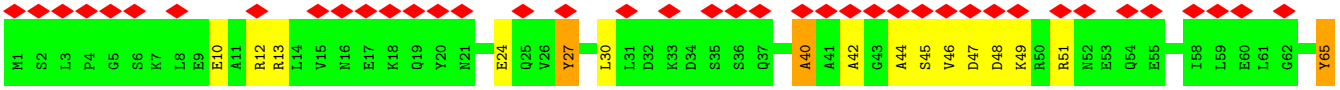


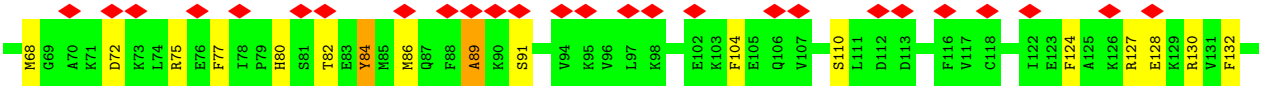


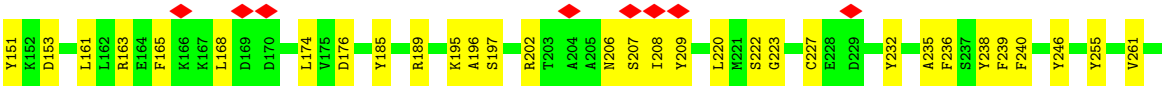


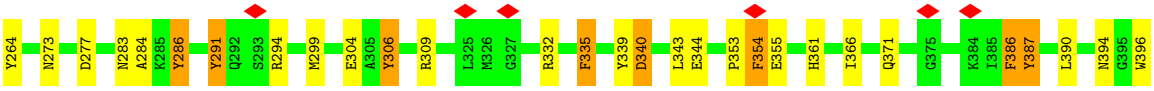
• Molecule 24: 26S proteasome regulatory subunit RPN6

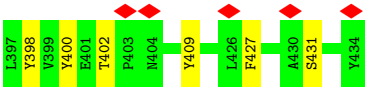






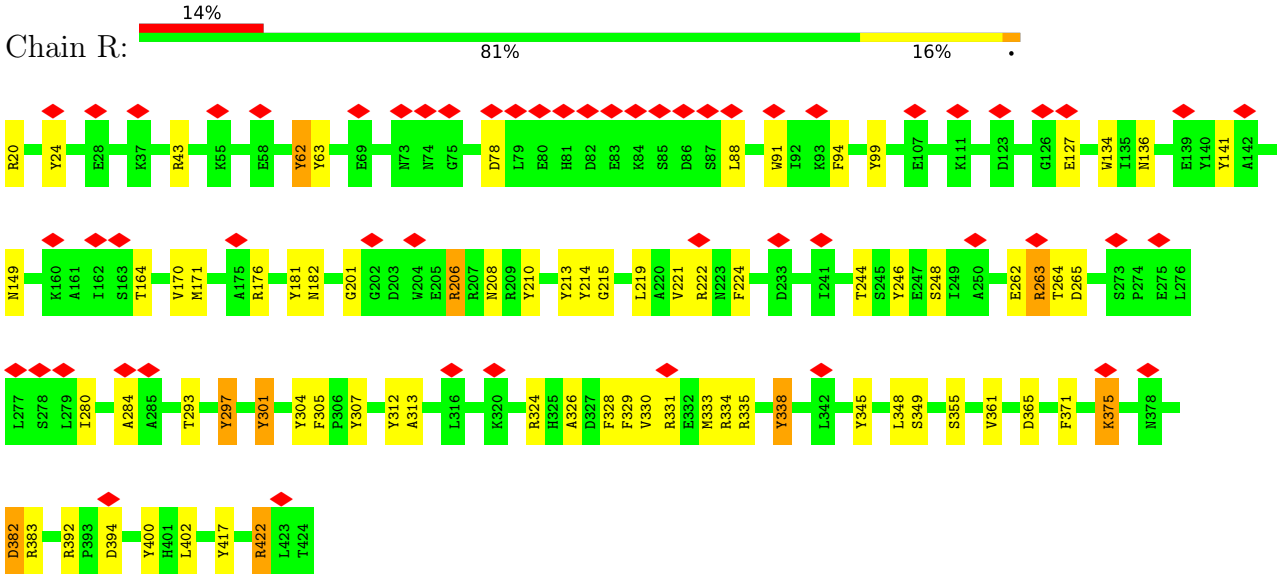






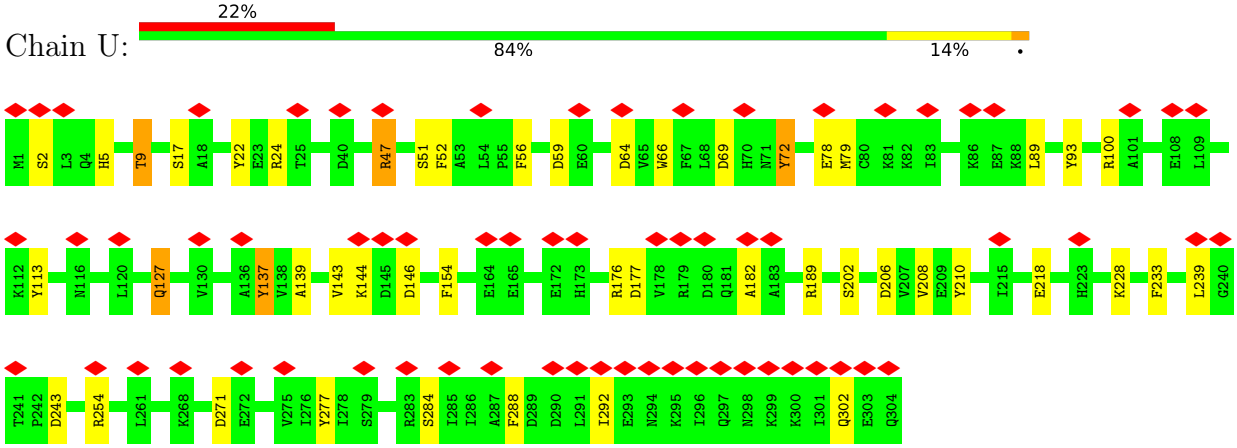
• Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R:



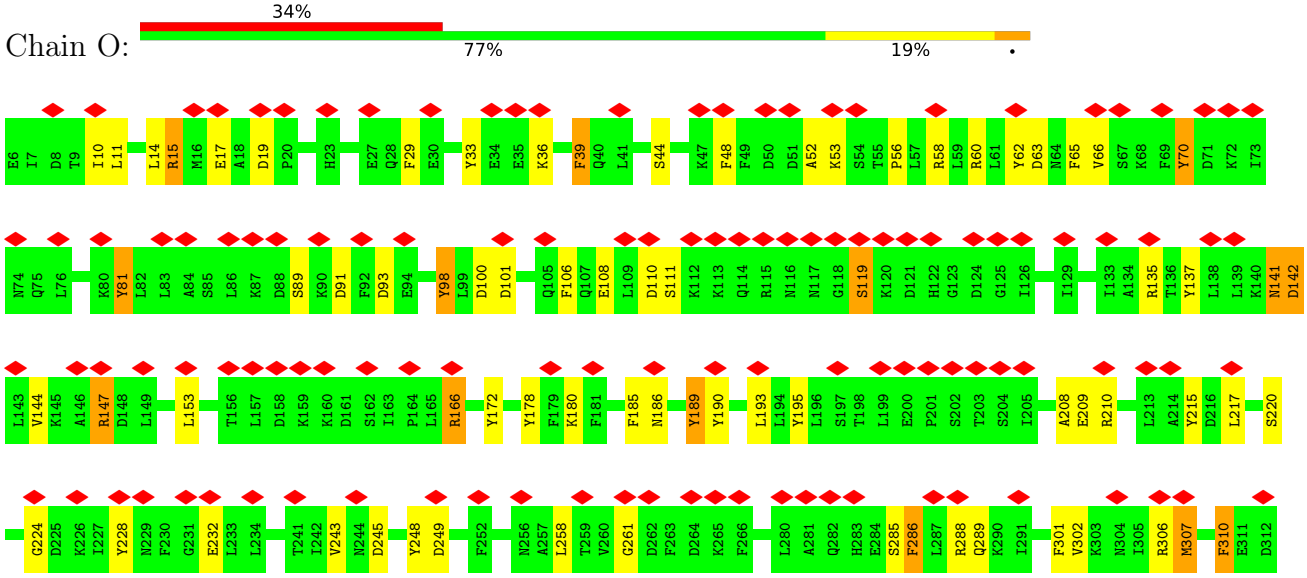
• Molecule 26: 26S proteasome regulatory subunit RPN8

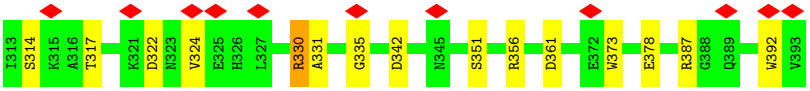
Chain U:



• Molecule 27: 26S proteasome regulatory subunit RPN9

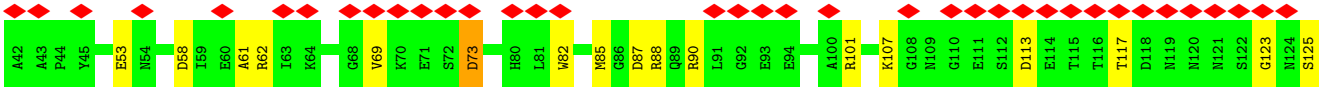
Chain O:

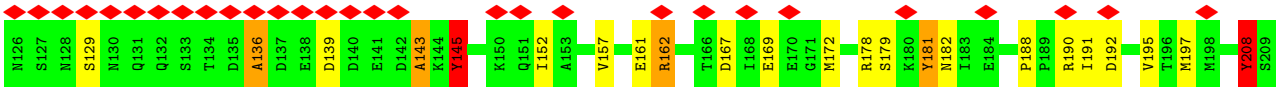


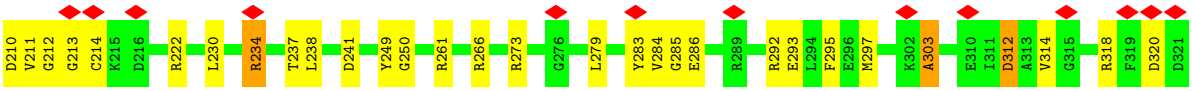


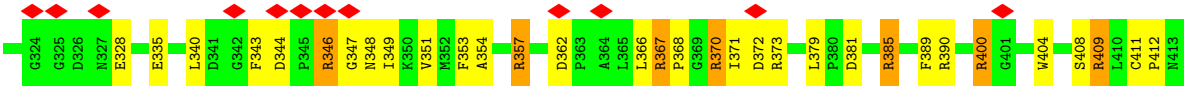
• Molecule 28: 26S proteasome regulatory subunit 7 homolog

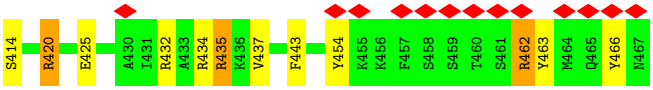
Chain H:





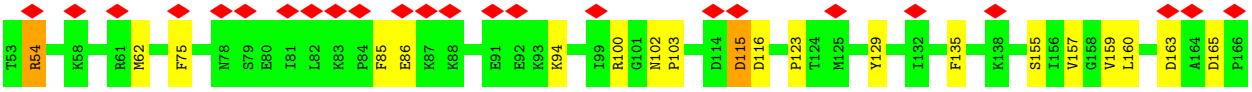


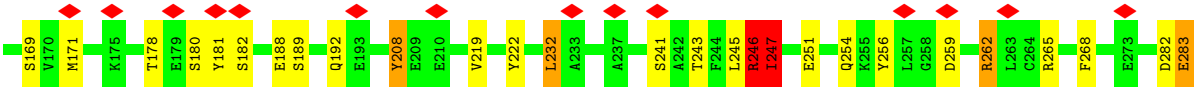


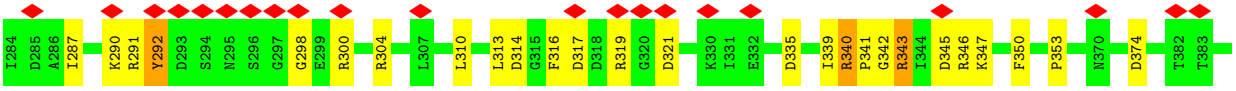


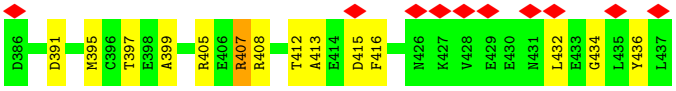
• Molecule 29: 26S proteasome regulatory subunit 4 homolog

Chain I:



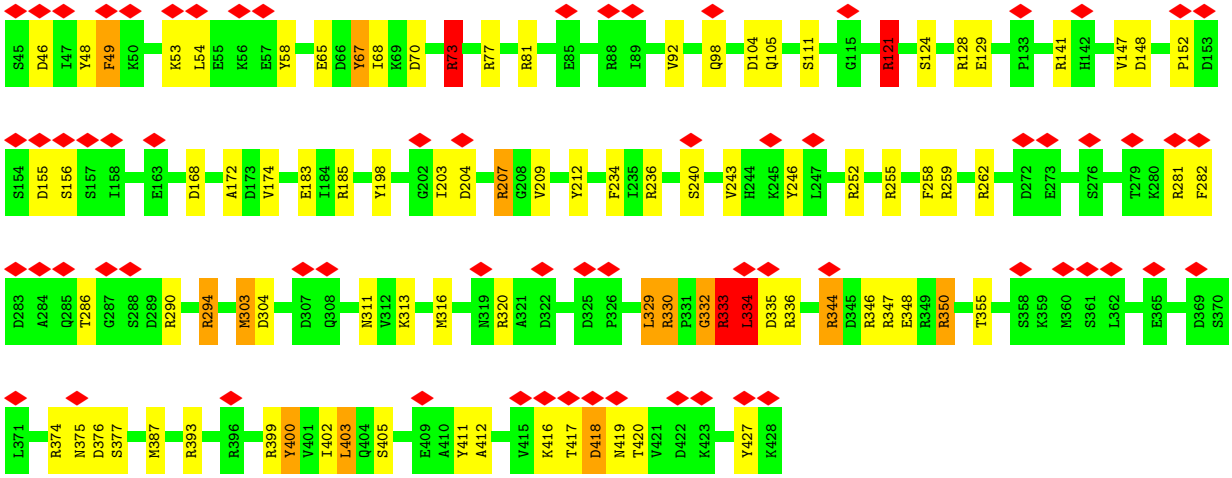




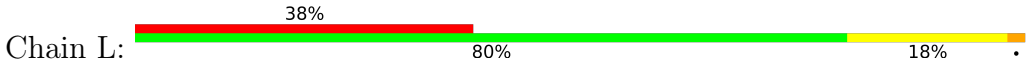


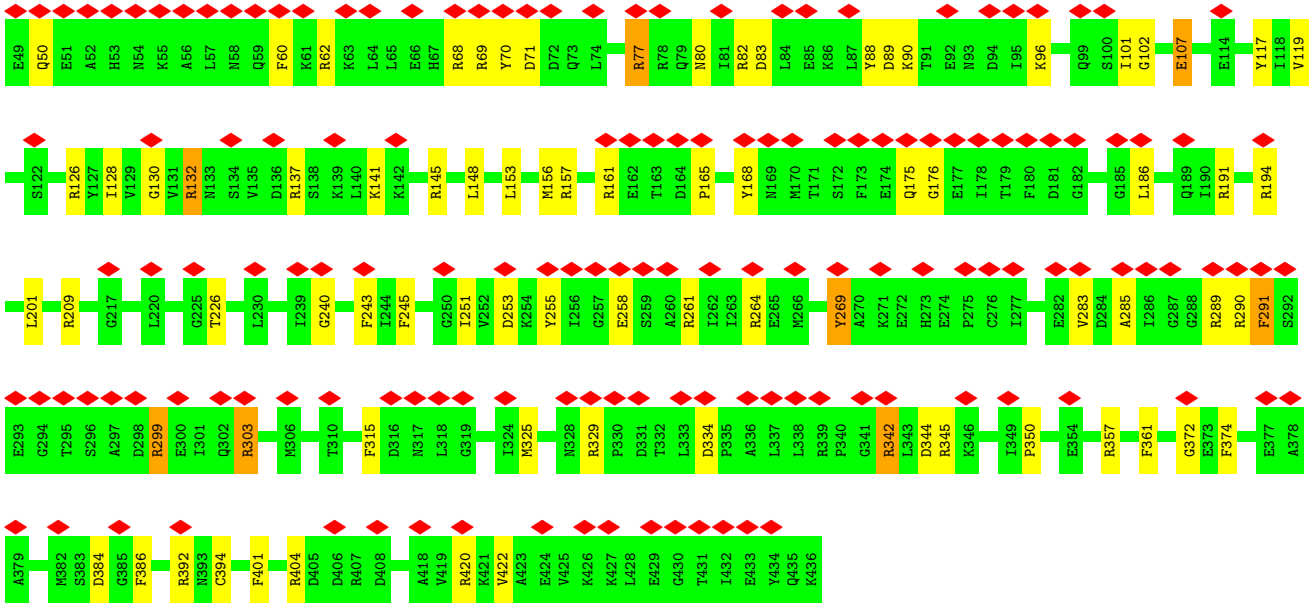
• Molecule 30: 26S proteasome regulatory subunit 6B homolog

Chain K:

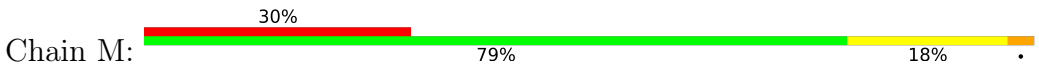


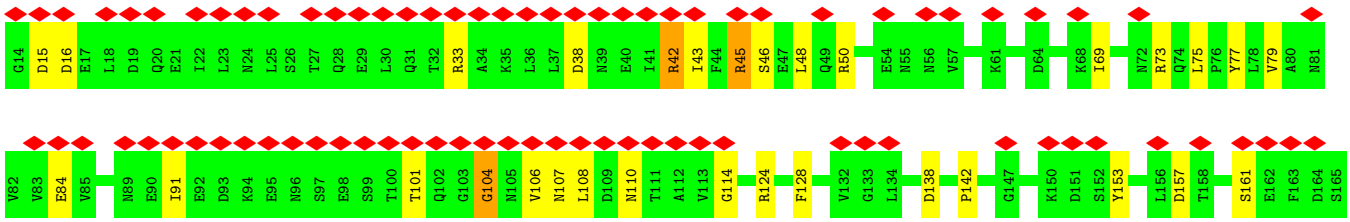
• Molecule 31: 26S proteasome subunit RPT4

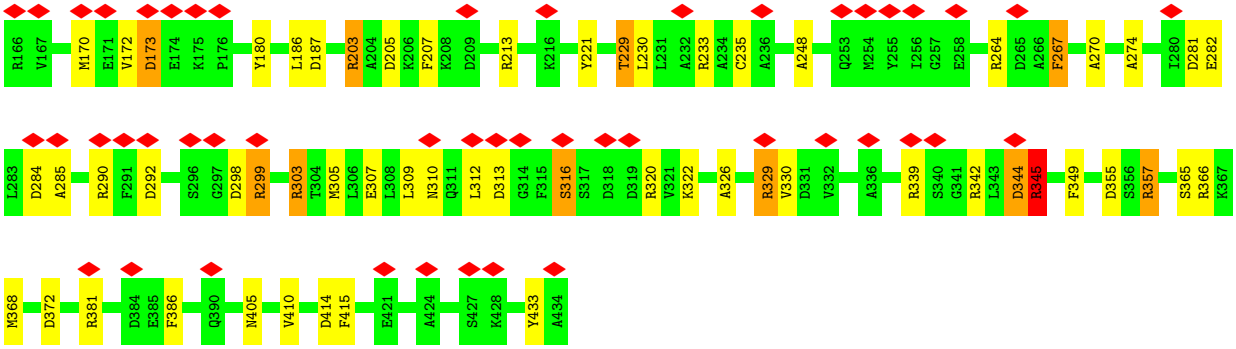




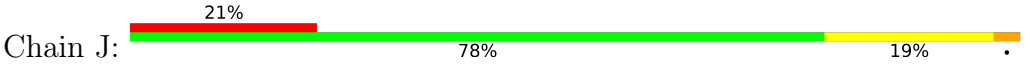
• Molecule 32: 26S proteasome regulatory subunit 6A

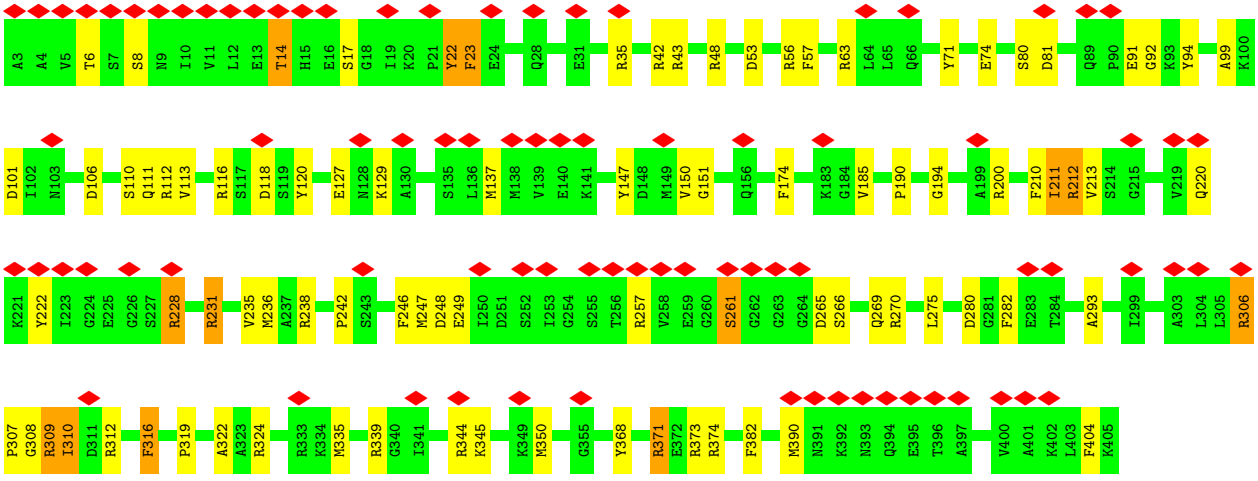






• Molecule 33: 26S proteasome regulatory subunit 8 homolog





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	351984	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 ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.223	Depositor
Minimum map value	-0.185	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.76	22/1962 (1.1%)	1.91	51/2656 (1.9%)
1	a	1.74	26/1962 (1.3%)	1.90	42/2656 (1.6%)
2	B	1.67	15/1929 (0.8%)	1.92	42/2611 (1.6%)
2	b	1.69	22/1929 (1.1%)	1.96	52/2611 (2.0%)
3	C	1.75	14/1914 (0.7%)	1.93	32/2591 (1.2%)
3	c	1.71	16/1914 (0.8%)	1.93	54/2591 (2.1%)
4	D	1.74	20/2016 (1.0%)	2.03	52/2723 (1.9%)
4	d	1.75	19/2016 (0.9%)	1.97	55/2723 (2.0%)
5	E	1.79	19/1915 (1.0%)	1.82	36/2579 (1.4%)
5	e	1.75	13/1915 (0.7%)	2.02	49/2579 (1.9%)
6	F	1.74	17/1811 (0.9%)	1.92	34/2447 (1.4%)
6	f	1.69	18/1811 (1.0%)	1.91	47/2447 (1.9%)
7	G	1.71	15/1945 (0.8%)	1.94	45/2625 (1.7%)
7	g	1.67	15/1945 (0.8%)	2.01	54/2625 (2.1%)
8	1	1.74	17/1541 (1.1%)	1.99	46/2087 (2.2%)
8	h	1.74	11/1541 (0.7%)	1.98	42/2087 (2.0%)
9	2	1.70	11/1751 (0.6%)	1.92	38/2373 (1.6%)
9	i	1.70	13/1751 (0.7%)	1.89	39/2373 (1.6%)
10	3	1.76	15/1611 (0.9%)	2.03	40/2174 (1.8%)
10	j	1.75	14/1611 (0.9%)	1.87	32/2174 (1.5%)
11	4	1.81	28/1590 (1.8%)	1.90	34/2142 (1.6%)
11	k	1.72	17/1590 (1.1%)	1.93	36/2142 (1.7%)
12	5	1.74	16/1681 (1.0%)	1.92	35/2274 (1.5%)
12	l	1.75	14/1681 (0.8%)	1.97	52/2274 (2.3%)
13	6	1.75	19/1795 (1.1%)	2.01	49/2420 (2.0%)
13	m	1.70	11/1795 (0.6%)	1.98	48/2420 (2.0%)
14	7	1.71	20/1821 (1.1%)	2.04	51/2470 (2.1%)
14	n	1.75	17/1847 (0.9%)	1.94	49/2503 (2.0%)
15	W	1.72	17/1558 (1.1%)	1.86	28/2111 (1.3%)
16	V	1.71	24/2309 (1.0%)	1.87	47/3115 (1.5%)
17	T	1.64	18/2236 (0.8%)	1.88	52/3017 (1.7%)
18	X	1.76	10/1059 (0.9%)	2.00	20/1432 (1.4%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
19	Y	1.69	8/741 (1.1%)	2.12	28/1000 (2.8%)
20	Z	1.67	56/7122 (0.8%)	1.88	167/9645 (1.7%)
21	N	1.69	61/7273 (0.8%)	1.89	159/9822 (1.6%)
22	S	1.69	33/3967 (0.8%)	1.99	99/5355 (1.8%)
23	P	1.65	31/3664 (0.8%)	1.89	82/4940 (1.7%)
24	Q	1.71	31/3556 (0.9%)	1.95	86/4787 (1.8%)
25	R	1.72	34/3314 (1.0%)	1.92	66/4469 (1.5%)
26	U	1.64	14/2461 (0.6%)	1.87	50/3327 (1.5%)
27	O	1.71	29/3247 (0.9%)	1.91	82/4380 (1.9%)
28	H	1.73	33/3363 (1.0%)	1.99	89/4532 (2.0%)
29	I	1.69	23/3061 (0.8%)	1.90	65/4121 (1.6%)
30	K	1.77	39/3084 (1.3%)	1.96	73/4162 (1.8%)
31	L	1.74	23/3129 (0.7%)	1.97	72/4204 (1.7%)
32	M	1.70	24/3323 (0.7%)	1.94	81/4478 (1.8%)
33	J	1.71	29/3197 (0.9%)	1.97	78/4296 (1.8%)
All	All	1.71	1011/112254 (0.9%)	1.93	2660/151570 (1.8%)

Chiral center outliers are detected by calculating the chiral volume of a chiral center and verifying if the center is modelled as a planar moiety or with the opposite hand.A planarity outlier is detected by checking planarity of atoms in a peptide group, atoms in a mainchain group or atoms of a sidechain that are expected to be planar.

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	7
1	a	0	5
2	B	0	4
2	b	0	8
3	C	0	15
3	c	0	7
4	D	0	9
4	d	0	8
5	E	0	7
5	e	0	3
6	F	0	4
6	f	0	8
7	G	0	6
7	g	0	7
8	1	0	5
8	h	0	5
9	2	0	7
9	i	0	6
10	3	0	3

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
10	j	0	3
11	4	0	5
11	k	0	4
12	5	0	6
12	l	0	6
13	6	0	4
13	m	0	9
14	7	0	7
14	n	0	8
15	W	0	4
16	V	0	8
17	T	0	5
18	X	0	7
19	Y	0	2
20	Z	0	12
21	N	0	21
22	S	0	16
23	P	0	12
24	Q	0	8
25	R	0	7
26	U	0	3
27	O	0	11
28	H	0	20
29	I	0	18
30	K	0	15
31	L	0	9
32	M	0	10
33	J	0	12
All	All	0	376

All (1011) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	355	SER	CA-CB	10.56	1.68	1.52
5	E	214	GLU	CG-CD	9.48	1.66	1.51
5	E	26	TYR	CG-CD2	9.46	1.51	1.39
29	I	405	ARG	NE-CZ	9.24	1.45	1.33
30	K	121	ARG	CD-NE	8.91	1.61	1.46
3	c	50	ARG	NE-CZ	8.79	1.44	1.33
14	n	162	TYR	CE1-CZ	8.47	1.49	1.38
14	7	161	ARG	CZ-NH2	8.41	1.44	1.33
23	P	92	SER	CA-CB	8.34	1.65	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	84	TYR	CG-CD2	8.30	1.50	1.39
24	Q	409	TYR	CE1-CZ	8.28	1.49	1.38
16	V	157	ARG	CZ-NH1	8.26	1.43	1.33
20	Z	759	ARG	CZ-NH2	8.20	1.43	1.33
3	C	92	ARG	NE-CZ	8.20	1.43	1.33
5	e	72	ARG	CD-NE	8.13	1.60	1.46
10	3	198	ARG	CZ-NH1	8.13	1.43	1.33
20	Z	753	GLY	CA-C	-8.12	1.38	1.51
18	X	103	GLU	CG-CD	8.06	1.64	1.51
2	b	240	SER	CA-CB	8.01	1.65	1.52
20	Z	371	SER	CA-CB	8.00	1.65	1.52
29	I	181	TYR	CE1-CZ	7.90	1.48	1.38
4	D	48	ARG	NE-CZ	7.87	1.43	1.33
6	F	171	TYR	CE2-CZ	7.87	1.48	1.38
33	J	368	TYR	CE1-CZ	7.87	1.48	1.38
4	d	181	ARG	CD-NE	7.75	1.59	1.46
4	d	108	TYR	CG-CD2	7.73	1.49	1.39
27	O	378	GLU	CD-OE2	7.73	1.34	1.25
30	K	128	ARG	CD-NE	7.72	1.59	1.46
3	c	114	ARG	CD-NE	7.71	1.59	1.46
5	e	128	SER	CA-CB	7.68	1.64	1.52
11	4	73	TYR	CZ-OH	7.65	1.50	1.37
26	U	51	SER	CA-CB	7.61	1.64	1.52
8	h	75	TYR	CE2-CZ	7.58	1.48	1.38
21	N	507	GLU	CD-OE2	7.55	1.33	1.25
32	M	73	ARG	NE-CZ	7.54	1.42	1.33
12	l	196	ARG	CZ-NH2	7.52	1.42	1.33
21	N	208	ARG	CD-NE	7.51	1.59	1.46
11	4	93	ARG	CD-NE	7.50	1.59	1.46
12	5	273	TRP	CD2-CE2	-7.48	1.32	1.41
2	B	130	PHE	CG-CD1	7.45	1.50	1.38
23	P	234	TYR	CG-CD1	7.45	1.48	1.39
9	i	208	GLU	CD-OE2	-7.44	1.17	1.25
2	b	128	ARG	NE-CZ	7.43	1.42	1.33
28	H	292	ARG	NE-CZ	7.43	1.42	1.33
30	K	141	ARG	NE-CZ	7.41	1.42	1.33
28	H	283	TYR	CE1-CZ	7.39	1.48	1.38
14	n	218	TYR	CG-CD2	-7.38	1.29	1.39
24	Q	400	TYR	CE2-CZ	7.37	1.48	1.38
16	V	100	ARG	NE-CZ	7.36	1.42	1.33
33	J	127	GLU	CB-CG	7.35	1.66	1.52
30	K	333	ARG	CD-NE	7.34	1.58	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	346	ARG	CZ-NH2	7.34	1.42	1.33
14	7	215	ARG	CZ-NH2	7.34	1.42	1.33
1	A	234	PHE	CG-CD1	7.33	1.49	1.38
4	d	111	ARG	NE-CZ	7.33	1.42	1.33
11	k	176	PHE	CG-CD1	7.33	1.49	1.38
23	P	310	ARG	CZ-NH1	7.31	1.42	1.33
13	6	99	ARG	CZ-NH1	7.30	1.42	1.33
11	k	93	ARG	CZ-NH1	7.30	1.42	1.33
6	F	3	ARG	CZ-NH2	7.29	1.42	1.33
22	S	287	SER	CA-CB	7.29	1.63	1.52
3	C	16	GLU	CG-CD	7.27	1.62	1.51
17	T	224	ARG	CD-NE	7.27	1.58	1.46
29	I	405	ARG	CD-NE	7.27	1.58	1.46
30	K	255	ARG	NE-CZ	7.26	1.42	1.33
21	N	162	ARG	CZ-NH2	7.25	1.42	1.33
29	I	181	TYR	CG-CD1	7.22	1.48	1.39
1	a	166	TYR	CG-CD2	7.22	1.48	1.39
12	5	94	ARG	NE-CZ	7.22	1.42	1.33
1	a	26	TYR	CZ-OH	7.21	1.50	1.37
28	H	273	ARG	CD-NE	7.21	1.58	1.46
21	N	109	TYR	CE1-CZ	7.20	1.48	1.38
20	Z	600	GLU	CG-CD	7.19	1.62	1.51
12	5	287	GLY	N-CA	-7.16	1.35	1.46
6	f	225	TYR	CG-CD1	7.16	1.48	1.39
2	B	83	ARG	CZ-NH1	7.11	1.42	1.33
27	O	335	GLY	N-CA	-7.10	1.35	1.46
20	Z	155	ARG	CZ-NH2	7.08	1.42	1.33
28	H	162	ARG	CZ-NH2	7.08	1.42	1.33
4	d	69	SER	CA-CB	7.07	1.63	1.52
32	M	124	ARG	NE-CZ	7.03	1.42	1.33
21	N	873	ARG	NE-CZ	7.03	1.42	1.33
28	H	408	SER	CA-CB	7.03	1.63	1.52
3	c	18	ARG	CZ-NH1	7.02	1.42	1.33
13	6	221	ARG	NE-CZ	7.02	1.42	1.33
1	a	14	ARG	NE-CZ	7.01	1.42	1.33
10	j	2	SER	CA-CB	7.00	1.63	1.52
12	l	262	TYR	CE1-CZ	7.00	1.47	1.38
32	M	366	ARG	CD-NE	6.97	1.58	1.46
21	N	299	TYR	CE1-CZ	6.94	1.47	1.38
33	J	344	ARG	CD-NE	6.94	1.58	1.46
14	7	134	TYR	CZ-OH	6.94	1.49	1.37
1	a	162	TYR	CE1-CZ	6.93	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	372	GLY	CA-C	-6.93	1.40	1.51
25	R	176	ARG	CZ-NH1	6.90	1.42	1.33
21	N	326	SER	CA-CB	6.89	1.63	1.52
15	W	43	SER	CA-CB	6.89	1.63	1.52
7	G	91	ARG	CZ-NH2	6.89	1.42	1.33
13	6	219	GLY	N-CA	-6.88	1.35	1.46
32	M	73	ARG	CD-NE	6.87	1.58	1.46
1	A	14	ARG	CD-NE	6.87	1.58	1.46
16	V	28	TYR	CG-CD2	6.87	1.48	1.39
20	Z	826	ARG	CZ-NH2	6.87	1.42	1.33
31	L	290	ARG	CD-NE	6.86	1.58	1.46
32	M	33	ARG	CZ-NH1	6.86	1.42	1.33
23	P	338	TRP	CD2-CE2	6.85	1.49	1.41
1	A	148	GLU	CG-CD	6.84	1.62	1.51
2	B	241	GLN	CG-CD	6.83	1.66	1.51
13	6	145	ARG	NE-CZ	6.83	1.42	1.33
7	g	149	TYR	CE1-CZ	6.83	1.47	1.38
23	P	312	PRO	N-CD	-6.82	1.38	1.47
24	Q	232	TYR	CE2-CZ	6.82	1.47	1.38
30	K	374	ARG	CZ-NH2	6.81	1.42	1.33
18	X	17	TYR	CB-CG	6.81	1.61	1.51
22	S	292	TYR	CE2-CZ	6.81	1.47	1.38
5	e	139	GLY	N-CA	-6.80	1.35	1.46
5	E	132	ARG	CZ-NH1	6.79	1.41	1.33
25	R	297	TYR	CE1-CZ	6.79	1.47	1.38
33	J	48	ARG	CD-NE	6.78	1.57	1.46
9	i	152	TYR	CE1-CZ	6.77	1.47	1.38
19	Y	22	GLU	CG-CD	6.77	1.62	1.51
30	K	252	ARG	NE-CZ	6.76	1.41	1.33
24	Q	10	GLU	CG-CD	6.73	1.62	1.51
5	e	166	ARG	CZ-NH1	6.73	1.41	1.33
30	K	290	ARG	CZ-NH1	6.73	1.41	1.33
22	S	367	TYR	CZ-OH	6.71	1.49	1.37
10	j	177	ARG	CD-NE	6.71	1.57	1.46
1	a	149	GLU	CD-OE1	6.70	1.33	1.25
33	J	374	ARG	CD-NE	6.69	1.57	1.46
3	C	213	PHE	CE1-CZ	6.68	1.50	1.37
6	F	162	GLY	CA-C	-6.68	1.41	1.51
20	Z	477	TYR	CE2-CZ	6.67	1.47	1.38
30	K	48	TYR	CE1-CZ	6.67	1.47	1.38
6	F	227	GLY	CA-C	-6.67	1.41	1.51
3	c	154	SER	CB-OG	6.66	1.50	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	235	PRO	N-CD	-6.66	1.38	1.47
2	B	246	ARG	NE-CZ	6.66	1.41	1.33
2	B	236	ARG	CD-NE	6.65	1.57	1.46
9	i	236	ARG	CZ-NH2	6.64	1.41	1.33
7	G	205	GLU	CD-OE2	6.64	1.32	1.25
13	6	131	TYR	CG-CD1	6.64	1.47	1.39
20	Z	928	ARG	CZ-NH2	6.64	1.41	1.33
21	N	651	PHE	CB-CG	6.63	1.62	1.51
30	K	294	ARG	CD-NE	6.63	1.57	1.46
14	n	194	ARG	CD-NE	6.63	1.57	1.46
22	S	255	SER	CA-CB	6.63	1.62	1.52
30	K	183	GLU	CB-CG	6.63	1.64	1.52
8	1	28	ARG	CZ-NH1	6.62	1.41	1.33
10	j	111	GLY	CA-C	-6.62	1.41	1.51
17	T	144	TYR	CG-CD2	6.62	1.47	1.39
4	D	141	ARG	CD-NE	6.61	1.57	1.46
6	F	164	ARG	NE-CZ	6.61	1.41	1.33
10	3	203	ARG	CD-NE	6.61	1.57	1.46
11	4	18	SER	CB-OG	6.61	1.50	1.42
20	Z	849	ARG	NE-CZ	6.59	1.41	1.33
25	R	304	TYR	CE2-CZ	6.59	1.47	1.38
31	L	194	ARG	NE-CZ	6.58	1.41	1.33
23	P	123	ARG	NE-CZ	6.58	1.41	1.33
30	K	236	ARG	CZ-NH2	6.57	1.41	1.33
24	Q	361	HIS	CB-CG	6.57	1.61	1.50
29	I	343	ARG	CD-NE	6.56	1.57	1.46
5	E	20	ARG	CD-NE	6.56	1.57	1.46
20	Z	138	ARG	CZ-NH1	6.56	1.41	1.33
4	d	197	ARG	CD-NE	6.56	1.57	1.46
1	a	91	ARG	CD-NE	6.55	1.57	1.46
29	I	304	ARG	NE-CZ	6.55	1.41	1.33
7	G	79	SER	CB-OG	6.55	1.50	1.42
31	L	82	ARG	NE-CZ	6.55	1.41	1.33
27	O	60	ARG	CZ-NH2	6.54	1.41	1.33
9	2	158	SER	CA-CB	6.54	1.62	1.52
27	O	111	SER	CA-CB	6.53	1.62	1.52
27	O	14	LEU	CA-CB	6.53	1.68	1.53
21	N	47	GLU	CB-CG	6.53	1.64	1.52
10	j	106	GLY	N-CA	-6.52	1.36	1.46
11	4	173	PRO	N-CA	-6.51	1.36	1.47
18	X	51	ARG	CZ-NH1	6.51	1.41	1.33
32	M	342	ARG	NE-CZ	6.51	1.41	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	166	ARG	NE-CZ	6.49	1.41	1.33
21	N	58	ARG	CZ-NH2	6.48	1.41	1.33
17	T	165	GLN	CG-CD	6.48	1.66	1.51
20	Z	103	TYR	CG-CD1	6.48	1.47	1.39
27	O	44	SER	CA-CB	6.47	1.62	1.52
33	J	80	SER	CA-CB	6.46	1.62	1.52
7	G	79	SER	CA-C	-6.46	1.36	1.52
17	T	81	TYR	CE1-CZ	6.46	1.47	1.38
4	D	211	GLU	CD-OE2	6.46	1.32	1.25
8	1	137	GLY	CA-C	-6.46	1.41	1.51
33	J	74	GLU	CG-CD	6.44	1.61	1.51
3	c	20	TYR	CG-CD1	6.44	1.47	1.39
21	N	776	TYR	CE2-CZ	6.43	1.47	1.38
17	T	91	SER	CA-CB	6.43	1.62	1.52
7	g	20	ARG	CZ-NH1	6.42	1.41	1.33
17	T	66	ALA	N-CA	-6.42	1.33	1.46
8	1	194	ARG	CD-NE	6.42	1.57	1.46
20	Z	296	SER	CA-CB	6.42	1.62	1.52
14	n	180	GLY	N-CA	-6.41	1.36	1.46
23	P	232	ARG	NE-CZ	6.41	1.41	1.33
20	Z	39	SER	CA-CB	6.41	1.62	1.52
31	L	420	ARG	NE-CZ	6.39	1.41	1.33
11	k	139	TYR	CG-CD2	6.39	1.47	1.39
28	H	432	ARG	CZ-NH1	6.38	1.41	1.33
5	e	10	ARG	CD-NE	6.38	1.57	1.46
20	Z	919	GLU	CG-CD	6.38	1.61	1.51
1	a	12	TYR	CG-CD1	6.38	1.47	1.39
20	Z	16	SER	CB-OG	-6.37	1.33	1.42
7	g	190	ARG	CZ-NH1	6.37	1.41	1.33
14	7	68	ARG	CZ-NH2	6.36	1.41	1.33
14	n	231	ALA	CA-CB	6.35	1.65	1.52
5	E	210	GLU	CA-CB	6.35	1.68	1.53
30	K	77	ARG	NE-CZ	6.34	1.41	1.33
13	m	110	PHE	CG-CD2	6.34	1.48	1.38
25	R	383	ARG	NE-CZ	6.34	1.41	1.33
15	W	113	PHE	CG-CD1	6.33	1.48	1.38
2	B	99	ARG	NE-CZ	6.32	1.41	1.33
26	U	189	ARG	CZ-NH1	6.32	1.41	1.33
32	M	77	TYR	CE2-CZ	6.32	1.46	1.38
20	Z	385	PHE	CG-CD1	6.32	1.48	1.38
25	R	206	ARG	NE-CZ	6.32	1.41	1.33
16	V	77	GLY	N-CA	-6.32	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	13	PHE	CG-CD2	6.31	1.48	1.38
27	O	189	TYR	CG-CD1	6.31	1.47	1.39
22	S	147	TRP	NE1-CE2	6.31	1.45	1.37
4	d	97	ARG	NE-CZ	6.30	1.41	1.33
25	R	334	ARG	NE-CZ	6.30	1.41	1.33
7	g	16	SER	CA-CB	6.30	1.62	1.52
23	P	221	TYR	CG-CD1	6.29	1.47	1.39
32	M	233	ARG	CZ-NH2	6.28	1.41	1.33
12	5	206	SER	CA-CB	6.28	1.62	1.52
5	E	165	TYR	CE2-CZ	6.28	1.46	1.38
31	L	165	PRO	N-CD	-6.27	1.39	1.47
8	1	187	LEU	N-CA	-6.26	1.33	1.46
18	X	132	SER	CA-CB	6.25	1.62	1.52
24	Q	255	TYR	CE2-CZ	6.25	1.46	1.38
24	Q	332	ARG	CZ-NH2	6.25	1.41	1.33
20	Z	244	ARG	CZ-NH2	6.25	1.41	1.33
25	R	91	TRP	CE3-CZ3	6.25	1.49	1.38
21	N	468	GLU	CG-CD	6.24	1.61	1.51
31	L	69	ARG	CD-NE	6.23	1.57	1.46
14	7	252	TRP	NE1-CE2	-6.22	1.29	1.37
20	Z	55	ARG	CZ-NH2	6.21	1.41	1.33
15	W	196	SER	CB-OG	6.21	1.50	1.42
9	i	146	GLY	CA-C	-6.20	1.42	1.51
15	W	32	SER	CA-CB	6.20	1.62	1.52
31	L	132	ARG	CZ-NH2	6.20	1.41	1.33
33	J	324	ARG	CZ-NH2	6.20	1.41	1.33
1	A	91	ARG	CZ-NH1	6.20	1.41	1.33
32	M	161	SER	CA-CB	6.20	1.62	1.52
20	Z	504	GLU	CD-OE2	6.19	1.32	1.25
21	N	711	ARG	CZ-NH2	6.19	1.41	1.33
20	Z	589	SER	CA-CB	6.19	1.62	1.52
28	H	182	ASN	CA-CB	6.18	1.69	1.53
11	4	36	ARG	NE-CZ	6.18	1.41	1.33
16	V	196	TYR	CG-CD1	6.17	1.47	1.39
32	M	233	ARG	NE-CZ	6.17	1.41	1.33
25	R	345	TYR	CB-CG	6.16	1.60	1.51
22	S	211	ARG	CZ-NH1	6.16	1.41	1.33
2	B	206	GLY	CA-C	-6.16	1.42	1.51
28	H	62	ARG	NE-CZ	6.16	1.41	1.33
20	Z	323	TYR	CB-CG	-6.15	1.42	1.51
21	N	561	GLY	CA-C	-6.15	1.42	1.51
21	N	709	GLY	C-N	6.15	1.44	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	256	LYS	N-CA	-6.15	1.34	1.46
13	m	142	GLU	CB-CG	6.14	1.63	1.52
22	S	228	GLU	CG-CD	6.14	1.61	1.51
7	g	20	ARG	NE-CZ	6.14	1.41	1.33
12	5	93	SER	CA-CB	6.14	1.62	1.52
28	H	101	ARG	CD-NE	6.14	1.56	1.46
2	b	236	ARG	CD-NE	6.13	1.56	1.46
4	d	49	ARG	NE-CZ	6.13	1.41	1.33
33	J	261	SER	C-N	6.13	1.44	1.33
32	M	299	ARG	CZ-NH1	6.13	1.41	1.33
7	G	213	GLU	CD-OE1	6.13	1.32	1.25
24	Q	161	LEU	N-CA	-6.13	1.34	1.46
22	S	196	ARG	CZ-NH2	6.12	1.41	1.33
6	f	59	TYR	CB-CG	-6.12	1.42	1.51
1	A	183	GLU	CD-OE2	6.12	1.32	1.25
4	d	228	GLU	CG-CD	6.11	1.61	1.51
10	3	103	TYR	CE1-CZ	6.11	1.46	1.38
24	Q	398	TYR	CG-CD2	6.11	1.47	1.39
2	b	4	ARG	NE-CZ	6.10	1.41	1.33
1	A	131	ARG	CZ-NH2	6.10	1.41	1.33
20	Z	703	SER	CA-CB	6.10	1.62	1.52
1	A	185	HIS	CA-CB	6.09	1.67	1.53
7	g	149	TYR	CD2-CE2	6.09	1.48	1.39
4	d	95	SER	CA-CB	6.09	1.62	1.52
23	P	351	ARG	CD-NE	6.08	1.56	1.46
24	Q	189	ARG	CZ-NH2	6.08	1.41	1.33
6	f	39	ARG	CZ-NH2	6.08	1.41	1.33
12	5	155	SER	CA-CB	6.08	1.62	1.52
15	W	101	ARG	CZ-NH2	6.08	1.41	1.33
4	d	166	ARG	CZ-NH1	6.08	1.41	1.33
12	5	253	TYR	CG-CD2	6.08	1.47	1.39
1	a	120	ARG	NE-CZ	6.07	1.41	1.33
11	4	98	TYR	CZ-OH	6.07	1.48	1.37
21	N	69	TYR	CB-CG	-6.06	1.42	1.51
11	4	147	HIS	CB-CG	6.06	1.60	1.50
13	6	75	ARG	NE-CZ	6.05	1.41	1.33
20	Z	169	VAL	CB-CG1	6.05	1.65	1.52
10	j	46	TYR	CE2-CZ	6.05	1.46	1.38
4	D	172	ARG	CD-NE	6.04	1.56	1.46
10	j	28	ARG	CZ-NH2	6.04	1.40	1.33
1	a	105	ARG	NE-CZ	6.03	1.40	1.33
24	Q	12	ARG	CZ-NH1	6.03	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	300	ARG	CZ-NH1	6.03	1.40	1.33
5	E	166	ARG	CZ-NH1	6.03	1.40	1.33
16	V	169	GLU	CD-OE2	6.02	1.32	1.25
12	l	234	ARG	NE-CZ	6.02	1.40	1.33
13	m	202	ARG	CD-NE	6.02	1.56	1.46
28	H	266	ARG	NE-CZ	6.02	1.40	1.33
20	Z	441	TYR	CZ-OH	6.02	1.48	1.37
1	A	96	ARG	NE-CZ	6.01	1.40	1.33
9	2	98	TYR	CB-CG	-6.01	1.42	1.51
24	Q	277	ASP	CB-CG	6.01	1.64	1.51
5	e	28	LEU	CA-C	-6.01	1.37	1.52
25	R	99	TYR	CE1-CZ	6.01	1.46	1.38
20	Z	752	ILE	C-N	6.00	1.43	1.33
8	1	45	ARG	CZ-NH2	5.99	1.40	1.33
23	P	138	ARG	CD-NE	5.99	1.56	1.46
4	d	248	LYS	CA-CB	5.98	1.67	1.53
22	S	55	ARG	NE-CZ	5.98	1.40	1.33
25	R	224	PHE	CG-CD1	5.98	1.47	1.38
33	J	266	SER	CA-CB	5.98	1.61	1.52
17	T	89	TYR	CD1-CE1	5.96	1.48	1.39
24	Q	223	GLY	CA-C	-5.96	1.42	1.51
3	C	43	GLY	CA-C	-5.96	1.42	1.51
6	f	51	ARG	NE-CZ	5.95	1.40	1.33
20	Z	838	TYR	CZ-OH	5.95	1.48	1.37
22	S	239	ARG	CZ-NH1	5.95	1.40	1.33
1	A	11	GLY	CA-C	-5.95	1.42	1.51
3	C	113	ARG	CZ-NH2	5.95	1.40	1.33
7	G	130	ARG	NE-CZ	5.95	1.40	1.33
23	P	150	GLU	CG-CD	5.95	1.60	1.51
21	N	788	TYR	CE2-CZ	5.94	1.46	1.38
14	n	68	ARG	NE-CZ	5.93	1.40	1.33
20	Z	623	ARG	CZ-NH2	5.93	1.40	1.33
29	I	343	ARG	CZ-NH1	5.93	1.40	1.33
1	A	55	SER	CA-CB	5.93	1.61	1.52
33	J	56	ARG	CZ-NH1	5.93	1.40	1.33
16	V	135	ARG	CD-NE	5.93	1.56	1.46
1	a	24	ARG	CD-NE	5.93	1.56	1.46
12	l	281	SER	CB-OG	5.93	1.50	1.42
33	J	112	ARG	CZ-NH1	5.92	1.40	1.33
21	N	188	TYR	CE1-CZ	5.92	1.46	1.38
29	I	291	ARG	NE-CZ	5.92	1.40	1.33
7	G	78	TYR	CG-CD2	5.92	1.46	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	69	PHE	CE2-CZ	5.92	1.48	1.37
31	L	209	ARG	CZ-NH1	5.92	1.40	1.33
23	P	103	TYR	CG-CD2	5.92	1.46	1.39
29	I	180	SER	CA-CB	5.91	1.61	1.52
13	6	133	PHE	CG-CD2	5.91	1.47	1.38
25	R	215	GLY	CA-C	5.91	1.61	1.51
12	5	230	TYR	CG-CD1	5.90	1.46	1.39
31	L	90	LYS	C-N	5.90	1.47	1.34
28	H	273	ARG	CZ-NH1	5.90	1.40	1.33
5	e	44	GLU	CD-OE1	5.89	1.32	1.25
31	L	299	ARG	CZ-NH2	5.89	1.40	1.33
16	V	61	TYR	CG-CD2	5.89	1.46	1.39
29	I	155	SER	CA-CB	-5.89	1.44	1.52
21	N	485	MET	C-N	5.88	1.43	1.33
25	R	62	TYR	CZ-OH	5.88	1.47	1.37
27	O	33	TYR	CE1-CZ	5.87	1.46	1.38
22	S	76	PHE	CG-CD2	5.87	1.47	1.38
20	Z	287	ARG	CZ-NH2	5.87	1.40	1.33
15	W	144	PHE	C-N	5.86	1.43	1.33
8	1	133	TYR	CG-CD2	5.86	1.46	1.39
16	V	273	ARG	CZ-NH1	5.86	1.40	1.33
24	Q	124	PHE	CG-CD1	5.85	1.47	1.38
21	N	208	ARG	CZ-NH1	5.85	1.40	1.33
22	S	346	TYR	CG-CD1	5.85	1.46	1.39
3	c	79	GLY	CA-C	-5.85	1.42	1.51
33	J	344	ARG	NE-CZ	5.85	1.40	1.33
26	U	284	SER	CA-CB	5.84	1.61	1.52
22	S	241	PHE	CG-CD1	5.84	1.47	1.38
26	U	56	PHE	CG-CD2	5.84	1.47	1.38
4	d	123	SER	CA-CB	5.84	1.61	1.52
11	k	167	GLU	CG-CD	5.84	1.60	1.51
21	N	723	GLY	N-CA	-5.84	1.37	1.46
7	g	157	TYR	CB-CG	-5.84	1.42	1.51
22	S	25	TYR	CE2-CZ	5.84	1.46	1.38
14	n	189	ARG	CZ-NH2	5.83	1.40	1.33
2	B	48	GLU	CG-CD	5.83	1.60	1.51
9	2	146	GLY	CA-C	-5.83	1.42	1.51
29	I	408	ARG	NE-CZ	5.83	1.40	1.33
14	7	124	TYR	CD2-CE2	-5.83	1.30	1.39
14	7	130	ALA	CA-CB	5.82	1.64	1.52
1	a	250	GLU	CD-OE1	5.82	1.32	1.25
7	g	115	ARG	CZ-NH1	5.82	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	98	TYR	CE1-CZ	5.82	1.46	1.38
4	D	179	TYR	CB-CG	-5.82	1.43	1.51
6	F	157	TYR	CE1-CZ	5.80	1.46	1.38
24	Q	91	SER	CA-CB	5.80	1.61	1.52
32	M	124	ARG	CD-NE	5.80	1.56	1.46
2	B	13	SER	CA-CB	5.80	1.61	1.52
3	c	14	SER	CB-OG	5.79	1.49	1.42
2	b	5	TYR	CE1-CZ	5.79	1.46	1.38
28	H	190	ARG	CZ-NH2	5.79	1.40	1.33
9	i	219	TYR	CG-CD1	5.78	1.46	1.39
19	Y	64	TRP	CZ2-CH2	5.78	1.48	1.37
30	K	243	VAL	CB-CG2	5.78	1.65	1.52
22	S	445	THR	N-CA	-5.78	1.34	1.46
30	K	65	GLU	CD-OE1	5.78	1.32	1.25
7	g	158	TRP	NE1-CE2	5.77	1.45	1.37
29	I	189	SER	CA-CB	5.77	1.61	1.52
5	E	138	PHE	N-CA	-5.77	1.34	1.46
21	N	188	TYR	CB-CG	-5.77	1.43	1.51
33	J	306	ARG	CG-CD	5.76	1.66	1.51
25	R	382	ASP	CB-CG	5.76	1.63	1.51
9	2	93	GLU	CB-CG	5.76	1.63	1.52
23	P	138	ARG	NE-CZ	5.75	1.40	1.33
2	B	201	GLU	CB-CG	5.75	1.63	1.52
16	V	61	TYR	CG-CD1	5.75	1.46	1.39
9	2	65	ARG	NE-CZ	5.75	1.40	1.33
21	N	861	TYR	CG-CD1	5.75	1.46	1.39
6	F	34	VAL	CA-CB	-5.74	1.42	1.54
21	N	653	ARG	CZ-NH2	5.74	1.40	1.33
17	T	220	PHE	CG-CD1	5.73	1.47	1.38
31	L	191	ARG	NE-CZ	5.73	1.40	1.33
21	N	597	ARG	CZ-NH2	5.73	1.40	1.33
1	A	135	ARG	CZ-NH2	5.73	1.40	1.33
8	1	87	ALA	N-CA	-5.72	1.34	1.46
19	Y	12	SER	CA-CB	5.72	1.61	1.52
23	P	403	GLU	CG-CD	5.72	1.60	1.51
13	6	75	ARG	CD-NE	5.72	1.56	1.46
31	L	290	ARG	CZ-NH1	5.72	1.40	1.33
30	K	73	ARG	NE-CZ	5.72	1.40	1.33
8	h	75	TYR	CG-CD2	5.72	1.46	1.39
6	f	101	ARG	CD-NE	5.71	1.56	1.46
22	S	114	TYR	CB-CG	5.70	1.60	1.51
8	h	163	PHE	CG-CD2	5.70	1.47	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	201	GLY	C-N	5.70	1.43	1.33
7	g	78	TYR	CE2-CZ	5.70	1.46	1.38
9	i	168	GLU	CD-OE2	5.70	1.31	1.25
20	Z	773	ARG	CZ-NH2	5.70	1.40	1.33
11	4	14	ILE	CA-CB	-5.69	1.41	1.54
20	Z	331	GLY	N-CA	-5.69	1.37	1.46
26	U	189	ARG	CD-NE	5.69	1.56	1.46
30	K	77	ARG	CD-NE	5.69	1.56	1.46
20	Z	962	ARG	NE-CZ	5.68	1.40	1.33
6	F	36	VAL	C-N	5.68	1.43	1.33
15	W	109	ARG	CZ-NH1	5.68	1.40	1.33
25	R	263	ARG	CD-NE	5.68	1.56	1.46
11	4	6	GLY	CA-C	-5.68	1.42	1.51
23	P	228	SER	CA-CB	5.68	1.61	1.52
8	1	93	GLU	N-CA	-5.68	1.34	1.46
14	7	141	ASN	N-CA	-5.68	1.34	1.46
6	F	51	ARG	CZ-NH2	5.67	1.40	1.33
21	N	457	SER	CB-OG	5.67	1.49	1.42
26	U	302	GLN	N-CA	-5.67	1.35	1.46
27	O	261	GLY	CA-C	-5.66	1.42	1.51
17	T	174	PHE	CG-CD2	5.66	1.47	1.38
7	G	115	ARG	CD-NE	5.66	1.56	1.46
28	H	123	GLY	CA-C	-5.66	1.42	1.51
16	V	194	ARG	CZ-NH1	5.65	1.40	1.33
11	4	178	GLY	N-CA	-5.65	1.37	1.46
23	P	6	PRO	N-CA	5.65	1.56	1.47
30	K	128	ARG	NE-CZ	5.65	1.40	1.33
10	j	98	ARG	CZ-NH1	5.65	1.40	1.33
3	c	129	ARG	CZ-NH2	5.64	1.40	1.33
9	2	98	TYR	CE2-CZ	5.64	1.45	1.38
21	N	312	GLY	CA-C	-5.64	1.42	1.51
10	j	97	GLU	CD-OE1	5.64	1.31	1.25
2	B	19	GLY	CA-C	-5.64	1.42	1.51
22	S	174	ARG	NE-CZ	5.64	1.40	1.33
22	S	345	TYR	CG-CD1	5.64	1.46	1.39
32	M	114	GLY	CA-C	-5.64	1.42	1.51
14	7	226	ARG	NE-CZ	5.63	1.40	1.33
2	b	178	ARG	CZ-NH2	5.63	1.40	1.33
4	D	22	TYR	CG-CD2	5.62	1.46	1.39
30	K	350	ARG	CZ-NH2	5.62	1.40	1.33
21	N	916	LEU	C-N	5.62	1.47	1.34
3	C	79	GLY	N-CA	-5.62	1.37	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	58	ARG	NE-CZ	5.61	1.40	1.33
20	Z	798	ARG	CZ-NH2	5.61	1.40	1.33
29	I	94	LYS	N-CA	-5.61	1.35	1.46
33	J	246	PHE	CB-CG	5.61	1.60	1.51
11	4	70	ARG	NE-CZ	5.61	1.40	1.33
31	L	291	PHE	CG-CD1	5.60	1.47	1.38
7	G	166	GLY	CA-C	-5.60	1.42	1.51
22	S	286	TYR	CZ-OH	5.60	1.47	1.37
20	Z	81	SER	CA-CB	5.60	1.61	1.52
20	Z	586	GLU	CD-OE2	5.60	1.31	1.25
27	O	166	ARG	CZ-NH2	5.60	1.40	1.33
1	a	198	SER	CA-CB	5.59	1.61	1.52
8	1	54	ARG	CZ-NH2	5.59	1.40	1.33
13	m	209	GLY	N-CA	-5.59	1.37	1.46
12	5	203	CYS	CB-SG	-5.59	1.72	1.81
17	T	12	SER	CA-CB	5.58	1.61	1.52
22	S	405	ARG	CG-CD	5.58	1.66	1.51
28	H	328	GLU	CB-CG	5.58	1.62	1.52
9	2	74	GLY	N-CA	-5.58	1.37	1.46
20	Z	138	ARG	CZ-NH2	5.58	1.40	1.33
21	N	741	TYR	CB-CG	-5.58	1.43	1.51
7	g	91	ARG	CD-NE	5.58	1.55	1.46
5	E	20	ARG	CZ-NH1	5.58	1.40	1.33
31	L	168	TYR	CG-CD1	5.57	1.46	1.39
4	d	6	ARG	CZ-NH1	5.57	1.40	1.33
8	1	85	GLU	CG-CD	5.57	1.60	1.51
27	O	186	ASN	CB-CG	5.57	1.63	1.51
21	N	281	GLY	N-CA	-5.57	1.37	1.46
7	G	159	GLY	N-CA	-5.57	1.37	1.46
33	J	373	ARG	NE-CZ	5.56	1.40	1.33
15	W	19	GLY	CA-C	-5.56	1.43	1.51
32	M	320	ARG	CZ-NH1	5.56	1.40	1.33
24	Q	264	TYR	CD1-CE1	5.56	1.47	1.39
7	G	20	ARG	NE-CZ	5.56	1.40	1.33
21	N	320	SER	CA-CB	5.55	1.61	1.52
30	K	53	LYS	N-CA	-5.55	1.35	1.46
2	b	233	PRO	N-CD	-5.55	1.40	1.47
5	E	10	ARG	CZ-NH2	5.55	1.40	1.33
11	4	190	ARG	NE-CZ	5.55	1.40	1.33
22	S	160	ARG	CD-NE	5.55	1.55	1.46
5	E	125	GLU	CD-OE1	5.55	1.31	1.25
16	V	157	ARG	CA-CB	5.54	1.66	1.53

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	82	ARG	CD-NE	5.54	1.55	1.46
13	6	109	ARG	CZ-NH1	5.54	1.40	1.33
30	K	350	ARG	NE-CZ	5.54	1.40	1.33
11	4	23	ARG	CZ-NH1	5.54	1.40	1.33
2	b	90	ARG	CZ-NH1	5.54	1.40	1.33
6	F	107	ARG	NE-CZ	5.54	1.40	1.33
21	N	50	TYR	CG-CD2	5.54	1.46	1.39
21	N	921	ARG	CZ-NH2	5.54	1.40	1.33
30	K	259	ARG	NE-CZ	5.54	1.40	1.33
1	a	217	GLU	CD-OE2	5.53	1.31	1.25
2	b	20	GLN	CG-CD	5.53	1.63	1.51
8	h	193	GLU	CB-CG	5.53	1.62	1.52
16	V	269	ARG	CD-NE	5.53	1.55	1.46
11	k	91	SER	CA-CB	5.53	1.61	1.52
20	Z	564	ARG	CZ-NH1	5.53	1.40	1.33
5	E	132	ARG	CZ-NH2	5.53	1.40	1.33
5	E	132	ARG	N-CA	-5.53	1.35	1.46
20	Z	295	ARG	CD-NE	5.53	1.55	1.46
25	R	127	GLU	CG-CD	5.53	1.60	1.51
28	H	435	ARG	CZ-NH1	5.52	1.40	1.33
12	l	221	TRP	CB-CG	5.51	1.60	1.50
16	V	129	PHE	CE2-CZ	5.51	1.47	1.37
8	h	133	TYR	CE2-CZ	5.50	1.45	1.38
2	b	201	GLU	CA-C	-5.50	1.38	1.52
14	7	39	VAL	CA-CB	-5.50	1.43	1.54
14	n	134	TYR	CB-CG	-5.50	1.43	1.51
26	U	113	TYR	CE2-CZ	5.50	1.45	1.38
11	4	72	ASP	CA-CB	5.50	1.66	1.53
16	V	31	SER	CB-OG	-5.50	1.35	1.42
31	L	156	MET	N-CA	-5.50	1.35	1.46
25	R	141	TYR	CG-CD1	5.49	1.46	1.39
20	Z	623	ARG	NE-CZ	5.49	1.40	1.33
20	Z	494	GLY	N-CA	-5.49	1.37	1.46
8	1	169	SER	CA-CB	5.48	1.61	1.52
4	d	148	TYR	CB-CG	-5.48	1.43	1.51
3	c	18	ARG	NE-CZ	5.48	1.40	1.33
10	j	100	PHE	CG-CD1	5.48	1.47	1.38
4	D	201	GLU	CG-CD	5.48	1.60	1.51
14	7	124	TYR	CG-CD2	5.48	1.46	1.39
16	V	48	GLU	CD-OE1	5.48	1.31	1.25
11	k	117	TYR	CB-CG	-5.48	1.43	1.51
8	1	152	ARG	NE-CZ	5.47	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	79	TYR	CZ-OH	5.47	1.47	1.37
9	i	112	LEU	N-CA	-5.47	1.35	1.46
16	V	230	TYR	CG-CD2	5.47	1.46	1.39
6	f	128	TYR	CG-CD1	5.47	1.46	1.39
20	Z	8	LYS	CA-CB	5.47	1.66	1.53
3	c	167	ALA	CA-CB	5.46	1.64	1.52
15	W	145	GLY	CA-C	-5.46	1.43	1.51
10	3	161	GLU	CG-CD	5.46	1.60	1.51
16	V	157	ARG	NE-CZ	5.46	1.40	1.33
5	e	153	TYR	CD1-CE1	5.46	1.47	1.39
17	T	245	TYR	CE2-CZ	5.46	1.45	1.38
23	P	95	TYR	CG-CD1	5.46	1.46	1.39
2	B	217	GLU	CD-OE2	5.45	1.31	1.25
21	N	282	TYR	CZ-OH	5.45	1.47	1.37
23	P	26	SER	CA-CB	5.45	1.61	1.52
30	K	234	PHE	CA-CB	5.45	1.66	1.53
25	R	297	TYR	CA-CB	5.45	1.66	1.53
33	J	42	ARG	NE-CZ	5.45	1.40	1.33
17	T	109	TYR	CE1-CZ	5.45	1.45	1.38
4	D	49	ARG	CD-NE	5.45	1.55	1.46
16	V	20	ARG	CD-NE	5.45	1.55	1.46
26	U	239	LEU	C-N	5.45	1.42	1.33
29	I	407	ARG	CD-NE	5.44	1.55	1.46
9	i	238	THR	N-CA	-5.44	1.35	1.46
10	j	186	VAL	N-CA	-5.44	1.35	1.46
11	4	106	GLY	N-CA	-5.44	1.37	1.46
22	S	271	ARG	NE-CZ	5.44	1.40	1.33
3	C	54	SER	CA-CB	5.44	1.61	1.52
6	F	3	ARG	CZ-NH1	5.44	1.40	1.33
20	Z	216	GLY	CA-C	-5.44	1.43	1.51
5	e	250	GLU	CB-CG	5.43	1.62	1.52
1	A	131	ARG	CZ-NH1	5.43	1.40	1.33
4	D	168	SER	CA-C	-5.43	1.38	1.52
24	Q	127	ARG	CZ-NH1	5.43	1.40	1.33
6	F	28	ALA	CA-CB	5.43	1.63	1.52
7	G	93	ARG	NE-CZ	5.43	1.40	1.33
32	M	339	ARG	CD-NE	5.43	1.55	1.46
32	M	405	ASN	C-N	5.43	1.42	1.33
27	O	33	TYR	CG-CD2	5.43	1.46	1.39
30	K	348	GLU	CG-CD	5.43	1.60	1.51
7	g	242	PHE	CG-CD1	5.43	1.46	1.38
1	A	120	ARG	NE-CZ	5.43	1.40	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	472	ASN	CB-CG	5.43	1.63	1.51
20	Z	64	TYR	CE2-CZ	5.43	1.45	1.38
27	O	285	SER	CA-CB	5.43	1.61	1.52
14	n	254	PHE	CE1-CZ	5.42	1.47	1.37
15	W	157	PHE	CG-CD1	5.42	1.46	1.38
33	J	312	ARG	CZ-NH2	5.42	1.40	1.33
11	k	93	ARG	CD-NE	5.42	1.55	1.46
20	Z	962	ARG	CD-NE	5.42	1.55	1.46
21	N	26	GLU	CG-CD	5.42	1.60	1.51
23	P	273	TYR	CG-CD2	5.42	1.46	1.39
30	K	294	ARG	CZ-NH1	5.42	1.40	1.33
26	U	202	SER	CB-OG	5.41	1.49	1.42
6	F	18	ARG	NE-CZ	5.41	1.40	1.33
12	5	165	TYR	CZ-OH	5.41	1.47	1.37
17	T	266	TYR	CG-CD2	5.41	1.46	1.39
22	S	342	LEU	N-CA	-5.41	1.35	1.46
33	J	71	TYR	CG-CD2	5.41	1.46	1.39
6	f	107	ARG	CZ-NH1	5.41	1.40	1.33
12	l	242	ARG	CZ-NH1	5.41	1.40	1.33
1	A	205	PHE	CA-CB	5.41	1.65	1.53
17	T	245	TYR	CG-CD2	5.41	1.46	1.39
14	7	123	SER	CA-CB	5.40	1.61	1.52
17	T	10	SER	CA-CB	5.39	1.61	1.52
1	a	186	PHE	CB-CG	-5.39	1.42	1.51
31	L	117	TYR	CE1-CZ	5.39	1.45	1.38
25	R	313	ALA	CA-CB	5.39	1.63	1.52
9	2	153	TYR	CG-CD2	5.39	1.46	1.39
2	b	4	ARG	CZ-NH2	5.39	1.40	1.33
11	4	135	TYR	CZ-OH	5.39	1.47	1.37
14	7	172	SER	CA-CB	5.39	1.61	1.52
1	a	128	TYR	CZ-OH	5.38	1.47	1.37
5	e	20	ARG	CZ-NH1	5.38	1.40	1.33
28	H	212	GLY	CA-C	-5.38	1.43	1.51
23	P	364	ARG	CZ-NH1	5.38	1.40	1.33
21	N	205	SER	CA-CB	-5.38	1.44	1.52
2	b	236	ARG	CZ-NH2	5.38	1.40	1.33
5	e	250	GLU	CD-OE2	5.38	1.31	1.25
22	S	332	PHE	CG-CD1	5.38	1.46	1.38
6	F	147	PHE	CG-CD2	5.37	1.46	1.38
26	U	47	ARG	NE-CZ	5.37	1.40	1.33
23	P	336	HIS	N-CA	-5.37	1.35	1.46
4	D	12	SER	CB-OG	5.37	1.49	1.42

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	g	138	PHE	CE2-CZ	5.37	1.47	1.37
24	Q	130	ARG	NE-CZ	5.37	1.40	1.33
33	J	63	ARG	NE-CZ	5.37	1.40	1.33
24	Q	75	ARG	CD-NE	5.37	1.55	1.46
6	f	107	ARG	CD-NE	5.36	1.55	1.46
32	M	79	VAL	CB-CG2	5.36	1.64	1.52
13	m	169	GLU	CD-OE2	5.36	1.31	1.25
22	S	475	TYR	CZ-OH	5.36	1.47	1.37
21	N	889	ARG	CZ-NH1	5.36	1.40	1.33
25	R	331	ARG	CD-NE	5.36	1.55	1.46
22	S	271	ARG	CZ-NH2	5.36	1.40	1.33
12	5	253	TYR	CG-CD1	-5.35	1.32	1.39
21	N	594	VAL	CB-CG1	5.35	1.64	1.52
29	I	298	GLY	CA-C	5.35	1.60	1.51
20	Z	819	GLY	CA-C	-5.35	1.43	1.51
2	B	224	TYR	CZ-OH	5.34	1.47	1.37
14	7	74	ARG	NE-CZ	5.34	1.40	1.33
11	k	149	ARG	CZ-NH2	5.34	1.40	1.33
10	3	123	GLY	CA-C	-5.34	1.43	1.51
26	U	59	ASP	CA-CB	5.34	1.65	1.53
28	H	285	GLY	N-CA	5.34	1.54	1.46
4	D	58	ARG	NE-CZ	5.34	1.40	1.33
20	Z	832	ARG	CZ-NH2	5.34	1.40	1.33
1	a	244	ARG	CD-NE	5.34	1.55	1.46
33	J	238	ARG	CZ-NH1	5.34	1.40	1.33
4	d	112	TYR	CG-CD2	5.33	1.46	1.39
11	k	23	ARG	CD-NE	5.33	1.55	1.46
10	3	102	PRO	CA-C	-5.33	1.42	1.52
28	H	411	CYS	CB-SG	5.33	1.91	1.82
31	L	175	GLN	C-N	5.33	1.42	1.33
1	a	173	PRO	CA-C	-5.33	1.42	1.52
6	f	6	TYR	CG-CD2	5.33	1.46	1.39
24	Q	110	SER	CA-CB	5.32	1.60	1.52
28	H	143	ALA	CA-CB	5.32	1.63	1.52
29	I	54	ARG	NE-CZ	5.32	1.40	1.33
24	Q	24	GLU	CG-CD	5.32	1.59	1.51
1	a	14	ARG	CZ-NH2	5.31	1.40	1.33
12	l	270	GLU	CD-OE2	5.31	1.31	1.25
30	K	281	ARG	CZ-NH1	5.31	1.40	1.33
33	J	92	GLY	N-CA	-5.31	1.38	1.46
1	a	120	ARG	CD-NE	5.31	1.55	1.46
8	h	146	TYR	CE1-CZ	5.31	1.45	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	73	GLU	CG-CD	5.31	1.59	1.51
14	n	126	PHE	CG-CD2	5.31	1.46	1.38
3	C	9	ARG	CZ-NH1	5.31	1.40	1.33
7	G	211	ASP	CB-CG	5.31	1.62	1.51
16	V	197	TYR	CG-CD1	5.31	1.46	1.39
29	I	268	PHE	CG-CD1	5.31	1.46	1.38
6	f	228	GLU	CD-OE2	5.31	1.31	1.25
1	a	234	PHE	CG-CD1	5.31	1.46	1.38
1	A	71	TYR	CE1-CZ	5.30	1.45	1.38
3	C	50	ARG	CZ-NH2	5.30	1.40	1.33
30	K	405	SER	CA-CB	5.30	1.60	1.52
13	m	36	ARG	CZ-NH2	5.30	1.40	1.33
11	4	77	PRO	N-CD	-5.30	1.40	1.47
13	6	82	TRP	CB-CG	5.30	1.59	1.50
23	P	359	ARG	NE-CZ	5.30	1.40	1.33
28	H	335	GLU	CD-OE2	5.30	1.31	1.25
6	f	162	GLY	N-CA	-5.30	1.38	1.46
14	n	83	VAL	N-CA	-5.30	1.35	1.46
10	3	33	SER	CA-C	-5.30	1.39	1.52
10	3	15	MET	N-CA	-5.29	1.35	1.46
25	R	338	TYR	CA-CB	5.29	1.65	1.53
28	H	101	ARG	CA-CB	5.29	1.65	1.53
12	5	192	SER	CA-CB	5.29	1.60	1.52
15	W	27	GLU	CG-CD	5.29	1.59	1.51
4	D	48	ARG	CZ-NH2	5.29	1.40	1.33
8	1	11	SER	CB-OG	5.28	1.49	1.42
10	3	203	ARG	CZ-NH2	5.28	1.40	1.33
1	A	166	TYR	CG-CD2	5.28	1.46	1.39
4	D	227	GLU	CG-CD	5.28	1.59	1.51
21	N	292	GLY	N-CA	-5.28	1.38	1.46
33	J	316	PHE	CB-CG	5.28	1.60	1.51
2	b	234	ARG	CZ-NH1	5.27	1.40	1.33
7	G	119	TYR	CE1-CZ	5.27	1.45	1.38
12	l	82	ARG	NE-CZ	5.27	1.40	1.33
29	I	408	ARG	CD-NE	5.27	1.55	1.46
33	J	309	ARG	CZ-NH1	5.27	1.39	1.33
11	k	85	ARG	CZ-NH1	5.27	1.39	1.33
10	j	80	ARG	CZ-NH2	5.26	1.39	1.33
14	7	220	ARG	NE-CZ	5.26	1.39	1.33
18	X	56	PRO	C-N	5.26	1.46	1.34
28	H	53	GLU	CB-CG	5.26	1.62	1.52
28	H	286	GLU	C-N	5.26	1.42	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	71	GLU	N-CA	-5.26	1.35	1.46
19	Y	22	GLU	CB-CG	5.26	1.62	1.52
21	N	604	ARG	CZ-NH2	5.26	1.39	1.33
21	N	251	GLU	CG-CD	5.26	1.59	1.51
8	1	174	TRP	NE1-CE2	-5.26	1.30	1.37
13	6	85	PHE	CG-CD2	5.26	1.46	1.38
29	I	347	LYS	N-CA	-5.25	1.35	1.46
4	d	90	ARG	CZ-NH1	5.25	1.39	1.33
11	4	139	TYR	CD2-CE2	5.25	1.47	1.39
15	W	101	ARG	NE-CZ	5.25	1.39	1.33
32	M	281	ASP	CA-CB	5.25	1.65	1.53
5	e	122	ARG	CZ-NH2	5.25	1.39	1.33
4	D	124	GLY	CA-C	-5.25	1.43	1.51
21	N	178	SER	CB-OG	5.25	1.49	1.42
12	5	226	GLU	CB-CG	5.25	1.62	1.52
11	4	149	ARG	CZ-NH2	5.24	1.39	1.33
1	a	234	PHE	CG-CD2	5.24	1.46	1.38
9	2	82	GLU	CG-CD	5.24	1.59	1.51
15	W	127	ARG	CZ-NH1	5.24	1.39	1.33
18	X	81	SER	CB-OG	-5.24	1.35	1.42
23	P	358	SER	CA-CB	5.24	1.60	1.52
30	K	400	TYR	CE2-CZ	5.24	1.45	1.38
5	E	167	TYR	CZ-OH	5.24	1.46	1.37
15	W	182	TYR	CE1-CZ	5.24	1.45	1.38
22	S	186	TYR	CD2-CE2	5.24	1.47	1.39
28	H	434	ARG	NE-CZ	5.24	1.39	1.33
31	L	255	TYR	CB-CG	-5.24	1.43	1.51
18	X	85	ARG	CZ-NH1	5.24	1.39	1.33
20	Z	202	ARG	CZ-NH2	5.24	1.39	1.33
3	C	137	TYR	CG-CD2	-5.23	1.32	1.39
27	O	15	ARG	NE-CZ	5.23	1.39	1.33
27	O	209	GLU	CD-OE2	-5.23	1.19	1.25
28	H	318	ARG	CZ-NH2	5.23	1.39	1.33
16	V	179	LEU	CA-CB	5.23	1.65	1.53
24	Q	366	ILE	N-CA	-5.23	1.35	1.46
15	W	167	GLU	CD-OE1	-5.23	1.19	1.25
27	O	288	ARG	CD-NE	5.23	1.55	1.46
21	N	434	SER	C-N	5.23	1.42	1.33
25	R	246	TYR	CD2-CE2	5.22	1.47	1.39
11	4	8	ARG	CZ-NH1	5.22	1.39	1.33
21	N	394	ARG	NE-CZ	5.22	1.39	1.33
27	O	210	ARG	CZ-NH1	5.22	1.39	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	29	GLU	CG-CD	5.22	1.59	1.51
10	3	136	PHE	CB-CG	-5.22	1.42	1.51
12	l	81	PHE	CD1-CE1	-5.22	1.28	1.39
5	E	210	GLU	CD-OE2	-5.22	1.20	1.25
18	X	11	ARG	CD-NE	5.22	1.55	1.46
9	2	126	TYR	CB-CG	-5.22	1.43	1.51
10	3	177	ARG	NE-CZ	5.22	1.39	1.33
9	i	225	ARG	CD-NE	5.22	1.55	1.46
11	k	70	ARG	NE-CZ	5.22	1.39	1.33
12	l	272	PHE	CB-CG	5.22	1.60	1.51
15	W	179	ARG	CD-NE	5.21	1.55	1.46
23	P	240	TYR	CZ-OH	5.21	1.46	1.37
24	Q	431	SER	CA-CB	5.21	1.60	1.52
14	n	78	VAL	N-CA	-5.21	1.35	1.46
30	K	393	ARG	CZ-NH2	5.21	1.39	1.33
33	J	231	ARG	CZ-NH1	5.21	1.39	1.33
8	h	202	TYR	CB-CG	-5.21	1.43	1.51
13	m	145	ARG	NE-CZ	5.21	1.39	1.33
13	6	229	ARG	CZ-NH2	5.21	1.39	1.33
11	4	147	HIS	CG-CD2	5.20	1.44	1.35
13	6	73	VAL	CB-CG1	5.20	1.63	1.52
21	N	162	ARG	CD-NE	5.20	1.55	1.46
1	a	97	ALA	N-CA	-5.20	1.35	1.46
10	3	68	ARG	NE-CZ	5.20	1.39	1.33
19	Y	86	ARG	CD-NE	5.20	1.55	1.46
27	O	135	ARG	CZ-NH1	5.20	1.39	1.33
20	Z	165	TYR	CE1-CZ	5.20	1.45	1.38
27	O	65	PHE	CG-CD1	5.20	1.46	1.38
5	E	95	ALA	CA-CB	5.20	1.63	1.52
21	N	105	SER	CA-CB	5.20	1.60	1.52
26	U	66	TRP	CZ3-CH2	5.20	1.48	1.40
18	X	84	GLY	CA-C	-5.19	1.43	1.51
11	k	60	ILE	N-CA	-5.19	1.35	1.46
31	L	60	PHE	CG-CD2	5.19	1.46	1.38
8	h	120	TYR	CE2-CZ	5.19	1.45	1.38
5	E	235	LYS	CA-CB	5.19	1.65	1.53
24	Q	294	ARG	NE-CZ	5.19	1.39	1.33
32	M	307	GLU	CG-CD	5.19	1.59	1.51
20	Z	174	GLU	CG-CD	5.19	1.59	1.51
17	T	128	TYR	CG-CD2	5.19	1.45	1.39
27	O	387	ARG	CZ-NH2	5.19	1.39	1.33
13	m	193	ARG	CD-NE	5.18	1.55	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	33	ARG	CD-NE	5.18	1.55	1.46
12	l	212	TYR	CE1-CZ	5.18	1.45	1.38
8	1	142	PHE	CG-CD2	5.18	1.46	1.38
27	O	108	GLU	CG-CD	5.18	1.59	1.51
13	m	114	TYR	CA-C	-5.18	1.39	1.52
1	A	186	PHE	CG-CD1	5.18	1.46	1.38
11	4	23	ARG	NE-CZ	5.18	1.39	1.33
2	b	232	GLY	N-CA	-5.18	1.38	1.46
12	l	196	ARG	NE-CZ	5.18	1.39	1.33
16	V	257	GLU	CD-OE2	5.18	1.31	1.25
6	F	3	ARG	CD-NE	5.17	1.55	1.46
24	Q	206	ASN	CA-C	-5.17	1.39	1.52
31	L	96	LYS	CA-CB	5.17	1.65	1.53
31	L	269	TYR	CZ-OH	5.17	1.46	1.37
20	Z	55	ARG	NE-CZ	5.17	1.39	1.33
3	c	98	TYR	CZ-OH	5.17	1.46	1.37
9	i	120	GLN	CA-CB	5.17	1.65	1.53
18	X	17	TYR	CG-CD1	5.17	1.45	1.39
1	a	42	SER	N-CA	-5.17	1.36	1.46
6	F	13	PHE	CG-CD2	5.16	1.46	1.38
4	d	141	ARG	CD-NE	5.16	1.55	1.46
2	b	6	SER	CA-CB	5.16	1.60	1.52
13	6	159	ASP	CB-CG	5.16	1.62	1.51
21	N	139	ARG	CD-NE	5.16	1.55	1.46
28	H	420	ARG	NE-CZ	5.16	1.39	1.33
6	f	27	GLU	CG-CD	-5.16	1.44	1.51
24	Q	202	ARG	NE-CZ	5.15	1.39	1.33
30	K	141	ARG	N-CA	-5.15	1.36	1.46
2	b	101	TYR	CE1-CZ	5.15	1.45	1.38
2	b	210	GLU	CD-OE2	5.15	1.31	1.25
4	D	111	ARG	NE-CZ	5.15	1.39	1.33
12	5	234	ARG	NE-CZ	5.15	1.39	1.33
21	N	786	ARG	CZ-NH2	5.15	1.39	1.33
22	S	22	GLU	CD-OE1	5.15	1.31	1.25
28	H	454	TYR	CG-CD1	5.15	1.45	1.39
2	b	128	ARG	CZ-NH2	5.15	1.39	1.33
7	g	149	TYR	CG-CD2	-5.15	1.32	1.39
4	d	25	GLU	CD-OE1	-5.15	1.20	1.25
28	H	370	ARG	CG-CD	5.15	1.64	1.51
23	P	282	HIS	CG-CD2	5.15	1.44	1.35
6	f	59	TYR	CG-CD1	5.14	1.45	1.39
20	Z	113	SER	CA-CB	5.14	1.60	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	198	TYR	CG-CD1	5.14	1.45	1.39
32	M	290	ARG	NE-CZ	5.14	1.39	1.33
13	6	83	TYR	CG-CD1	-5.14	1.32	1.39
24	Q	344	GLU	CB-CG	5.14	1.61	1.52
14	7	226	ARG	CZ-NH2	5.14	1.39	1.33
23	P	356	TYR	CG-CD1	5.13	1.45	1.39
24	Q	197	SER	CB-OG	5.13	1.49	1.42
21	N	743	PHE	CG-CD2	5.13	1.46	1.38
11	k	58	GLU	CB-CG	5.13	1.61	1.52
25	R	307	TYR	CG-CD2	5.13	1.45	1.39
12	l	100	TRP	CE3-CZ3	5.13	1.47	1.38
25	R	349	SER	CA-CB	5.13	1.60	1.52
6	f	82	ARG	CZ-NH2	5.13	1.39	1.33
20	Z	358	TYR	CE1-CZ	5.13	1.45	1.38
20	Z	912	PHE	CG-CD1	5.13	1.46	1.38
21	N	870	ASN	CB-CG	5.13	1.62	1.51
30	K	121	ARG	NE-CZ	5.13	1.39	1.33
20	Z	34	GLU	CD-OE2	5.12	1.31	1.25
22	S	382	ARG	CZ-NH2	5.12	1.39	1.33
6	f	55	GLU	CG-CD	5.12	1.59	1.51
16	V	128	SER	CB-OG	-5.12	1.35	1.42
32	M	203	ARG	CZ-NH2	5.12	1.39	1.33
3	c	160	TRP	NE1-CE2	-5.12	1.30	1.37
11	4	82	SER	CB-OG	5.12	1.49	1.42
3	C	13	PHE	CE2-CZ	5.12	1.47	1.37
4	D	103	PRO	N-CD	-5.12	1.40	1.47
2	b	160	LYS	CD-CE	5.12	1.64	1.51
20	Z	384	SER	CA-CB	5.12	1.60	1.52
22	S	25	TYR	CD1-CE1	5.12	1.47	1.39
22	S	147	TRP	CZ2-CH2	5.12	1.47	1.37
5	E	231	TYR	CG-CD2	5.12	1.45	1.39
7	G	8	TYR	CG-CD1	5.12	1.45	1.39
23	P	159	ILE	CA-CB	5.11	1.66	1.54
28	H	234	ARG	CZ-NH2	5.11	1.39	1.33
30	K	262	ARG	NE-CZ	5.11	1.39	1.33
32	M	339	ARG	NE-CZ	5.11	1.39	1.33
21	N	291	SER	C-N	5.11	1.42	1.33
30	K	129	GLU	CD-OE1	5.11	1.31	1.25
2	B	62	SER	CB-OG	-5.11	1.35	1.42
8	1	70	TYR	CE1-CZ	5.11	1.45	1.38
1	a	24	ARG	CZ-NH1	5.11	1.39	1.33
8	h	87	ALA	CA-CB	5.11	1.63	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	142	GLU	CG-CD	-5.11	1.44	1.51
2	b	83	ARG	NE-CZ	5.11	1.39	1.33
4	D	137	GLY	N-CA	-5.11	1.38	1.46
25	R	246	TYR	CE2-CZ	5.10	1.45	1.38
7	g	86	ARG	CZ-NH2	5.10	1.39	1.33
11	k	139	TYR	CE1-CZ	5.10	1.45	1.38
3	C	28	SER	CB-OG	5.10	1.48	1.42
17	T	83	ASN	N-CA	-5.10	1.36	1.46
25	R	181	TYR	CB-CG	5.10	1.59	1.51
11	k	121	TYR	CB-CG	5.10	1.59	1.51
23	P	245	TYR	CZ-OH	5.10	1.46	1.37
33	J	231	ARG	CD-NE	5.10	1.55	1.46
12	l	189	TYR	CG-CD1	5.10	1.45	1.39
10	3	65	GLU	CA-CB	5.10	1.65	1.53
24	Q	232	TYR	CE1-CZ	5.10	1.45	1.38
30	K	172	ALA	CA-CB	5.10	1.63	1.52
31	L	77	ARG	CZ-NH2	5.09	1.39	1.33
3	c	137	TYR	CG-CD2	5.09	1.45	1.39
1	A	55	SER	CB-OG	5.09	1.48	1.42
1	A	200	GLU	CG-CD	5.09	1.59	1.51
19	Y	31	GLU	CA-CB	5.09	1.65	1.53
23	P	19	GLU	CD-OE1	-5.09	1.20	1.25
11	4	81	SER	CA-CB	5.09	1.60	1.52
11	4	98	TYR	CE1-CZ	5.09	1.45	1.38
6	f	123	TYR	CE2-CZ	5.09	1.45	1.38
8	h	20	GLY	CA-C	-5.09	1.43	1.51
30	K	246	TYR	CZ-OH	5.09	1.46	1.37
33	J	247	MET	CA-CB	5.09	1.65	1.53
14	n	74	ARG	CZ-NH1	5.08	1.39	1.33
26	U	292	ILE	N-CA	-5.08	1.36	1.46
21	N	139	ARG	CZ-NH1	5.08	1.39	1.33
6	F	233	TYR	CB-CG	-5.08	1.44	1.51
4	d	154	GLY	N-CA	-5.08	1.38	1.46
25	R	210	TYR	CZ-OH	5.08	1.46	1.37
21	N	565	ASN	CB-CG	5.08	1.62	1.51
21	N	912	GLU	CG-CD	5.08	1.59	1.51
27	O	232	GLU	CG-CD	5.08	1.59	1.51
25	R	222	ARG	CZ-NH2	5.07	1.39	1.33
13	6	193	ARG	CZ-NH2	5.07	1.39	1.33
17	T	60	ARG	NE-CZ	5.07	1.39	1.33
27	O	248	TYR	CE1-CZ	5.07	1.45	1.38
9	i	95	HIS	CB-CG	5.07	1.59	1.50

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	96	SER	CA-CB	5.07	1.60	1.52
27	O	220	SER	CA-CB	-5.07	1.45	1.52
28	H	425	GLU	CB-CG	5.07	1.61	1.52
11	4	130	TYR	CD2-CE2	5.06	1.47	1.39
27	O	17	GLU	CD-OE1	5.06	1.31	1.25
27	O	119	SER	CB-OG	-5.06	1.35	1.42
6	f	6	TYR	CE2-CZ	5.06	1.45	1.38
3	c	166	GLY	N-CA	-5.06	1.38	1.46
4	D	97	ARG	CZ-NH2	5.06	1.39	1.33
24	Q	195	LYS	CA-CB	5.06	1.65	1.53
3	c	16	GLU	CG-CD	5.05	1.59	1.51
19	Y	38	PHE	CG-CD2	5.05	1.46	1.38
25	R	62	TYR	CG-CD1	5.05	1.45	1.39
14	7	170	TYR	CE1-CZ	5.05	1.45	1.38
30	K	427	TYR	CZ-OH	5.05	1.46	1.37
25	R	219	LEU	C-N	5.05	1.45	1.34
11	k	39	SER	CA-CB	5.05	1.60	1.52
25	R	43	ARG	CD-NE	5.05	1.55	1.46
28	H	463	TYR	CG-CD1	5.05	1.45	1.39
29	I	346	ARG	CZ-NH1	5.05	1.39	1.33
3	c	234	GLU	CD-OE1	-5.05	1.20	1.25
14	n	151	GLY	N-CA	-5.05	1.38	1.46
13	6	106	TYR	CD2-CE2	5.05	1.47	1.39
13	6	114	TYR	CE1-CZ	5.05	1.45	1.38
10	j	5	SER	CB-OG	-5.04	1.35	1.42
4	D	29	ARG	NE-CZ	5.04	1.39	1.33
21	N	813	ARG	CD-NE	5.04	1.55	1.46
9	i	217	ARG	NE-CZ	5.04	1.39	1.33
10	j	103	TYR	CG-CD1	5.04	1.45	1.39
15	W	41	ARG	N-CA	-5.04	1.36	1.46
2	B	52	SER	CA-CB	5.04	1.60	1.52
4	D	92	GLU	CD-OE1	5.04	1.31	1.25
22	S	440	ASP	C-N	5.04	1.42	1.33
10	j	155	GLU	CG-CD	5.04	1.59	1.51
11	4	76	SER	CA-CB	5.04	1.60	1.52
14	7	261	TYR	C-N	5.03	1.42	1.33
28	H	82	TRP	CD2-CE3	-5.03	1.32	1.40
14	n	74	ARG	CZ-NH2	5.03	1.39	1.33
2	b	42	GLY	CA-C	5.03	1.59	1.51
14	n	73	GLU	CB-CG	5.03	1.61	1.52
33	J	235	VAL	CB-CG1	5.03	1.63	1.52
10	3	25	CYS	N-CA	-5.03	1.36	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	504	TYR	CZ-OH	5.03	1.46	1.37
2	b	148	TYR	CG-CD2	5.03	1.45	1.39
1	A	192	ASP	CB-CG	5.03	1.62	1.51
3	C	144	TYR	CZ-OH	5.03	1.46	1.37
27	O	330	ARG	CD-NE	5.03	1.54	1.46
29	I	434	GLY	CA-C	-5.02	1.43	1.51
1	a	189	SER	CA-CB	5.02	1.60	1.52
21	N	414	GLY	CA-C	-5.02	1.43	1.51
28	H	125	SER	CA-CB	5.02	1.60	1.52
30	K	346	ARG	CZ-NH1	5.02	1.39	1.33
5	E	20	ARG	NE-CZ	5.01	1.39	1.33
10	3	154	TYR	CE2-CZ	5.01	1.45	1.38
21	N	526	TYR	CB-CG	5.01	1.59	1.51
25	R	312	TYR	CB-CG	5.01	1.59	1.51
33	J	91	GLU	N-CA	-5.01	1.36	1.46
11	k	96	ARG	NE-CZ	5.01	1.39	1.33
14	7	49	TYR	CG-CD2	5.01	1.45	1.39
13	m	113	TYR	CG-CD2	5.01	1.45	1.39
1	A	251	GLN	C-O	5.01	1.32	1.23
13	m	171	GLY	CA-C	-5.01	1.43	1.51
21	N	168	SER	CB-OG	5.01	1.48	1.42
23	P	117	SER	CA-CB	5.01	1.60	1.52
27	O	356	ARG	CD-NE	5.01	1.54	1.46
21	N	836	GLU	CD-OE2	5.01	1.31	1.25
12	5	163	TYR	CZ-OH	5.01	1.46	1.37
26	U	100	ARG	CZ-NH1	5.01	1.39	1.33
32	M	267	PHE	CA-CB	5.01	1.65	1.53
19	Y	60	TRP	CZ2-CH2	5.00	1.46	1.37
20	Z	426	TYR	CG-CD1	5.00	1.45	1.39
25	R	20	ARG	CZ-NH2	5.00	1.39	1.33
1	a	91	ARG	CZ-NH1	5.00	1.39	1.33
8	1	120	TYR	CG-CD2	5.00	1.45	1.39
23	P	77	GLU	CD-OE2	5.00	1.31	1.25
29	I	319	ARG	CD-NE	5.00	1.54	1.46
16	V	282	GLU	CB-CG	5.00	1.61	1.52
20	Z	136	ARG	CZ-NH2	5.00	1.39	1.33

All (2660) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	6	ARG	NE-CZ-NH1	-20.22	110.19	120.30
4	D	6	ARG	NE-CZ-NH2	18.42	129.51	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	259	TYR	CB-CG-CD2	18.40	132.04	121.00
5	e	231	TYR	CB-CG-CD2	18.27	131.96	121.00
5	e	136	ARG	NE-CZ-NH1	16.91	128.75	120.30
31	L	357	ARG	NE-CZ-NH2	-16.89	111.86	120.30
10	3	203	ARG	NE-CZ-NH2	-16.84	111.88	120.30
24	Q	51	ARG	NE-CZ-NH2	-16.59	112.01	120.30
1	a	131	ARG	NE-CZ-NH2	-16.57	112.02	120.30
22	S	292	TYR	CB-CG-CD2	-16.38	111.17	121.00
24	Q	398	TYR	CB-CG-CD1	-16.05	111.37	121.00
8	h	151	PHE	CB-CG-CD2	15.97	131.98	120.80
6	F	3	ARG	NE-CZ-NH1	15.97	128.28	120.30
3	C	24	TYR	CB-CG-CD2	-15.90	111.46	121.00
4	D	22	TYR	CB-CG-CD2	-15.90	111.46	121.00
20	Z	574	TYR	CB-CG-CD2	-15.67	111.60	121.00
31	L	82	ARG	NE-CZ-NH2	-15.44	112.58	120.30
20	Z	439	TYR	CB-CG-CD1	15.29	130.17	121.00
14	7	223	ARG	NE-CZ-NH2	-15.13	112.73	120.30
14	7	124	TYR	CB-CG-CD2	-15.00	112.00	121.00
14	7	137	ARG	NE-CZ-NH1	14.88	127.74	120.30
1	a	163	TYR	CB-CG-CD1	14.71	129.82	121.00
9	2	236	ARG	NE-CZ-NH2	-14.70	112.95	120.30
8	h	151	PHE	CB-CG-CD1	-14.63	110.56	120.80
27	O	195	TYR	CB-CG-CD1	-14.43	112.34	121.00
18	X	59	ARG	NE-CZ-NH2	14.43	127.51	120.30
5	e	231	TYR	CB-CG-CD1	-14.39	112.37	121.00
7	G	86	ARG	NE-CZ-NH2	-14.38	113.11	120.30
4	D	111	ARG	NE-CZ-NH1	14.35	127.48	120.30
25	R	307	TYR	CB-CG-CD1	14.24	129.55	121.00
22	S	367	TYR	CB-CG-CD2	14.17	129.50	121.00
32	M	342	ARG	NE-CZ-NH2	-14.09	113.25	120.30
22	S	425	ARG	NE-CZ-NH1	14.05	127.33	120.30
31	L	191	ARG	NE-CZ-NH1	-14.05	113.27	120.30
20	Z	574	TYR	CB-CG-CD1	14.03	129.42	121.00
30	K	207	ARG	NE-CZ-NH2	-14.02	113.29	120.30
23	P	47	ARG	NE-CZ-NH1	13.84	127.22	120.30
24	Q	286	TYR	CB-CG-CD1	-13.82	112.71	121.00
14	7	124	TYR	CB-CG-CD1	13.78	129.27	121.00
12	l	82	ARG	NE-CZ-NH2	-13.78	113.41	120.30
14	n	74	ARG	NE-CZ-NH1	13.73	127.17	120.30
22	S	119	TYR	CB-CG-CD2	-13.66	112.80	121.00
22	S	25	TYR	CB-CG-CD1	-13.56	112.86	121.00
21	N	298	TYR	CB-CG-CD1	13.56	129.13	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	338	TYR	CB-CG-CD1	13.52	129.11	121.00
3	C	137	TYR	CB-CG-CD1	-13.37	112.98	121.00
22	S	467	PHE	CB-CG-CD1	13.32	130.12	120.80
23	P	234	TYR	CB-CG-CD1	-13.30	113.02	121.00
12	l	148	ARG	NE-CZ-NH1	13.25	126.93	120.30
21	N	81	TYR	CB-CG-CD2	13.23	128.94	121.00
12	5	179	TYR	CB-CG-CD2	-13.20	113.08	121.00
11	k	70	ARG	NE-CZ-NH1	13.20	126.90	120.30
22	S	119	TYR	CB-CG-CD1	13.16	128.90	121.00
20	Z	385	PHE	CB-CG-CD2	-13.14	111.60	120.80
7	g	157	TYR	CB-CG-CD1	-13.12	113.13	121.00
21	N	282	TYR	CB-CG-CD1	-13.06	113.16	121.00
21	N	471	TYR	CB-CG-CD2	-13.05	113.17	121.00
19	Y	73	PHE	CB-CG-CD2	13.04	129.93	120.80
19	Y	84	TYR	CB-CG-CD2	-13.02	113.19	121.00
32	M	207	PHE	CB-CG-CD1	-12.99	111.70	120.80
10	3	69	TYR	CB-CG-CD1	12.98	128.79	121.00
20	Z	269	TYR	CB-CG-CD2	-12.87	113.28	121.00
7	g	130	ARG	NE-CZ-NH2	-12.83	113.88	120.30
20	Z	264	PHE	CB-CG-CD2	-12.79	111.85	120.80
22	S	25	TYR	CB-CG-CD2	12.72	128.63	121.00
7	G	8	TYR	CB-CG-CD1	-12.71	113.37	121.00
32	M	264	ARG	NE-CZ-NH1	12.68	126.64	120.30
22	S	259	TYR	CB-CG-CD1	-12.64	113.41	121.00
2	B	101	TYR	CB-CG-CD2	12.64	128.59	121.00
4	D	148	TYR	CB-CG-CD2	-12.57	113.46	121.00
30	K	207	ARG	NE-CZ-NH1	12.55	126.58	120.30
19	Y	73	PHE	CB-CG-CD1	-12.54	112.02	120.80
21	N	504	TYR	CB-CG-CD1	12.49	128.50	121.00
3	c	180	TYR	CB-CG-CD1	-12.49	113.51	121.00
3	C	24	TYR	CB-CG-CD1	12.48	128.49	121.00
4	d	83	ARG	NE-CZ-NH1	12.48	126.54	120.30
20	Z	103	TYR	CB-CG-CD1	12.47	128.48	121.00
31	L	77	ARG	NE-CZ-NH2	-12.47	114.07	120.30
1	a	30	TYR	CB-CG-CD1	12.43	128.46	121.00
23	P	3	ARG	NE-CZ-NH2	-12.43	114.08	120.30
29	I	317	ASP	CB-CG-OD2	12.43	129.48	118.30
24	Q	240	PHE	CB-CG-CD1	12.41	129.49	120.80
1	a	131	ARG	NE-CZ-NH1	12.35	126.47	120.30
31	L	168	TYR	CB-CG-CD2	-12.35	113.59	121.00
20	Z	738	TYR	CB-CG-CD1	12.29	128.38	121.00
25	R	417	TYR	CB-CG-CD2	-12.29	113.63	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	189	TYR	CB-CG-CD1	-12.28	113.63	121.00
7	g	20	ARG	NE-CZ-NH1	-12.23	114.19	120.30
8	h	194	ARG	NE-CZ-NH1	12.20	126.40	120.30
22	S	467	PHE	CB-CG-CD2	-12.20	112.26	120.80
13	6	75	ARG	NE-CZ-NH1	-12.19	114.21	120.30
31	L	126	ARG	NE-CZ-NH2	-12.18	114.21	120.30
32	M	207	PHE	CB-CG-CD2	12.17	129.32	120.80
28	H	463	TYR	CB-CG-CD1	-12.15	113.71	121.00
20	Z	96	TYR	CB-CG-CD1	-12.15	113.71	121.00
27	O	286	PHE	CB-CG-CD2	-12.13	112.31	120.80
32	M	320	ARG	NE-CZ-NH2	-12.10	114.25	120.30
7	g	119	TYR	CB-CG-CD2	-12.07	113.76	121.00
31	L	269	TYR	CB-CG-CD2	-12.07	113.76	121.00
4	D	22	TYR	CB-CG-CD1	12.05	128.23	121.00
29	I	304	ARG	NE-CZ-NH2	-12.05	114.28	120.30
28	H	343	PHE	CB-CG-CD2	-11.97	112.42	120.80
32	M	357	ARG	NE-CZ-NH2	11.94	126.27	120.30
9	i	152	TYR	CB-CG-CD1	11.94	128.16	121.00
27	O	62	TYR	CB-CG-CD2	-11.93	113.84	121.00
29	I	319	ARG	NE-CZ-NH2	-11.92	114.34	120.30
14	7	68	ARG	NE-CZ-NH2	-11.91	114.34	120.30
32	M	213	ARG	NE-CZ-NH2	-11.91	114.34	120.30
24	Q	189	ARG	NE-CZ-NH1	11.82	126.21	120.30
6	F	225	TYR	CB-CG-CD2	-11.80	113.92	121.00
32	M	320	ARG	NE-CZ-NH1	11.77	126.18	120.30
1	A	46	ARG	NE-CZ-NH2	-11.75	114.42	120.30
30	K	141	ARG	NE-CZ-NH2	-11.73	114.44	120.30
23	P	51	ASP	CB-CG-OD2	-11.72	107.75	118.30
27	O	286	PHE	CB-CG-CD1	11.70	128.99	120.80
1	a	163	TYR	CB-CG-CD2	-11.69	113.98	121.00
2	b	82	TYR	CB-CG-CD2	-11.66	114.00	121.00
13	m	109	ARG	NE-CZ-NH1	11.64	126.12	120.30
11	k	85	ARG	NE-CZ-NH2	-11.63	114.49	120.30
7	g	22	PHE	CB-CG-CD2	-11.59	112.69	120.80
4	D	148	TYR	CB-CG-CD1	11.58	127.95	121.00
3	c	180	TYR	CB-CG-CD2	11.52	127.91	121.00
11	k	85	ARG	NE-CZ-NH1	11.48	126.04	120.30
33	J	371	ARG	NE-CZ-NH1	11.47	126.04	120.30
1	A	205	PHE	CB-CG-CD1	-11.47	112.77	120.80
26	U	154	PHE	CB-CG-CD2	-11.46	112.78	120.80
33	J	56	ARG	NE-CZ-NH1	-11.46	114.57	120.30
24	Q	400	TYR	CB-CG-CD1	-11.45	114.13	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	101	TYR	CB-CG-CD1	-11.43	114.14	121.00
28	H	454	TYR	CB-CG-CD2	11.41	127.85	121.00
21	N	711	ARG	NE-CZ-NH1	11.39	125.99	120.30
31	L	264	ARG	NE-CZ-NH1	11.37	125.98	120.30
31	L	137	ARG	NE-CZ-NH2	-11.35	114.63	120.30
7	g	130	ARG	NE-CZ-NH1	11.34	125.97	120.30
8	1	142	PHE	CB-CG-CD1	-11.31	112.88	120.80
28	H	234	ARG	NE-CZ-NH2	-11.27	114.67	120.30
20	Z	55	ARG	NE-CZ-NH1	11.25	125.92	120.30
25	R	181	TYR	CB-CG-CD2	-11.25	114.25	121.00
20	Z	928	ARG	NE-CZ-NH2	-11.25	114.68	120.30
33	J	371	ARG	NE-CZ-NH2	-11.23	114.69	120.30
11	k	135	TYR	CB-CG-CD2	-11.21	114.28	121.00
4	D	97	ARG	NE-CZ-NH1	11.19	125.89	120.30
22	S	51	ARG	NE-CZ-NH2	-11.15	114.72	120.30
24	Q	130	ARG	NE-CZ-NH2	11.15	125.87	120.30
30	K	262	ARG	NE-CZ-NH2	-11.14	114.73	120.30
26	U	254	ARG	NE-CZ-NH2	-11.13	114.74	120.30
4	d	58	ARG	NE-CZ-NH2	-11.12	114.74	120.30
9	2	225	ARG	NE-CZ-NH1	11.12	125.86	120.30
10	3	103	TYR	CB-CG-CD1	-11.11	114.33	121.00
27	O	387	ARG	NE-CZ-NH1	11.07	125.83	120.30
28	H	181	TYR	CB-CG-CD2	-11.04	114.37	121.00
15	W	127	ARG	NE-CZ-NH1	11.03	125.81	120.30
33	J	373	ARG	NE-CZ-NH2	-11.02	114.79	120.30
23	P	13	TYR	CB-CG-CD2	-11.01	114.39	121.00
17	T	81	TYR	CB-CG-CD2	-11.00	114.40	121.00
33	J	368	TYR	CB-CG-CD2	-11.00	114.40	121.00
29	I	304	ARG	NE-CZ-NH1	10.99	125.79	120.30
22	S	425	ARG	NE-CZ-NH2	-10.95	114.83	120.30
23	P	123	ARG	NE-CZ-NH1	-10.93	114.83	120.30
33	J	248	ASP	CB-CG-OD1	-10.92	108.47	118.30
33	J	120	TYR	CB-CG-CD1	10.91	127.54	121.00
6	f	3	ARG	NE-CZ-NH1	10.86	125.73	120.30
11	4	141	PHE	CB-CG-CD1	10.85	128.40	120.80
28	H	261	ARG	NE-CZ-NH2	-10.85	114.87	120.30
28	H	454	TYR	CB-CG-CD1	-10.85	114.49	121.00
32	M	303	ARG	NE-CZ-NH1	-10.84	114.88	120.30
1	A	26	TYR	CB-CG-CD1	10.81	127.48	121.00
1	A	162	TYR	CB-CG-CD2	10.80	127.48	121.00
10	j	199	TYR	CB-CG-CD1	10.77	127.46	121.00
33	J	63	ARG	NE-CZ-NH1	10.76	125.68	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	266	ARG	NE-CZ-NH2	-10.74	114.93	120.30
20	Z	843	ASP	CB-CG-OD2	-10.71	108.66	118.30
24	Q	255	TYR	CB-CG-CD1	-10.71	114.57	121.00
21	N	81	TYR	CB-CG-CD1	-10.67	114.60	121.00
22	S	367	TYR	CB-CG-CD1	-10.66	114.60	121.00
22	S	114	TYR	CB-CG-CD2	-10.64	114.61	121.00
10	3	203	ARG	NE-CZ-NH1	10.63	125.61	120.30
2	B	145	PHE	CB-CG-CD1	-10.63	113.36	120.80
20	Z	137	TYR	CB-CG-CD1	10.61	127.36	121.00
4	d	232	TYR	CB-CG-CD1	10.59	127.35	121.00
28	H	390	ARG	NE-CZ-NH2	-10.58	115.01	120.30
33	J	210	PHE	CB-CG-CD1	-10.56	113.41	120.80
27	O	306	ARG	NE-CZ-NH1	-10.51	115.05	120.30
21	N	282	TYR	CB-CG-CD2	10.50	127.30	121.00
22	S	51	ARG	NE-CZ-NH1	10.48	125.54	120.30
19	Y	84	TYR	CB-CG-CD1	10.48	127.29	121.00
22	S	211	ARG	NE-CZ-NH2	-10.47	115.06	120.30
33	J	312	ARG	NE-CZ-NH1	10.47	125.53	120.30
20	Z	339	PHE	CB-CG-CD2	-10.46	113.47	120.80
30	K	346	ARG	NE-CZ-NH1	10.45	125.53	120.30
18	X	11	ARG	NE-CZ-NH2	-10.45	115.08	120.30
2	b	4	ARG	NE-CZ-NH2	-10.44	115.08	120.30
17	T	186	ARG	NE-CZ-NH2	-10.43	115.09	120.30
12	l	148	ARG	NE-CZ-NH2	-10.40	115.10	120.30
17	T	172	SER	N-CA-CB	10.40	126.10	110.50
4	d	218	ASP	CB-CG-OD1	-10.38	108.96	118.30
20	Z	970	TYR	CB-CG-CD1	-10.37	114.78	121.00
2	b	142	PHE	CB-CG-CD2	-10.36	113.55	120.80
9	2	152	TYR	CB-CG-CD1	-10.35	114.79	121.00
15	W	41	ARG	NE-CZ-NH2	-10.35	115.13	120.30
13	6	139	TYR	CB-CG-CD1	-10.34	114.79	121.00
28	H	432	ARG	NE-CZ-NH1	-10.33	115.13	120.30
32	M	357	ARG	NE-CZ-NH1	-10.33	115.13	120.30
7	g	20	ARG	NE-CZ-NH2	10.33	125.46	120.30
2	b	246	ARG	NE-CZ-NH1	10.32	125.46	120.30
4	d	83	ARG	NE-CZ-NH2	-10.31	115.14	120.30
13	6	46	ARG	NE-CZ-NH1	10.31	125.45	120.30
10	3	136	PHE	CB-CG-CD1	-10.30	113.59	120.80
5	e	26	TYR	CB-CG-CD1	-10.30	114.82	121.00
21	N	298	TYR	CB-CG-CD2	-10.29	114.83	121.00
20	Z	774	ARG	NE-CZ-NH1	10.29	125.44	120.30
7	G	8	TYR	CB-CG-CD2	10.27	127.16	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	68	ARG	NE-CZ-NH1	10.27	125.44	120.30
17	T	245	TYR	CB-CG-CD2	10.26	127.16	121.00
30	K	400	TYR	CB-CG-CD2	-10.25	114.85	121.00
4	d	156	TYR	CB-CG-CD1	-10.20	114.88	121.00
21	N	743	PHE	CB-CG-CD2	10.20	127.94	120.80
31	L	82	ARG	NE-CZ-NH1	10.20	125.40	120.30
4	D	111	ARG	NE-CZ-NH2	-10.19	115.20	120.30
14	n	126	PHE	CB-CG-CD1	10.17	127.92	120.80
19	Y	86	ARG	NE-CZ-NH1	10.17	125.39	120.30
11	4	36	ARG	NE-CZ-NH2	-10.17	115.22	120.30
22	S	480	ARG	NE-CZ-NH1	10.15	125.38	120.30
6	f	82	ARG	NE-CZ-NH2	-10.15	115.23	120.30
22	S	95	PHE	CB-CG-CD1	10.12	127.88	120.80
11	k	70	ARG	NE-CZ-NH2	-10.11	115.24	120.30
30	K	344	ARG	NE-CZ-NH2	-10.11	115.25	120.30
33	J	71	TYR	CB-CG-CD2	-10.09	114.94	121.00
26	U	79	MET	CG-SD-CE	-10.07	84.08	100.20
33	J	324	ARG	NE-CZ-NH1	10.07	125.34	120.30
5	e	167	TYR	CB-CG-CD2	-10.06	114.97	121.00
29	I	317	ASP	CB-CG-OD1	-10.04	109.27	118.30
21	N	161	TYR	CB-CG-CD2	-10.03	114.98	121.00
24	Q	48	ASP	CB-CG-OD2	10.02	127.31	118.30
5	e	16	SER	N-CA-CB	10.01	125.51	110.50
14	7	137	ARG	NE-CZ-NH2	-10.00	115.30	120.30
25	R	333	MET	CG-SD-CE	-10.00	84.20	100.20
20	Z	137	TYR	CB-CG-CD2	-9.99	115.01	121.00
31	L	261	ARG	NE-CZ-NH1	9.98	125.29	120.30
8	1	111	TYR	CB-CG-CD1	9.98	126.99	121.00
2	b	179	TRP	CB-CG-CD2	-9.97	113.63	126.60
29	I	208	TYR	CB-CG-CD1	-9.97	115.02	121.00
13	m	157	PHE	CB-CG-CD2	-9.93	113.85	120.80
17	T	109	TYR	CB-CG-CD1	-9.91	115.05	121.00
29	I	408	ARG	NE-CZ-NH1	-9.90	115.35	120.30
33	J	63	ARG	NE-CZ-NH2	-9.90	115.35	120.30
28	H	373	ARG	NE-CZ-NH2	-9.86	115.37	120.30
24	Q	75	ARG	NE-CZ-NH2	9.85	125.23	120.30
23	P	351	ARG	NE-CZ-NH1	9.84	125.22	120.30
8	1	202	TYR	CB-CG-CD2	-9.83	115.10	121.00
23	P	266	TYR	CB-CG-CD2	-9.83	115.10	121.00
10	3	136	PHE	CB-CG-CD2	9.82	127.68	120.80
24	Q	398	TYR	CB-CG-CD2	9.82	126.89	121.00
28	H	181	TYR	CB-CG-CD1	9.73	126.84	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	420	ARG	NE-CZ-NH2	-9.73	115.44	120.30
8	1	152	ARG	NE-CZ-NH2	-9.72	115.44	120.30
25	R	392	ARG	NE-CZ-NH1	9.72	125.16	120.30
21	N	242	PHE	CB-CG-CD1	-9.72	114.00	120.80
8	h	111	TYR	CB-CG-CD1	-9.71	115.17	121.00
29	I	208	TYR	CB-CG-CD2	9.71	126.83	121.00
31	L	88	TYR	CB-CG-CD2	9.71	126.83	121.00
21	N	597	ARG	NE-CZ-NH2	-9.71	115.45	120.30
4	d	90	ARG	NE-CZ-NH2	-9.70	115.45	120.30
12	l	139	ARG	NE-CZ-NH1	9.70	125.15	120.30
16	V	100	ARG	NE-CZ-NH2	-9.69	115.45	120.30
25	R	24	TYR	CB-CG-CD2	9.69	126.81	121.00
32	M	203	ARG	NE-CZ-NH1	9.68	125.14	120.30
22	S	440	ASP	CB-CG-OD1	-9.68	109.59	118.30
30	K	376	ASP	CB-CG-OD1	9.68	127.01	118.30
10	j	147	PHE	CB-CG-CD1	-9.67	114.03	120.80
20	Z	248	TYR	CB-CG-CD2	-9.67	115.20	121.00
24	Q	239	PHE	CB-CG-CD2	-9.66	114.03	120.80
25	R	328	PHE	CB-CG-CD1	-9.63	114.06	120.80
30	K	58	TYR	CB-CG-CD1	-9.62	115.23	121.00
9	2	101	ARG	NE-CZ-NH1	9.62	125.11	120.30
7	G	169	ARG	NE-CZ-NH1	9.62	125.11	120.30
30	K	252	ARG	NE-CZ-NH2	-9.60	115.50	120.30
10	3	98	ARG	NE-CZ-NH1	9.57	125.08	120.30
21	N	234	ASP	CB-CG-OD1	-9.54	109.71	118.30
28	H	73	ASP	CB-CG-OD2	9.53	126.88	118.30
1	A	218	PHE	CB-CG-CD2	-9.53	114.13	120.80
15	W	17	ARG	NE-CZ-NH2	-9.53	115.54	120.30
26	U	113	TYR	CB-CG-CD1	-9.52	115.29	121.00
22	S	95	PHE	CB-CG-CD2	-9.50	114.15	120.80
27	O	39	PHE	CB-CG-CD2	-9.50	114.15	120.80
7	g	22	PHE	CB-CG-CD1	9.47	127.43	120.80
11	4	141	PHE	CB-CG-CD2	-9.46	114.18	120.80
9	i	126	TYR	CB-CG-CD2	9.45	126.67	121.00
6	f	3	ARG	NE-CZ-NH2	-9.45	115.58	120.30
32	M	329	ARG	NE-CZ-NH2	-9.44	115.58	120.30
20	Z	738	TYR	CB-CG-CD2	-9.43	115.34	121.00
25	R	334	ARG	NE-CZ-NH2	-9.42	115.59	120.30
33	J	35	ARG	NE-CZ-NH1	-9.41	115.59	120.30
5	e	20	ARG	NE-CZ-NH1	-9.41	115.60	120.30
29	I	75	PHE	CB-CG-CD1	9.41	127.39	120.80
17	T	81	TYR	CB-CG-CD1	9.40	126.64	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	338	TYR	CB-CG-CD2	-9.39	115.36	121.00
23	P	266	TYR	CB-CG-CD1	9.38	126.63	121.00
14	n	161	ARG	NE-CZ-NH1	9.36	124.98	120.30
22	S	186	TYR	CB-CG-CD2	9.35	126.61	121.00
20	Z	385	PHE	CB-CG-CD1	9.34	127.34	120.80
32	M	267	PHE	CB-CG-CD1	9.34	127.34	120.80
32	M	342	ARG	NE-CZ-NH1	9.34	124.97	120.30
9	i	219	TYR	CB-CG-CD2	-9.33	115.40	121.00
28	H	373	ARG	NE-CZ-NH1	9.33	124.97	120.30
10	j	136	PHE	CB-CG-CD1	-9.33	114.27	120.80
20	Z	759	ARG	NE-CZ-NH1	9.33	124.96	120.30
2	B	7	PHE	CB-CG-CD2	9.31	127.32	120.80
7	G	72	ARG	NE-CZ-NH1	9.31	124.95	120.30
21	N	208	ARG	NE-CZ-NH1	9.30	124.95	120.30
24	Q	151	TYR	CB-CG-CD1	-9.30	115.42	121.00
7	G	149	TYR	CB-CG-CD2	-9.29	115.42	121.00
28	H	432	ARG	NE-CZ-NH2	9.29	124.95	120.30
20	Z	153	TYR	CB-CG-CD2	-9.28	115.43	121.00
23	P	31	ASP	CB-CG-OD2	9.27	126.64	118.30
30	K	185	ARG	NE-CZ-NH2	-9.27	115.67	120.30
28	H	357	ARG	NE-CZ-NH2	-9.26	115.67	120.30
21	N	784	TYR	CB-CG-CD2	9.26	126.55	121.00
13	6	125	ASP	CB-CG-OD2	-9.24	109.98	118.30
21	N	776	TYR	CB-CG-CD2	-9.24	115.45	121.00
33	J	324	ARG	NE-CZ-NH2	-9.24	115.68	120.30
4	d	97	ARG	NE-CZ-NH1	9.23	124.91	120.30
8	h	54	ARG	NE-CZ-NH2	-9.23	115.69	120.30
14	7	220	ARG	NE-CZ-NH2	-9.22	115.69	120.30
21	N	504	TYR	CB-CG-CD2	-9.21	115.47	121.00
1	a	244	ARG	NE-CZ-NH1	9.18	124.89	120.30
3	C	149	TYR	CB-CG-CD2	-9.17	115.50	121.00
6	F	101	ARG	NE-CZ-NH2	-9.17	115.72	120.30
23	P	267	PHE	CB-CG-CD2	-9.17	114.38	120.80
27	O	137	TYR	CG-CD2-CE2	9.16	128.63	121.30
23	P	310	ARG	NE-CZ-NH2	9.16	124.88	120.30
6	f	7	ASP	CB-CG-OD2	-9.15	110.06	118.30
28	H	466	TYR	CB-CG-CD1	-9.15	115.51	121.00
7	g	157	TYR	CB-CG-CD2	9.14	126.48	121.00
2	B	236	ARG	NE-CZ-NH1	9.13	124.87	120.30
33	J	71	TYR	CB-CG-CD1	9.12	126.47	121.00
4	D	138	PHE	CB-CG-CD2	-9.11	114.42	120.80
5	e	151	ASP	CB-CG-OD2	9.10	126.49	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	169	ARG	NE-CZ-NH2	-9.10	115.75	120.30
15	W	179	ARG	NE-CZ-NH1	9.08	124.84	120.30
19	Y	83	ARG	NE-CZ-NH2	-9.08	115.76	120.30
2	B	12	PHE	CB-CG-CD1	-9.07	114.45	120.80
20	Z	928	ARG	NE-CZ-NH1	9.05	124.83	120.30
10	3	104	PHE	CB-CG-CD2	9.05	127.13	120.80
33	J	222	TYR	CB-CG-CD1	-9.05	115.57	121.00
8	h	183	ARG	NE-CZ-NH1	9.04	124.82	120.30
13	m	157	PHE	CB-CG-CD1	9.04	127.13	120.80
13	6	15	ASP	CB-CG-OD1	9.04	126.44	118.30
30	K	427	TYR	CB-CG-CD2	-9.03	115.58	121.00
25	R	301	TYR	CB-CG-CD1	-9.02	115.59	121.00
1	a	30	TYR	CB-CG-CD2	-9.02	115.59	121.00
32	M	33	ARG	NE-CZ-NH1	9.00	124.80	120.30
23	P	220	TYR	CB-CG-CD1	-8.99	115.61	121.00
8	1	163	PHE	CB-CG-CD1	8.99	127.09	120.80
6	f	171	TYR	CB-CG-CD2	8.98	126.39	121.00
20	Z	103	TYR	CB-CG-CD2	-8.98	115.61	121.00
25	R	329	PHE	CB-CG-CD2	8.98	127.09	120.80
10	j	199	TYR	CB-CG-CD2	-8.98	115.61	121.00
22	S	461	PHE	CB-CG-CD2	8.98	127.08	120.80
31	L	168	TYR	CB-CG-CD1	8.97	126.38	121.00
17	T	144	TYR	CG-CD2-CE2	-8.96	114.13	121.30
4	d	181	ARG	NE-CZ-NH1	8.96	124.78	120.30
26	U	288	PHE	CB-CG-CD1	-8.96	114.53	120.80
23	P	47	ARG	NE-CZ-NH2	-8.95	115.82	120.30
21	N	628	ALA	N-CA-CB	8.95	122.63	110.10
19	Y	83	ARG	NE-CZ-NH1	8.95	124.77	120.30
27	O	288	ARG	NE-CZ-NH2	-8.93	115.84	120.30
33	J	120	TYR	CB-CG-CD2	-8.93	115.64	121.00
7	g	190	ARG	NE-CZ-NH2	8.92	124.76	120.30
24	Q	72	ASP	CB-CG-OD1	-8.91	110.28	118.30
5	E	122	ARG	NE-CZ-NH1	8.91	124.75	120.30
10	3	188	TYR	CB-CG-CD1	-8.91	115.65	121.00
20	Z	513	ALA	CB-CA-C	8.91	123.46	110.10
21	N	593	PHE	CB-CG-CD2	-8.90	114.57	120.80
22	S	292	TYR	CB-CG-CD1	8.89	126.34	121.00
3	c	188	ASP	CB-CG-OD2	-8.88	110.31	118.30
20	Z	298	PHE	CB-CG-CD1	8.88	127.02	120.80
20	Z	264	PHE	CB-CG-CD1	8.87	127.01	120.80
21	N	202	PHE	CB-CG-CD1	8.86	127.00	120.80
5	e	148	ASP	CB-CG-OD2	8.86	126.28	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	409	TYR	CD1-CE1-CZ	-8.86	111.83	119.80
14	7	219	TYR	CB-CG-CD2	-8.86	115.69	121.00
13	6	36	ARG	NE-CZ-NH2	8.85	124.73	120.30
2	b	83	ARG	NE-CZ-NH2	-8.85	115.88	120.30
20	Z	912	PHE	CB-CG-CD2	8.84	126.99	120.80
31	L	361	PHE	CB-CG-CD2	-8.84	114.61	120.80
30	K	73	ARG	NE-CZ-NH2	8.84	124.72	120.30
17	T	89	TYR	CB-CG-CD2	-8.83	115.70	121.00
26	U	100	ARG	NE-CZ-NH1	8.83	124.71	120.30
4	D	4	TYR	CB-CG-CD1	-8.81	115.71	121.00
28	H	101	ARG	NE-CZ-NH1	8.81	124.71	120.30
2	b	179	TRP	CB-CG-CD1	8.80	138.44	127.00
15	W	11	ASP	CB-CG-OD2	-8.80	110.38	118.30
32	M	42	ARG	NE-CZ-NH1	8.79	124.69	120.30
10	j	203	ARG	NE-CZ-NH2	-8.78	115.91	120.30
23	P	69	ARG	NE-CZ-NH2	-8.76	115.92	120.30
23	P	179	PHE	CB-CG-CD2	-8.75	114.68	120.80
26	U	288	PHE	CB-CG-CD2	8.75	126.92	120.80
7	G	242	PHE	CB-CG-CD1	8.74	126.92	120.80
5	e	167	TYR	CG-CD2-CE2	-8.72	114.32	121.30
20	Z	439	TYR	CB-CG-CD2	-8.72	115.77	121.00
10	j	3	ASP	CB-CG-OD2	8.70	126.13	118.30
2	b	83	ARG	NE-CZ-NH1	8.70	124.65	120.30
1	a	128	TYR	CB-CG-CD2	-8.69	115.78	121.00
27	O	215	TYR	CB-CG-CD1	-8.69	115.78	121.00
2	B	224	TYR	CB-CG-CD2	-8.68	115.79	121.00
7	G	190	ARG	NE-CZ-NH1	8.68	124.64	120.30
13	m	168	TYR	CB-CG-CD2	8.66	126.19	121.00
28	H	381	ASP	CB-CG-OD1	8.66	126.09	118.30
21	N	653	ARG	NE-CZ-NH2	8.65	124.63	120.30
27	O	29	PHE	CB-CG-CD2	-8.65	114.74	120.80
7	g	24	VAL	CA-CB-CG2	-8.65	97.93	110.90
29	I	343	ARG	NE-CZ-NH1	8.65	124.62	120.30
12	5	94	ARG	NE-CZ-NH2	-8.64	115.98	120.30
31	L	88	TYR	CB-CG-CD1	-8.64	115.82	121.00
1	A	77	ARG	NE-CZ-NH2	-8.63	115.98	120.30
28	H	303	ALA	N-CA-CB	8.62	122.17	110.10
9	i	152	TYR	CB-CG-CD2	-8.61	115.83	121.00
9	2	219	TYR	CB-CG-CD2	-8.61	115.84	121.00
25	R	400	TYR	CB-CG-CD1	-8.61	115.84	121.00
3	C	137	TYR	CB-CG-CD2	8.60	126.16	121.00
16	V	135	ARG	NE-CZ-NH1	8.59	124.60	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	10	THR	CA-CB-CG2	-8.59	100.38	112.40
5	E	42	THR	N-CA-CB	8.57	126.59	110.30
21	N	202	PHE	CB-CG-CD2	-8.57	114.80	120.80
15	W	101	ARG	NE-CZ-NH1	8.57	124.58	120.30
32	M	45	ARG	NE-CZ-NH2	-8.57	116.02	120.30
8	1	70	TYR	CB-CG-CD2	-8.56	115.87	121.00
21	N	890	PHE	CB-CG-CD2	8.55	126.79	120.80
31	L	392	ARG	NE-CZ-NH2	-8.55	116.02	120.30
30	K	316	MET	CG-SD-CE	8.55	113.88	100.20
21	N	857	TYR	CB-CG-CD2	-8.54	115.88	121.00
8	1	111	TYR	CB-CG-CD2	-8.54	115.88	121.00
14	7	136	ARG	NE-CZ-NH2	-8.53	116.03	120.30
20	Z	722	ASP	CB-CG-OD1	8.53	125.98	118.30
28	H	385	ARG	NE-CZ-NH1	-8.53	116.03	120.30
32	M	221	TYR	CB-CG-CD2	-8.53	115.88	121.00
30	K	320	ARG	NE-CZ-NH2	-8.53	116.03	120.30
5	e	26	TYR	CG-CD2-CE2	-8.52	114.48	121.30
14	7	170	TYR	CB-CG-CD2	-8.52	115.89	121.00
21	N	75	TYR	CB-CG-CD1	-8.52	115.89	121.00
29	I	416	PHE	CB-CG-CD2	8.52	126.76	120.80
4	d	166	ARG	NE-CZ-NH1	-8.52	116.04	120.30
8	1	70	TYR	CB-CG-CD1	8.50	126.10	121.00
12	5	262	TYR	CB-CG-CD2	-8.50	115.90	121.00
26	U	22	TYR	CB-CG-CD2	-8.49	115.91	121.00
7	g	15	PHE	CB-CG-CD2	-8.49	114.86	120.80
25	R	63	TYR	CB-CG-CD2	-8.48	115.91	121.00
12	5	262	TYR	CG-CD1-CE1	-8.46	114.53	121.30
21	N	234	ASP	CB-CG-OD2	8.46	125.91	118.30
13	6	182	TYR	CB-CG-CD2	-8.45	115.93	121.00
18	X	10	PHE	CB-CG-CD1	-8.45	114.89	120.80
1	a	192	ASP	CB-CG-OD1	8.45	125.90	118.30
4	D	141	ARG	NE-CZ-NH2	-8.44	116.08	120.30
26	U	52	PHE	CB-CG-CD1	8.43	126.70	120.80
33	J	43	ARG	NE-CZ-NH1	8.43	124.51	120.30
21	N	222	TYR	CB-CG-CD2	-8.42	115.95	121.00
2	b	104	TYR	CB-CG-CD1	-8.41	115.96	121.00
8	1	79	TYR	CB-CG-CD2	-8.40	115.96	121.00
20	Z	4	GLU	N-CA-CB	8.40	125.72	110.60
20	Z	244	ARG	NE-CZ-NH1	8.39	124.50	120.30
30	K	246	TYR	CB-CG-CD2	-8.39	115.97	121.00
10	3	199	TYR	CB-CG-CD2	-8.36	115.98	121.00
11	4	190	ARG	NE-CZ-NH2	8.36	124.48	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	221	ARG	NE-CZ-NH2	-8.36	116.12	120.30
25	R	176	ARG	NE-CZ-NH1	8.34	124.47	120.30
9	i	117	PHE	CB-CG-CD1	-8.34	114.96	120.80
13	m	46	ARG	NE-CZ-NH2	8.33	124.47	120.30
17	T	139	ASP	CB-CG-OD1	8.33	125.80	118.30
12	5	168	ALA	N-CA-CB	8.33	121.76	110.10
1	A	218	PHE	CB-CG-CD1	8.31	126.62	120.80
3	C	193	ALA	N-CA-CB	8.31	121.74	110.10
22	S	88	PHE	CB-CG-CD2	8.31	126.62	120.80
14	7	161	ARG	NE-CZ-NH2	-8.31	116.14	120.30
22	S	211	ARG	NE-CZ-NH1	8.30	124.45	120.30
1	A	162	TYR	CB-CG-CD1	-8.30	116.02	121.00
13	6	141	ARG	NE-CZ-NH1	8.30	124.45	120.30
31	L	299	ARG	NE-CZ-NH1	8.29	124.44	120.30
8	h	54	ARG	NE-CZ-NH1	8.27	124.43	120.30
3	c	9	ARG	NE-CZ-NH1	8.26	124.43	120.30
14	n	126	PHE	CB-CG-CD2	-8.26	115.02	120.80
13	m	75	ARG	NE-CZ-NH1	-8.26	116.17	120.30
26	U	24	ARG	NE-CZ-NH1	-8.26	116.17	120.30
12	l	227	ASP	CB-CG-OD2	-8.26	110.87	118.30
30	K	58	TYR	CB-CG-CD2	8.25	125.95	121.00
1	A	105	ARG	NE-CZ-NH1	-8.24	116.18	120.30
21	N	739	PHE	CB-CG-CD1	8.24	126.57	120.80
28	H	312	ASP	CB-CG-OD1	8.24	125.72	118.30
33	J	212	ARG	NE-CZ-NH2	-8.24	116.18	120.30
21	N	559	TYR	CB-CG-CD2	8.23	125.94	121.00
21	N	570	ARG	NE-CZ-NH2	-8.23	116.19	120.30
11	k	138	PHE	CB-CG-CD1	8.22	126.56	120.80
27	O	93	ASP	CB-CG-OD2	8.21	125.69	118.30
8	1	75	TYR	CB-CG-CD1	-8.21	116.07	121.00
32	M	233	ARG	NE-CZ-NH2	-8.21	116.20	120.30
26	U	113	TYR	CB-CG-CD2	8.21	125.92	121.00
1	a	91	ARG	NE-CZ-NH2	8.20	124.40	120.30
32	M	50	ARG	NE-CZ-NH2	8.20	124.40	120.30
29	I	246	ARG	CA-C-N	-8.19	99.17	117.20
24	Q	339	TYR	CB-CG-CD2	-8.18	116.09	121.00
8	1	194	ARG	NE-CZ-NH2	8.18	124.39	120.30
26	U	24	ARG	NE-CZ-NH2	8.18	124.39	120.30
11	4	190	ARG	NE-CZ-NH1	-8.17	116.21	120.30
16	V	268	THR	CA-CB-CG2	-8.16	100.97	112.40
13	6	10	PHE	CB-CG-CD1	-8.16	115.09	120.80
11	4	44	MET	CG-SD-CE	-8.15	87.16	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	335	PHE	CB-CG-CD2	-8.15	115.09	120.80
17	T	174	PHE	CB-CG-CD1	8.15	126.50	120.80
28	H	167	ASP	CB-CG-OD2	-8.13	110.98	118.30
10	3	124	PHE	CB-CG-CD2	-8.13	115.11	120.80
18	X	125	MET	CG-SD-CE	-8.13	87.20	100.20
2	b	159	TRP	CB-CG-CD2	-8.12	116.05	126.60
6	F	77	LEU	CB-CG-CD1	8.12	124.80	111.00
22	S	114	TYR	CB-CG-CD1	8.12	125.87	121.00
16	V	160	ASP	CB-CG-OD1	8.11	125.60	118.30
2	B	82	TYR	CB-CG-CD2	-8.11	116.14	121.00
4	D	179	TYR	CB-CG-CD2	-8.11	116.14	121.00
7	G	242	PHE	CB-CG-CD2	-8.11	115.13	120.80
27	O	100	ASP	CB-CG-OD2	-8.10	111.01	118.30
21	N	776	TYR	CB-CG-CD1	8.10	125.86	121.00
24	Q	27	TYR	CB-CG-CD1	8.09	125.86	121.00
20	Z	272	TYR	CB-CG-CD2	8.09	125.85	121.00
32	M	73	ARG	NE-CZ-NH2	-8.09	116.26	120.30
21	N	584	ARG	NE-CZ-NH2	-8.08	116.26	120.30
2	b	90	ARG	NE-CZ-NH2	8.07	124.34	120.30
21	N	515	ARG	NE-CZ-NH2	-8.07	116.27	120.30
23	P	364	ARG	NE-CZ-NH1	8.06	124.33	120.30
24	Q	189	ARG	NE-CZ-NH2	-8.06	116.27	120.30
9	2	57	ASP	CB-CG-OD1	-8.06	111.04	118.30
6	F	87	TYR	CB-CG-CD2	-8.06	116.17	121.00
14	n	223	ARG	NE-CZ-NH1	-8.05	116.27	120.30
21	N	124	TYR	CB-CG-CD1	-8.05	116.17	121.00
22	S	452	TYR	CZ-CE2-CD2	-8.05	112.56	119.80
7	g	103	TYR	CB-CG-CD1	8.03	125.82	121.00
6	f	18	ARG	NE-CZ-NH1	-8.03	116.29	120.30
11	k	95	ARG	NE-CZ-NH1	8.02	124.31	120.30
1	A	110	TYR	CB-CG-CD1	-8.02	116.19	121.00
10	j	198	ARG	NE-CZ-NH1	8.01	124.31	120.30
21	N	463	TYR	CB-CG-CD1	8.00	125.80	121.00
6	F	203	ASP	CB-CG-OD1	-8.00	111.10	118.30
3	c	143	ARG	NE-CZ-NH1	8.00	124.30	120.30
14	n	183	MET	CG-SD-CE	-8.00	87.41	100.20
1	a	162	TYR	CB-CG-CD2	-7.99	116.20	121.00
24	Q	264	TYR	CB-CG-CD2	-7.99	116.21	121.00
33	J	101	ASP	CB-CG-OD2	-7.99	111.11	118.30
21	N	33	ASP	CB-CG-OD1	-7.99	111.11	118.30
15	W	26	PHE	CB-CG-CD2	-7.98	115.21	120.80
6	F	20	PHE	CB-CG-CD2	-7.97	115.22	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	294	ARG	NE-CZ-NH1	-7.97	116.31	120.30
17	T	88	TYR	N-CA-CB	7.96	124.93	110.60
21	N	348	PHE	CB-CG-CD1	-7.96	115.23	120.80
29	I	268	PHE	CB-CG-CD1	7.95	126.37	120.80
30	K	427	TYR	CG-CD1-CE1	-7.95	114.94	121.30
33	J	23	PHE	CB-CG-CD1	7.95	126.37	120.80
30	K	387	MET	CG-SD-CE	-7.94	87.49	100.20
5	e	165	TYR	CB-CG-CD2	7.94	125.76	121.00
13	6	225	TYR	CB-CG-CD1	-7.94	116.24	121.00
21	N	438	ASP	CB-CG-OD2	7.94	125.44	118.30
18	X	50	TRP	N-CA-CB	7.94	124.89	110.60
13	6	36	ARG	NE-CZ-NH1	-7.93	116.33	120.30
30	K	212	TYR	CB-CG-CD1	7.93	125.76	121.00
27	O	195	TYR	CB-CG-CD2	7.93	125.76	121.00
24	Q	176	ASP	CB-CG-OD1	-7.92	111.17	118.30
31	L	69	ARG	NE-CZ-NH1	7.92	124.26	120.30
21	N	471	TYR	CB-CG-CD1	7.92	125.75	121.00
23	P	357	TYR	CB-CG-CD2	-7.91	116.25	121.00
31	L	243	PHE	CB-CG-CD2	7.90	126.33	120.80
3	C	217	ARG	NE-CZ-NH2	-7.90	116.35	120.30
26	U	206	ASP	CB-CG-OD2	7.90	125.41	118.30
32	M	368	MET	CG-SD-CE	-7.90	87.57	100.20
10	3	69	TYR	CB-CG-CD2	-7.89	116.27	121.00
20	Z	48	ASP	CB-CG-OD2	-7.89	111.20	118.30
2	B	4	ARG	NE-CZ-NH1	7.88	124.24	120.30
12	l	210	PHE	CB-CG-CD2	7.88	126.32	120.80
13	6	224	PHE	CB-CG-CD1	-7.88	115.28	120.80
25	R	417	TYR	CB-CG-CD1	7.88	125.73	121.00
20	Z	242	PHE	CB-CG-CD2	-7.87	115.29	120.80
3	c	217	ARG	NE-CZ-NH1	-7.87	116.37	120.30
14	n	189	ARG	NE-CZ-NH2	-7.87	116.37	120.30
12	l	83	PHE	CB-CG-CD2	-7.86	115.30	120.80
21	N	502	PHE	CB-CG-CD1	-7.86	115.30	120.80
3	c	5	ARG	NE-CZ-NH2	-7.86	116.37	120.30
13	m	141	ARG	NE-CZ-NH2	-7.86	116.37	120.30
19	Y	82	ASP	CB-CG-OD1	-7.86	111.23	118.30
21	N	584	ARG	NE-CZ-NH1	7.85	124.22	120.30
3	C	180	TYR	CB-CG-CD1	7.84	125.71	121.00
10	j	139	SER	N-CA-CB	7.84	122.26	110.50
30	K	400	TYR	CB-CG-CD1	7.84	125.70	121.00
28	H	85	MET	CG-SD-CE	-7.83	87.67	100.20
9	i	140	PHE	CB-CG-CD2	7.82	126.28	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	170	MET	CG-SD-CE	-7.82	87.68	100.20
5	e	41	ALA	N-CA-CB	7.82	121.05	110.10
28	H	357	ARG	NE-CZ-NH1	7.82	124.21	120.30
20	Z	441	TYR	CB-CG-CD1	7.80	125.68	121.00
2	B	156	TYR	CB-CG-CD1	-7.80	116.32	121.00
12	5	181	ARG	NE-CZ-NH2	-7.79	116.41	120.30
13	m	37	ASN	N-CA-CB	7.77	124.59	110.60
17	T	266	TYR	CB-CG-CD2	7.77	125.66	121.00
7	G	72	ARG	NE-CZ-NH2	-7.77	116.42	120.30
30	K	262	ARG	NE-CZ-NH1	7.77	124.19	120.30
7	g	241	ASP	CB-CG-OD2	-7.76	111.31	118.30
25	R	392	ARG	NE-CZ-NH2	-7.76	116.42	120.30
13	6	182	TYR	CG-CD2-CE2	-7.76	115.09	121.30
10	j	3	ASP	CB-CG-OD1	-7.76	111.32	118.30
12	5	175	MET	CG-SD-CE	-7.75	87.79	100.20
22	S	461	PHE	CB-CG-CD1	-7.75	115.38	120.80
25	R	307	TYR	CG-CD1-CE1	7.74	127.49	121.30
3	c	122	TYR	CD1-CE1-CZ	-7.74	112.83	119.80
17	T	15	PHE	CB-CG-CD1	-7.74	115.38	120.80
6	f	54	ASP	CB-CG-OD2	-7.74	111.34	118.30
20	Z	202	ARG	NE-CZ-NH2	-7.74	116.43	120.30
1	A	104	PHE	CB-CG-CD1	-7.73	115.39	120.80
22	S	440	ASP	CB-CG-OD2	7.73	125.25	118.30
13	6	145	ARG	NE-CZ-NH1	-7.72	116.44	120.30
10	3	199	TYR	CA-CB-CG	-7.72	98.73	113.40
9	2	101	ARG	NE-CZ-NH2	-7.72	116.44	120.30
31	L	137	ARG	NE-CZ-NH1	7.71	124.16	120.30
31	L	80	ASN	N-CA-CB	7.70	124.47	110.60
5	e	132	ARG	NE-CZ-NH1	7.70	124.15	120.30
12	l	144	ARG	NE-CZ-NH1	7.70	124.15	120.30
28	H	90	ARG	NE-CZ-NH1	7.69	124.15	120.30
4	d	232	TYR	CB-CG-CD2	-7.69	116.38	121.00
8	h	45	ARG	NE-CZ-NH1	-7.69	116.46	120.30
33	J	374	ARG	NE-CZ-NH2	7.69	124.14	120.30
28	H	443	PHE	CB-CG-CD2	7.68	126.18	120.80
3	C	54	SER	N-CA-CB	7.68	122.02	110.50
22	S	82	TYR	CB-CG-CD1	-7.68	116.39	121.00
7	g	218	TRP	CB-CG-CD1	7.67	136.97	127.00
28	H	362	ASP	CB-CG-OD2	-7.67	111.40	118.30
4	D	97	ARG	NE-CZ-NH2	-7.67	116.47	120.30
21	N	682	PHE	CB-CG-CD2	-7.67	115.43	120.80
16	V	100	ARG	NE-CZ-NH1	7.67	124.13	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	240	TYR	CB-CG-CD2	-7.67	116.40	121.00
26	U	154	PHE	CB-CG-CD1	7.67	126.17	120.80
27	O	228	TYR	CG-CD1-CE1	7.67	127.43	121.30
21	N	230	VAL	CA-CB-CG2	-7.66	99.41	110.90
29	I	54	ARG	NE-CZ-NH1	7.66	124.13	120.30
7	g	78	TYR	CG-CD2-CE2	7.65	127.42	121.30
5	E	93	ARG	NE-CZ-NH2	7.65	124.12	120.30
30	K	347	ARG	NE-CZ-NH1	7.65	124.12	120.30
33	J	6	THR	CA-CB-CG2	-7.65	101.69	112.40
14	n	74	ARG	NE-CZ-NH2	-7.65	116.48	120.30
24	Q	176	ASP	CB-CG-OD2	7.65	125.18	118.30
13	m	114	TYR	CB-CG-CD2	7.64	125.59	121.00
20	Z	767	TYR	CB-CG-CD1	7.64	125.58	121.00
25	R	329	PHE	CB-CG-CD1	-7.64	115.45	120.80
9	i	215	TYR	CG-CD1-CE1	-7.64	115.19	121.30
22	S	52	TYR	CB-CG-CD1	7.64	125.58	121.00
24	Q	400	TYR	CG-CD2-CE2	-7.64	115.19	121.30
24	Q	130	ARG	NE-CZ-NH1	-7.64	116.48	120.30
27	O	58	ARG	NE-CZ-NH2	7.63	124.12	120.30
6	f	51	ARG	NE-CZ-NH1	-7.63	116.48	120.30
19	Y	86	ARG	NE-CZ-NH2	-7.63	116.49	120.30
13	m	120	ALA	N-CA-CB	7.62	120.77	110.10
20	Z	175	ASP	CB-CG-OD2	-7.62	111.44	118.30
1	a	145	SER	N-CA-CB	7.62	121.93	110.50
33	J	118	ASP	CB-CG-OD1	-7.62	111.44	118.30
24	Q	332	ARG	NE-CZ-NH1	7.62	124.11	120.30
3	C	208	TYR	CB-CG-CD2	-7.61	116.43	121.00
26	U	93	TYR	CG-CD2-CE2	7.61	127.39	121.30
4	d	197	ARG	NE-CZ-NH2	-7.61	116.50	120.30
1	A	115	ASP	CB-CG-OD2	-7.60	111.46	118.30
17	T	220	PHE	CB-CG-CD2	7.60	126.12	120.80
13	m	224	PHE	CB-CG-CD2	7.60	126.12	120.80
30	K	418	ASP	N-CA-CB	7.59	124.27	110.60
29	I	116	ASP	CB-CG-OD1	-7.59	111.47	118.30
7	g	160	TYR	CB-CG-CD1	-7.59	116.45	121.00
21	N	528	ARG	NE-CZ-NH2	-7.58	116.51	120.30
28	H	101	ARG	NE-CZ-NH2	-7.58	116.51	120.30
14	n	49	TYR	CB-CG-CD1	-7.58	116.45	121.00
21	N	618	ARG	NE-CZ-NH1	7.57	124.08	120.30
23	P	344	ARG	NE-CZ-NH1	7.56	124.08	120.30
1	A	106	TYR	CA-CB-CG	-7.56	99.04	113.40
9	i	219	TYR	CB-CG-CD1	7.56	125.53	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	174	ARG	NE-CZ-NH1	-7.55	116.52	120.30
12	5	245	TYR	CB-CG-CD1	7.55	125.53	121.00
13	m	75	ARG	NE-CZ-NH2	7.55	124.07	120.30
31	L	77	ARG	NE-CZ-NH1	7.54	124.07	120.30
24	Q	387	TYR	CB-CG-CD1	-7.54	116.48	121.00
16	V	295	VAL	CA-CB-CG1	7.54	122.20	110.90
31	L	243	PHE	CB-CG-CD1	-7.53	115.53	120.80
7	g	212	PHE	CB-CG-CD2	7.53	126.07	120.80
5	E	53	ARG	NE-CZ-NH2	-7.53	116.54	120.30
21	N	299	TYR	CB-CG-CD1	7.52	125.51	121.00
3	c	102	TYR	CB-CG-CD2	-7.51	116.49	121.00
30	K	204	ASP	CB-CG-OD1	7.50	125.05	118.30
8	1	183	ARG	NE-CZ-NH2	-7.50	116.55	120.30
31	L	325	MET	CG-SD-CE	-7.50	88.20	100.20
5	E	13	SER	C-N-CA	7.50	140.44	121.70
14	n	197	ASP	CB-CG-OD2	7.49	125.04	118.30
26	U	277	TYR	CB-CG-CD1	7.49	125.49	121.00
21	N	455	MET	CG-SD-CE	-7.48	88.23	100.20
9	i	215	TYR	CB-CG-CD2	-7.48	116.51	121.00
27	O	137	TYR	CZ-CE2-CD2	-7.47	113.07	119.80
32	M	386	PHE	CB-CG-CD1	-7.47	115.57	120.80
20	Z	153	TYR	CB-CG-CD1	7.47	125.48	121.00
21	N	438	ASP	CB-CG-OD1	-7.47	111.58	118.30
9	i	140	PHE	CB-CG-CD1	-7.46	115.58	120.80
4	D	127	ARG	NE-CZ-NH1	7.45	124.03	120.30
33	J	212	ARG	NE-CZ-NH1	7.45	124.03	120.30
11	4	195	PHE	CB-CG-CD1	-7.45	115.58	120.80
4	D	139	ASP	CB-CG-OD2	-7.44	111.60	118.30
33	J	248	ASP	CB-CG-OD2	7.44	125.00	118.30
25	R	345	TYR	CB-CG-CD2	-7.43	116.54	121.00
4	D	179	TYR	CB-CG-CD1	7.42	125.45	121.00
2	b	142	PHE	CB-CG-CD1	7.42	126.00	120.80
20	Z	408	TYR	CB-CG-CD1	7.42	125.45	121.00
7	g	86	ARG	NE-CZ-NH1	7.42	124.01	120.30
31	L	132	ARG	NE-CZ-NH2	-7.41	116.59	120.30
9	2	232	TYR	CB-CG-CD2	-7.41	116.55	121.00
6	F	20	PHE	CB-CG-CD1	7.41	125.99	120.80
4	d	120	TYR	CB-CG-CD2	7.41	125.44	121.00
14	7	63	TYR	CB-CG-CD2	-7.41	116.56	121.00
28	H	169	GLU	N-CA-CB	7.38	123.89	110.60
28	H	192	ASP	CB-CG-OD1	-7.38	111.66	118.30
4	D	66	LYS	N-CA-CB	7.38	123.89	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	651	PHE	CB-CG-CD1	-7.38	115.63	120.80
25	R	305	PHE	CB-CG-CD1	-7.38	115.64	120.80
28	H	463	TYR	CB-CG-CD2	7.38	125.43	121.00
2	b	60	THR	CA-CB-CG2	-7.37	102.08	112.40
8	h	96	TYR	CB-CG-CD1	-7.37	116.58	121.00
23	P	221	TYR	CB-CG-CD2	7.37	125.42	121.00
1	a	46	ARG	NE-CZ-NH1	-7.37	116.62	120.30
21	N	921	ARG	NE-CZ-NH1	7.37	123.98	120.30
5	E	16	SER	N-CA-CB	7.37	121.55	110.50
7	G	160	TYR	CB-CG-CD2	-7.36	116.58	121.00
9	2	231	SER	N-CA-CB	7.35	121.53	110.50
22	S	265	SER	N-CA-CB	7.35	121.53	110.50
8	h	134	ALA	N-CA-CB	7.35	120.39	110.10
6	F	233	TYR	CB-CG-CD2	7.34	125.41	121.00
13	m	35	THR	CA-CB-CG2	-7.34	102.13	112.40
29	I	391	ASP	CB-CG-OD2	-7.33	111.70	118.30
21	N	857	TYR	CZ-CE2-CD2	7.33	126.39	119.80
20	Z	798	ARG	NE-CZ-NH2	-7.32	116.64	120.30
30	K	333	ARG	C-N-CA	7.32	140.01	121.70
33	J	280	ASP	CB-CG-OD1	-7.32	111.71	118.30
11	k	176	PHE	CB-CG-CD2	7.32	125.92	120.80
12	5	179	TYR	CG-CD2-CE2	-7.32	115.45	121.30
32	M	213	ARG	NE-CZ-NH1	7.31	123.96	120.30
21	N	735	MET	CG-SD-CE	-7.30	88.52	100.20
21	N	502	PHE	CB-CG-CD2	7.29	125.91	120.80
26	U	243	ASP	CB-CG-OD2	-7.29	111.74	118.30
7	g	26	TYR	CB-CG-CD2	-7.29	116.63	121.00
27	O	147	ARG	NE-CZ-NH1	-7.29	116.66	120.30
10	j	34	LEU	CB-CG-CD2	7.29	123.39	111.00
23	P	351	ARG	NE-CZ-NH2	-7.28	116.66	120.30
21	N	69	TYR	CG-CD1-CE1	-7.28	115.48	121.30
28	H	318	ARG	NE-CZ-NH1	7.28	123.94	120.30
13	m	223	GLU	N-CA-CB	7.28	123.70	110.60
12	5	196	ARG	NE-CZ-NH2	7.28	123.94	120.30
20	Z	603	VAL	CA-CB-CG2	-7.28	99.98	110.90
1	a	234	PHE	CB-CG-CD1	-7.28	115.71	120.80
6	F	6	TYR	CB-CG-CD2	-7.27	116.64	121.00
4	d	119	ARG	NE-CZ-NH1	7.27	123.93	120.30
2	b	104	TYR	CB-CG-CD2	7.27	125.36	121.00
3	c	9	ARG	NE-CZ-NH2	-7.27	116.67	120.30
21	N	771	PHE	CB-CG-CD2	-7.27	115.71	120.80
5	E	86	ARG	NE-CZ-NH2	-7.26	116.67	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4	ARG	NE-CZ-NH2	-7.26	116.67	120.30
14	7	74	ARG	NE-CZ-NH1	-7.25	116.67	120.30
33	J	35	ARG	NE-CZ-NH2	7.25	123.93	120.30
9	2	132	VAL	CA-CB-CG1	-7.25	100.02	110.90
22	S	82	TYR	CG-CD1-CE1	-7.25	115.50	121.30
13	m	114	TYR	CB-CG-CD1	-7.25	116.65	121.00
13	6	93	SER	N-CA-CB	7.25	121.37	110.50
23	P	213	TYR	CB-CG-CD2	7.25	125.35	121.00
32	M	84	GLU	N-CA-CB	7.25	123.64	110.60
30	K	393	ARG	NE-CZ-NH1	-7.24	116.68	120.30
7	G	160	TYR	CG-CD1-CE1	-7.24	115.51	121.30
17	T	139	ASP	CB-CG-OD2	-7.24	111.79	118.30
6	F	126	ARG	NE-CZ-NH2	-7.23	116.68	120.30
23	P	168	TYR	CA-CB-CG	-7.23	99.66	113.40
2	b	23	TYR	CB-CG-CD2	-7.23	116.66	121.00
1	A	131	ARG	NE-CZ-NH2	-7.23	116.69	120.30
26	U	271	ASP	CB-CG-OD1	-7.22	111.80	118.30
4	D	29	ARG	NE-CZ-NH2	-7.22	116.69	120.30
20	Z	231	ASP	CB-CG-OD2	-7.22	111.80	118.30
33	J	312	ARG	NE-CZ-NH2	-7.22	116.69	120.30
16	V	108	TYR	CG-CD1-CE1	-7.21	115.53	121.30
2	b	178	ARG	NE-CZ-NH2	-7.21	116.69	120.30
20	Z	723	ASP	CB-CG-OD1	7.21	124.79	118.30
17	T	220	PHE	CB-CG-CD1	-7.21	115.75	120.80
32	M	366	ARG	NE-CZ-NH1	-7.21	116.69	120.30
15	W	25	ARG	NE-CZ-NH2	-7.21	116.70	120.30
12	5	245	TYR	CG-CD1-CE1	7.21	127.06	121.30
31	L	384	ASP	CB-CG-OD1	-7.21	111.81	118.30
20	Z	574	TYR	CZ-CE2-CD2	7.20	126.28	119.80
28	H	136	ALA	N-CA-CB	7.20	120.18	110.10
4	D	4	TYR	CG-CD1-CE1	-7.20	115.54	121.30
8	1	28	ARG	NE-CZ-NH1	7.19	123.90	120.30
12	l	165	TYR	CB-CG-CD2	-7.18	116.69	121.00
4	d	141	ARG	NE-CZ-NH2	-7.18	116.71	120.30
10	j	74	TYR	CB-CG-CD2	7.18	125.31	121.00
25	R	305	PHE	N-CA-CB	7.17	123.51	110.60
26	U	17	SER	N-CA-CB	7.17	121.26	110.50
3	c	208	TYR	CB-CG-CD2	7.17	125.30	121.00
14	7	126	PHE	CB-CG-CD1	7.17	125.82	120.80
32	M	153	TYR	CB-CG-CD2	7.16	125.29	121.00
9	2	225	ARG	NE-CZ-NH2	-7.15	116.72	120.30
6	f	39	ARG	NE-CZ-NH1	7.15	123.87	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	66	LEU	CB-CG-CD2	7.15	123.15	111.00
18	X	51	ARG	NE-CZ-NH1	7.14	123.87	120.30
29	I	246	ARG	CA-C-O	-7.14	105.11	120.10
25	R	422	ARG	NE-CZ-NH1	7.13	123.86	120.30
3	C	98	TYR	CB-CG-CD2	-7.12	116.73	121.00
10	3	19	ASP	CB-CG-OD2	-7.12	111.89	118.30
3	c	210	ARG	NE-CZ-NH2	7.12	123.86	120.30
29	I	243	THR	CA-CB-CG2	-7.12	102.43	112.40
28	H	466	TYR	CB-CG-CD2	7.11	125.27	121.00
28	H	434	ARG	CD-NE-CZ	7.11	133.56	123.60
14	7	109	TYR	CB-CG-CD1	-7.11	116.73	121.00
25	R	304	TYR	CB-CG-CD1	-7.11	116.74	121.00
3	c	157	TYR	CD1-CE1-CZ	7.10	126.19	119.80
1	A	73	PHE	CB-CG-CD1	-7.10	115.83	120.80
14	7	109	TYR	CB-CG-CD2	7.10	125.26	121.00
21	N	706	MET	N-CA-CB	7.10	123.37	110.60
3	c	13	PHE	CB-CG-CD1	7.09	125.77	120.80
31	L	255	TYR	CG-CD1-CE1	-7.09	115.63	121.30
31	L	342	ARG	NE-CZ-NH1	7.09	123.84	120.30
12	l	94	ARG	NE-CZ-NH2	7.08	123.84	120.30
22	S	446	THR	CA-CB-CG2	7.08	122.32	112.40
4	d	54	LEU	CB-CG-CD2	7.08	123.03	111.00
14	7	98	ARG	NE-CZ-NH1	7.08	123.84	120.30
4	d	70	HIS	O-C-N	7.08	134.02	122.70
4	d	148	TYR	CG-CD1-CE1	-7.07	115.64	121.30
7	G	93	ARG	NE-CZ-NH1	-7.07	116.77	120.30
10	3	40	PHE	CB-CG-CD2	-7.07	115.85	120.80
11	4	73	TYR	CB-CG-CD1	-7.07	116.76	121.00
21	N	906	ARG	NE-CZ-NH2	-7.07	116.77	120.30
9	i	240	ALA	N-CA-CB	7.06	119.98	110.10
20	Z	613	ASP	CB-CG-OD2	7.06	124.65	118.30
22	S	241	PHE	CB-CG-CD2	7.06	125.74	120.80
13	m	106	TYR	CB-CG-CD2	7.05	125.23	121.00
8	1	175	ASP	CB-CG-OD2	-7.04	111.96	118.30
22	S	137	PHE	CB-CG-CD1	7.04	125.73	120.80
6	f	82	ARG	NE-CZ-NH1	7.04	123.82	120.30
20	Z	565	PHE	CB-CG-CD2	-7.04	115.88	120.80
14	7	161	ARG	NE-CZ-NH1	7.03	123.82	120.30
20	Z	843	ASP	CB-CG-OD1	7.03	124.63	118.30
22	S	78	VAL	CA-CB-CG2	-7.03	100.35	110.90
22	S	399	TYR	CB-CG-CD2	-7.03	116.78	121.00
27	O	228	TYR	CB-CG-CD1	7.03	125.22	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	291	TYR	CB-CG-CD2	7.03	125.22	121.00
25	R	263	ARG	NE-CZ-NH2	-7.03	116.79	120.30
1	A	110	TYR	CB-CG-CD2	7.02	125.21	121.00
28	H	190	ARG	NE-CZ-NH1	-7.02	116.79	120.30
3	c	162	ALA	N-CA-CB	7.02	119.93	110.10
3	c	122	TYR	CB-CG-CD1	-7.01	116.79	121.00
9	2	153	TYR	CG-CD1-CE1	-7.01	115.69	121.30
29	I	316	PHE	CB-CG-CD2	-7.01	115.89	120.80
5	e	166	ARG	NE-CZ-NH2	-7.01	116.79	120.30
21	N	75	TYR	CB-CG-CD2	7.01	125.20	121.00
22	S	52	TYR	CB-CG-CD2	-7.01	116.79	121.00
22	S	428	ARG	NE-CZ-NH1	7.01	123.81	120.30
26	U	47	ARG	NE-CZ-NH2	-7.01	116.80	120.30
30	K	67	TYR	CG-CD1-CE1	7.01	126.91	121.30
4	d	220	ASP	CB-CG-OD2	-7.00	112.00	118.30
20	Z	564	ARG	NE-CZ-NH2	-7.00	116.80	120.30
7	g	181	ASP	CB-CG-OD2	-7.00	112.00	118.30
29	I	75	PHE	CB-CG-CD2	-7.00	115.90	120.80
3	c	28	SER	N-CA-CB	7.00	121.00	110.50
27	O	36	LYS	N-CA-CB	7.00	123.20	110.60
5	E	78	MET	CG-SD-CE	-7.00	89.00	100.20
27	O	60	ARG	NE-CZ-NH1	-7.00	116.80	120.30
22	S	271	ARG	NE-CZ-NH2	-6.99	116.81	120.30
25	R	284	ALA	N-CA-CB	6.99	119.88	110.10
6	f	157	TYR	CG-CD1-CE1	-6.98	115.71	121.30
10	j	136	PHE	CB-CG-CD2	6.98	125.69	120.80
17	T	197	TYR	CB-CG-CD1	-6.98	116.81	121.00
12	5	234	ARG	NE-CZ-NH1	6.98	123.79	120.30
4	d	174	PHE	CB-CG-CD2	-6.97	115.92	120.80
9	2	45	ALA	CB-CA-C	-6.97	99.65	110.10
6	F	201	LEU	CB-CG-CD2	6.96	122.84	111.00
27	O	185	PHE	CB-CG-CD1	6.96	125.67	120.80
12	l	210	PHE	CB-CG-CD1	-6.96	115.93	120.80
27	O	89	SER	N-CA-CB	6.96	120.94	110.50
14	7	215	ARG	NE-CZ-NH2	6.96	123.78	120.30
20	Z	825	ALA	N-CA-CB	6.95	119.83	110.10
21	N	23	TYR	CB-CG-CD2	-6.95	116.83	121.00
21	N	549	TYR	CB-CG-CD2	-6.95	116.83	121.00
5	e	98	THR	CA-CB-CG2	-6.94	102.68	112.40
27	O	119	SER	N-CA-CB	6.94	120.91	110.50
1	A	155	TYR	CB-CG-CD2	-6.94	116.84	121.00
6	F	87	TYR	CB-CG-CD1	6.94	125.16	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	89	ALA	N-CA-CB	6.93	119.81	110.10
8	h	28	ARG	NE-CZ-NH1	-6.93	116.83	120.30
20	Z	826	ARG	NE-CZ-NH1	6.93	123.76	120.30
5	E	228	PHE	CB-CG-CD1	-6.92	115.95	120.80
9	i	80	ASP	CB-CG-OD1	6.92	124.53	118.30
30	K	333	ARG	NE-CZ-NH2	-6.91	116.84	120.30
29	I	314	ASP	CB-CG-OD1	6.90	124.51	118.30
33	J	270	ARG	NE-CZ-NH2	-6.90	116.85	120.30
6	F	94	TYR	CB-CG-CD1	-6.89	116.86	121.00
7	g	160	TYR	CB-CG-CD2	6.88	125.13	121.00
7	g	84	ASP	CB-CG-OD2	-6.88	112.11	118.30
18	X	97	TYR	CB-CG-CD1	-6.88	116.87	121.00
1	A	139	VAL	CA-CB-CG1	-6.87	100.59	110.90
13	6	109	ARG	NE-CZ-NH2	-6.87	116.86	120.30
2	B	90	ARG	NE-CZ-NH2	-6.87	116.86	120.30
11	4	23	ARG	NE-CZ-NH1	-6.87	116.87	120.30
22	S	64	ARG	NE-CZ-NH2	6.87	123.73	120.30
24	Q	151	TYR	CG-CD2-CE2	-6.87	115.81	121.30
27	O	310	PHE	CB-CG-CD1	6.86	125.60	120.80
12	l	189	TYR	CB-CG-CD2	-6.86	116.88	121.00
25	R	383	ARG	NE-CZ-NH2	-6.86	116.87	120.30
26	U	69	ASP	CB-CG-OD1	6.86	124.47	118.30
26	U	182	ALA	N-CA-CB	6.86	119.70	110.10
20	Z	912	PHE	CB-CG-CD1	-6.86	116.00	120.80
7	g	202	LEU	CB-CG-CD1	6.85	122.64	111.00
14	7	98	ARG	NE-CZ-NH2	-6.85	116.88	120.30
10	3	40	PHE	CB-CG-CD1	6.85	125.59	120.80
25	R	221	VAL	CG1-CB-CG2	6.84	121.84	110.90
5	E	85	ALA	CB-CA-C	-6.84	99.84	110.10
21	N	788	TYR	CB-CG-CD1	-6.84	116.90	121.00
29	I	246	ARG	CA-CB-CG	6.84	128.44	113.40
2	B	220	ASP	CB-CG-OD2	6.83	124.45	118.30
13	m	52	PHE	CB-CG-CD1	-6.83	116.02	120.80
1	A	131	ARG	NE-CZ-NH1	6.83	123.71	120.30
4	D	232	TYR	CB-CG-CD2	-6.83	116.90	121.00
10	3	147	PHE	CB-CG-CD2	-6.83	116.02	120.80
6	f	149	PRO	N-CA-CB	6.82	111.49	103.30
29	I	232	LEU	CB-CG-CD2	6.82	122.59	111.00
21	N	788	TYR	CD1-CG-CD2	6.82	125.40	117.90
8	1	60	ASP	CB-CG-OD1	6.82	124.43	118.30
8	h	112	ASP	CB-CG-OD1	-6.81	112.17	118.30
9	i	224	VAL	CA-CB-CG2	-6.81	100.68	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	220	ARG	NE-CZ-NH2	-6.80	116.90	120.30
28	H	249	TYR	N-CA-CB	6.80	122.84	110.60
8	h	79	TYR	CB-CG-CD1	-6.80	116.92	121.00
31	L	386	PHE	CB-CG-CD2	-6.79	116.04	120.80
2	b	159	TRP	CB-CG-CD1	6.79	135.82	127.00
28	H	261	ARG	NE-CZ-NH1	6.78	123.69	120.30
11	k	165	VAL	CA-CB-CG1	6.77	121.06	110.90
7	G	201	TYR	CB-CG-CD2	6.77	125.06	121.00
17	T	157	TYR	CA-CB-CG	-6.77	100.53	113.40
4	d	247	ASP	CB-CG-OD1	-6.77	112.21	118.30
21	N	543	ASP	CB-CG-OD2	6.77	124.39	118.30
26	U	47	ARG	NE-CZ-NH1	6.77	123.68	120.30
4	d	172	ARG	NE-CZ-NH2	-6.76	116.92	120.30
27	O	306	ARG	NH1-CZ-NH2	6.76	126.84	119.40
33	J	118	ASP	CB-CG-OD2	6.76	124.39	118.30
6	f	83	VAL	CA-CB-CG1	6.76	121.04	110.90
11	4	98	TYR	CB-CG-CD2	-6.75	116.95	121.00
24	Q	261	VAL	CA-CB-CG2	-6.75	100.77	110.90
22	S	186	TYR	CG-CD1-CE1	6.75	126.70	121.30
13	m	65	PHE	CB-CG-CD1	-6.74	116.08	120.80
4	D	90	ARG	NE-CZ-NH1	6.74	123.67	120.30
14	n	226	ARG	NE-CZ-NH1	6.74	123.67	120.30
23	P	379	TYR	CB-CG-CD2	-6.74	116.96	121.00
20	Z	165	TYR	CB-CG-CD2	6.74	125.04	121.00
21	N	713	VAL	CA-CB-CG2	-6.73	100.80	110.90
5	e	115	SER	N-CA-CB	6.73	120.59	110.50
12	l	230	TYR	CB-CG-CD2	-6.72	116.97	121.00
4	D	232	TYR	CG-CD2-CE2	-6.72	115.92	121.30
23	P	428	THR	CA-CB-CG2	-6.72	102.98	112.40
4	d	56	ASP	CB-CG-OD1	-6.72	112.25	118.30
22	S	215	MET	CG-SD-CE	6.72	110.95	100.20
21	N	310	ASP	CB-CG-OD1	-6.72	112.25	118.30
24	Q	246	TYR	CB-CG-CD1	-6.71	116.97	121.00
22	S	452	TYR	CG-CD1-CE1	-6.71	115.93	121.30
10	j	90	LEU	CB-CG-CD1	6.70	122.39	111.00
2	B	128	ARG	N-CA-CB	6.70	122.66	110.60
23	P	201	ARG	NE-CZ-NH2	-6.70	116.95	120.30
8	1	19	ASP	CB-CG-OD1	6.70	124.33	118.30
12	l	202	PHE	CB-CG-CD2	6.70	125.49	120.80
21	N	743	PHE	CB-CG-CD1	-6.70	116.11	120.80
5	e	153	TYR	CG-CD1-CE1	-6.69	115.94	121.30
33	J	249	GLU	N-CA-C	-6.69	92.93	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	386	VAL	CA-CB-CG2	-6.69	100.87	110.90
28	H	349	ILE	N-CA-C	-6.69	92.94	111.00
32	M	205	ASP	CB-CG-OD2	-6.69	112.28	118.30
14	n	220	ARG	NE-CZ-NH1	6.69	123.64	120.30
4	d	156	TYR	CB-CG-CD2	6.68	125.01	121.00
30	K	329	LEU	CB-CG-CD2	-6.68	99.64	111.00
4	D	49	ARG	NE-CZ-NH2	-6.68	116.96	120.30
27	O	248	TYR	CG-CD1-CE1	-6.68	115.96	121.30
3	c	222	ASP	CB-CG-OD2	-6.67	112.30	118.30
18	X	99	PHE	CB-CG-CD2	6.67	125.47	120.80
25	R	324	ARG	NE-CZ-NH1	6.67	123.64	120.30
23	P	234	TYR	CG-CD1-CE1	-6.67	115.97	121.30
2	b	130	PHE	CB-CG-CD1	-6.67	116.13	120.80
13	6	182	TYR	CD1-CG-CD2	6.66	125.23	117.90
26	U	137	TYR	CG-CD2-CE2	-6.66	115.97	121.30
24	Q	27	TYR	CG-CD2-CE2	6.66	126.63	121.30
2	b	82	TYR	CG-CD2-CE2	-6.66	115.97	121.30
12	5	179	TYR	CB-CG-CD1	6.66	124.99	121.00
5	E	53	ARG	NE-CZ-NH1	-6.65	116.97	120.30
13	6	30	VAL	CA-CB-CG2	6.65	120.88	110.90
5	E	153	TYR	CB-CG-CD2	-6.65	117.01	121.00
12	l	189	TYR	CG-CD1-CE1	-6.64	115.98	121.30
13	m	109	ARG	NE-CZ-NH2	-6.64	116.98	120.30
33	J	22	TYR	CB-CG-CD1	6.64	124.98	121.00
7	G	11	SER	N-CA-CB	6.64	120.46	110.50
7	g	180	VAL	CA-CB-CG1	6.63	120.85	110.90
20	Z	231	ASP	CB-CG-OD1	6.63	124.27	118.30
25	R	335	ARG	NE-CZ-NH2	6.63	123.61	120.30
10	3	68	ARG	NE-CZ-NH1	-6.63	116.99	120.30
26	U	59	ASP	CB-CG-OD1	6.62	124.26	118.30
7	G	91	ARG	NE-CZ-NH2	6.62	123.61	120.30
8	1	202	TYR	CB-CG-CD1	6.62	124.97	121.00
24	Q	75	ARG	NH1-CZ-NH2	-6.62	112.12	119.40
5	E	123	PHE	CB-CG-CD1	6.62	125.43	120.80
25	R	176	ARG	NE-CZ-NH2	-6.62	116.99	120.30
28	H	58	ASP	CB-CG-OD1	6.62	124.25	118.30
11	4	107	TYR	CB-CG-CD1	-6.61	117.03	121.00
8	1	163	PHE	N-CA-CB	-6.61	98.70	110.60
20	Z	544	THR	CA-CB-CG2	-6.61	103.14	112.40
19	Y	65	ASP	CB-CG-OD2	-6.61	112.35	118.30
23	P	240	TYR	CG-CD2-CE2	-6.61	116.01	121.30
30	K	376	ASP	CB-CG-OD2	-6.61	112.35	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	304	TYR	CG-CD2-CE2	-6.61	116.02	121.30
6	F	107	ARG	NE-CZ-NH1	-6.60	117.00	120.30
21	N	406	TYR	CB-CG-CD1	6.60	124.96	121.00
26	U	189	ARG	NE-CZ-NH2	6.60	123.60	120.30
33	J	111	GLN	N-CA-C	-6.59	93.20	111.00
2	b	5	TYR	CB-CG-CD1	-6.59	117.05	121.00
8	1	152	ARG	NE-CZ-NH1	6.58	123.59	120.30
24	Q	309	ARG	NE-CZ-NH1	6.58	123.59	120.30
21	N	740	TRP	CB-CG-CD2	-6.58	118.05	126.60
15	W	21	PHE	CB-CG-CD2	-6.58	116.19	120.80
21	N	642	ASP	CB-CG-OD2	-6.58	112.38	118.30
2	B	245	ASP	CB-CG-OD1	6.58	124.22	118.30
7	G	157	TYR	CG-CD2-CE2	-6.58	116.04	121.30
9	2	57	ASP	CB-CG-OD2	6.58	124.22	118.30
18	X	129	LEU	CB-CG-CD2	6.58	122.18	111.00
5	e	123	PHE	CB-CG-CD2	-6.57	116.20	120.80
22	S	399	TYR	CB-CG-CD1	6.57	124.94	121.00
6	F	138	ASP	CB-CG-OD1	-6.57	112.39	118.30
13	6	13	TYR	CB-CG-CD2	-6.57	117.06	121.00
30	K	416	LYS	CB-CA-C	6.57	123.53	110.40
10	3	80	ARG	N-CA-CB	6.57	122.42	110.60
5	E	30	ALA	CB-CA-C	-6.56	100.25	110.10
12	5	200	ASP	CB-CG-OD2	-6.56	112.39	118.30
13	m	155	MET	CG-SD-CE	6.56	110.69	100.20
25	R	222	ARG	NE-CZ-NH1	6.55	123.58	120.30
11	k	152	MET	CG-SD-CE	-6.55	89.72	100.20
13	m	89	ASP	CB-CG-OD1	-6.55	112.41	118.30
7	g	119	TYR	CD1-CE1-CZ	6.55	125.69	119.80
5	E	231	TYR	CB-CG-CD1	-6.55	117.07	121.00
17	T	161	TRP	CH2-CZ2-CE2	6.54	123.94	117.40
4	d	127	ARG	NE-CZ-NH1	6.54	123.57	120.30
20	Z	167	ASP	CB-CG-OD2	6.54	124.19	118.30
20	Z	312	TYR	CG-CD1-CE1	6.54	126.53	121.30
5	E	72	ARG	NE-CZ-NH2	6.54	123.57	120.30
1	A	26	TYR	CB-CG-CD2	-6.54	117.08	121.00
12	l	144	ARG	CD-NE-CZ	-6.53	114.45	123.60
1	A	133	TYR	CG-CD2-CE2	-6.53	116.08	121.30
8	h	25	ALA	CB-CA-C	-6.52	100.32	110.10
21	N	370	SER	CB-CA-C	-6.52	97.71	110.10
28	H	346	ARG	NE-CZ-NH2	6.52	123.56	120.30
25	R	365	ASP	CB-CG-OD2	6.52	124.17	118.30
10	j	131	ASP	CB-CG-OD2	6.52	124.17	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	TYR	CZ-CE2-CD2	6.51	125.66	119.80
27	O	310	PHE	CB-CG-CD2	-6.51	116.24	120.80
32	M	248	ALA	CA-C-O	-6.51	106.42	120.10
14	n	261	TYR	CG-CD1-CE1	6.51	126.51	121.30
3	c	13	PHE	CB-CG-CD2	-6.51	116.24	120.80
30	K	399	ARG	NE-CZ-NH2	-6.51	117.05	120.30
20	Z	767	TYR	CG-CD1-CE1	6.50	126.50	121.30
6	F	225	TYR	CB-CG-CD1	6.50	124.90	121.00
25	R	402	LEU	CB-CG-CD2	6.50	122.06	111.00
5	E	153	TYR	CB-CG-CD1	6.50	124.90	121.00
29	I	182	SER	N-CA-CB	6.50	120.25	110.50
2	B	145	PHE	CB-CG-CD2	6.50	125.35	120.80
23	P	136	ARG	NE-CZ-NH2	-6.50	117.05	120.30
29	I	291	ARG	NE-CZ-NH1	6.50	123.55	120.30
5	e	169	ALA	N-CA-CB	6.50	119.20	110.10
12	l	82	ARG	NE-CZ-NH1	6.49	123.55	120.30
6	f	24	TYR	CB-CG-CD2	-6.49	117.11	121.00
2	b	80	PRO	N-CA-CB	6.49	111.08	103.30
10	j	67	PHE	CB-CA-C	-6.48	97.44	110.40
12	l	267	ASP	CB-CG-OD1	6.48	124.13	118.30
18	X	51	ARG	NE-CZ-NH2	6.48	123.54	120.30
8	1	61	THR	CA-CB-OG1	6.48	122.60	109.00
3	C	217	ARG	NH1-CZ-NH2	6.47	126.52	119.40
6	f	83	VAL	CA-CB-CG2	-6.47	101.20	110.90
28	H	409	ARG	NE-CZ-NH1	6.47	123.53	120.30
2	b	236	ARG	NE-CZ-NH2	6.46	123.53	120.30
20	Z	1	MET	CG-SD-CE	-6.46	89.86	100.20
23	P	95	TYR	CB-CG-CD2	-6.46	117.12	121.00
18	X	87	PHE	CB-CG-CD2	6.46	125.32	120.80
22	S	428	ARG	NH1-CZ-NH2	-6.46	112.30	119.40
33	J	220	GLN	N-CA-CB	6.46	122.22	110.60
8	h	75	TYR	CB-CG-CD1	6.45	124.87	121.00
14	7	133	MET	CG-SD-CE	-6.45	89.87	100.20
16	V	251	TYR	CB-CG-CD2	-6.45	117.13	121.00
6	F	89	ARG	NE-CZ-NH1	6.45	123.53	120.30
21	N	422	TYR	CD1-CE1-CZ	-6.45	113.99	119.80
2	B	128	ARG	NE-CZ-NH1	6.45	123.53	120.30
24	Q	291	TYR	CB-CG-CD1	-6.45	117.13	121.00
27	O	178	TYR	CG-CD2-CE2	-6.45	116.14	121.30
6	f	104	ALA	N-CA-CB	6.45	119.13	110.10
20	Z	790	MET	N-CA-CB	6.45	122.21	110.60
30	K	334	LEU	N-CA-CB	6.45	123.29	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	2	SER	N-CA-CB	6.45	120.17	110.50
20	Z	837	TYR	CB-CG-CD1	6.44	124.87	121.00
21	N	604	ARG	NE-CZ-NH2	-6.44	117.08	120.30
7	g	149	TYR	CB-CG-CD2	6.44	124.86	121.00
21	N	653	ARG	NH1-CZ-NH2	-6.44	112.31	119.40
27	O	19	ASP	CB-CG-OD1	-6.44	112.50	118.30
27	O	189	TYR	CB-CG-CD2	6.44	124.86	121.00
22	S	84	ASP	CB-CG-OD1	-6.44	112.51	118.30
24	Q	304	GLU	N-CA-CB	6.44	122.19	110.60
11	k	133	HIS	CB-CA-C	-6.43	97.53	110.40
24	Q	89	ALA	N-CA-CB	6.43	119.10	110.10
7	G	112	PHE	CB-CG-CD2	-6.43	116.30	120.80
6	F	101	ARG	NE-CZ-NH1	6.42	123.51	120.30
4	D	64	VAL	CG1-CB-CG2	6.42	121.18	110.90
13	m	151	ALA	N-CA-CB	6.42	119.09	110.10
8	1	151	PHE	CB-CG-CD1	6.42	125.29	120.80
15	W	155	ASP	CB-CG-OD2	-6.42	112.53	118.30
17	T	150	ARG	NE-CZ-NH2	-6.42	117.09	120.30
24	Q	13	ARG	NE-CZ-NH1	6.42	123.51	120.30
3	C	217	ARG	NE-CZ-NH1	-6.41	117.09	120.30
4	D	224	LEU	CB-CG-CD2	6.41	121.90	111.00
26	U	51	SER	N-CA-CB	6.41	120.12	110.50
29	I	62	MET	CG-SD-CE	-6.41	89.94	100.20
25	R	265	ASP	CB-CA-C	-6.41	97.58	110.40
32	M	187	ASP	C-N-CA	6.41	137.72	121.70
1	A	135	ARG	NE-CZ-NH1	6.41	123.50	120.30
7	g	149	TYR	CB-CG-CD1	-6.41	117.16	121.00
20	Z	970	TYR	CB-CG-CD2	6.41	124.84	121.00
29	I	115	ASP	N-CA-CB	6.41	122.13	110.60
30	K	46	ASP	CB-CG-OD2	-6.41	112.53	118.30
7	G	9	ASP	CB-CG-OD1	6.40	124.06	118.30
25	R	365	ASP	CB-CG-OD1	-6.40	112.54	118.30
12	l	81	PHE	CB-CG-CD2	-6.40	116.32	120.80
20	Z	780	MET	CG-SD-CE	-6.40	89.97	100.20
21	N	473	ASP	N-CA-CB	6.39	122.11	110.60
32	M	38	ASP	CB-CG-OD1	-6.39	112.55	118.30
22	S	155	LEU	CB-CG-CD1	6.39	121.86	111.00
3	C	208	TYR	CG-CD2-CE2	-6.39	116.19	121.30
6	F	6	TYR	CB-CG-CD1	6.39	124.83	121.00
1	a	155	TYR	CB-CG-CD2	-6.39	117.17	121.00
33	J	350	MET	CG-SD-CE	-6.39	89.98	100.20
10	3	103	TYR	CG-CD2-CE2	-6.38	116.19	121.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	234	ARG	NE-CZ-NH1	6.38	123.49	120.30
20	Z	441	TYR	CA-CB-CG	-6.38	101.29	113.40
3	C	135	PHE	CB-CG-CD2	-6.37	116.34	120.80
32	M	284	ASP	CB-CG-OD1	-6.37	112.57	118.30
12	l	188	TYR	CG-CD1-CE1	-6.37	116.20	121.30
1	a	155	TYR	CB-CG-CD1	6.37	124.82	121.00
3	c	149	TYR	CB-CA-C	-6.37	97.66	110.40
17	T	20	TYR	CB-CG-CD1	6.37	124.82	121.00
16	V	28	TYR	CB-CG-CD1	6.37	124.82	121.00
5	e	136	ARG	NE-CZ-NH2	-6.36	117.12	120.30
12	l	202	PHE	CB-CG-CD1	-6.36	116.35	120.80
20	Z	608	TYR	CB-CG-CD2	-6.36	117.18	121.00
28	H	367	ARG	CB-CA-C	-6.36	97.68	110.40
14	n	109	TYR	CB-CG-CD1	-6.36	117.19	121.00
8	1	196	ILE	CG1-CB-CG2	6.35	125.38	111.40
16	V	270	TYR	CB-CG-CD2	6.35	124.81	121.00
6	F	3	ARG	NH1-CZ-NH2	-6.35	112.41	119.40
22	S	137	PHE	CB-CG-CD2	-6.35	116.35	120.80
33	J	247	MET	CG-SD-CE	-6.35	90.04	100.20
5	e	151	ASP	CB-CG-OD1	-6.35	112.58	118.30
4	d	75	PHE	CB-CG-CD1	6.35	125.24	120.80
13	6	182	TYR	CG-CD1-CE1	-6.35	116.22	121.30
17	T	128	TYR	CB-CG-CD2	-6.35	117.19	121.00
24	Q	335	PHE	CB-CG-CD1	6.35	125.24	120.80
15	W	123	ASP	CB-CG-OD1	6.35	124.01	118.30
1	a	12	TYR	CB-CG-CD2	6.34	124.80	121.00
4	D	138	PHE	CB-CG-CD1	6.33	125.23	120.80
13	6	68	ASP	CB-CG-OD2	-6.33	112.60	118.30
23	P	294	GLU	OE1-CD-OE2	-6.33	115.70	123.30
1	a	67	THR	CA-CB-CG2	-6.33	103.54	112.40
9	i	57	ASP	CB-CG-OD1	-6.33	112.60	118.30
11	k	95	ARG	N-CA-CB	6.33	121.99	110.60
12	l	139	ARG	NH1-CZ-NH2	-6.33	112.44	119.40
14	7	61	GLY	N-CA-C	-6.33	97.28	113.10
33	J	368	TYR	CD1-CE1-CZ	-6.33	114.11	119.80
6	f	126	ARG	NE-CZ-NH2	6.32	123.46	120.30
1	A	24	ARG	NE-CZ-NH1	6.32	123.46	120.30
21	N	724	THR	N-CA-CB	6.32	122.31	110.30
11	k	148	TYR	CB-CG-CD1	-6.32	117.21	121.00
22	S	170	TYR	CD1-CE1-CZ	-6.32	114.11	119.80
12	5	209	THR	CA-CB-CG2	-6.32	103.56	112.40
27	O	324	VAL	CA-CB-CG2	-6.32	101.43	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	58	GLU	N-CA-CB	6.31	121.96	110.60
21	N	788	TYR	CG-CD2-CE2	-6.31	116.25	121.30
29	I	163	ASP	CB-CG-OD2	-6.31	112.62	118.30
4	d	194	LEU	CB-CG-CD1	6.31	121.73	111.00
6	f	168	ALA	N-CA-CB	-6.31	101.27	110.10
24	Q	264	TYR	CG-CD1-CE1	-6.31	116.25	121.30
12	5	115	PHE	CB-CG-CD2	-6.30	116.39	120.80
27	O	106	PHE	CB-CG-CD1	6.30	125.21	120.80
24	Q	371	GLN	CB-CA-C	-6.30	97.80	110.40
20	Z	426	TYR	CB-CG-CD1	6.30	124.78	121.00
21	N	841	THR	N-CA-C	-6.30	94.00	111.00
16	V	269	ARG	NE-CZ-NH2	-6.29	117.15	120.30
9	i	217	ARG	NE-CZ-NH2	6.29	123.45	120.30
23	P	414	GLU	N-CA-CB	-6.29	99.27	110.60
30	K	168	ASP	CB-CG-OD2	-6.29	112.64	118.30
3	C	117	ASP	CB-CG-OD1	6.29	123.96	118.30
4	D	127	ARG	NE-CZ-NH2	-6.29	117.16	120.30
9	i	46	ASP	CB-CG-OD2	-6.29	112.64	118.30
22	S	292	TYR	CG-CD2-CE2	-6.29	116.27	121.30
24	Q	196	ALA	CB-CA-C	-6.28	100.68	110.10
32	M	16	ASP	CB-CG-OD2	6.28	123.95	118.30
24	Q	339	TYR	CG-CD2-CE2	-6.28	116.28	121.30
6	f	157	TYR	CD1-CE1-CZ	6.28	125.45	119.80
2	B	128	ARG	CB-CA-C	-6.28	97.85	110.40
20	Z	838	TYR	CG-CD1-CE1	6.27	126.32	121.30
6	f	26	LEU	CB-CG-CD1	6.27	121.66	111.00
31	L	285	ALA	CB-CA-C	-6.27	100.70	110.10
33	J	246	PHE	CB-CG-CD2	-6.27	116.41	120.80
33	J	309	ARG	C-N-CA	6.27	137.37	121.70
23	P	224	LEU	CB-CA-C	-6.27	98.30	110.20
7	g	56	SER	N-CA-CB	6.26	119.89	110.50
5	E	233	ASN	CB-CA-C	-6.26	97.88	110.40
28	H	443	PHE	CB-CG-CD1	-6.26	116.42	120.80
5	E	10	ARG	NE-CZ-NH1	6.26	123.43	120.30
16	V	108	TYR	CB-CG-CD2	-6.25	117.25	121.00
19	Y	72	ASP	CB-CG-OD2	-6.25	112.67	118.30
16	V	228	TYR	CB-CG-CD2	6.25	124.75	121.00
16	V	154	ASP	CA-CB-CG	-6.25	99.65	113.40
21	N	739	PHE	CB-CG-CD2	-6.25	116.43	120.80
5	e	210	GLU	N-CA-CB	6.25	121.84	110.60
9	2	71	TRP	CG-CD2-CE3	-6.25	128.28	133.90
12	5	139	ARG	NE-CZ-NH1	6.24	123.42	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	370	ASP	N-CA-CB	6.24	121.84	110.60
20	Z	210	TYR	CB-CG-CD1	6.24	124.74	121.00
31	L	345	ARG	NE-CZ-NH1	-6.24	117.18	120.30
3	C	172	ALA	CB-CA-C	-6.24	100.74	110.10
6	F	89	ARG	NE-CZ-NH2	-6.24	117.18	120.30
4	d	148	TYR	CB-CG-CD1	-6.24	117.26	121.00
27	O	331	ALA	CB-CA-C	-6.24	100.75	110.10
28	H	145	TYR	N-CA-CB	6.23	121.82	110.60
22	S	433	GLU	N-CA-CB	6.23	121.82	110.60
29	I	335	ASP	CB-CG-OD1	-6.23	112.69	118.30
32	M	233	ARG	NE-CZ-NH1	6.23	123.42	120.30
8	1	142	PHE	CB-CG-CD2	6.23	125.16	120.80
20	Z	269	TYR	CG-CD2-CE2	-6.23	116.32	121.30
23	P	115	ARG	NE-CZ-NH1	-6.23	117.19	120.30
11	k	83	PHE	CB-CG-CD1	-6.22	116.44	120.80
18	X	51	ARG	NH1-CZ-NH2	-6.22	112.55	119.40
24	Q	51	ARG	NH1-CZ-NH2	6.22	126.25	119.40
7	G	46	VAL	N-CA-CB	6.22	125.19	111.50
10	3	159	GLU	OE1-CD-OE2	6.22	130.77	123.30
14	7	128	TYR	CB-CG-CD2	6.22	124.73	121.00
12	5	88	ILE	CB-CA-C	-6.22	99.16	111.60
16	V	160	ASP	CB-CG-OD2	-6.22	112.70	118.30
25	R	305	PHE	CG-CD1-CE1	-6.22	113.96	120.80
17	T	151	TRP	CA-CB-CG	6.22	125.51	113.70
27	O	245	ASP	N-CA-CB	6.22	121.79	110.60
10	3	96	TYR	CB-CG-CD1	-6.21	117.27	121.00
22	S	273	PHE	CB-CG-CD1	-6.21	116.45	120.80
11	4	130	TYR	CG-CD2-CE2	-6.21	116.33	121.30
5	e	93	ARG	NE-CZ-NH2	-6.21	117.20	120.30
15	W	155	ASP	CB-CG-OD1	6.21	123.89	118.30
27	O	302	VAL	CA-CB-CG1	-6.21	101.59	110.90
10	j	120	PHE	CB-CG-CD1	6.21	125.14	120.80
29	I	171	MET	CG-SD-CE	-6.21	90.27	100.20
3	c	76	ALA	CB-CA-C	-6.20	100.80	110.10
14	7	145	ASN	CB-CA-C	-6.20	97.99	110.40
20	Z	476	ASP	CB-CG-OD1	6.20	123.88	118.30
28	H	172	MET	CG-SD-CE	-6.20	90.28	100.20
7	G	108	PRO	N-CA-CB	6.20	110.74	103.30
22	S	184	TRP	CG-CD2-CE3	-6.20	128.32	133.90
31	L	261	ARG	NH1-CZ-NH2	-6.20	112.58	119.40
31	L	329	ARG	NE-CZ-NH1	6.20	123.40	120.30
2	b	157	PHE	CB-CG-CD2	6.20	125.14	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	104	ALA	CB-CA-C	-6.20	100.81	110.10
17	T	265	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	b	239	THR	CA-CB-CG2	-6.19	103.73	112.40
26	U	233	PHE	CB-CG-CD2	-6.19	116.46	120.80
12	l	118	GLY	N-CA-C	-6.19	97.62	113.10
21	N	575	ALA	N-CA-CB	6.19	118.77	110.10
24	Q	286	TYR	CB-CG-CD2	6.19	124.71	121.00
5	e	26	TYR	CB-CG-CD2	6.18	124.71	121.00
6	f	225	TYR	CB-CG-CD1	6.18	124.71	121.00
2	B	203	GLU	CB-CG-CD	-6.18	97.51	114.20
22	S	184	TRP	CE2-CD2-CG	6.18	112.25	107.30
6	f	171	TYR	CB-CG-CD1	-6.18	117.29	121.00
6	f	80	ASP	CB-CG-OD2	-6.18	112.74	118.30
9	i	232	TYR	CA-CB-CG	-6.18	101.66	113.40
20	Z	298	PHE	CG-CD2-CE2	6.17	127.59	120.80
17	T	89	TYR	CB-CG-CD1	6.17	124.70	121.00
29	I	256	TYR	CG-CD1-CE1	-6.17	116.36	121.30
8	1	174	TRP	CB-CG-CD1	6.17	135.02	127.00
14	n	98	ARG	N-CA-CB	6.17	121.70	110.60
33	J	228	ARG	NE-CZ-NH1	6.17	123.38	120.30
7	g	218	TRP	CB-CG-CD2	-6.17	118.59	126.60
8	h	120	TYR	CB-CG-CD2	6.16	124.70	121.00
32	M	107	ASN	N-CA-CB	6.16	121.69	110.60
31	L	240	GLY	N-CA-C	-6.16	97.70	113.10
7	g	103	TYR	CB-CG-CD2	-6.16	117.31	121.00
3	C	7	ASP	CB-CG-OD1	-6.16	112.76	118.30
13	6	27	ASP	CB-CG-OD2	-6.16	112.76	118.30
6	f	179	PHE	N-CA-CB	6.15	121.68	110.60
19	Y	7	ALA	CB-CA-C	6.15	119.33	110.10
5	e	72	ARG	NE-CZ-NH1	-6.14	117.23	120.30
32	M	345	ARG	NE-CZ-NH2	-6.14	117.23	120.30
24	Q	27	TYR	CB-CA-C	-6.14	98.12	110.40
21	N	23	TYR	CG-CD2-CE2	-6.14	116.39	121.30
4	D	199	LEU	O-C-N	-6.14	112.88	122.70
2	b	98	LYS	N-CA-CB	6.13	121.64	110.60
29	I	350	PHE	CB-CG-CD2	-6.13	116.51	120.80
13	m	89	ASP	CB-CG-OD2	6.13	123.82	118.30
26	U	176	ARG	NE-CZ-NH2	-6.13	117.23	120.30
25	R	246	TYR	CZ-CE2-CD2	-6.13	114.28	119.80
21	N	549	TYR	CG-CD1-CE1	-6.13	116.40	121.30
33	J	228	ARG	NE-CZ-NH2	-6.13	117.24	120.30
11	k	176	PHE	CB-CG-CD1	-6.13	116.51	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	396	TRP	CE2-CD2-CE3	6.12	126.05	118.70
23	P	3	ARG	NE-CZ-NH1	6.12	123.36	120.30
29	I	407	ARG	N-CA-CB	6.12	121.62	110.60
5	e	50	VAL	CA-CB-CG2	6.12	120.08	110.90
17	T	249	MET	CG-SD-CE	-6.12	90.41	100.20
31	L	303	ARG	NE-CZ-NH1	-6.12	117.24	120.30
4	d	237	GLU	CB-CA-C	-6.12	98.17	110.40
12	l	79	LEU	CB-CG-CD2	6.12	121.40	111.00
2	B	84	VAL	O-C-N	-6.12	112.91	122.70
8	1	148	ASP	CB-CG-OD2	6.11	123.80	118.30
32	M	101	THR	CA-CB-CG2	-6.11	103.84	112.40
3	c	99	LEU	CB-CG-CD1	6.11	121.39	111.00
32	M	235	CYS	C-N-CA	6.11	136.97	121.70
8	1	133	TYR	CB-CG-CD2	6.11	124.66	121.00
4	d	120	TYR	CD1-CG-CD2	-6.11	111.18	117.90
20	Z	623	ARG	NE-CZ-NH1	6.11	123.35	120.30
28	H	414	SER	CB-CA-C	-6.11	98.50	110.10
22	S	119	TYR	CD1-CE1-CZ	6.10	125.29	119.80
31	L	117	TYR	CZ-CE2-CD2	6.10	125.29	119.80
31	L	394	CYS	N-CA-CB	6.10	121.58	110.60
25	R	348	LEU	CB-CG-CD2	6.10	121.37	111.00
32	M	285	ALA	CB-CA-C	-6.10	100.95	110.10
30	K	104	ASP	CB-CG-OD1	-6.10	112.81	118.30
9	2	117	PHE	CB-CG-CD1	-6.09	116.53	120.80
13	6	180	LEU	N-CA-CB	6.09	122.59	110.40
3	c	71	ASP	CB-CG-OD1	-6.09	112.82	118.30
14	n	228	PHE	N-CA-CB	6.09	121.56	110.60
30	K	333	ARG	NE-CZ-NH1	6.08	123.34	120.30
13	m	53	ASP	CB-CG-OD2	6.08	123.77	118.30
21	N	765	ASP	O-C-N	-6.08	112.97	122.70
4	d	90	ARG	NE-CZ-NH1	6.08	123.34	120.30
1	a	234	PHE	CB-CG-CD2	6.08	125.05	120.80
10	j	83	GLU	N-CA-CB	6.08	121.54	110.60
21	N	857	TYR	CG-CD2-CE2	-6.08	116.44	121.30
24	Q	153	ASP	CB-CG-OD2	-6.08	112.83	118.30
27	O	314	SER	N-CA-CB	6.07	119.61	110.50
3	C	26	LEU	CB-CG-CD1	6.07	121.32	111.00
16	V	45	VAL	CA-CB-CG1	6.07	120.00	110.90
33	J	81	ASP	CB-CG-OD2	6.07	123.76	118.30
22	S	382	ARG	NE-CZ-NH2	6.06	123.33	120.30
2	b	229	THR	CA-CB-CG2	-6.06	103.92	112.40
20	Z	803	ALA	N-CA-CB	6.06	118.58	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	204	ASP	CB-CG-OD2	6.06	123.75	118.30
29	I	374	ASP	CB-CG-OD1	6.06	123.75	118.30
31	L	255	TYR	CB-CG-CD2	-6.06	117.36	121.00
14	n	109	TYR	CG-CD1-CE1	-6.06	116.45	121.30
5	E	86	ARG	NE-CZ-NH1	6.06	123.33	120.30
20	Z	774	ARG	NE-CZ-NH2	-6.06	117.27	120.30
3	c	149	TYR	CB-CG-CD2	-6.05	117.37	121.00
1	A	108	TYR	CB-CG-CD1	-6.05	117.37	121.00
17	T	222	LEU	CB-CG-CD2	6.05	121.28	111.00
15	W	151	THR	CA-CB-CG2	-6.05	103.93	112.40
19	Y	1	MET	CG-SD-CE	-6.05	90.53	100.20
33	J	94	TYR	CG-CD2-CE2	-6.05	116.46	121.30
14	n	63	TYR	CB-CG-CD1	-6.04	117.37	121.00
14	n	81	ASN	O-C-N	-6.04	113.03	122.70
6	f	96	SER	O-C-N	-6.04	113.04	122.70
30	K	67	TYR	CB-CG-CD1	-6.04	117.38	121.00
3	c	22	VAL	CA-CB-CG1	6.04	119.95	110.90
19	Y	17	THR	CA-CB-CG2	-6.04	103.95	112.40
21	N	348	PHE	CG-CD1-CE1	-6.03	114.17	120.80
23	P	96	MET	CG-SD-CE	6.03	109.85	100.20
16	V	251	TYR	CB-CG-CD1	6.03	124.62	121.00
29	I	291	ARG	NE-CZ-NH2	-6.03	117.28	120.30
7	G	86	ARG	NE-CZ-NH1	6.03	123.31	120.30
21	N	789	GLU	OE1-CD-OE2	6.03	130.53	123.30
22	S	452	TYR	CB-CG-CD1	-6.03	117.39	121.00
8	h	159	GLU	OE1-CD-OE2	-6.02	116.07	123.30
21	N	862	SER	N-CA-CB	6.02	119.53	110.50
10	3	67	PHE	CB-CG-CD1	-6.02	116.58	120.80
27	O	189	TYR	CG-CD2-CE2	-6.02	116.48	121.30
8	h	109	ALA	N-CA-CB	6.02	118.53	110.10
20	Z	406	TRP	CE2-CD2-CE3	6.02	125.92	118.70
23	P	192	ASP	CB-CG-OD2	-6.02	112.88	118.30
19	Y	68	GLU	C-N-CA	6.01	136.73	121.70
24	Q	72	ASP	CB-CG-OD2	6.01	123.71	118.30
7	g	26	TYR	CB-CG-CD1	6.01	124.61	121.00
13	m	213	LEU	N-CA-CB	6.01	122.42	110.40
27	O	307	MET	N-CA-C	-6.01	94.78	111.00
14	7	116	ALA	N-CA-CB	6.00	118.50	110.10
21	N	84	ALA	CB-CA-C	-6.00	101.10	110.10
31	L	315	PHE	CB-CG-CD1	-6.00	116.60	120.80
1	a	163	TYR	CD1-CE1-CZ	-6.00	114.40	119.80
2	B	83	ARG	CB-CA-C	-6.00	98.40	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	69	TYR	CB-CG-CD1	-6.00	117.40	121.00
27	O	317	THR	CA-CB-CG2	-6.00	104.00	112.40
1	A	70	SER	N-CA-CB	6.00	119.50	110.50
21	N	367	ALA	CB-CA-C	-6.00	101.10	110.10
7	g	230	PHE	CB-CG-CD2	-6.00	116.60	120.80
1	A	147	ASP	N-CA-CB	6.00	121.39	110.60
25	R	284	ALA	CB-CA-C	-6.00	101.11	110.10
26	U	64	ASP	N-CA-CB	5.99	121.39	110.60
23	P	51	ASP	CB-CG-OD1	5.99	123.69	118.30
4	d	68	ASP	CB-CG-OD1	5.99	123.69	118.30
23	P	287	ASP	CB-CG-OD1	-5.99	112.91	118.30
27	O	62	TYR	CB-CG-CD1	5.99	124.59	121.00
33	J	42	ARG	NE-CZ-NH1	-5.99	117.30	120.30
3	c	74	ALA	N-CA-CB	5.99	118.48	110.10
3	c	78	ALA	N-CA-CB	5.99	118.48	110.10
2	B	156	TYR	CB-CG-CD2	5.99	124.59	121.00
11	k	75	LEU	CB-CG-CD2	5.99	121.17	111.00
23	P	221	TYR	CB-CG-CD1	-5.99	117.41	121.00
27	O	322	ASP	CB-CG-OD2	-5.99	112.91	118.30
8	h	146	TYR	CB-CG-CD1	-5.98	117.41	121.00
15	W	23	ARG	CG-CD-NE	-5.98	99.24	111.80
21	N	722	THR	CA-CB-CG2	-5.98	104.03	112.40
13	m	10	PHE	CB-CG-CD1	5.98	124.99	120.80
27	O	310	PHE	CB-CA-C	-5.98	98.44	110.40
4	d	116	VAL	CA-CB-CG2	-5.98	101.93	110.90
14	7	134	TYR	CB-CG-CD1	-5.98	117.41	121.00
1	a	244	ARG	CB-CG-CD	5.98	127.14	111.60
6	f	32	GLY	O-C-N	5.98	132.26	122.70
27	O	307	MET	CA-CB-CG	5.97	123.45	113.30
30	K	111	SER	N-CA-CB	5.97	119.46	110.50
20	Z	206	ASP	CB-CG-OD1	5.97	123.67	118.30
32	M	153	TYR	CB-CG-CD1	-5.97	117.42	121.00
5	e	54	ALA	N-CA-CB	5.97	118.45	110.10
24	Q	390	LEU	CB-CG-CD1	5.97	121.15	111.00
5	e	20	ARG	NH1-CZ-NH2	5.97	125.96	119.40
12	5	129	PHE	CB-CG-CD2	5.97	124.98	120.80
25	R	214	TYR	CB-CG-CD2	5.97	124.58	121.00
26	U	139	ALA	N-CA-CB	5.97	118.45	110.10
27	O	245	ASP	CB-CG-OD1	5.97	123.67	118.30
31	L	119	VAL	CA-CB-CG2	-5.97	101.95	110.90
30	K	49	PHE	N-CA-CB	5.96	121.34	110.60
8	h	70	TYR	CB-CG-CD2	-5.96	117.42	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	174	ASP	N-CA-CB	5.96	121.33	110.60
22	S	28	GLU	OE1-CD-OE2	5.96	130.45	123.30
6	F	114	ASP	CB-CG-OD2	-5.96	112.94	118.30
30	K	234	PHE	CB-CG-CD1	-5.96	116.63	120.80
31	L	291	PHE	CB-CG-CD2	5.95	124.97	120.80
29	I	346	ARG	NE-CZ-NH2	-5.95	117.33	120.30
11	k	46	PHE	CB-CG-CD2	-5.95	116.64	120.80
14	n	118	GLU	N-CA-C	-5.95	94.94	111.00
14	n	131	THR	N-CA-CB	5.95	121.60	110.30
2	B	168	SER	N-CA-CB	5.95	119.42	110.50
21	N	365	PHE	CB-CG-CD2	-5.95	116.64	120.80
24	Q	185	TYR	CB-CG-CD1	5.95	124.57	121.00
27	O	93	ASP	CB-CG-OD1	-5.95	112.95	118.30
28	H	295	PHE	CB-CG-CD1	5.95	124.96	120.80
12	l	239	ALA	CB-CA-C	-5.95	101.18	110.10
12	l	162	VAL	CA-CB-CG1	-5.94	101.99	110.90
26	U	210	TYR	CB-CG-CD2	-5.94	117.44	121.00
3	c	157	TYR	CB-CG-CD2	-5.94	117.44	121.00
17	T	172	SER	CB-CA-C	-5.94	98.81	110.10
20	Z	777	PRO	N-CA-CB	5.94	110.43	103.30
14	n	57	ALA	CB-CA-C	-5.94	101.19	110.10
8	1	85	GLU	OE1-CD-OE2	5.94	130.42	123.30
22	S	345	TYR	CG-CD1-CE1	-5.94	116.55	121.30
28	H	139	ASP	CB-CG-OD2	5.94	123.64	118.30
2	B	236	ARG	NE-CZ-NH2	-5.94	117.33	120.30
5	E	24	VAL	CA-CB-CG1	5.94	119.80	110.90
4	d	220	ASP	CB-CG-OD1	5.93	123.64	118.30
10	3	177	ARG	NE-CZ-NH1	-5.93	117.33	120.30
16	V	53	MET	CG-SD-CE	5.93	109.69	100.20
11	k	135	TYR	CB-CG-CD1	5.93	124.56	121.00
22	S	428	ARG	NE-CZ-NH2	5.93	123.27	120.30
24	Q	235	ALA	N-CA-CB	5.93	118.40	110.10
29	I	397	THR	N-CA-CB	5.93	121.56	110.30
30	K	335	ASP	CB-CG-OD2	-5.93	112.96	118.30
31	L	71	ASP	CB-CG-OD2	5.93	123.64	118.30
9	2	83	ALA	N-CA-CB	5.93	118.40	110.10
20	Z	63	LEU	CB-CG-CD1	5.93	121.08	111.00
20	Z	300	ALA	N-CA-CB	5.93	118.40	110.10
2	b	163	ALA	N-CA-CB	5.92	118.40	110.10
12	l	188	TYR	CB-CG-CD1	-5.92	117.45	121.00
28	H	197	MET	CG-SD-CE	-5.92	90.72	100.20
29	I	262	ARG	CB-CA-C	-5.92	98.55	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	170	VAL	CA-CB-CG2	-5.92	102.02	110.90
9	i	119	TYR	CB-CG-CD2	5.92	124.55	121.00
10	3	183	TRP	CB-CG-CD2	-5.92	118.91	126.60
14	7	145	ASN	N-CA-CB	5.92	121.25	110.60
26	U	143	VAL	CA-CB-CG1	-5.92	102.03	110.90
8	h	175	ASP	N-CA-CB	5.92	121.25	110.60
31	L	201	LEU	N-CA-CB	-5.92	98.57	110.40
23	P	402	PHE	CB-CG-CD2	-5.91	116.66	120.80
22	S	248	ASP	CB-CG-OD1	-5.91	112.98	118.30
24	Q	151	TYR	CG-CD1-CE1	-5.91	116.57	121.30
30	K	204	ASP	N-CA-CB	5.91	121.23	110.60
1	A	143	PHE	CB-CG-CD1	5.91	124.94	120.80
12	5	181	ARG	NE-CZ-NH1	5.91	123.25	120.30
14	7	203	VAL	CA-CB-CG1	5.91	119.76	110.90
4	D	112	TYR	CA-CB-CG	-5.90	102.18	113.40
5	e	22	PHE	CB-CG-CD1	-5.90	116.67	120.80
21	N	313	LEU	CB-CG-CD1	5.90	121.03	111.00
22	S	119	TYR	CG-CD1-CE1	-5.90	116.58	121.30
28	H	400	ARG	NE-CZ-NH2	5.90	123.25	120.30
31	L	168	TYR	CG-CD1-CE1	-5.90	116.58	121.30
16	V	139	VAL	CA-CB-CG1	-5.90	102.05	110.90
20	Z	301	THR	CA-CB-CG2	-5.90	104.14	112.40
23	P	47	ARG	CD-NE-CZ	5.90	131.86	123.60
8	h	96	TYR	CB-CG-CD2	5.89	124.54	121.00
30	K	148	ASP	CB-CG-OD2	-5.89	113.00	118.30
13	6	155	MET	CG-SD-CE	-5.89	90.77	100.20
21	N	755	PRO	N-CD-CG	5.89	112.04	103.20
3	c	13	PHE	CB-CA-C	-5.89	98.62	110.40
24	Q	283	ASN	CA-CB-CG	-5.89	100.45	113.40
14	n	241	PHE	CD1-CE1-CZ	-5.88	113.04	120.10
20	Z	894	MET	CG-SD-CE	5.88	109.61	100.20
28	H	368	PRO	N-CA-CB	5.88	110.36	103.30
11	4	36	ARG	NE-CZ-NH1	5.88	123.24	120.30
33	J	266	SER	N-CA-CB	5.88	119.32	110.50
8	1	17	PHE	CB-CG-CD2	5.88	124.92	120.80
11	k	98	TYR	CB-CG-CD1	-5.88	117.47	121.00
13	6	194	ASP	CB-CG-OD2	-5.88	113.01	118.30
23	P	298	SER	N-CA-CB	5.87	119.31	110.50
33	J	339	ARG	NE-CZ-NH1	-5.87	117.36	120.30
25	R	134	TRP	CB-CG-CD2	-5.87	118.97	126.60
29	I	123	PRO	N-CA-CB	5.87	110.34	103.30
4	D	232	TYR	CZ-CE2-CD2	5.87	125.08	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	154	THR	CA-CB-CG2	-5.87	104.19	112.40
24	Q	82	THR	CA-CB-CG2	-5.87	104.19	112.40
26	U	59	ASP	N-CA-C	-5.87	95.17	111.00
22	S	76	PHE	CG-CD2-CE2	-5.86	114.35	120.80
23	P	257	TRP	CA-CB-CG	5.86	124.84	113.70
9	i	112	LEU	CB-CG-CD2	5.86	120.97	111.00
6	f	122	SER	N-CA-CB	5.86	119.29	110.50
12	5	272	PHE	CB-CG-CD2	-5.86	116.70	120.80
20	Z	42	ASP	CB-CG-OD1	5.86	123.57	118.30
22	S	70	ASN	O-C-N	-5.86	113.33	122.70
7	g	99	PHE	CB-CG-CD1	5.86	124.90	120.80
16	V	117	TRP	CG-CD2-CE3	-5.86	128.63	133.90
29	I	262	ARG	NE-CZ-NH1	-5.86	117.37	120.30
3	c	193	ALA	CB-CA-C	5.85	118.88	110.10
1	A	244	ARG	NE-CZ-NH2	5.85	123.23	120.30
3	c	6	TYR	CB-CG-CD2	-5.85	117.49	121.00
30	K	255	ARG	NE-CZ-NH2	-5.85	117.38	120.30
8	h	87	ALA	N-CA-CB	5.85	118.29	110.10
6	F	222	PHE	CB-CG-CD2	-5.84	116.71	120.80
2	b	27	ALA	N-CA-CB	5.84	118.28	110.10
5	e	78	MET	CG-SD-CE	5.84	109.54	100.20
9	i	139	LEU	CB-CG-CD1	5.84	120.93	111.00
30	K	258	PHE	N-CA-CB	5.84	121.11	110.60
1	a	234	PHE	N-CA-CB	5.84	121.11	110.60
28	H	107	LYS	C-N-CA	5.83	134.55	122.30
3	c	188	ASP	CB-CG-OD1	5.83	123.55	118.30
2	B	173	THR	CA-CB-CG2	-5.83	104.24	112.40
2	B	246	ARG	NE-CZ-NH1	5.83	123.22	120.30
22	S	472	HIS	CA-CB-CG	5.83	123.51	113.60
7	g	170	GLN	CG-CD-OE1	-5.83	109.94	121.60
21	N	553	PHE	CB-CG-CD1	-5.83	116.72	120.80
27	O	63	ASP	CB-CG-OD1	-5.83	113.05	118.30
20	Z	909	ARG	NE-CZ-NH2	5.83	123.21	120.30
10	j	68	ARG	NE-CZ-NH2	-5.83	117.39	120.30
27	O	98	TYR	CA-CB-CG	-5.83	102.33	113.40
28	H	230	LEU	CB-CG-CD1	5.83	120.91	111.00
7	g	162	GLY	N-CA-C	-5.82	98.54	113.10
13	m	46	ARG	NE-CZ-NH1	-5.82	117.39	120.30
8	h	184	MET	N-CA-CB	5.82	121.08	110.60
20	Z	815	MET	CG-SD-CE	5.82	109.51	100.20
12	l	263	HIS	N-CA-CB	5.82	121.08	110.60
11	4	194	ASP	CB-CG-OD2	-5.82	113.06	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	303	VAL	CA-CB-CG1	-5.82	102.17	110.90
20	Z	889	VAL	CA-CB-CG1	5.82	119.63	110.90
20	Z	565	PHE	CB-CA-C	-5.82	98.77	110.40
27	O	331	ALA	N-CA-CB	5.82	118.24	110.10
16	V	129	PHE	CB-CG-CD1	-5.81	116.73	120.80
3	c	205	ALA	CB-CA-C	-5.81	101.38	110.10
7	g	95	GLU	OE1-CD-OE2	5.81	130.28	123.30
14	7	80	ASP	CB-CG-OD2	-5.81	113.07	118.30
24	Q	398	TYR	CG-CD1-CE1	-5.81	116.65	121.30
26	U	127	GLN	N-CA-CB	5.81	121.06	110.60
28	H	372	ASP	CB-CG-OD2	-5.81	113.07	118.30
22	S	183	LEU	N-CA-CB	5.81	122.02	110.40
14	7	241	PHE	CB-CG-CD2	-5.81	116.73	120.80
18	X	40	GLU	CB-CA-C	-5.81	98.78	110.40
24	Q	151	TYR	CD1-CG-CD2	5.81	124.29	117.90
8	1	91	PHE	CB-CG-CD1	-5.81	116.73	120.80
20	Z	612	GLY	O-C-N	5.81	131.99	122.70
29	I	100	ARG	NE-CZ-NH2	-5.81	117.40	120.30
33	J	222	TYR	CB-CG-CD2	5.81	124.48	121.00
2	b	73	ALA	N-CA-CB	5.81	118.23	110.10
5	e	13	SER	CB-CA-C	5.80	121.13	110.10
29	I	208	TYR	O-C-N	5.80	131.99	122.70
30	K	81	ARG	CG-CD-NE	-5.80	99.61	111.80
13	m	47	TYR	CZ-CE2-CD2	-5.80	114.58	119.80
13	6	140	GLU	N-CA-CB	5.80	121.04	110.60
16	V	20	ARG	NE-CZ-NH2	-5.80	117.40	120.30
19	Y	25	ASN	N-CA-CB	5.80	121.04	110.60
5	e	101	LEU	CB-CG-CD2	-5.80	101.14	111.00
30	K	152	PRO	N-CA-CB	5.80	110.26	103.30
5	e	155	LEU	CB-CG-CD1	5.80	120.85	111.00
11	4	62	ALA	N-CA-CB	5.80	118.21	110.10
15	W	48	THR	CA-CB-CG2	-5.80	104.29	112.40
28	H	210	ASP	C-N-CA	5.79	136.19	121.70
12	l	233	LYS	N-CA-CB	5.79	121.03	110.60
13	m	227	LEU	CB-CG-CD2	5.79	120.85	111.00
7	G	112	PHE	CB-CG-CD1	5.79	124.86	120.80
12	5	165	TYR	CB-CG-CD2	-5.79	117.53	121.00
16	V	163	ALA	N-CA-CB	5.79	118.21	110.10
17	T	147	LYS	O-C-N	-5.79	113.43	122.70
10	3	28	ARG	NE-CZ-NH2	5.79	123.19	120.30
21	N	52	ASP	CB-CG-OD1	5.79	123.51	118.30
8	1	63	ALA	N-CA-CB	5.79	118.20	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	128	PHE	CG-CD2-CE2	-5.79	114.44	120.80
3	c	122	TYR	CG-CD1-CE1	5.79	125.93	121.30
10	3	28	ARG	NE-CZ-NH1	-5.78	117.41	120.30
1	A	236	LEU	CB-CG-CD2	5.78	120.83	111.00
33	J	151	GLY	O-C-N	-5.78	113.37	123.20
13	m	53	ASP	CB-CG-OD1	-5.78	113.10	118.30
21	N	771	PHE	CB-CG-CD1	5.78	124.84	120.80
12	l	204	VAL	CA-CB-CG2	-5.78	102.24	110.90
9	2	179	GLU	N-CA-CB	5.78	121.00	110.60
16	V	254	ARG	NE-CZ-NH1	5.78	123.19	120.30
22	S	108	ALA	N-CA-CB	5.77	118.18	110.10
32	M	138	ASP	CB-CG-OD1	5.77	123.50	118.30
3	C	145	GLY	O-C-N	5.77	131.94	122.70
27	O	330	ARG	NE-CZ-NH1	5.77	123.19	120.30
31	L	132	ARG	NE-CZ-NH1	5.77	123.19	120.30
4	D	155	ILE	N-CA-C	-5.77	95.42	111.00
10	j	99	ARG	O-C-N	-5.77	113.47	122.70
20	Z	96	TYR	CB-CG-CD2	5.77	124.46	121.00
28	H	162	ARG	NE-CZ-NH2	5.77	123.18	120.30
2	B	53	SER	N-CA-CB	5.76	119.15	110.50
14	7	128	TYR	CB-CG-CD1	-5.76	117.54	121.00
21	N	50	TYR	CG-CD2-CE2	-5.76	116.69	121.30
12	5	78	THR	N-CA-C	-5.76	95.44	111.00
32	M	355	ASP	CB-CG-OD2	5.76	123.49	118.30
1	A	24	ARG	NE-CZ-NH2	-5.76	117.42	120.30
12	5	243	ASP	CB-CG-OD1	-5.76	113.12	118.30
6	F	233	TYR	CB-CG-CD1	-5.76	117.55	121.00
30	K	67	TYR	CD1-CE1-CZ	-5.76	114.62	119.80
32	M	345	ARG	N-CA-CB	5.76	120.97	110.60
17	T	88	TYR	CB-CA-C	-5.76	98.89	110.40
17	T	96	LEU	N-CA-CB	5.76	121.91	110.40
8	h	17	PHE	CB-CG-CD2	-5.75	116.77	120.80
20	Z	218	GLU	N-CA-CB	5.75	120.96	110.60
15	W	142	ILE	N-CA-C	-5.75	95.47	111.00
30	K	67	TYR	CB-CG-CD2	5.75	124.45	121.00
14	n	50	ASP	CB-CG-OD2	5.75	123.48	118.30
31	L	130	GLY	N-CA-C	-5.75	98.72	113.10
6	f	123	TYR	CB-CG-CD1	5.75	124.45	121.00
16	V	142	ASP	N-CA-C	-5.75	95.47	111.00
20	Z	189	ALA	CB-CA-C	-5.75	101.47	110.10
26	U	137	TYR	CB-CG-CD2	-5.75	117.55	121.00
27	O	58	ARG	NE-CZ-NH1	-5.75	117.42	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	88	ILE	N-CA-C	-5.75	95.48	111.00
12	l	129	PHE	N-CA-CB	-5.75	100.25	110.60
22	S	333	PHE	CB-CG-CD2	5.75	124.82	120.80
7	g	201	TYR	CB-CG-CD2	5.74	124.45	121.00
21	N	92	ASP	CB-CG-OD1	-5.74	113.13	118.30
27	O	15	ARG	NE-CZ-NH1	5.74	123.17	120.30
20	Z	476	ASP	CB-CG-OD2	-5.74	113.13	118.30
14	n	218	TYR	CG-CD1-CE1	-5.74	116.71	121.30
5	E	53	ARG	NH1-CZ-NH2	5.74	125.72	119.40
6	f	6	TYR	CB-CG-CD2	5.74	124.44	121.00
12	l	225	VAL	CA-CB-CG1	5.74	119.50	110.90
10	j	166	THR	CA-CB-CG2	-5.73	104.38	112.40
3	C	48	ALA	N-CA-CB	5.73	118.12	110.10
13	m	116	HIS	N-CA-C	-5.73	95.53	111.00
8	h	48	ASP	CB-CG-OD1	5.73	123.46	118.30
3	C	5	ARG	NE-CZ-NH2	5.73	123.17	120.30
9	i	65	ARG	NE-CZ-NH2	-5.73	117.44	120.30
7	G	134	VAL	CA-CB-CG1	-5.73	102.31	110.90
6	f	80	ASP	CB-CG-OD1	5.73	123.45	118.30
29	I	416	PHE	CB-CG-CD1	-5.73	116.79	120.80
23	P	2	SER	CB-CA-C	-5.72	99.22	110.10
31	L	401	PHE	CB-CG-CD1	5.72	124.81	120.80
5	e	103	TYR	CD1-CE1-CZ	-5.72	114.65	119.80
4	d	179	TYR	CZ-CE2-CD2	-5.72	114.66	119.80
4	D	44	LEU	CB-CG-CD2	5.72	120.72	111.00
20	Z	386	VAL	CG1-CB-CG2	5.72	120.05	110.90
21	N	161	TYR	CG-CD2-CE2	-5.72	116.73	121.30
27	O	100	ASP	CB-CG-OD1	5.72	123.44	118.30
17	T	99	SER	N-CA-CB	5.71	119.07	110.50
3	c	106	ILE	N-CA-CB	5.71	123.93	110.80
19	Y	82	ASP	CB-CG-OD2	5.71	123.44	118.30
1	a	104	PHE	CB-CG-CD2	5.71	124.80	120.80
2	B	46	ALA	N-CA-CB	5.71	118.09	110.10
10	3	84	PRO	N-CA-CB	5.71	110.15	103.30
18	X	85	ARG	NE-CZ-NH1	-5.71	117.45	120.30
27	O	301	PHE	CB-CG-CD1	-5.71	116.80	120.80
4	D	33	ALA	N-CA-CB	5.71	118.09	110.10
9	2	187	ALA	CB-CA-C	-5.71	101.54	110.10
11	4	155	GLU	OE1-CD-OE2	-5.71	116.45	123.30
12	l	161	LEU	CB-CG-CD2	5.71	120.70	111.00
25	R	400	TYR	CB-CG-CD2	5.71	124.42	121.00
8	h	108	VAL	CG1-CB-CG2	5.70	120.03	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	297	TYR	CB-CG-CD2	5.70	124.42	121.00
10	j	193	ASP	CB-CG-OD2	-5.70	113.17	118.30
13	6	188	VAL	CA-CB-CG2	-5.70	102.35	110.90
17	T	151	TRP	CE2-CD2-CE3	5.70	125.54	118.70
5	e	13	SER	C-N-CA	5.70	135.94	121.70
27	O	11	LEU	CB-CG-CD1	-5.70	101.31	111.00
2	b	132	VAL	C-N-CA	5.70	135.94	121.70
12	5	165	TYR	CB-CG-CD1	5.70	124.42	121.00
21	N	222	TYR	CB-CG-CD1	5.69	124.42	121.00
23	P	329	PHE	CB-CG-CD1	-5.69	116.81	120.80
32	M	292	ASP	O-C-N	-5.69	113.59	122.70
2	b	4	ARG	NE-CZ-NH1	5.69	123.15	120.30
22	S	259	TYR	CD1-CE1-CZ	-5.69	114.68	119.80
14	n	123	SER	CB-CA-C	-5.69	99.29	110.10
11	k	41	HIS	CA-CB-CG	-5.69	103.93	113.60
14	n	128	TYR	CB-CG-CD1	-5.69	117.59	121.00
2	b	83	ARG	CA-CB-CG	-5.69	100.89	113.40
23	P	138	ARG	NE-CZ-NH1	5.69	123.14	120.30
21	N	903	VAL	CG1-CB-CG2	5.69	120.00	110.90
4	d	158	SER	N-CA-CB	5.68	119.03	110.50
9	2	190	ALA	N-CA-CB	5.68	118.06	110.10
24	Q	427	PHE	CB-CG-CD2	-5.68	116.82	120.80
3	c	102	TYR	CB-CG-CD1	5.68	124.41	121.00
29	I	155	SER	N-CA-CB	5.68	119.02	110.50
5	e	132	ARG	NE-CZ-NH2	-5.67	117.46	120.30
25	R	149	ASN	N-CA-CB	5.67	120.81	110.60
28	H	297	MET	CG-SD-CE	-5.67	91.12	100.20
16	V	238	LEU	N-CA-CB	5.67	121.75	110.40
27	O	228	TYR	CZ-CE2-CD2	5.67	124.91	119.80
28	H	210	ASP	CB-CG-OD1	-5.67	113.20	118.30
30	K	70	ASP	CB-CG-OD2	-5.67	113.20	118.30
16	V	238	LEU	CB-CG-CD2	-5.67	101.36	111.00
12	5	250	VAL	CG1-CB-CG2	5.67	119.97	110.90
12	l	133	TRP	CB-CG-CD1	5.67	134.37	127.00
33	J	8	SER	N-CA-CB	5.67	119.00	110.50
32	M	322	LYS	N-CA-CB	5.67	120.80	110.60
7	G	56	SER	N-CA-C	-5.66	95.71	111.00
8	h	44	THR	CA-CB-CG2	-5.66	104.47	112.40
6	F	85	SER	N-CA-CB	5.66	118.99	110.50
6	F	187	ASP	CB-CG-OD2	-5.66	113.20	118.30
21	N	762	ARG	NE-CZ-NH1	-5.66	117.47	120.30
19	Y	41	ASP	O-C-N	5.66	131.75	122.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	282	PHE	CB-CG-CD2	-5.66	116.84	120.80
20	Z	295	ARG	CD-NE-CZ	5.66	131.52	123.60
20	Z	849	ARG	N-CA-CB	5.66	120.78	110.60
29	I	282	ASP	CB-CG-OD1	-5.66	113.21	118.30
16	V	28	TYR	CB-CG-CD2	-5.65	117.61	121.00
21	N	581	ASP	CB-CG-OD2	5.65	123.39	118.30
18	X	99	PHE	N-CA-CB	5.65	120.77	110.60
33	J	14	THR	N-CA-CB	5.65	121.03	110.30
4	D	234	THR	CA-CB-CG2	-5.64	104.50	112.40
3	c	222	ASP	N-CA-CB	5.64	120.76	110.60
20	Z	23	GLN	CB-CG-CD	-5.64	96.93	111.60
31	L	299	ARG	NH1-CZ-NH2	-5.64	113.19	119.40
7	G	116	LEU	CB-CG-CD2	5.64	120.59	111.00
11	k	72	ASP	N-CA-CB	5.64	120.75	110.60
11	4	130	TYR	CZ-CE2-CD2	5.64	124.87	119.80
6	f	177	ASP	CB-CG-OD1	5.63	123.37	118.30
15	W	140	ASP	N-CA-CB	5.63	120.74	110.60
29	I	350	PHE	CG-CD1-CE1	-5.63	114.60	120.80
9	2	176	THR	CA-CB-CG2	-5.63	104.52	112.40
27	O	361	ASP	CB-CG-OD2	5.63	123.37	118.30
18	X	114	LEU	CB-CG-CD1	-5.63	101.43	111.00
20	Z	421	SER	N-CA-CB	5.63	118.94	110.50
22	S	145	PHE	CB-CG-CD1	5.63	124.74	120.80
22	S	194	LEU	CB-CG-CD1	5.63	120.57	111.00
26	U	93	TYR	CZ-CE2-CD2	-5.63	114.73	119.80
11	k	67	TYR	CB-CG-CD2	-5.62	117.62	121.00
20	Z	900	LEU	CB-CG-CD1	5.62	120.56	111.00
17	T	85	LEU	CB-CG-CD1	5.62	120.56	111.00
30	K	374	ARG	NE-CZ-NH1	-5.62	117.49	120.30
32	M	69	ILE	CA-CB-CG1	-5.62	100.31	111.00
11	k	120	ASP	CB-CG-OD1	-5.62	113.24	118.30
4	D	218	ASP	CB-CG-OD1	-5.62	113.24	118.30
20	Z	155	ARG	CD-NE-CZ	5.62	131.47	123.60
32	M	173	ASP	N-CA-CB	5.62	120.72	110.60
7	G	177	GLU	OE1-CD-OE2	5.62	130.04	123.30
20	Z	607	ALA	CB-CA-C	-5.62	101.67	110.10
6	f	153	VAL	N-CA-CB	5.62	123.86	111.50
14	7	58	ASP	CB-CG-OD2	-5.62	113.24	118.30
20	Z	564	ARG	NE-CZ-NH1	5.62	123.11	120.30
9	i	163	ALA	CB-CA-C	-5.62	101.67	110.10
22	S	315	LYS	CB-CA-C	-5.62	99.17	110.40
2	b	18	LEU	CB-CA-C	-5.61	99.54	110.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	220	THR	N-CA-CB	5.61	120.97	110.30
2	B	140	ASP	CB-CG-OD1	-5.61	113.25	118.30
15	W	79	THR	CA-CB-OG1	5.61	120.79	109.00
32	M	298	ASP	CB-CG-OD1	5.61	123.35	118.30
20	Z	491	LEU	N-CA-CB	5.61	121.61	110.40
4	d	141	ARG	NE-CZ-NH1	5.61	123.10	120.30
20	Z	206	ASP	CB-CG-OD2	-5.61	113.25	118.30
21	N	134	THR	CA-CB-CG2	-5.61	104.55	112.40
22	S	423	VAL	CG1-CB-CG2	-5.61	101.93	110.90
27	O	302	VAL	CA-CB-CG2	5.61	119.31	110.90
32	M	248	ALA	CA-C-N	5.61	132.80	117.10
24	Q	80	HIS	O-C-N	5.60	131.67	122.70
2	b	53	SER	N-CA-CB	5.60	118.90	110.50
25	R	371	PHE	CB-CG-CD1	-5.60	116.88	120.80
7	G	119	TYR	CG-CD1-CE1	5.60	125.78	121.30
7	G	230	PHE	CB-CG-CD2	-5.60	116.88	120.80
20	Z	151	HIS	CB-CA-C	-5.60	99.21	110.40
2	b	250	LEU	N-CA-C	-5.59	95.89	111.00
6	f	18	ARG	O-C-N	-5.59	113.75	122.70
12	l	79	LEU	N-CA-CB	5.59	121.59	110.40
13	m	146	ALA	N-CA-CB	5.59	117.93	110.10
16	V	28	TYR	CA-CB-CG	-5.59	102.77	113.40
4	d	120	TYR	CD1-CE1-CZ	5.59	124.83	119.80
3	C	60	ASP	CB-CG-OD1	-5.59	113.27	118.30
14	7	261	TYR	CB-CG-CD2	-5.59	117.64	121.00
28	H	250	GLY	N-CA-C	-5.59	99.12	113.10
31	L	404	ARG	NE-CZ-NH1	5.59	123.10	120.30
7	g	91	ARG	NE-CZ-NH2	-5.59	117.51	120.30
11	k	31	SER	N-CA-CB	5.59	118.88	110.50
13	6	229	ARG	NE-CZ-NH1	5.59	123.09	120.30
23	P	221	TYR	CD1-CE1-CZ	5.59	124.83	119.80
14	n	216	VAL	CA-CB-CG2	-5.59	102.52	110.90
20	Z	175	ASP	CB-CG-OD1	5.59	123.33	118.30
24	Q	222	SER	O-C-N	5.58	132.69	123.20
2	B	250	LEU	CB-CG-CD2	5.58	120.49	111.00
8	1	28	ARG	NE-CZ-NH2	-5.58	117.51	120.30
20	Z	97	PRO	N-CA-CB	5.58	110.00	103.30
16	V	135	ARG	NE-CZ-NH2	-5.58	117.51	120.30
17	T	150	ARG	CD-NE-CZ	-5.58	115.79	123.60
20	Z	798	ARG	NE-CZ-NH1	5.58	123.09	120.30
28	H	320	ASP	CA-CB-CG	-5.58	101.14	113.40
8	1	34	TYR	CB-CG-CD2	-5.57	117.66	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	94	PHE	N-CA-CB	5.57	120.63	110.60
7	g	185	GLU	N-CA-CB	5.57	120.63	110.60
15	W	35	PHE	CB-CG-CD1	-5.57	116.90	120.80
5	e	156	PHE	CA-CB-CG	-5.57	100.53	113.90
27	O	19	ASP	CB-CG-OD2	5.57	123.31	118.30
5	e	187	TRP	CH2-CZ2-CE2	5.56	122.96	117.40
9	i	150	VAL	N-CA-C	-5.56	95.98	111.00
33	J	231	ARG	NE-CZ-NH2	5.56	123.08	120.30
14	n	259	LYS	CB-CA-C	-5.56	99.27	110.40
23	P	13	TYR	CG-CD2-CE2	-5.56	116.85	121.30
24	Q	409	TYR	CB-CG-CD2	-5.56	117.66	121.00
30	K	336	ARG	NE-CZ-NH1	5.56	123.08	120.30
30	K	412	ALA	N-CA-CB	5.56	117.89	110.10
32	M	433	TYR	CG-CD1-CE1	-5.56	116.85	121.30
19	Y	16	LEU	CB-CG-CD2	-5.56	101.55	111.00
20	Z	118	VAL	CA-CB-CG1	5.56	119.24	110.90
3	C	222	ASP	N-CA-CB	5.56	120.60	110.60
9	2	152	TYR	CG-CD1-CE1	-5.56	116.85	121.30
30	K	346	ARG	NE-CZ-NH2	-5.56	117.52	120.30
12	5	163	TYR	CG-CD1-CE1	5.55	125.74	121.30
2	b	65	SER	N-CA-CB	5.55	118.83	110.50
12	5	251	ASN	N-CA-CB	5.55	120.59	110.60
20	Z	339	PHE	CB-CG-CD1	5.55	124.69	120.80
32	M	349	PHE	N-CA-CB	5.55	120.59	110.60
7	g	78	TYR	CZ-CE2-CD2	-5.55	114.81	119.80
13	m	149	ALA	CB-CA-C	-5.55	101.78	110.10
16	V	107	TRP	CG-CD2-CE3	-5.55	128.91	133.90
25	R	141	TYR	CG-CD2-CE2	-5.55	116.86	121.30
9	i	207	MET	CG-SD-CE	-5.54	91.33	100.20
4	d	97	ARG	NE-CZ-NH2	-5.54	117.53	120.30
17	T	105	LEU	CB-CA-C	-5.54	99.67	110.20
26	U	243	ASP	CB-CG-OD1	5.54	123.29	118.30
21	N	124	TYR	CG-CD1-CE1	-5.54	116.87	121.30
3	c	157	TYR	CG-CD1-CE1	-5.54	116.87	121.30
20	Z	426	TYR	CD1-CE1-CZ	-5.54	114.81	119.80
23	P	171	MET	CA-CB-CG	5.54	122.72	113.30
27	O	10	ILE	CB-CA-C	-5.54	100.53	111.60
2	b	101	TYR	CZ-CE2-CD2	5.53	124.78	119.80
4	d	159	TRP	CB-CG-CD1	5.53	134.19	127.00
14	n	228	PHE	CB-CG-CD2	-5.53	116.93	120.80
20	Z	129	ASN	C-N-CA	5.53	133.92	122.30
29	I	94	LYS	N-CA-CB	5.53	120.56	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	81	ASP	CB-CG-OD2	5.53	123.28	118.30
2	B	178	ARG	NE-CZ-NH1	5.53	123.07	120.30
20	Z	889	VAL	CA-CB-CG2	-5.53	102.60	110.90
1	a	249	ALA	N-CA-CB	5.53	117.84	110.10
7	g	10	LEU	N-CA-CB	5.53	121.46	110.40
8	h	25	ALA	N-CA-CB	5.53	117.84	110.10
11	k	138	PHE	CB-CG-CD2	-5.53	116.93	120.80
8	1	134	ALA	N-CA-CB	5.53	117.84	110.10
22	S	442	PHE	N-CA-CB	5.53	120.55	110.60
24	Q	168	LEU	CB-CG-CD1	5.53	120.40	111.00
24	Q	238	TYR	CG-CD2-CE2	5.53	125.72	121.30
27	O	302	VAL	N-CA-CB	5.53	123.67	111.50
17	T	175	ASP	CB-CG-OD1	5.53	123.28	118.30
14	n	215	ARG	NE-CZ-NH2	5.53	123.06	120.30
20	Z	58	GLU	CB-CA-C	-5.53	99.34	110.40
10	3	74	TYR	CD1-CE1-CZ	5.53	124.77	119.80
29	I	129	TYR	CZ-CE2-CD2	5.53	124.77	119.80
8	1	19	ASP	CB-CG-OD2	-5.52	113.33	118.30
20	Z	167	ASP	CB-CG-OD1	-5.52	113.33	118.30
20	Z	293	MET	CG-SD-CE	-5.52	91.36	100.20
24	Q	306	TYR	CG-CD2-CE2	5.52	125.72	121.30
8	1	60	ASP	CB-CG-OD2	-5.52	113.33	118.30
17	T	175	ASP	CB-CG-OD2	-5.52	113.33	118.30
21	N	788	TYR	CB-CG-CD2	-5.52	117.69	121.00
27	O	142	ASP	N-CA-C	-5.52	96.09	111.00
12	l	144	ARG	NE-CZ-NH2	-5.52	117.54	120.30
13	m	210	LEU	CB-CG-CD2	-5.52	101.62	111.00
24	Q	354	PHE	CB-CG-CD1	5.52	124.66	120.80
31	L	145	ARG	NE-CZ-NH1	-5.52	117.54	120.30
17	T	234	TYR	CZ-CE2-CD2	-5.51	114.84	119.80
14	n	137	ARG	NE-CZ-NH1	-5.51	117.55	120.30
16	V	45	VAL	CA-CB-CG2	-5.51	102.63	110.90
5	e	15	PHE	C-N-CA	5.51	135.47	121.70
10	j	110	ALA	N-CA-CB	5.51	117.81	110.10
7	g	182	HIS	CA-CB-CG	-5.51	104.24	113.60
32	M	326	ALA	N-CA-CB	5.51	117.81	110.10
1	A	134	MET	N-CA-CB	5.50	120.51	110.60
8	1	120	TYR	CG-CD2-CE2	-5.50	116.90	121.30
21	N	685	VAL	CG1-CB-CG2	-5.50	102.09	110.90
11	4	175	ASP	CB-CG-OD2	-5.50	113.35	118.30
23	P	201	ARG	CG-CD-NE	-5.50	100.24	111.80
11	k	150	PRO	CA-N-CD	5.50	119.40	111.70

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2	202	VAL	CA-CB-CG2	-5.50	102.65	110.90
30	K	198	TYR	CB-CG-CD2	-5.50	117.70	121.00
7	g	119	TYR	CA-CB-CG	-5.50	102.95	113.40
28	H	222	ARG	NE-CZ-NH1	5.50	123.05	120.30
12	l	263	HIS	CA-CB-CG	-5.50	104.26	113.60
21	N	424	LYS	N-CA-CB	5.50	120.49	110.60
21	N	908	ARG	NE-CZ-NH2	-5.50	117.55	120.30
30	K	124	SER	C-N-CA	5.50	135.44	121.70
1	A	110	TYR	C-N-CA	5.49	135.44	121.70
1	A	161	GLY	CA-C-O	-5.49	110.71	120.60
31	L	62	ARG	NE-CZ-NH1	5.49	123.05	120.30
31	L	258	GLU	C-N-CA	5.49	135.43	121.70
20	Z	272	TYR	CG-CD1-CE1	5.49	125.69	121.30
33	J	249	GLU	N-CA-CB	5.49	120.49	110.60
8	h	141	THR	CA-CB-CG2	-5.49	104.71	112.40
20	Z	265	LEU	CB-CA-C	-5.49	99.77	110.20
20	Z	530	LEU	O-C-N	-5.49	113.92	122.70
21	N	463	TYR	CB-CG-CD2	-5.49	117.71	121.00
21	N	474	SER	N-CA-CB	5.49	118.74	110.50
30	K	98	GLN	N-CA-C	-5.49	96.18	111.00
8	1	133	TYR	N-CA-CB	5.49	120.48	110.60
20	Z	349	THR	CA-CB-CG2	-5.49	104.72	112.40
14	7	110	ASP	CB-CG-OD1	-5.49	113.36	118.30
9	2	232	TYR	CB-CG-CD1	5.48	124.29	121.00
13	6	26	GLU	OE1-CD-OE2	-5.48	116.72	123.30
33	J	310	ILE	N-CA-CB	5.48	123.41	110.80
20	Z	963	ALA	CB-CA-C	-5.48	101.88	110.10
21	N	685	VAL	CA-CB-CG1	5.48	119.12	110.90
25	R	78	ASP	CB-CG-OD2	5.48	123.23	118.30
8	1	169	SER	CB-CA-C	-5.48	99.69	110.10
4	D	186	ALA	N-CA-CB	-5.48	102.43	110.10
7	G	145	GLY	N-CA-C	-5.48	99.41	113.10
16	V	225	LEU	CB-CG-CD1	-5.48	101.69	111.00
2	b	138	GLY	O-C-N	5.47	131.46	122.70
12	l	282	PHE	CB-CG-CD1	-5.47	116.97	120.80
14	7	179	PHE	CB-CG-CD2	-5.47	116.97	120.80
28	H	87	ASP	CB-CA-C	-5.47	99.45	110.40
1	a	42	SER	N-CA-CB	5.47	118.71	110.50
10	j	177	ARG	NE-CZ-NH1	5.47	123.04	120.30
32	M	372	ASP	CB-CG-OD1	5.47	123.22	118.30
6	f	7	ASP	CB-CG-OD1	5.47	123.22	118.30
4	d	78	LEU	CB-CG-CD1	5.47	120.30	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	415	ASP	CB-CG-OD1	5.47	123.22	118.30
30	K	246	TYR	CG-CD1-CE1	-5.47	116.92	121.30
23	P	234	TYR	CB-CG-CD2	5.47	124.28	121.00
2	b	219	PRO	C-N-CA	5.47	135.37	121.70
4	d	172	ARG	NE-CZ-NH1	5.47	123.03	120.30
15	W	67	ALA	N-CA-CB	5.46	117.75	110.10
21	N	168	SER	CB-CA-C	-5.46	99.72	110.10
31	L	283	VAL	CG1-CB-CG2	5.46	119.64	110.90
1	a	162	TYR	CB-CG-CD1	5.46	124.28	121.00
13	m	49	PRO	N-CA-CB	5.46	109.85	103.30
19	Y	53	ALA	N-CA-CB	5.46	117.74	110.10
27	O	224	GLY	O-C-N	5.46	131.43	122.70
20	Z	356	ASP	CB-CG-OD1	5.46	123.21	118.30
19	Y	7	ALA	N-CA-CB	-5.45	102.47	110.10
11	4	26	SER	O-C-N	5.45	131.42	122.70
20	Z	467	VAL	CA-CB-CG2	-5.45	102.72	110.90
2	b	175	LEU	CB-CG-CD1	-5.45	101.74	111.00
14	n	241	PHE	CG-CD1-CE1	5.45	126.79	120.80
11	4	107	TYR	N-CA-CB	5.45	120.41	110.60
6	f	6	TYR	CG-CD1-CE1	5.45	125.66	121.30
23	P	245	TYR	CB-CG-CD1	5.45	124.27	121.00
9	2	162	ALA	CB-CA-C	-5.45	101.93	110.10
10	3	100	PHE	CB-CG-CD2	-5.45	116.99	120.80
20	Z	619	ASP	CB-CG-OD2	-5.45	113.40	118.30
22	S	354	LEU	CB-CG-CD2	5.45	120.26	111.00
31	L	168	TYR	CZ-CE2-CD2	5.45	124.70	119.80
5	e	148	ASP	CB-CG-OD1	-5.44	113.40	118.30
14	n	131	THR	CA-CB-CG2	5.44	120.02	112.40
8	h	17	PHE	CB-CG-CD1	5.44	124.61	120.80
6	F	175	THR	N-CA-CB	-5.44	99.96	110.30
16	V	108	TYR	CD1-CE1-CZ	5.44	124.70	119.80
21	N	813	ARG	CG-CD-NE	-5.44	100.37	111.80
29	I	283	GLU	N-CA-CB	5.44	120.40	110.60
30	K	209	VAL	CG1-CB-CG2	-5.44	102.19	110.90
3	c	217	ARG	N-CA-CB	5.44	120.39	110.60
1	A	71	TYR	CB-CG-CD1	-5.44	117.73	121.00
21	N	210	SER	N-CA-CB	5.44	118.66	110.50
11	4	194	ASP	CB-CG-OD1	5.44	123.19	118.30
20	Z	901	PHE	CB-CG-CD1	-5.44	116.99	120.80
29	I	135	PHE	CB-CG-CD1	5.44	124.61	120.80
30	K	185	ARG	NE-CZ-NH1	5.44	123.02	120.30
31	L	245	PHE	CB-CG-CD1	5.44	124.61	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	186	PHE	CB-CG-CD1	5.44	124.61	120.80
2	B	170	ALA	N-CA-CB	5.43	117.71	110.10
5	E	232	ASP	CB-CG-OD2	-5.43	113.41	118.30
21	N	481	ALA	CB-CA-C	-5.43	101.95	110.10
22	S	195	ALA	N-CA-CB	5.43	117.70	110.10
31	L	253	ASP	CB-CG-OD2	-5.43	113.41	118.30
1	a	234	PHE	CD1-CE1-CZ	-5.43	113.58	120.10
4	D	82	SER	CB-CA-C	-5.43	99.78	110.10
4	D	108	TYR	CB-CG-CD1	-5.43	117.74	121.00
12	5	188	TYR	CA-CB-CG	-5.43	103.08	113.40
21	N	331	ALA	CB-CA-C	-5.43	101.96	110.10
9	i	100	SER	CB-CA-C	5.43	120.41	110.10
1	a	71	TYR	N-CA-CB	5.43	120.37	110.60
16	V	273	ARG	NE-CZ-NH1	-5.43	117.59	120.30
3	c	160	TRP	CG-CD1-NE1	-5.42	104.68	110.10
26	U	9	THR	CA-CB-CG2	-5.42	104.81	112.40
1	A	42	SER	N-CA-CB	5.42	118.63	110.50
8	1	163	PHE	CD1-CE1-CZ	-5.42	113.59	120.10
31	L	386	PHE	CB-CG-CD1	5.42	124.59	120.80
31	L	89	ASP	CB-CG-OD1	-5.42	113.42	118.30
8	h	202	TYR	N-CA-CB	5.42	120.35	110.60
4	D	136	ALA	N-CA-CB	5.42	117.68	110.10
33	J	53	ASP	CB-CG-OD2	5.42	123.17	118.30
14	n	244	ASN	N-CA-CB	5.41	120.34	110.60
16	V	153	ILE	N-CA-C	-5.41	96.38	111.00
6	f	179	PHE	CG-CD1-CE1	-5.41	114.85	120.80
13	m	56	ASP	N-CA-CB	5.41	120.34	110.60
18	X	102	GLN	N-CA-CB	5.41	120.34	110.60
13	6	131	TYR	CA-CB-CG	-5.41	103.12	113.40
29	I	241	SER	N-CA-CB	5.41	118.61	110.50
4	d	101	GLU	N-CA-CB	5.41	120.33	110.60
9	2	219	TYR	CB-CG-CD1	5.41	124.24	121.00
5	E	141	ALA	N-CA-CB	5.41	117.67	110.10
14	7	35	GLN	N-CA-CB	5.41	120.33	110.60
24	Q	104	PHE	CB-CG-CD1	-5.41	117.02	120.80
32	M	339	ARG	NE-CZ-NH2	5.41	123.00	120.30
7	G	54	ILE	N-CA-C	-5.40	96.41	111.00
30	K	282	PHE	CB-CG-CD2	-5.40	117.02	120.80
8	h	161	VAL	CA-CB-CG2	-5.40	102.80	110.90
11	k	107	TYR	CB-CG-CD2	-5.40	117.76	121.00
21	N	45	ASP	CB-CG-OD1	-5.40	113.44	118.30
21	N	865	PRO	N-CD-CG	5.40	111.30	103.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	289	ARG	NE-CZ-NH1	-5.40	117.60	120.30
17	T	96	LEU	C-N-CA	5.40	135.19	121.70
20	Z	60	ASP	N-CA-CB	5.39	120.31	110.60
28	H	286	GLU	CB-CG-CD	-5.39	99.63	114.20
9	i	119	TYR	CB-CG-CD1	-5.39	117.76	121.00
23	P	10	ASP	CB-CG-OD2	-5.39	113.45	118.30
12	5	82	ARG	CD-NE-CZ	-5.39	116.06	123.60
15	W	165	GLN	N-CA-CB	5.39	120.30	110.60
24	Q	30	LEU	CB-CA-C	-5.39	99.96	110.20
33	J	101	ASP	CB-CG-OD1	5.39	123.15	118.30
3	C	183	ASP	CB-CG-OD2	-5.39	113.45	118.30
3	C	207	THR	CA-CB-CG2	-5.39	104.86	112.40
18	X	68	LEU	CB-CG-CD1	5.39	120.16	111.00
24	Q	340	ASP	N-CA-CB	5.39	120.29	110.60
32	M	381	ARG	CD-NE-CZ	5.39	131.14	123.60
3	c	157	TYR	CB-CG-CD1	5.38	124.23	121.00
13	6	114	TYR	CG-CD2-CE2	5.38	125.61	121.30
33	J	174	PHE	CZ-CE2-CD2	-5.38	113.64	120.10
12	l	175	MET	CG-SD-CE	5.38	108.81	100.20
4	D	37	LYS	CB-CA-C	-5.38	99.63	110.40
20	Z	15	GLN	CG-CD-OE1	-5.38	110.83	121.60
20	Z	838	TYR	CB-CG-CD1	5.38	124.23	121.00
5	e	205	LYS	N-CA-CB	5.38	120.29	110.60
12	l	100	TRP	CB-CG-CD1	5.38	134.00	127.00
5	E	15	PHE	O-C-N	-5.38	114.09	122.70
7	G	181	ASP	CB-CG-OD2	5.38	123.14	118.30
21	N	370	SER	N-CA-CB	5.38	118.57	110.50
10	j	188	TYR	CB-CG-CD2	5.38	124.23	121.00
14	7	84	VAL	CA-CB-CG1	5.38	118.97	110.90
23	P	303	PHE	CB-CG-CD2	-5.38	117.03	120.80
6	f	51	ARG	NH1-CZ-NH2	5.38	125.31	119.40
33	J	81	ASP	N-CA-CB	5.38	120.28	110.60
12	5	227	ASP	CB-CG-OD1	5.38	123.14	118.30
28	H	354	ALA	N-CA-CB	5.38	117.63	110.10
30	K	68	ILE	CB-CA-C	5.38	122.35	111.60
31	L	128	ILE	N-CA-C	-5.37	96.49	111.00
7	g	119	TYR	CB-CG-CD1	5.37	124.22	121.00
21	N	422	TYR	CZ-CE2-CD2	-5.37	114.97	119.80
32	M	203	ARG	CD-NE-CZ	-5.37	116.08	123.60
14	7	93	MET	CG-SD-CE	-5.37	91.61	100.20
28	H	208	TYR	CB-CG-CD1	5.37	124.22	121.00
7	g	97	ALA	CB-CA-C	-5.36	102.05	110.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	213	GLU	N-CA-C	-5.36	96.52	111.00
1	A	201	LYS	CB-CA-C	-5.36	99.67	110.40
9	2	51	GLN	N-CA-C	-5.36	96.52	111.00
9	2	98	TYR	CD1-CG-CD2	5.36	123.80	117.90
24	Q	353	PRO	N-CA-CB	5.36	109.74	103.30
32	M	15	ASP	N-CA-CB	5.36	120.26	110.60
4	d	98	LEU	CB-CG-CD1	5.36	120.11	111.00
1	A	153	SER	N-CA-CB	5.36	118.54	110.50
30	K	333	ARG	N-CA-CB	5.36	120.25	110.60
26	U	89	LEU	CB-CG-CD2	5.36	120.11	111.00
23	P	171	MET	CG-SD-CE	-5.36	91.63	100.20
23	P	293	LEU	N-CA-C	-5.36	96.53	111.00
24	Q	132	PHE	N-CA-CB	5.36	120.24	110.60
13	m	27	ASP	CB-CG-OD1	-5.36	113.48	118.30
22	S	259	TYR	CG-CD1-CE1	5.36	125.58	121.30
33	J	106	ASP	CB-CG-OD2	-5.36	113.48	118.30
20	Z	299	ASP	CB-CG-OD2	-5.35	113.48	118.30
9	2	243	LYS	N-CA-CB	5.35	120.23	110.60
28	H	381	ASP	N-CA-CB	5.35	120.23	110.60
7	G	243	ALA	CB-CA-C	-5.35	102.07	110.10
10	3	16	THR	N-CA-CB	5.35	120.47	110.30
19	Y	52	ASN	N-CA-CB	5.35	120.23	110.60
1	A	234	PHE	N-CA-CB	5.35	120.23	110.60
20	Z	397	ASP	CB-CG-OD1	5.35	123.11	118.30
20	Z	428	TRP	CG-CD2-CE3	-5.35	129.09	133.90
21	N	588	VAL	CA-CB-CG2	-5.35	102.88	110.90
2	b	135	LEU	N-CA-CB	5.35	121.09	110.40
24	Q	48	ASP	N-CA-CB	5.35	120.22	110.60
14	7	165	LEU	CB-CG-CD2	5.34	120.08	111.00
22	S	414	ASP	CB-CG-OD2	-5.34	113.49	118.30
6	f	123	TYR	CG-CD2-CE2	5.34	125.57	121.30
4	D	4	TYR	CD1-CE1-CZ	5.34	124.61	119.80
13	6	41	TYR	CA-CB-CG	-5.34	103.25	113.40
17	T	86	LYS	CA-C-N	5.34	132.06	117.10
2	b	246	ARG	NH1-CZ-NH2	-5.34	113.53	119.40
1	A	150	LEU	C-N-CA	5.34	133.51	122.30
21	N	246	LYS	CA-CB-CG	5.34	125.15	113.40
22	S	76	PHE	CB-CG-CD1	-5.34	117.06	120.80
5	E	15	PHE	CB-CG-CD2	-5.34	117.06	120.80
13	6	105	LEU	O-C-N	-5.34	114.16	122.70
14	7	219	TYR	CG-CD1-CE1	-5.34	117.03	121.30
25	R	171	MET	CG-SD-CE	-5.34	91.66	100.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	91	ARG	NE-CZ-NH1	5.33	122.97	120.30
14	7	126	PHE	CG-CD1-CE1	5.33	126.67	120.80
21	N	621	THR	CA-CB-CG2	5.33	119.87	112.40
20	Z	112	LYS	CA-CB-CG	5.33	125.13	113.40
27	O	190	TYR	CB-CG-CD1	-5.33	117.80	121.00
4	D	187	THR	N-CA-CB	5.33	120.43	110.30
7	g	137	ILE	CB-CA-C	-5.33	100.94	111.60
8	h	205	LEU	CB-CG-CD1	5.33	120.06	111.00
17	T	151	TRP	CG-CD2-CE3	-5.33	129.10	133.90
16	V	61	TYR	CG-CD2-CE2	-5.33	117.04	121.30
18	X	34	GLU	N-CA-CB	5.33	120.19	110.60
20	Z	323	TYR	CB-CG-CD1	-5.33	117.81	121.00
29	I	222	TYR	CB-CG-CD2	-5.33	117.81	121.00
3	c	160	TRP	CD1-NE1-CE2	5.32	113.79	109.00
10	j	40	PHE	CB-CG-CD1	-5.32	117.07	120.80
12	l	77	THR	N-CA-C	-5.32	96.63	111.00
13	6	31	LEU	N-CA-CB	5.32	121.05	110.40
21	N	585	ARG	NE-CZ-NH2	5.32	122.96	120.30
28	H	90	ARG	NE-CZ-NH2	-5.32	117.64	120.30
28	H	230	LEU	CB-CG-CD2	-5.32	101.95	111.00
8	h	155	MET	N-CA-CB	5.32	120.18	110.60
1	a	32	PHE	N-CA-CB	5.32	120.17	110.60
14	n	141	ASN	N-CA-CB	5.32	120.18	110.60
7	G	167	LYS	CA-CB-CG	5.32	125.11	113.40
33	J	137	MET	CG-SD-CE	-5.32	91.69	100.20
2	b	9	LEU	CB-CG-CD1	5.32	120.04	111.00
2	B	82	TYR	CB-CG-CD1	5.32	124.19	121.00
7	g	99	PHE	CB-CG-CD2	-5.32	117.08	120.80
12	l	214	VAL	CA-CB-CG2	-5.32	102.92	110.90
20	Z	269	TYR	CD1-CE1-CZ	-5.32	115.01	119.80
25	R	164	THR	CA-CB-CG2	-5.32	104.96	112.40
27	O	172	TYR	CB-CG-CD2	5.32	124.19	121.00
9	i	245	SER	CB-CA-C	-5.32	100.00	110.10
25	R	136	ASN	CA-CB-CG	-5.32	101.71	113.40
8	1	119	VAL	CA-CB-CG1	-5.31	102.93	110.90
6	f	128	TYR	CG-CD1-CE1	-5.31	117.05	121.30
8	h	201	GLU	O-C-N	-5.31	114.20	122.70
7	G	97	ALA	N-CA-CB	5.31	117.54	110.10
1	a	19	PHE	CB-CA-C	-5.31	99.78	110.40
11	k	98	TYR	CB-CG-CD2	5.31	124.18	121.00
11	k	139	TYR	CB-CG-CD2	-5.31	117.82	121.00
31	L	264	ARG	NE-CZ-NH2	-5.31	117.65	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	189	ALA	CB-CA-C	-5.31	102.14	110.10
7	G	22	PHE	CB-CG-CD1	5.30	124.51	120.80
31	L	153	LEU	N-CA-CB	5.30	121.01	110.40
5	e	60	GLU	OE1-CD-OE2	-5.30	116.94	123.30
17	T	186	ARG	CD-NE-CZ	5.30	131.02	123.60
32	M	381	ARG	NE-CZ-NH1	-5.30	117.65	120.30
1	a	197	GLU	N-CA-CB	5.30	120.14	110.60
9	2	152	TYR	CD1-CE1-CZ	5.30	124.57	119.80
14	7	240	THR	CA-CB-CG2	-5.30	104.98	112.40
22	S	60	LEU	CB-CG-CD1	-5.30	101.99	111.00
23	P	257	TRP	N-CA-CB	5.30	120.14	110.60
28	H	343	PHE	CB-CG-CD1	5.30	124.51	120.80
3	c	171	ALA	CB-CA-C	-5.30	102.15	110.10
19	Y	84	TYR	CD1-CE1-CZ	-5.30	115.03	119.80
20	Z	269	TYR	CD1-CG-CD2	5.30	123.73	117.90
25	R	264	THR	CA-CB-CG2	-5.30	104.98	112.40
31	L	344	ASP	CB-CG-OD2	5.30	123.07	118.30
6	f	159	THR	N-CA-CB	5.30	120.37	110.30
8	h	66	ASP	CB-CG-OD1	5.30	123.07	118.30
13	m	52	PHE	CG-CD1-CE1	-5.30	114.97	120.80
17	T	51	TYR	CA-CB-CG	5.30	123.46	113.40
17	T	246	GLU	OE1-CD-OE2	-5.30	116.94	123.30
25	R	91	TRP	CG-CD2-CE3	-5.30	129.13	133.90
27	O	141	ASN	N-CA-CB	5.30	120.13	110.60
13	6	29	ALA	N-CA-CB	5.29	117.51	110.10
15	W	44	ASN	N-CA-CB	5.29	120.13	110.60
20	Z	145	ASP	N-CA-CB	5.29	120.13	110.60
21	N	348	PHE	CD1-CE1-CZ	5.29	126.45	120.10
2	b	207	ASP	N-CA-CB	5.29	120.13	110.60
28	H	389	PHE	CB-CG-CD1	-5.29	117.09	120.80
32	M	104	GLY	CA-C-O	5.29	130.12	120.60
33	J	94	TYR	CZ-CE2-CD2	5.29	124.56	119.80
33	J	390	MET	CG-SD-CE	-5.29	91.73	100.20
11	4	96	ARG	CG-CD-NE	-5.29	100.69	111.80
20	Z	316	ALA	N-CA-CB	5.29	117.50	110.10
21	N	526	TYR	CB-CG-CD1	5.29	124.17	121.00
3	C	54	SER	CB-CA-C	-5.29	100.05	110.10
21	N	758	VAL	CA-C-O	5.29	131.21	120.10
21	N	651	PHE	CB-CG-CD2	5.29	124.50	120.80
6	f	13	PHE	CG-CD2-CE2	-5.29	114.99	120.80
14	n	67	LEU	N-CA-CB	5.29	120.97	110.40
16	V	296	LEU	CB-CG-CD1	5.29	119.98	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	269	GLN	N-CA-CB	5.29	120.11	110.60
23	P	397	ALA	N-CA-CB	5.28	117.50	110.10
12	5	115	PHE	CB-CG-CD1	5.28	124.50	120.80
15	W	122	ARG	NE-CZ-NH2	-5.28	117.66	120.30
17	T	32	ILE	CA-CB-CG2	-5.28	100.34	110.90
28	H	353	PHE	CB-CG-CD1	5.28	124.50	120.80
3	c	141	ASP	CB-CG-OD1	-5.28	113.55	118.30
1	A	46	ARG	NE-CZ-NH1	5.28	122.94	120.30
13	6	89	ASP	N-CA-CB	5.28	120.10	110.60
22	S	375	ASP	CB-CG-OD2	-5.28	113.55	118.30
8	h	62	GLN	N-CA-CB	5.28	120.09	110.60
2	B	236	ARG	N-CA-C	-5.28	96.75	111.00
31	L	422	VAL	CA-CB-CG1	5.28	118.81	110.90
6	f	85	SER	N-CA-CB	5.27	118.41	110.50
9	i	179	GLU	O-C-N	-5.27	114.26	122.70
13	m	215	VAL	O-C-N	5.27	131.13	122.70
14	n	63	TYR	CD1-CG-CD2	5.27	123.70	117.90
22	S	244	ASN	N-CA-CB	5.27	120.09	110.60
13	6	79	SER	N-CA-CB	5.27	118.41	110.50
16	V	135	ARG	CG-CD-NE	-5.27	100.73	111.80
22	S	382	ARG	NE-CZ-NH1	-5.27	117.67	120.30
11	k	96	ARG	CA-CB-CG	5.27	125.00	113.40
28	H	346	ARG	NE-CZ-NH1	-5.27	117.67	120.30
9	i	50	THR	CA-CB-CG2	-5.27	105.03	112.40
8	1	153	GLU	OE1-CD-OE2	5.27	129.62	123.30
20	Z	893	PHE	CG-CD1-CE1	-5.27	115.01	120.80
23	P	279	ASP	CB-CG-OD2	5.27	123.04	118.30
12	l	258	ASP	CB-CG-OD1	-5.26	113.56	118.30
14	n	146	ALA	N-CA-CB	5.26	117.47	110.10
11	4	145	ASP	CB-CG-OD1	-5.26	113.56	118.30
11	4	195	PHE	CB-CG-CD2	5.26	124.48	120.80
9	i	215	TYR	CD1-CG-CD2	5.26	123.69	117.90
29	I	399	ALA	CB-CA-C	-5.26	102.21	110.10
33	J	116	ARG	NE-CZ-NH2	-5.26	117.67	120.30
14	n	185	ASN	CA-C-O	-5.26	109.06	120.10
20	Z	868	ASN	CB-CA-C	-5.26	99.88	110.40
21	N	125	THR	CA-CB-CG2	-5.26	105.04	112.40
33	J	368	TYR	CB-CG-CD1	5.26	124.16	121.00
1	A	162	TYR	CD1-CE1-CZ	-5.26	115.07	119.80
14	n	218	TYR	CG-CD2-CE2	5.26	125.50	121.30
3	C	31	HIS	N-CA-CB	5.26	120.06	110.60
15	W	113	PHE	CB-CG-CD1	5.26	124.48	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	238	TYR	CZ-CE2-CD2	-5.26	115.07	119.80
26	U	22	TYR	CD1-CG-CD2	5.26	123.68	117.90
33	J	185	VAL	CA-CB-CG1	-5.26	103.02	110.90
17	T	62	LEU	CB-CG-CD2	5.25	119.93	111.00
1	A	229	THR	N-CA-C	-5.25	96.81	111.00
14	n	243	LYS	CB-CA-C	-5.25	99.90	110.40
4	D	156	TYR	CG-CD2-CE2	-5.25	117.10	121.30
13	6	16	ASN	N-CA-CB	5.25	120.05	110.60
20	Z	757	SER	N-CA-CB	5.25	118.38	110.50
23	P	168	TYR	N-CA-CB	5.25	120.05	110.60
26	U	137	TYR	N-CA-CB	5.25	120.05	110.60
28	H	241	ASP	N-CA-C	-5.25	96.82	111.00
28	H	368	PRO	C-N-CA	5.25	133.33	122.30
31	L	83	ASP	CB-CG-OD2	5.25	123.03	118.30
9	i	120	GLN	N-CA-CB	5.25	120.05	110.60
27	O	373	TRP	O-C-N	-5.25	114.30	122.70
20	Z	792	VAL	CA-CB-CG1	5.25	118.77	110.90
13	6	194	ASP	CB-CG-OD1	5.25	123.02	118.30
21	N	906	ARG	NH1-CZ-NH2	5.24	125.17	119.40
9	i	49	SER	N-CA-C	-5.24	96.85	111.00
16	V	92	MET	CG-SD-CE	-5.24	91.81	100.20
6	f	119	ASN	CB-CA-C	-5.24	99.92	110.40
9	i	57	ASP	N-CA-CB	5.24	120.03	110.60
27	O	306	ARG	NE-CZ-NH2	-5.24	117.68	120.30
4	d	217	PRO	N-CA-CB	5.24	109.58	103.30
1	A	105	ARG	NH1-CZ-NH2	5.24	125.16	119.40
1	A	160	ALA	CB-CA-C	-5.24	102.25	110.10
5	E	8	TYR	CB-CG-CD1	5.24	124.14	121.00
25	R	326	ALA	O-C-N	-5.24	114.33	122.70
29	I	129	TYR	CG-CD2-CE2	-5.24	117.11	121.30
30	K	129	GLU	N-CA-CB	5.23	120.02	110.60
14	n	49	TYR	N-CA-CB	5.23	120.02	110.60
2	B	6	SER	N-CA-C	-5.23	96.88	111.00
21	N	839	ARG	NE-CZ-NH1	5.23	122.92	120.30
26	U	146	ASP	CB-CG-OD1	5.23	123.01	118.30
33	J	174	PHE	CB-CG-CD1	-5.23	117.14	120.80
12	l	267	ASP	CB-CG-OD2	-5.23	113.59	118.30
28	H	385	ARG	N-CA-CB	5.23	120.01	110.60
5	e	53	ARG	NE-CZ-NH2	-5.23	117.69	120.30
7	g	242	PHE	CB-CA-C	5.23	120.86	110.40
25	R	246	TYR	CB-CG-CD2	-5.23	117.86	121.00
8	1	17	PHE	CG-CD2-CE2	5.22	126.55	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	147	ASP	CB-CG-OD1	5.22	123.00	118.30
22	S	344	PRO	N-CA-CB	5.22	109.57	103.30
29	I	313	LEU	CB-CG-CD1	5.22	119.88	111.00
2	b	90	ARG	NE-CZ-NH1	-5.22	117.69	120.30
24	Q	163	ARG	O-C-N	-5.22	114.35	122.70
9	2	233	LYS	N-CA-CB	5.22	120.00	110.60
21	N	23	TYR	CD1-CG-CD2	5.22	123.64	117.90
31	L	334	ASP	CB-CG-OD2	-5.22	113.60	118.30
20	Z	195	PHE	CB-CG-CD1	5.22	124.45	120.80
11	k	30	ASP	CB-CA-C	-5.22	99.97	110.40
4	d	155	ILE	CB-CA-C	-5.21	101.17	111.60
10	3	112	ILE	N-CA-C	-5.21	96.92	111.00
21	N	786	ARG	NE-CZ-NH2	-5.21	117.69	120.30
5	e	22	PHE	CG-CD2-CE2	-5.21	115.07	120.80
1	a	133	TYR	CG-CD2-CE2	-5.21	117.13	121.30
22	S	484	ASP	CB-CG-OD1	-5.21	113.61	118.30
2	B	56	ALA	N-CA-CB	5.21	117.39	110.10
28	H	295	PHE	CB-CG-CD2	-5.21	117.15	120.80
29	I	343	ARG	CD-NE-CZ	-5.21	116.31	123.60
31	L	80	ASN	CB-CA-C	-5.21	99.98	110.40
32	M	285	ALA	N-CA-CB	5.21	117.39	110.10
16	V	194	ARG	NE-CZ-NH2	5.21	122.90	120.30
30	K	375	ASN	CB-CA-C	-5.21	99.99	110.40
7	G	15	PHE	N-CA-CB	5.20	119.97	110.60
10	3	189	ILE	N-CA-C	-5.20	96.95	111.00
14	7	223	ARG	NH1-CZ-NH2	5.20	125.12	119.40
24	Q	77	PHE	CB-CG-CD1	5.20	124.44	120.80
32	M	309	LEU	CB-CG-CD1	-5.20	102.16	111.00
28	H	192	ASP	CA-C-N	5.20	131.67	117.10
13	m	13	TYR	CB-CG-CD1	5.20	124.12	121.00
13	6	51	VAL	CG1-CB-CG2	5.20	119.22	110.90
1	A	201	LYS	N-CA-CB	5.20	119.96	110.60
21	N	756	THR	CA-CB-CG2	-5.20	105.12	112.40
22	S	272	TYR	CG-CD1-CE1	-5.20	117.14	121.30
23	P	143	LEU	CB-CA-C	-5.20	100.32	110.20
2	b	22	ASP	CB-CG-OD1	-5.20	113.62	118.30
26	U	78	GLU	CB-CA-C	-5.20	100.01	110.40
3	c	18	ARG	NE-CZ-NH2	-5.20	117.70	120.30
10	3	45	HIS	CA-CB-CG	5.20	122.43	113.60
11	4	46	PHE	CB-CG-CD1	-5.20	117.16	120.80
15	W	21	PHE	N-CA-C	-5.20	96.97	111.00
33	J	71	TYR	CZ-CE2-CD2	-5.20	115.12	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	12	TYR	CB-CG-CD1	-5.19	117.88	121.00
9	i	139	LEU	N-CA-C	-5.19	96.98	111.00
20	Z	145	ASP	CB-CG-OD2	5.19	122.97	118.30
4	D	48	ARG	N-CA-CB	-5.19	101.25	110.60
21	N	706	MET	CG-SD-CE	5.19	108.50	100.20
26	U	137	TYR	CZ-CE2-CD2	5.19	124.47	119.80
26	U	22	TYR	CG-CD2-CE2	-5.19	117.15	121.30
32	M	274	ALA	CB-CA-C	-5.19	102.32	110.10
29	I	165	ASP	CA-C-N	5.19	131.62	117.10
9	2	98	TYR	CG-CD1-CE1	-5.19	117.15	121.30
32	M	274	ALA	CA-C-O	-5.19	109.21	120.10
10	3	199	TYR	CB-CG-CD1	5.18	124.11	121.00
32	M	46	SER	N-CA-CB	5.18	118.28	110.50
32	M	48	LEU	CB-CA-C	-5.18	100.35	110.20
33	J	345	LYS	N-CA-CB	5.18	119.93	110.60
1	a	91	ARG	NH1-CZ-NH2	-5.18	113.70	119.40
3	c	122	TYR	CB-CG-CD2	5.18	124.11	121.00
24	Q	283	ASN	N-CA-C	-5.18	97.01	111.00
7	G	132	PHE	CG-CD1-CE1	-5.18	115.10	120.80
11	4	138	PHE	CZ-CE2-CD2	5.18	126.32	120.10
1	a	234	PHE	CE1-CZ-CE2	5.18	129.32	120.00
23	P	221	TYR	CG-CD1-CE1	-5.18	117.16	121.30
4	D	48	ARG	NE-CZ-NH2	-5.18	117.71	120.30
5	E	102	TYR	CG-CD1-CE1	-5.18	117.16	121.30
12	l	179	TYR	CB-CG-CD2	-5.18	117.89	121.00
27	O	190	TYR	CA-CB-CG	-5.18	103.57	113.40
3	c	7	ASP	CB-CG-OD2	-5.17	113.64	118.30
13	6	28	PHE	N-CA-C	-5.17	97.03	111.00
20	Z	408	TYR	CG-CD2-CE2	5.17	125.44	121.30
21	N	422	TYR	CG-CD2-CE2	5.17	125.44	121.30
27	O	70	TYR	CB-CG-CD1	-5.17	117.89	121.00
27	O	110	ASP	CB-CG-OD2	-5.17	113.64	118.30
24	Q	400	TYR	CD1-CG-CD2	5.17	123.59	117.90
32	M	73	ARG	NE-CZ-NH1	5.17	122.89	120.30
10	j	183	TRP	N-CA-CB	5.17	119.91	110.60
11	4	33	ASP	CB-CG-OD2	-5.17	113.65	118.30
11	4	38	LEU	CB-CG-CD2	5.17	119.79	111.00
20	Z	823	ASN	CB-CG-OD1	-5.17	111.26	121.60
23	P	220	TYR	CB-CG-CD2	5.17	124.10	121.00
28	H	293	GLU	N-CA-CB	5.17	119.90	110.60
10	3	22	ALA	CB-CA-C	5.17	117.85	110.10
20	Z	200	THR	CA-CB-CG2	-5.17	105.17	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	436	ASP	CB-CG-OD1	5.17	122.95	118.30
21	N	741	TYR	CB-CG-CD1	-5.17	117.90	121.00
24	Q	202	ARG	N-CA-CB	5.17	119.90	110.60
1	A	231	ASP	CB-CG-OD1	-5.17	113.65	118.30
30	K	54	LEU	CB-CG-CD1	5.17	119.78	111.00
1	a	249	ALA	CB-CA-C	-5.16	102.35	110.10
8	1	148	ASP	CB-CG-OD1	-5.16	113.65	118.30
9	2	98	TYR	CB-CG-CD2	-5.16	117.90	121.00
21	N	422	TYR	CB-CA-C	-5.16	100.07	110.40
29	I	157	VAL	CB-CA-C	5.16	121.21	111.40
32	M	124	ARG	NE-CZ-NH2	-5.16	117.72	120.30
3	c	123	THR	CA-CB-CG2	-5.16	105.17	112.40
11	k	143	LEU	CB-CG-CD1	5.16	119.78	111.00
20	Z	164	VAL	O-C-N	-5.16	114.44	122.70
10	j	120	PHE	CB-CG-CD2	-5.16	117.19	120.80
5	E	113	THR	CA-CB-OG1	5.16	119.83	109.00
26	U	228	LYS	CA-CB-CG	5.16	124.75	113.40
5	E	249	ALA	N-CA-CB	5.16	117.32	110.10
3	C	237	ASP	CB-CG-OD1	5.16	122.94	118.30
20	Z	340	LEU	N-CA-C	-5.16	97.08	111.00
23	P	329	PHE	CZ-CE2-CD2	-5.16	113.91	120.10
29	I	169	SER	CB-CA-C	-5.16	100.31	110.10
30	K	240	SER	N-CA-CB	5.15	118.23	110.50
8	h	79	TYR	CB-CG-CD2	5.15	124.09	121.00
2	B	220	ASP	CB-CG-OD1	-5.15	113.66	118.30
20	Z	837	TYR	CB-CG-CD2	-5.15	117.91	121.00
21	N	441	VAL	CA-CB-CG2	-5.15	103.17	110.90
12	5	252	LEU	CB-CA-C	-5.15	100.42	110.20
14	7	134	TYR	CB-CG-CD2	5.15	124.09	121.00
20	Z	243	GLN	CG-CD-OE1	-5.15	111.30	121.60
31	L	107	GLU	N-CA-CB	5.15	119.87	110.60
8	1	168	LEU	CB-CA-C	-5.15	100.42	110.20
11	k	95	ARG	NE-CZ-NH2	-5.15	117.73	120.30
32	M	108	LEU	CB-CG-CD2	-5.15	102.25	111.00
32	M	310	ASN	N-CA-CB	5.15	119.87	110.60
2	B	135	LEU	N-CA-C	-5.15	97.11	111.00
32	M	433	TYR	CD1-CE1-CZ	5.15	124.43	119.80
4	D	161	ALA	N-CA-CB	5.14	117.30	110.10
17	T	64	VAL	CA-CB-CG1	-5.14	103.19	110.90
23	P	329	PHE	CB-CG-CD2	5.14	124.40	120.80
5	E	93	ARG	NH1-CZ-NH2	-5.14	113.74	119.40
22	S	384	ARG	N-CA-CB	5.14	119.86	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	119	TYR	CG-CD1-CE1	-5.14	117.19	121.30
9	i	212	ASP	CB-CG-OD1	5.14	122.93	118.30
5	E	92	ALA	CB-CA-C	-5.14	102.39	110.10
11	4	18	SER	N-CA-CB	-5.14	102.79	110.50
21	N	559	TYR	CB-CG-CD1	-5.14	117.92	121.00
31	L	68	ARG	NE-CZ-NH2	5.14	122.87	120.30
1	a	104	PHE	CG-CD2-CE2	5.14	126.45	120.80
1	A	44	ALA	N-CA-CB	5.14	117.30	110.10
23	P	213	TYR	CB-CG-CD1	-5.14	117.92	121.00
20	Z	406	TRP	CG-CD2-CE3	-5.14	129.28	133.90
21	N	191	THR	C-N-CA	5.14	134.55	121.70
4	d	4	TYR	CG-CD2-CE2	-5.14	117.19	121.30
10	j	54	THR	CA-CB-CG2	-5.13	105.21	112.40
10	j	68	ARG	NE-CZ-NH1	-5.13	117.73	120.30
24	Q	165	PHE	CG-CD2-CE2	5.13	126.45	120.80
5	E	169	ALA	CB-CA-C	-5.13	102.40	110.10
25	R	307	TYR	CB-CG-CD2	-5.13	117.92	121.00
2	b	101	TYR	CB-CG-CD2	5.13	124.08	121.00
11	k	28	LEU	CB-CG-CD1	5.13	119.72	111.00
12	5	94	ARG	NH1-CZ-NH2	5.13	125.04	119.40
14	7	60	LEU	CB-CA-C	-5.13	100.45	110.20
23	P	55	SER	N-CA-CB	5.13	118.19	110.50
3	c	30	SER	CB-CA-C	-5.13	100.36	110.10
17	T	161	TRP	CZ3-CH2-CZ2	-5.13	115.45	121.60
4	D	214	VAL	CA-CB-CG2	-5.12	103.22	110.90
7	G	175	GLU	CB-CA-C	-5.12	100.16	110.40
20	Z	813	PHE	CB-CG-CD2	-5.12	117.21	120.80
21	N	570	ARG	NE-CZ-NH1	5.12	122.86	120.30
31	L	168	TYR	CD1-CE1-CZ	5.12	124.41	119.80
32	M	281	ASP	CB-CA-C	-5.12	100.15	110.40
13	m	145	ARG	CG-CD-NE	-5.12	101.05	111.80
7	G	165	THR	CA-CB-CG2	5.12	119.57	112.40
20	Z	967	THR	CA-C-N	-5.12	105.93	117.20
24	Q	40	ALA	N-CA-CB	5.12	117.27	110.10
29	I	432	LEU	CB-CG-CD1	5.12	119.70	111.00
9	i	49	SER	N-CA-CB	5.12	118.18	110.50
26	U	72	TYR	CZ-CE2-CD2	-5.12	115.19	119.80
26	U	208	VAL	CG1-CB-CG2	-5.12	102.71	110.90
33	J	316	PHE	CB-CG-CD1	-5.12	117.22	120.80
2	B	12	PHE	CB-CG-CD2	5.12	124.38	120.80
2	B	176	GLU	N-CA-CB	5.12	119.81	110.60
12	l	146	LYS	N-CA-CB	5.11	119.81	110.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	83	TYR	CG-CD2-CE2	-5.11	117.21	121.30
13	m	168	TYR	CB-CG-CD1	-5.11	117.93	121.00
2	B	127	VAL	N-CA-C	-5.11	97.19	111.00
5	e	120	ALA	N-CA-CB	5.11	117.25	110.10
12	l	200	ASP	CB-CG-OD2	5.11	122.90	118.30
5	E	48	LEU	N-CA-C	-5.11	97.20	111.00
14	7	252	TRP	CZ3-CH2-CZ2	-5.11	115.47	121.60
21	N	832	HIS	N-CA-CB	5.11	119.80	110.60
23	P	16	ILE	O-C-N	-5.11	114.53	122.70
25	R	224	PHE	CB-CG-CD2	5.11	124.38	120.80
29	I	268	PHE	CG-CD2-CE2	5.11	126.42	120.80
33	J	265	ASP	CB-CG-OD2	-5.11	113.70	118.30
7	G	15	PHE	CB-CA-C	-5.11	100.18	110.40
23	P	275	ASN	CA-CB-CG	-5.11	102.17	113.40
22	S	158	PHE	CB-CG-CD1	5.11	124.37	120.80
23	P	273	TYR	CB-CG-CD1	-5.11	117.94	121.00
8	h	125	GLY	C-N-CA	5.10	133.02	122.30
33	J	404	PHE	CB-CG-CD1	-5.10	117.23	120.80
4	d	130	GLY	N-CA-C	-5.10	100.34	113.10
11	k	112	ASN	CB-CG-OD1	-5.10	111.40	121.60
13	6	193	ARG	NE-CZ-NH2	-5.10	117.75	120.30
12	l	219	TYR	CD1-CE1-CZ	5.10	124.39	119.80
13	m	13	TYR	CB-CG-CD2	-5.10	117.94	121.00
4	D	30	GLY	C-N-CA	5.10	134.45	121.70
23	P	367	GLU	CB-CG-CD	-5.10	100.43	114.20
29	I	395	MET	CA-CB-CG	5.10	121.97	113.30
32	M	316	SER	CB-CA-C	5.10	119.79	110.10
32	M	330	VAL	CA-CB-CG2	5.10	118.55	110.90
13	m	220	VAL	CG1-CB-CG2	-5.10	102.74	110.90
11	4	145	ASP	CB-CG-OD2	5.10	122.89	118.30
14	7	250	MET	CG-SD-CE	-5.10	92.04	100.20
19	Y	9	GLN	O-C-N	-5.10	114.54	122.70
21	N	284	PRO	N-CD-CG	5.10	110.85	103.20
27	O	17	GLU	O-C-N	5.10	130.86	122.70
27	O	91	ASP	N-CA-C	-5.10	97.23	111.00
4	d	12	SER	N-CA-CB	5.10	118.14	110.50
13	m	79	SER	N-CA-CB	5.10	118.15	110.50
15	W	162	ASN	N-CA-CB	5.10	119.77	110.60
22	S	56	SER	O-C-N	-5.10	114.54	122.70
23	P	21	PHE	CB-CG-CD2	-5.10	117.23	120.80
30	K	303	MET	CG-SD-CE	-5.10	92.04	100.20
7	G	10	LEU	N-CA-CB	5.10	120.59	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	293	ALA	N-CA-C	-5.10	97.24	111.00
20	Z	882	LEU	CB-CG-CD1	-5.09	102.34	111.00
28	H	69	VAL	CA-CB-CG2	-5.09	103.26	110.90
29	I	314	ASP	CB-CG-OD2	-5.09	113.71	118.30
32	M	270	ALA	CB-CA-C	-5.09	102.46	110.10
17	T	49	ASP	CB-CG-OD2	5.09	122.88	118.30
20	Z	341	TYR	CG-CD1-CE1	-5.09	117.23	121.30
23	P	234	TYR	CG-CD2-CE2	-5.09	117.23	121.30
29	I	265	ARG	O-C-N	-5.09	114.55	122.70
2	B	59	GLU	CG-CD-OE2	-5.09	108.12	118.30
6	F	53	ALA	CB-CA-C	-5.09	102.46	110.10
20	Z	363	ASP	CB-CG-OD2	-5.09	113.72	118.30
4	d	44	LEU	N-CA-C	-5.09	97.26	111.00
10	j	192	LYS	O-C-N	-5.09	114.56	122.70
10	3	193	ASP	CB-CG-OD2	-5.09	113.72	118.30
13	6	138	SER	N-CA-CB	5.09	118.13	110.50
21	N	336	ASN	CB-CA-C	-5.09	100.22	110.40
2	b	234	ARG	NE-CZ-NH2	5.09	122.84	120.30
6	F	130	VAL	CG1-CB-CG2	5.09	119.04	110.90
17	T	210	PHE	CB-CG-CD1	-5.09	117.24	120.80
24	Q	235	ALA	CB-CA-C	-5.09	102.47	110.10
2	b	156	TYR	CG-CD2-CE2	-5.08	117.23	121.30
4	d	127	ARG	CG-CD-NE	-5.08	101.13	111.80
28	H	462	ARG	NE-CZ-NH1	5.08	122.84	120.30
5	e	238	GLU	OE1-CD-OE2	5.08	129.40	123.30
8	h	198	TYR	CG-CD1-CE1	-5.08	117.23	121.30
20	Z	199	ASP	CB-CG-OD1	-5.08	113.73	118.30
27	O	208	ALA	CB-CA-C	-5.08	102.48	110.10
13	6	131	TYR	CG-CD2-CE2	-5.08	117.24	121.30
19	Y	3	THR	C-N-CA	5.08	134.40	121.70
21	N	784	TYR	CG-CD1-CE1	5.08	125.36	121.30
10	j	99	ARG	NE-CZ-NH1	-5.08	117.76	120.30
11	k	54	VAL	CA-CB-CG1	-5.08	103.28	110.90
15	W	17	ARG	NE-CZ-NH1	5.08	122.84	120.30
11	4	62	ALA	CB-CA-C	-5.08	102.48	110.10
32	M	344	ASP	CB-CG-OD2	-5.08	113.73	118.30
13	m	97	ALA	N-CA-CB	5.08	117.21	110.10
10	3	57	ALA	N-CA-CB	-5.08	102.99	110.10
14	7	88	GLY	N-CA-C	-5.08	100.41	113.10
27	O	153	LEU	CB-CG-CD1	5.08	119.63	111.00
31	L	157	ARG	N-CA-CB	5.08	119.73	110.60
4	D	131	VAL	CA-C-O	5.07	130.75	120.10

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	111	LEU	CA-CB-CG	-5.07	103.63	115.30
20	Z	924	LYS	O-C-N	-5.07	114.58	122.70
27	O	342	ASP	N-CA-CB	5.07	119.73	110.60
30	K	333	ARG	CA-C-N	5.07	128.36	117.20
16	V	68	VAL	CA-CB-CG2	5.07	118.50	110.90
20	Z	74	SER	CB-CA-C	-5.07	100.47	110.10
25	R	382	ASP	O-C-N	5.07	130.81	122.70
23	P	168	TYR	CB-CG-CD1	-5.07	117.96	121.00
33	J	322	ALA	N-CA-CB	-5.07	103.00	110.10
13	6	45	SER	CB-CA-C	-5.07	100.47	110.10
20	Z	193	PHE	CB-CG-CD1	-5.07	117.25	120.80
20	Z	460	SER	N-CA-CB	5.07	118.10	110.50
7	G	187	LEU	CB-CG-CD1	5.06	119.61	111.00
16	V	87	PHE	CD1-CE1-CZ	-5.06	114.02	120.10
22	S	110	LEU	CB-CG-CD2	5.06	119.61	111.00
3	C	239	LEU	CB-CG-CD1	5.06	119.61	111.00
19	Y	2	SER	CB-CA-C	5.06	119.72	110.10
20	Z	219	ASP	CB-CG-OD2	5.06	122.86	118.30
21	N	417	ARG	N-CA-CB	5.06	119.71	110.60
21	N	653	ARG	NE-CZ-NH1	5.06	122.83	120.30
25	R	375	LYS	N-CA-CB	5.06	119.71	110.60
28	H	61	ALA	CB-CA-C	-5.06	102.51	110.10
28	H	404	TRP	CD1-CG-CD2	5.06	110.35	106.30
14	n	163	VAL	N-CA-C	-5.06	97.33	111.00
9	2	126	TYR	CZ-CE2-CD2	-5.06	115.25	119.80
22	S	246	GLU	C-N-CA	5.06	134.35	121.70
23	P	299	LEU	CB-CG-CD1	5.06	119.60	111.00
19	Y	56	GLN	N-CA-CB	5.06	119.71	110.60
23	P	203	ILE	N-CA-C	-5.06	97.34	111.00
1	a	133	TYR	CZ-CE2-CD2	5.06	124.35	119.80
12	l	95	ALA	N-CA-C	-5.06	97.34	111.00
14	n	132	VAL	CA-CB-CG2	-5.06	103.31	110.90
14	7	94	GLN	N-CA-CB	5.06	119.70	110.60
21	N	598	ASP	CB-CG-OD2	5.06	122.85	118.30
21	N	676	ALA	N-CA-CB	5.06	117.18	110.10
27	O	285	SER	CB-CA-C	-5.06	100.49	110.10
32	M	229	THR	N-CA-CB	5.06	119.91	110.30
9	2	152	TYR	CG-CD2-CE2	-5.06	117.25	121.30
24	Q	236	PHE	CB-CG-CD2	-5.06	117.26	120.80
25	R	345	TYR	N-CA-CB	5.06	119.70	110.60
1	a	199	TRP	CD1-NE1-CE2	-5.05	104.45	109.00
5	E	14	THR	N-CA-CB	5.05	119.90	110.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	140	MET	CG-SD-CE	-5.05	92.11	100.20
24	Q	286	TYR	CD1-CE1-CZ	-5.05	115.25	119.80
25	R	331	ARG	N-CA-CB	5.05	119.70	110.60
5	e	42	THR	N-CA-CB	5.05	119.90	110.30
7	G	201	TYR	CB-CG-CD1	-5.05	117.97	121.00
24	Q	47	ASP	N-CA-CB	5.05	119.70	110.60
11	4	2	ASP	CB-CG-OD1	-5.05	113.75	118.30
18	X	122	TYR	CB-CG-CD2	5.05	124.03	121.00
6	F	225	TYR	CZ-CE2-CD2	5.05	124.34	119.80
9	2	239	THR	CA-CB-CG2	-5.05	105.33	112.40
11	4	46	PHE	CB-CG-CD2	5.05	124.33	120.80
17	T	199	PHE	CB-CG-CD1	5.05	124.33	120.80
28	H	237	THR	CA-CB-CG2	-5.05	105.33	112.40
19	Y	43	TRP	CB-CG-CD2	-5.05	120.04	126.60
3	c	141	ASP	N-CA-C	-5.05	97.37	111.00
3	c	226	TYR	N-CA-CB	5.05	119.68	110.60
30	K	174	VAL	CA-CB-CG2	-5.05	103.33	110.90
4	d	151	GLU	OE1-CD-OE2	-5.04	117.25	123.30
13	6	30	VAL	CG1-CB-CG2	-5.04	102.83	110.90
21	N	157	ALA	CB-CA-C	-5.04	102.53	110.10
4	d	229	ILE	CA-CB-CG2	-5.04	100.81	110.90
12	l	139	ARG	CB-CG-CD	5.04	124.71	111.60
3	C	143	ARG	NE-CZ-NH2	5.04	122.82	120.30
27	O	81	TYR	N-CA-CB	5.04	119.68	110.60
32	M	43	ILE	C-N-CA	5.04	134.31	121.70
23	P	249	ALA	N-CA-CB	5.04	117.16	110.10
8	1	94	LEU	CB-CG-CD2	5.04	119.57	111.00
16	V	216	LEU	N-CA-C	-5.04	97.40	111.00
20	Z	491	LEU	O-C-N	-5.04	114.64	123.20
6	F	178	THR	N-CA-CB	5.04	119.87	110.30
8	1	52	CYS	CA-CB-SG	-5.04	104.94	114.00
27	O	144	VAL	CA-CB-CG1	-5.04	103.35	110.90
1	a	17	THR	CA-CB-CG2	-5.03	105.35	112.40
10	3	130	ILE	O-C-N	5.03	130.75	122.70
14	7	144	TRP	CD2-CE3-CZ3	-5.03	112.26	118.80
9	2	155	SER	N-CA-CB	5.03	118.05	110.50
24	Q	132	PHE	CB-CG-CD2	-5.03	117.28	120.80
9	i	170	HIS	C-N-CA	-5.03	109.12	121.70
14	n	43	SER	N-CA-CB	5.03	118.05	110.50
13	6	13	TYR	CB-CG-CD1	5.03	124.02	121.00
20	Z	522	THR	CA-CB-CG2	-5.03	105.36	112.40
23	P	253	ASP	CA-CB-CG	-5.03	102.33	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	180	TYR	N-CA-CB	5.03	119.66	110.60
12	l	90	ALA	N-CA-CB	5.03	117.14	110.10
9	2	203	ASP	N-CA-CB	5.03	119.65	110.60
20	Z	52	LEU	CB-CG-CD2	5.03	119.55	111.00
22	S	456	ASP	CB-CG-OD1	-5.03	113.77	118.30
24	Q	299	MET	O-C-N	-5.03	114.66	122.70
28	H	351	VAL	CA-CB-CG1	-5.03	103.36	110.90
2	b	17	LYS	CB-CG-CD	5.03	124.66	111.60
14	n	230	LEU	CB-CG-CD1	-5.03	102.45	111.00
4	D	220	ASP	CB-CG-OD2	-5.03	113.78	118.30
25	R	330	VAL	C-N-CA	5.03	134.26	121.70
4	d	204	GLN	N-CA-CB	5.02	119.64	110.60
10	3	195	VAL	CA-CB-CG2	-5.02	103.36	110.90
22	S	60	LEU	C-N-CA	5.02	134.26	121.70
24	Q	65	TYR	CD1-CE1-CZ	5.02	124.32	119.80
3	c	207	THR	C-N-CA	5.02	134.26	121.70
13	m	36	ARG	CG-CD-NE	-5.02	101.25	111.80
16	V	206	THR	CA-CB-CG2	-5.02	105.37	112.40
22	S	217	PHE	CG-CD2-CE2	-5.02	115.28	120.80
10	j	67	PHE	N-CA-CB	5.02	119.64	110.60
21	N	242	PHE	CB-CG-CD2	5.02	124.31	120.80
21	N	386	MET	CG-SD-CE	-5.02	92.17	100.20
33	J	57	PHE	CB-CG-CD2	5.02	124.31	120.80
8	h	91	PHE	CB-CG-CD1	5.02	124.31	120.80
14	n	128	TYR	CZ-CE2-CD2	5.02	124.32	119.80
13	6	188	VAL	CA-CB-CG1	5.02	118.42	110.90
28	H	279	LEU	CB-CA-C	-5.02	100.67	110.20
23	P	422	LEU	CB-CA-C	5.02	119.73	110.20
3	c	17	GLY	C-N-CA	5.01	134.24	121.70
9	i	154	LEU	CA-C-O	5.01	130.63	120.10
16	V	106	GLY	N-CA-C	-5.01	100.56	113.10
5	e	167	TYR	CD1-CG-CD2	5.01	123.42	117.90
27	O	166	ARG	NE-CZ-NH2	-5.01	117.79	120.30
31	L	71	ASP	CB-CG-OD1	-5.01	113.79	118.30
15	W	163	ASN	N-CA-C	-5.01	97.47	111.00
20	Z	119	LEU	CB-CG-CD2	-5.01	102.48	111.00
25	R	219	LEU	CB-CG-CD1	5.01	119.52	111.00
1	a	132	ALA	N-CA-CB	5.01	117.11	110.10
1	a	225	VAL	CA-CB-CG2	-5.01	103.39	110.90
1	A	46	ARG	N-CA-CB	5.01	119.62	110.60
12	5	119	THR	N-CA-CB	5.01	119.82	110.30
27	O	70	TYR	CB-CG-CD2	5.01	124.01	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	202	ARG	O-C-N	5.01	130.71	122.70
32	M	73	ARG	N-CA-CB	5.01	119.61	110.60
6	f	138	ASP	CB-CG-OD2	-5.01	113.80	118.30
7	g	88	LEU	O-C-N	5.01	130.71	122.70
30	K	355	THR	N-CA-CB	5.01	119.81	110.30
33	J	23	PHE	CG-CD1-CE1	5.01	126.31	120.80
7	g	78	TYR	N-CA-CB	5.00	119.61	110.60
2	b	82	TYR	CD1-CG-CD2	5.00	123.41	117.90
11	4	12	SER	N-CA-CB	5.00	118.01	110.50
21	N	149	GLU	N-CA-C	-5.00	97.49	111.00
21	N	354	PRO	O-C-N	5.00	130.71	122.70
5	E	219	LEU	CB-CG-CD1	5.00	119.50	111.00

There are no chirality outliers.

All (376) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	144	TYR	Sidechain
8	1	146	TYR	Sidechain
8	1	198	TYR	Sidechain
8	1	202	TYR	Sidechain
8	1	34	TYR	Sidechain
9	2	101	ARG	Sidechain
9	2	153	TYR	Sidechain
9	2	217	ARG	Sidechain
9	2	232	TYR	Sidechain
9	2	236	ARG	Sidechain
9	2	37	PHE	Sidechain
9	2	98	TYR	Sidechain
10	3	154	TYR	Sidechain
10	3	69	TYR	Sidechain
10	3	74	TYR	Sidechain
11	4	121	TYR	Sidechain
11	4	135	TYR	Sidechain
11	4	139	TYR	Sidechain
11	4	8	ARG	Sidechain
11	4	98	TYR	Sidechain
12	5	129	PHE	Sidechain
12	5	165	TYR	Sidechain
12	5	189	TYR	Sidechain
12	5	230	TYR	Sidechain
12	5	253	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
12	5	282	PHE	Sidechain
13	6	139	TYR	Sidechain
13	6	229	ARG	Sidechain
13	6	41	TYR	Sidechain
13	6	47	TYR	Sidechain
14	7	128	TYR	Sidechain
14	7	161	ARG	Sidechain
14	7	162	TYR	Sidechain
14	7	170	TYR	Sidechain
14	7	215	ARG	Sidechain
14	7	254	PHE	Sidechain
14	7	49	TYR	Sidechain
1	A	106	TYR	Sidechain
1	A	108	TYR	Sidechain
1	A	11	GLY	Peptide
1	A	12	TYR	Peptide,Sidechain
1	A	162	TYR	Sidechain
1	A	233	PHE	Sidechain
2	B	23	TYR	Sidechain
2	B	7	PHE	Peptide
2	B	75	TYR	Sidechain
2	B	82	TYR	Sidechain
3	C	10	THR	Mainchain
3	C	102	TYR	Sidechain
3	C	114	ARG	Sidechain
3	C	122	TYR	Sidechain
3	C	129	ARG	Peptide,Sidechain
3	C	135	PHE	Sidechain
3	C	140	TYR	Sidechain
3	C	146	TYR	Sidechain
3	C	157	TYR	Sidechain
3	C	24	TYR	Sidechain
3	C	6	TYR	Peptide,Sidechain
3	C	67	TYR	Sidechain
3	C	98	TYR	Sidechain
4	D	111	ARG	Sidechain
4	D	120	TYR	Sidechain
4	D	156	TYR	Sidechain
4	D	166	ARG	Sidechain
4	D	179	TYR	Sidechain
4	D	29	ARG	Sidechain
4	D	3	GLY	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
4	D	48	ARG	Sidechain
4	D	90	ARG	Sidechain
5	E	102	TYR	Sidechain
5	E	12	VAL	Mainchain
5	E	13	SER	Peptide
5	E	142	LEU	Peptide
5	E	165	TYR	Sidechain
5	E	22	PHE	Sidechain
5	E	86	ARG	Sidechain
6	F	126	ARG	Sidechain
6	F	18	ARG	Peptide
6	F	225	TYR	Sidechain
6	F	4	ASN	Peptide
7	G	123	HIS	Sidechain
7	G	15	PHE	Sidechain
7	G	230	PHE	Sidechain
7	G	78	TYR	Sidechain
7	G	8	TYR	Peptide
7	G	91	ARG	Sidechain
28	H	145	TYR	Sidechain
28	H	178	ARG	Sidechain
28	H	181	TYR	Sidechain
28	H	208	TYR	Sidechain
28	H	213	GLY	Peptide
28	H	234	ARG	Sidechain
28	H	344	ASP	Peptide
28	H	346	ARG	Peptide,Sidechain
28	H	357	ARG	Sidechain
28	H	366	LEU	Peptide
28	H	367	ARG	Sidechain
28	H	370	ARG	Peptide,Sidechain
28	H	385	ARG	Sidechain
28	H	400	ARG	Sidechain
28	H	409	ARG	Sidechain
28	H	435	ARG	Sidechain
28	H	462	ARG	Sidechain
28	H	88	ARG	Sidechain
29	I	178	THR	Peptide
29	I	208	TYR	Sidechain
29	I	245	LEU	Peptide,Mainchain
29	I	246	ARG	Peptide,Mainchain
29	I	247	ILE	Mainchain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
29	I	262	ARG	Sidechain
29	I	292	TYR	Sidechain
29	I	339	ILE	Peptide
29	I	340	ARG	Peptide
29	I	342	GLY	Peptide
29	I	345	ASP	Peptide
29	I	407	ARG	Sidechain
29	I	412	THR	Peptide
29	I	436	TYR	Sidechain
29	I	54	ARG	Sidechain
29	I	85	PHE	Sidechain
33	J	147	TYR	Sidechain
33	J	200	ARG	Sidechain
33	J	211	ILE	Peptide
33	J	212	ARG	Peptide
33	J	23	PHE	Sidechain
33	J	231	ARG	Sidechain
33	J	261	SER	Peptide
33	J	306	ARG	Peptide
33	J	308	GLY	Peptide
33	J	309	ARG	Peptide
33	J	371	ARG	Sidechain
33	J	382	PHE	Sidechain
30	K	121	ARG	Sidechain
30	K	207	ARG	Sidechain
30	K	294	ARG	Sidechain
30	K	303	MET	Peptide
30	K	329	LEU	Peptide
30	K	332	GLY	Peptide
30	K	333	ARG	Peptide,Sidechain
30	K	350	ARG	Sidechain
30	K	400	TYR	Sidechain
30	K	402	ILE	Peptide
30	K	411	TYR	Sidechain
30	K	49	PHE	Sidechain
30	K	67	TYR	Sidechain
30	K	73	ARG	Sidechain
31	L	132	ARG	Sidechain
31	L	161	ARG	Sidechain
31	L	176	GLY	Peptide
31	L	186	LEU	Peptide
31	L	269	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
31	L	299	ARG	Sidechain
31	L	303	ARG	Sidechain
31	L	342	ARG	Sidechain
31	L	70	TYR	Sidechain
32	M	203	ARG	Sidechain
32	M	229	THR	Peptide
32	M	299	ARG	Sidechain
32	M	303	ARG	Sidechain
32	M	312	LEU	Peptide
32	M	329	ARG	Sidechain
32	M	345	ARG	Sidechain
32	M	357	ARG	Sidechain
32	M	42	ARG	Sidechain
32	M	45	ARG	Sidechain
21	N	14	ARG	Sidechain
21	N	161	TYR	Sidechain
21	N	188	TYR	Sidechain
21	N	208	ARG	Sidechain
21	N	23	TYR	Sidechain
21	N	298	TYR	Sidechain
21	N	299	TYR	Sidechain
21	N	412	TYR	Sidechain
21	N	50	TYR	Sidechain
21	N	515	ARG	Sidechain
21	N	528	ARG	Sidechain
21	N	549	TYR	Sidechain
21	N	553	PHE	Sidechain
21	N	597	ARG	Sidechain
21	N	599	TYR	Sidechain
21	N	739	PHE	Sidechain
21	N	75	TYR	Sidechain
21	N	809	ARG	Sidechain
21	N	873	ARG	Sidechain
21	N	896	PHE	Sidechain
21	N	908	ARG	Sidechain
27	O	147	ARG	Sidechain
27	O	15	ARG	Sidechain
27	O	166	ARG	Sidechain
27	O	189	TYR	Sidechain
27	O	286	PHE	Sidechain
27	O	310	PHE	Sidechain
27	O	330	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
27	O	39	PHE	Sidechain
27	O	48	PHE	Sidechain
27	O	81	TYR	Sidechain
27	O	98	TYR	Sidechain
23	P	109	SER	Peptide
23	P	115	ARG	Sidechain
23	P	13	TYR	Sidechain
23	P	168	TYR	Sidechain
23	P	201	ARG	Sidechain
23	P	213	TYR	Sidechain
23	P	240	TYR	Sidechain
23	P	266	TYR	Sidechain
23	P	282	HIS	Sidechain
23	P	318	TYR	Sidechain
23	P	348	HIS	Sidechain
23	P	357	TYR	Sidechain
24	Q	209	TYR	Sidechain
24	Q	27	TYR	Sidechain
24	Q	291	TYR	Sidechain
24	Q	306	TYR	Sidechain
24	Q	386	PHE	Sidechain
24	Q	387	TYR	Sidechain
24	Q	65	TYR	Sidechain
24	Q	84	TYR	Sidechain
25	R	206	ARG	Sidechain
25	R	213	TYR	Sidechain
25	R	297	TYR	Sidechain
25	R	301	TYR	Sidechain
25	R	338	TYR	Sidechain
25	R	422	ARG	Sidechain
25	R	62	TYR	Sidechain
22	S	114	TYR	Sidechain
22	S	119	TYR	Sidechain
22	S	171	TYR	Sidechain
22	S	188	TYR	Sidechain
22	S	239	ARG	Sidechain
22	S	253	PHE	Sidechain
22	S	286	TYR	Sidechain
22	S	332	PHE	Sidechain
22	S	345	TYR	Sidechain
22	S	360	PHE	Sidechain
22	S	367	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
22	S	425	ARG	Sidechain
22	S	438	HIS	Sidechain
22	S	442	PHE	Sidechain
22	S	472	HIS	Sidechain
22	S	52	TYR	Sidechain
17	T	128	TYR	Sidechain
17	T	266	TYR	Sidechain
17	T	60	ARG	Sidechain
17	T	82	PHE	Sidechain
17	T	89	TYR	Sidechain
26	U	137	TYR	Sidechain
26	U	47	ARG	Sidechain
26	U	72	TYR	Sidechain
16	V	108	TYR	Sidechain
16	V	129	PHE	Sidechain
16	V	157	ARG	Sidechain
16	V	20	ARG	Sidechain
16	V	228	TYR	Sidechain
16	V	269	ARG	Sidechain
16	V	270	TYR	Sidechain
16	V	28	TYR	Sidechain
15	W	144	PHE	Sidechain
15	W	15	TYR	Sidechain
15	W	157	PHE	Sidechain
15	W	182	TYR	Sidechain
18	X	10	PHE	Sidechain
18	X	22	ARG	Sidechain
18	X	27	ILE	Peptide
18	X	51	ARG	Sidechain
18	X	59	ARG	Sidechain
18	X	98	PHE	Sidechain
18	X	99	PHE	Sidechain
19	Y	38	PHE	Sidechain
19	Y	84	TYR	Sidechain
20	Z	132	HIS	Sidechain
20	Z	210	TYR	Sidechain
20	Z	269	TYR	Sidechain
20	Z	312	TYR	Sidechain
20	Z	323	TYR	Sidechain
20	Z	385	PHE	Sidechain
20	Z	394	TYR	Sidechain
20	Z	426	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
20	Z	477	TYR	Sidechain
20	Z	773	ARG	Sidechain
20	Z	774	ARG	Sidechain
20	Z	849	ARG	Sidechain
1	a	106	TYR	Sidechain
1	a	11	GLY	Peptide
1	a	12	TYR	Peptide
1	a	131	ARG	Sidechain
1	a	96	ARG	Sidechain
2	b	145	PHE	Sidechain
2	b	224	TYR	Sidechain
2	b	23	TYR	Sidechain
2	b	234	ARG	Sidechain
2	b	246	ARG	Sidechain
2	b	5	TYR	Peptide
2	b	7	PHE	Peptide
2	b	97	TYR	Sidechain
3	c	102	TYR	Sidechain
3	c	122	TYR	Sidechain
3	c	131	PHE	Sidechain
3	c	135	PHE	Sidechain
3	c	143	ARG	Sidechain
3	c	157	TYR	Sidechain
3	c	6	TYR	Sidechain
4	d	108	TYR	Sidechain
4	d	120	TYR	Sidechain
4	d	179	TYR	Sidechain
4	d	22	TYR	Sidechain
4	d	232	TYR	Sidechain
4	d	3	GLY	Peptide
4	d	90	ARG	Sidechain
4	d	97	ARG	Sidechain
5	e	13	SER	Peptide
5	e	132	ARG	Sidechain
5	e	147	HIS	Sidechain
6	f	123	TYR	Sidechain
6	f	137	TYR	Sidechain
6	f	18	ARG	Peptide
6	f	233	TYR	Sidechain
6	f	4	ASN	Peptide
6	f	59	TYR	Sidechain
6	f	89	ARG	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
6	f	94	TYR	Sidechain
7	g	103	TYR	Sidechain
7	g	126	TYR	Sidechain
7	g	160	TYR	Sidechain
7	g	169	ARG	Sidechain
7	g	26	TYR	Sidechain
7	g	72	ARG	Sidechain
7	g	8	TYR	Peptide
8	h	198	TYR	Sidechain
8	h	45	ARG	Sidechain
8	h	70	TYR	Sidechain
8	h	79	TYR	Sidechain
8	h	96	TYR	Sidechain
9	i	104	ARG	Sidechain
9	i	117	PHE	Sidechain
9	i	122	HIS	Peptide
9	i	152	TYR	Sidechain
9	i	215	TYR	Sidechain
9	i	37	PHE	Sidechain
10	j	45	HIS	Sidechain
10	j	46	TYR	Sidechain
10	j	68	ARG	Sidechain
11	k	171	ARG	Sidechain
11	k	190	ARG	Sidechain
11	k	67	TYR	Sidechain
11	k	96	ARG	Sidechain
12	l	165	TYR	Sidechain
12	l	179	TYR	Sidechain
12	l	188	TYR	Sidechain
12	l	202	PHE	Sidechain
12	l	245	TYR	Sidechain
12	l	253	TYR	Sidechain
13	m	106	TYR	Sidechain
13	m	113	TYR	Sidechain
13	m	114	TYR	Sidechain
13	m	13	TYR	Sidechain
13	m	139	TYR	Sidechain
13	m	28	PHE	Sidechain
13	m	36	ARG	Sidechain
13	m	41	TYR	Sidechain
13	m	75	ARG	Sidechain
14	n	124	TYR	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
14	n	126	PHE	Sidechain
14	n	162	TYR	Sidechain
14	n	219	TYR	Sidechain
14	n	228	PHE	Sidechain
14	n	261	TYR	Sidechain
14	n	69	PHE	Sidechain
14	n	98	ARG	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	242/244 (99%)	231 (96%)	9 (4%)	2 (1%)	19 60
1	a	242/244 (99%)	227 (94%)	13 (5%)	2 (1%)	19 60
2	B	245/247 (99%)	232 (95%)	12 (5%)	1 (0%)	34 72
2	b	245/247 (99%)	231 (94%)	11 (4%)	3 (1%)	13 50
3	C	239/241 (99%)	222 (93%)	15 (6%)	2 (1%)	19 60
3	c	239/241 (99%)	227 (95%)	11 (5%)	1 (0%)	34 72
4	D	250/252 (99%)	238 (95%)	8 (3%)	4 (2%)	9 45
4	d	250/252 (99%)	235 (94%)	11 (4%)	4 (2%)	9 45
5	E	243/245 (99%)	226 (93%)	13 (5%)	4 (2%)	9 45
5	e	243/245 (99%)	225 (93%)	14 (6%)	4 (2%)	9 45
6	F	230/232 (99%)	219 (95%)	11 (5%)	0	100 100
6	f	230/232 (99%)	220 (96%)	10 (4%)	0	100 100
7	G	243/245 (99%)	225 (93%)	14 (6%)	4 (2%)	9 45

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
7	g	243/245 (99%)	226 (93%)	10 (4%)	7 (3%)	4 32
8	1	194/196 (99%)	185 (95%)	8 (4%)	1 (0%)	29 68
8	h	194/196 (99%)	182 (94%)	11 (6%)	1 (0%)	29 68
9	2	224/226 (99%)	211 (94%)	7 (3%)	6 (3%)	5 34
9	i	224/226 (99%)	209 (93%)	12 (5%)	3 (1%)	12 48
10	3	202/204 (99%)	188 (93%)	9 (4%)	5 (2%)	5 35
10	j	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	29 68
11	4	193/195 (99%)	183 (95%)	10 (5%)	0	100 100
11	k	193/195 (99%)	177 (92%)	12 (6%)	4 (2%)	7 39
12	5	210/212 (99%)	204 (97%)	6 (3%)	0	100 100
12	l	210/212 (99%)	196 (93%)	14 (7%)	0	100 100
13	6	220/222 (99%)	204 (93%)	13 (6%)	3 (1%)	11 47
13	m	220/222 (99%)	206 (94%)	10 (4%)	4 (2%)	8 42
14	7	227/232 (98%)	209 (92%)	15 (7%)	3 (1%)	12 48
14	n	230/232 (99%)	215 (94%)	12 (5%)	3 (1%)	12 48
15	W	195/197 (99%)	174 (89%)	14 (7%)	7 (4%)	3 28
16	V	287/289 (99%)	261 (91%)	22 (8%)	4 (1%)	11 47
17	T	264/266 (99%)	244 (92%)	15 (6%)	5 (2%)	8 41
18	X	125/127 (98%)	96 (77%)	20 (16%)	9 (7%)	1 16
19	Y	87/89 (98%)	74 (85%)	7 (8%)	6 (7%)	1 17
20	Z	902/970 (93%)	813 (90%)	66 (7%)	23 (2%)	5 35
21	N	920/922 (100%)	851 (92%)	51 (6%)	18 (2%)	7 40
22	S	473/475 (100%)	437 (92%)	21 (4%)	15 (3%)	4 30
23	P	438/440 (100%)	414 (94%)	20 (5%)	4 (1%)	17 56
24	Q	432/434 (100%)	395 (91%)	20 (5%)	17 (4%)	3 26
25	R	403/405 (100%)	375 (93%)	22 (6%)	6 (2%)	10 46
26	U	302/304 (99%)	290 (96%)	8 (3%)	4 (1%)	12 48
27	O	386/388 (100%)	364 (94%)	14 (4%)	8 (2%)	7 39
28	H	424/426 (100%)	369 (87%)	33 (8%)	22 (5%)	2 22
29	I	383/385 (100%)	341 (89%)	30 (8%)	12 (3%)	4 31
30	K	382/384 (100%)	339 (89%)	27 (7%)	16 (4%)	3 25

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
31	L	386/388 (100%)	361 (94%)	18 (5%)	7 (2%)	8 42
32	M	419/421 (100%)	379 (90%)	28 (7%)	12 (3%)	4 32
33	J	401/403 (100%)	351 (88%)	40 (10%)	10 (2%)	5 35
All	All	13936/14099 (99%)	12868 (92%)	791 (6%)	277 (2%)	11 40

All (277) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	10	ALA
2	b	53	SER
4	d	204	GLN
5	e	14	THR
5	e	16	SER
13	m	208	ASP
1	A	10	ALA
3	C	54	SER
5	E	16	SER
7	G	209	GLU
9	2	233	LYS
10	3	40	PHE
13	6	27	ASP
18	X	110	PRO
20	Z	24	THR
20	Z	82	MET
20	Z	85	VAL
21	N	750	SER
21	N	791	ALA
21	N	832	HIS
21	N	862	SER
22	S	84	ASP
22	S	107	SER
24	Q	46	VAL
24	Q	284	ALA
25	R	244	THR
27	O	52	ALA
28	H	136	ALA
28	H	211	VAL
28	H	214	CYS
28	H	371	ILE
29	I	102	ASN
29	I	115	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	I	246	ARG
29	I	247	ILE
30	K	304	ASP
30	K	334	LEU
30	K	403	LEU
30	K	419	ASN
32	M	186	LEU
32	M	230	LEU
33	J	213	VAL
33	J	257	ARG
33	J	307	PRO
33	J	310	ILE
7	g	63	LYS
9	i	174	ASP
11	k	11	ASP
13	m	27	ASP
14	n	80	ASP
14	n	116	ALA
1	A	49	ASP
3	C	184	MET
4	D	68	ASP
9	2	222	PRO
13	6	40	ASP
14	7	224	SER
15	W	3	LEU
15	W	147	ILE
15	W	191	ILE
16	V	47	MET
16	V	170	PRO
17	T	257	THR
18	X	29	VAL
18	X	81	SER
18	X	82	LYS
20	Z	142	ASP
20	Z	233	LEU
20	Z	802	ASP
20	Z	870	ALA
21	N	97	PHE
21	N	123	PHE
21	N	361	ASN
21	N	739	PHE
22	S	69	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	S	433	GLU
23	P	88	GLN
23	P	89	LEU
23	P	167	THR
24	Q	44	ALA
24	Q	89	ALA
24	Q	128	GLU
24	Q	354	PHE
25	R	182	ASN
25	R	280	ILE
25	R	394	ASP
26	U	218	GLU
28	H	73	ASP
28	H	117	THR
28	H	143	ALA
28	H	162	ARG
28	H	191	ILE
28	H	303	ALA
28	H	347	GLY
29	I	343	ARG
30	K	105	GLN
30	K	333	ARG
30	K	417	THR
31	L	101	ILE
31	L	251	ILE
31	L	291	PHE
31	L	374	PHE
32	M	282	GLU
32	M	313	ASP
33	J	211	ILE
3	c	221	ASN
4	d	14	ASP
4	d	70	HIS
7	g	72	ARG
9	i	222	PRO
11	k	34	LYS
11	k	72	ASP
13	m	40	ASP
13	m	138	SER
4	D	204	GLN
8	1	142	PHE
10	3	4	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	3	6	SER
14	7	116	ALA
15	W	180	LEU
17	T	93	ASN
18	X	42	GLU
18	X	95	GLU
19	Y	2	SER
19	Y	4	ASP
19	Y	32	ASP
19	Y	56	GLN
20	Z	377	ALA
20	Z	513	ALA
20	Z	578	GLY
20	Z	887	GLY
20	Z	926	ASN
20	Z	940	GLY
20	Z	947	GLY
21	N	88	ARG
21	N	233	ASN
21	N	416	GLY
21	N	564	ASN
22	S	46	LEU
22	S	47	THR
24	Q	42	ALA
24	Q	68	MET
24	Q	207	SER
24	Q	273	ASN
24	Q	394	ASN
25	R	88	LEU
26	U	5	HIS
26	U	144	LYS
27	O	70	TYR
27	O	119	SER
27	O	141	ASN
28	H	129	SER
28	H	284	VAL
28	H	348	ASN
29	I	341	PRO
29	I	413	ALA
30	K	156	SER
30	K	418	ASP
32	M	106	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	M	110	ASN
32	M	173	ASP
33	J	17	SER
33	J	194	GLY
2	b	41	ASN
5	e	71	ASP
7	g	13	SER
7	g	225	ASN
8	h	175	ASP
10	j	192	LYS
11	k	9	VAL
4	D	70	HIS
5	E	14	THR
9	2	200	SER
9	2	251	ASP
14	7	58	ASP
16	V	113	GLY
16	V	262	THR
17	T	45	SER
17	T	94	HIS
18	X	92	SER
20	Z	25	PRO
20	Z	237	VAL
20	Z	366	LYS
20	Z	557	GLU
20	Z	825	ALA
21	N	473	ASP
21	N	842	ASN
22	S	44	THR
22	S	116	ALA
22	S	153	GLU
22	S	304	SER
22	S	491	GLU
24	Q	386	PHE
27	O	392	TRP
28	H	113	ASP
28	H	145	TYR
28	H	314	VAL
29	I	283	GLU
29	I	321	ASP
30	K	311	ASN
30	K	332	GLY

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	L	50	GLN
32	M	316	SER
33	J	335	MET
1	a	60	PRO
2	b	205	ASN
4	d	144	GLU
5	e	73	HIS
7	g	11	SER
7	g	71	ASP
9	i	200	SER
2	B	53	SER
5	E	73	HIS
5	E	210	GLU
7	G	10	LEU
7	G	187	LEU
9	2	174	ASP
9	2	224	VAL
10	3	5	SER
10	3	157	ASN
15	W	81	ILE
15	W	179	ARG
17	T	210	PHE
18	X	41	GLU
18	X	55	LYS
19	Y	31	GLU
19	Y	52	ASN
20	Z	65	GLU
20	Z	463	HIS
21	N	381	GLU
21	N	748	PHE
22	S	98	SER
22	S	118	PHE
22	S	127	THR
22	S	150	LYS
23	P	130	ILE
24	Q	40	ALA
24	Q	49	LYS
24	Q	286	TYR
28	H	179	SER
28	H	312	ASP
28	H	340	LEU
29	I	160	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
30	K	344	ARG
30	K	420	THR
32	M	91	ILE
32	M	172	VAL
32	M	345	ARG
33	J	99	ALA
33	J	228	ARG
7	g	187	LEU
4	D	40	ASN
7	G	63	LYS
15	W	144	PHE
20	Z	728	LYS
21	N	666	GLN
21	N	864	LYS
24	Q	355	GLU
25	R	375	LYS
26	U	127	GLN
27	O	56	PRO
27	O	243	VAL
27	O	351	SER
29	I	188	GLU
30	K	377	SER
32	M	104	GLY
24	Q	208	ILE
14	n	262	GLY
29	I	287	ILE
30	K	92	VAL
31	L	350	PRO
13	6	48	GLU
20	Z	86	PRO
28	H	152	ILE
28	H	412	PRO
31	L	102	GLY
30	K	330	ARG

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	207/207 (100%)	203 (98%)	4 (2%)	57	75
1	a	207/207 (100%)	201 (97%)	6 (3%)	42	64
2	B	206/206 (100%)	200 (97%)	6 (3%)	42	64
2	b	206/206 (100%)	202 (98%)	4 (2%)	57	75
3	C	201/201 (100%)	193 (96%)	8 (4%)	31	56
3	c	201/201 (100%)	195 (97%)	6 (3%)	41	63
4	D	224/224 (100%)	217 (97%)	7 (3%)	40	63
4	d	224/224 (100%)	213 (95%)	11 (5%)	25	51
5	E	201/201 (100%)	197 (98%)	4 (2%)	55	73
5	e	201/201 (100%)	198 (98%)	3 (2%)	65	80
6	F	191/191 (100%)	184 (96%)	7 (4%)	34	59
6	f	191/191 (100%)	185 (97%)	6 (3%)	40	63
7	G	202/202 (100%)	195 (96%)	7 (4%)	36	60
7	g	202/202 (100%)	193 (96%)	9 (4%)	27	54
8	1	162/162 (100%)	159 (98%)	3 (2%)	57	75
8	h	162/162 (100%)	158 (98%)	4 (2%)	47	68
9	2	185/185 (100%)	181 (98%)	4 (2%)	52	71
9	i	185/185 (100%)	180 (97%)	5 (3%)	44	66
10	3	172/172 (100%)	165 (96%)	7 (4%)	30	56
10	j	172/172 (100%)	167 (97%)	5 (3%)	42	64
11	4	173/173 (100%)	167 (96%)	6 (4%)	36	60
11	k	173/173 (100%)	167 (96%)	6 (4%)	36	60
12	5	169/169 (100%)	164 (97%)	5 (3%)	41	63
12	l	169/169 (100%)	164 (97%)	5 (3%)	41	63
13	6	185/185 (100%)	178 (96%)	7 (4%)	33	58
13	m	185/185 (100%)	182 (98%)	3 (2%)	62	79
14	7	195/198 (98%)	187 (96%)	8 (4%)	30	56
14	n	198/198 (100%)	194 (98%)	4 (2%)	55	73
15	W	171/171 (100%)	167 (98%)	4 (2%)	50	70
16	V	253/253 (100%)	247 (98%)	6 (2%)	49	69
17	T	249/249 (100%)	245 (98%)	4 (2%)	62	79
18	X	116/116 (100%)	112 (97%)	4 (3%)	37	61

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
19	Y	81/81 (100%)	77 (95%)	4 (5%)	25 51
20	Z	773/828 (93%)	745 (96%)	28 (4%)	35 60
21	N	776/776 (100%)	759 (98%)	17 (2%)	52 71
22	S	447/447 (100%)	435 (97%)	12 (3%)	44 66
23	P	412/412 (100%)	408 (99%)	4 (1%)	76 86
24	Q	391/391 (100%)	382 (98%)	9 (2%)	50 70
25	R	356/356 (100%)	349 (98%)	7 (2%)	55 73
26	U	277/277 (100%)	275 (99%)	2 (1%)	84 90
27	O	363/363 (100%)	352 (97%)	11 (3%)	41 63
28	H	361/361 (100%)	351 (97%)	10 (3%)	43 65
29	I	342/342 (100%)	327 (96%)	15 (4%)	28 54
30	K	337/337 (100%)	327 (97%)	10 (3%)	41 63
31	L	332/332 (100%)	327 (98%)	5 (2%)	65 80
32	M	364/364 (100%)	354 (97%)	10 (3%)	44 66
33	J	350/350 (100%)	338 (97%)	12 (3%)	37 61
All	All	12100/12158 (100%)	11766 (97%)	334 (3%)	46 65

All (334) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	12	TYR
1	a	110	TYR
1	a	126	GLN
1	a	130	GLN
1	a	147	ASP
1	a	192	ASP
2	b	4	ARG
2	b	50	LYS
2	b	205	ASN
2	b	211	LEU
3	c	66	LEU
3	c	70	ASN
3	c	96	GLN
3	c	133	VAL
3	c	177	GLN
3	c	183	ASP
4	d	11	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	d	14	ASP
4	d	24	LEU
4	d	53	LYS
4	d	71	VAL
4	d	104	VAL
4	d	134	LEU
4	d	140	PRO
4	d	143	ASP
4	d	171	VAL
4	d	208	LYS
5	e	36	THR
5	e	116	VAL
5	e	214	GLU
6	f	33	SER
6	f	57	SER
6	f	72	LEU
6	f	74	LEU
6	f	134	ILE
6	f	178	THR
7	g	9	ASP
7	g	12	ASN
7	g	88	LEU
7	g	107	ILE
7	g	109	ILE
7	g	136	THR
7	g	185	GLU
7	g	206	ASP
7	g	218	TRP
8	h	84	THR
8	h	114	LYS
8	h	135	ILE
8	h	152	ARG
9	i	42	VAL
9	i	84	VAL
9	i	94	LEU
9	i	212	ASP
9	i	245	SER
10	j	13	VAL
10	j	20	CYS
10	j	147	PHE
10	j	183	TRP
10	j	196	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	k	54	VAL
11	k	101	ASN
11	k	112	ASN
11	k	126	VAL
11	k	145	ASP
11	k	161	LEU
12	l	79	LEU
12	l	84	GLN
12	l	106	VAL
12	l	146	LYS
12	l	222	ASP
13	m	106	TYR
13	m	109	ARG
13	m	127	LYS
14	n	80	ASP
14	n	220	ARG
14	n	226	ARG
14	n	230	LEU
1	A	126	GLN
1	A	169	THR
1	A	209	HIS
1	A	234	PHE
2	B	4	ARG
2	B	6	SER
2	B	8	SER
2	B	41	ASN
2	B	97	TYR
2	B	199	SER
3	C	66	LEU
3	C	70	ASN
3	C	96	GLN
3	C	115	LEU
3	C	177	GLN
3	C	186	VAL
3	C	206	LEU
3	C	232	PRO
4	D	5	ASP
4	D	19	GLN
4	D	24	LEU
4	D	40	ASN
4	D	53	LYS
4	D	71	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	D	139	ASP
5	E	18	GLU
5	E	36	THR
5	E	164	PHE
5	E	213	ASP
6	F	18	ARG
6	F	26	LEU
6	F	68	GLU
6	F	72	LEU
6	F	177	ASP
6	F	209	ASP
6	F	228	GLU
7	G	43	ASN
7	G	82	ILE
7	G	88	LEU
7	G	185	GLU
7	G	218	TRP
7	G	224	THR
7	G	241	ASP
8	1	30	THR
8	1	124	LEU
8	1	188	THR
9	2	68	PRO
9	2	118	LYS
9	2	153	TYR
9	2	161	LEU
10	3	11	ILE
10	3	13	VAL
10	3	45	HIS
10	3	77	LYS
10	3	80	ARG
10	3	99	ARG
10	3	147	PHE
11	4	78	GLN
11	4	126	VAL
11	4	151	ASP
11	4	159	ASP
11	4	168	LEU
11	4	186	LYS
12	5	79	LEU
12	5	109	VAL
12	5	179	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	5	251	ASN
12	5	252	LEU
13	6	15	ASP
13	6	30	VAL
13	6	31	LEU
13	6	59	VAL
13	6	89	ASP
13	6	91	LYS
13	6	125	ASP
14	7	53	VAL
14	7	80	ASP
14	7	89	ASP
14	7	115	ASP
14	7	165	LEU
14	7	197	ASP
14	7	220	ARG
14	7	221	ASP
15	W	53	SER
15	W	60	ARG
15	W	81	ILE
15	W	182	TYR
16	V	45	VAL
16	V	50	MET
16	V	92	MET
16	V	147	VAL
16	V	263	GLU
16	V	274	GLN
17	T	30	ILE
17	T	51	TYR
17	T	242	LYS
17	T	266	TYR
18	X	11	ARG
18	X	30	GLN
18	X	39	GLU
18	X	51	ARG
19	Y	42	THR
19	Y	66	ASP
19	Y	68	GLU
19	Y	88	ASN
20	Z	27	LYS
20	Z	29	ASP
20	Z	30	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
20	Z	81	SER
20	Z	93	ARG
20	Z	171	LYS
20	Z	185	ASP
20	Z	187	SER
20	Z	222	ASP
20	Z	236	PHE
20	Z	354	PRO
20	Z	402	ASP
20	Z	411	LYS
20	Z	434	GLN
20	Z	445	PRO
20	Z	548	ASP
20	Z	557	GLU
20	Z	563	VAL
20	Z	566	LEU
20	Z	609	THR
20	Z	703	SER
20	Z	756	MET
20	Z	767	TYR
20	Z	797	THR
20	Z	842	GLN
20	Z	874	ASN
20	Z	878	LEU
20	Z	910	PRO
21	N	76	GLU
21	N	87	ASP
21	N	223	LEU
21	N	282	TYR
21	N	310	ASP
21	N	360	GLN
21	N	361	ASN
21	N	418	ASP
21	N	505	SER
21	N	599	TYR
21	N	739	PHE
21	N	774	ASN
21	N	835	LYS
21	N	860	LYS
21	N	873	ARG
21	N	888	ASP
21	N	889	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	S	34	LEU
22	S	119	TYR
22	S	131	THR
22	S	144	LEU
22	S	155	LEU
22	S	165	PRO
22	S	244	ASN
22	S	313	SER
22	S	327	ILE
22	S	388	ILE
22	S	425	ARG
22	S	429	ASP
23	P	25	ASP
23	P	47	ARG
23	P	139	VAL
23	P	158	ASP
24	Q	45	SER
24	Q	86	MET
24	Q	174	LEU
24	Q	220	LEU
24	Q	227	CYS
24	Q	335	PHE
24	Q	340	ASP
24	Q	343	LEU
24	Q	402	THR
25	R	208	ASN
25	R	248	SER
25	R	262	GLU
25	R	263	ARG
25	R	293	THR
25	R	361	VAL
25	R	382	ASP
26	U	9	THR
26	U	177	ASP
27	O	53	LYS
27	O	66	VAL
27	O	101	ASP
27	O	142	ASP
27	O	180	LYS
27	O	193	LEU
27	O	217	LEU
27	O	249	ASP

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
27	O	258	LEU
27	O	289	GLN
27	O	307	MET
28	H	145	TYR
28	H	157	VAL
28	H	161	GLU
28	H	188	PRO
28	H	195	VAL
28	H	208	TYR
28	H	238	LEU
28	H	379	LEU
28	H	420	ARG
28	H	437	VAL
29	I	86	GLU
29	I	103	PRO
29	I	159	VAL
29	I	192	GLN
29	I	219	VAL
29	I	232	LEU
29	I	247	ILE
29	I	251	GLU
29	I	254	GLN
29	I	259	ASP
29	I	290	LYS
29	I	292	TYR
29	I	310	LEU
29	I	340	ARG
29	I	353	PRO
30	K	73	ARG
30	K	121	ARG
30	K	147	VAL
30	K	155	ASP
30	K	203	ILE
30	K	286	THR
30	K	313	LYS
30	K	330	ARG
30	K	334	LEU
30	K	403	LEU
31	L	77	ARG
31	L	107	GLU
31	L	141	LYS
31	L	148	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	L	226	THR
32	M	75	LEU
32	M	142	PRO
32	M	157	ASP
32	M	267	PHE
32	M	305	MET
32	M	344	ASP
32	M	365	SER
32	M	410	VAL
32	M	414	ASP
32	M	415	PHE
33	J	14	THR
33	J	22	TYR
33	J	110	SER
33	J	113	VAL
33	J	129	LYS
33	J	150	VAL
33	J	190	PRO
33	J	236	MET
33	J	242	PRO
33	J	275	LEU
33	J	316	PHE
33	J	319	PRO

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (147) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	193	HIS
1	a	209	HIS
2	b	139	HIS
3	c	21	GLN
3	c	31	HIS
3	c	96	GLN
3	c	120	GLN
5	e	91	HIS
6	f	121	GLN
6	f	143	HIS
6	f	148	GLN
7	g	23	GLN
7	g	64	ASN
7	g	123	HIS
7	g	147	HIS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	i	95	HIS
10	j	89	GLN
10	j	145	GLN
10	j	169	GLN
11	k	133	HIS
11	k	191	GLN
12	l	137	GLN
12	l	241	HIS
12	l	254	HIS
12	l	263	HIS
12	l	283	ASN
12	l	284	ASN
13	m	57	ASN
14	n	236	ASN
14	n	264	GLN
1	A	126	GLN
1	A	181	ASN
2	B	190	HIS
2	B	244	ASN
3	C	31	HIS
3	C	96	GLN
3	C	125	HIS
3	C	177	GLN
4	D	149	GLN
4	D	178	ASN
4	D	209	ASN
5	E	23	GLN
5	E	147	HIS
5	E	188	HIS
5	E	215	ASN
6	F	60	GLN
6	F	121	GLN
6	F	143	HIS
7	G	87	HIS
7	G	182	HIS
7	G	204	HIS
8	1	47	HIS
8	1	154	ASN
10	3	38	ASN
10	3	113	ASN
10	3	169	GLN
10	3	173	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	5	141	HIS
13	6	37	ASN
14	7	36	GLN
15	W	100	HIS
15	W	103	ASN
16	V	190	HIS
17	T	165	GLN
17	T	170	ASN
18	X	18	ASN
18	X	30	GLN
19	Y	9	GLN
19	Y	56	GLN
19	Y	88	ASN
20	Z	15	GLN
20	Z	129	ASN
20	Z	156	HIS
20	Z	214	HIS
20	Z	215	ASN
20	Z	247	GLN
20	Z	307	HIS
20	Z	317	GLN
20	Z	823	ASN
20	Z	829	GLN
21	N	288	ASN
21	N	329	HIS
21	N	340	HIS
21	N	361	ASN
21	N	378	ASN
21	N	614	ASN
21	N	654	GLN
21	N	672	ASN
21	N	688	ASN
21	N	690	HIS
22	S	79	ASN
22	S	166	ASN
22	S	225	HIS
22	S	312	GLN
22	S	317	HIS
22	S	334	HIS
22	S	437	ASN
23	P	38	GLN
23	P	128	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
23	P	222	ASN
23	P	337	HIS
23	P	417	HIS
24	Q	37	GLN
24	Q	145	HIS
24	Q	226	HIS
24	Q	253	ASN
24	Q	361	HIS
24	Q	392	GLN
25	R	81	HIS
25	R	130	GLN
25	R	136	ASN
25	R	223	ASN
25	R	323	ASN
25	R	415	GLN
26	U	5	HIS
26	U	21	HIS
26	U	127	GLN
26	U	302	GLN
26	U	304	GLN
27	O	40	GLN
27	O	122	HIS
27	O	318	HIS
28	H	130	ASN
28	H	131	GLN
28	H	265	ASN
28	H	281	GLN
28	H	339	GLN
28	H	467	ASN
29	I	78	ASN
29	I	254	GLN
29	I	365	HIS
29	I	393	GLN
30	K	106	ASN
30	K	180	GLN
30	K	302	GLN
30	K	414	GLN
31	L	175	GLN
31	L	203	ASN
31	L	302	GLN
32	M	110	ASN
32	M	328	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
32	M	364	HIS
33	J	25	GLN
33	J	205	HIS
33	J	287	ASN
33	J	351	ASN
33	J	394	GLN

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	K	501	35	24,29,29	1.86	7 (29%)	29,45,45	2.11	6 (20%)
34	ATP	H	501	35	26,33,33	1.27	2 (7%)	31,52,52	1.87	5 (16%)
34	ATP	M	501	35	26,33,33	1.28	2 (7%)	31,52,52	1.85	7 (22%)
36	ADP	L	501	35	24,29,29	2.04	5 (20%)	29,45,45	2.12	5 (17%)
34	ATP	I	501	35	26,33,33	1.49	5 (19%)	31,52,52	1.81	4 (12%)
34	ATP	J	501	35	26,33,33	1.63	3 (11%)	31,52,52	2.57	5 (16%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ADP	K	501	35	-	4/12/32/32	0/3/3/3
34	ATP	H	501	35	-	4/18/38/38	0/3/3/3
34	ATP	M	501	35	-	5/18/38/38	0/3/3/3
36	ADP	L	501	35	-	3/12/32/32	0/3/3/3
34	ATP	I	501	35	-	7/18/38/38	0/3/3/3
34	ATP	J	501	35	-	3/18/38/38	0/3/3/3

All (24) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	L	501	ADP	C2-N3	6.07	1.41	1.32
36	L	501	ADP	O4'-C1'	5.60	1.48	1.41
34	J	501	ATP	C4-N3	-5.29	1.28	1.35
36	K	501	ADP	C2'-C1'	-4.36	1.47	1.53
34	J	501	ATP	O4'-C1'	3.84	1.46	1.41
34	I	501	ATP	C8-N7	-3.38	1.28	1.34
34	M	501	ATP	C8-N7	-3.31	1.28	1.34
36	K	501	ADP	C4-N3	-3.31	1.31	1.35
34	H	501	ATP	C8-N7	-3.29	1.28	1.34
36	K	501	ADP	O2'-C2'	-3.12	1.35	1.43
36	K	501	ADP	O4'-C1'	2.98	1.45	1.41
36	L	501	ADP	C5-N7	-2.70	1.29	1.39
34	J	501	ATP	C6-N6	2.68	1.43	1.34
34	I	501	ATP	O2'-C2'	-2.59	1.36	1.43
36	K	501	ADP	C8-N7	-2.54	1.30	1.34
34	I	501	ATP	O3'-C3'	-2.53	1.37	1.43
36	K	501	ADP	C2-N3	2.53	1.36	1.32
34	I	501	ATP	C2'-C1'	-2.51	1.49	1.53
36	L	501	ADP	PB-O2B	-2.40	1.45	1.54
34	H	501	ATP	C2'-C3'	-2.30	1.47	1.53
34	M	501	ATP	C3'-C4'	2.18	1.58	1.53
34	I	501	ATP	O4'-C1'	2.14	1.44	1.41
36	L	501	ADP	O4'-C4'	-2.04	1.40	1.45
36	K	501	ADP	C6-N6	2.02	1.41	1.34

All (32) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	J	501	ATP	PA-O3A-PB	9.61	165.81	132.83
36	K	501	ADP	PA-O3A-PB	8.39	161.62	132.83
36	L	501	ADP	PA-O3A-PB	8.24	161.11	132.83
34	M	501	ATP	PB-O3B-PG	6.57	155.36	132.83
34	H	501	ATP	PA-O3A-PB	5.98	153.35	132.83
34	I	501	ATP	PB-O3B-PG	5.80	152.71	132.83
34	J	501	ATP	PB-O3B-PG	5.76	152.60	132.83
34	J	501	ATP	N6-C6-N1	5.65	130.29	118.57
34	H	501	ATP	PB-O3B-PG	5.18	150.60	132.83
34	I	501	ATP	PA-O3A-PB	4.77	149.18	132.83
34	M	501	ATP	N6-C6-N1	4.12	127.13	118.57
34	J	501	ATP	C5-C6-N1	-3.92	111.47	120.35
36	L	501	ADP	N6-C6-N1	3.63	126.10	118.57
36	K	501	ADP	C3'-C2'-C1'	3.52	106.28	100.98
36	K	501	ADP	C2'-C3'-C4'	-3.44	95.96	102.64
36	L	501	ADP	C5-C6-N1	-3.20	113.10	120.35
34	H	501	ATP	C5-C6-N1	-3.14	113.24	120.35
34	H	501	ATP	N6-C6-N1	3.12	125.04	118.57
34	H	501	ATP	O5'-C5'-C4'	2.98	119.23	108.99
34	I	501	ATP	N6-C6-N1	2.89	124.57	118.57
34	M	501	ATP	PA-O3A-PB	2.74	142.22	132.83
36	K	501	ADP	N6-C6-N1	2.68	124.13	118.57
34	M	501	ATP	C5-C6-N1	-2.65	114.36	120.35
34	J	501	ATP	O3G-PG-O2G	2.57	117.47	107.64
36	L	501	ADP	O5'-C5'-C4'	2.57	117.83	108.99
34	M	501	ATP	O3G-PG-O2G	2.54	117.33	107.64
36	K	501	ADP	O3B-PB-O2B	2.40	116.82	107.64
34	I	501	ATP	O4'-C1'-C2'	-2.31	103.55	106.93
36	K	501	ADP	C5-C6-N1	-2.11	115.57	120.35
36	L	501	ADP	O2A-PA-O1A	2.03	122.27	112.24
34	M	501	ATP	O3'-C3'-C4'	-2.01	105.24	111.05
34	M	501	ATP	C2'-C3'-C4'	-2.00	98.75	102.64

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	H	501	ATP	C5'-O5'-PA-O2A
34	H	501	ATP	C5'-O5'-PA-O3A
34	I	501	ATP	C5'-O5'-PA-O1A
34	I	501	ATP	C5'-O5'-PA-O2A
34	M	501	ATP	C5'-O5'-PA-O2A
34	M	501	ATP	C5'-O5'-PA-O3A

Continued on next page...

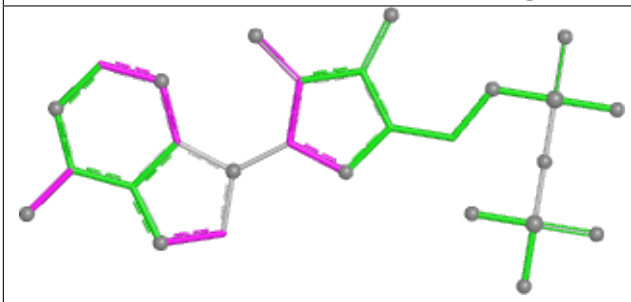
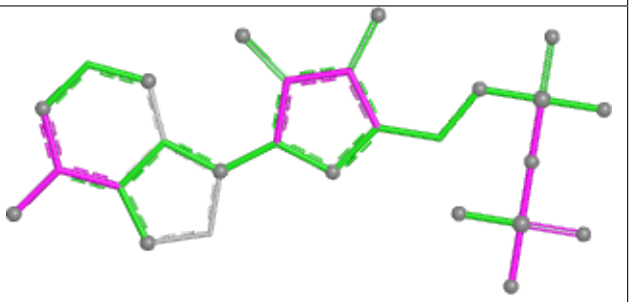
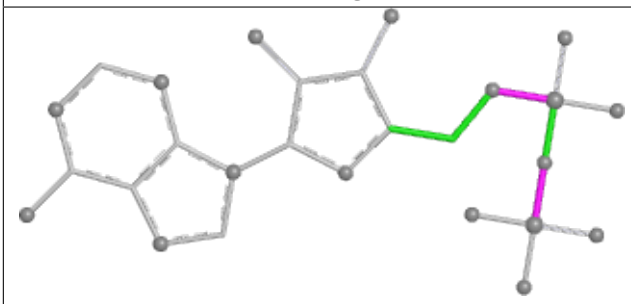
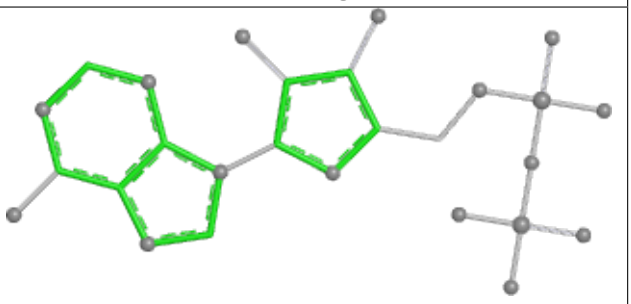
Continued from previous page...

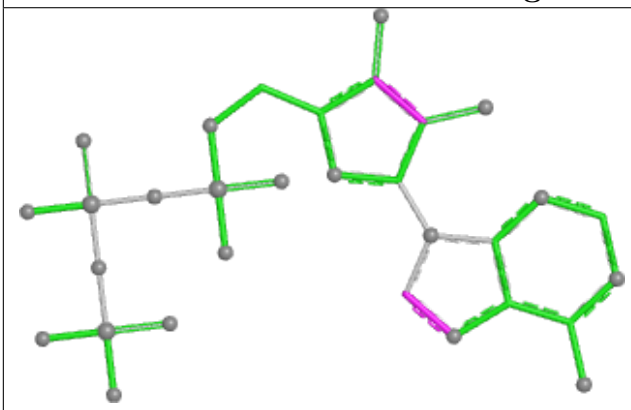
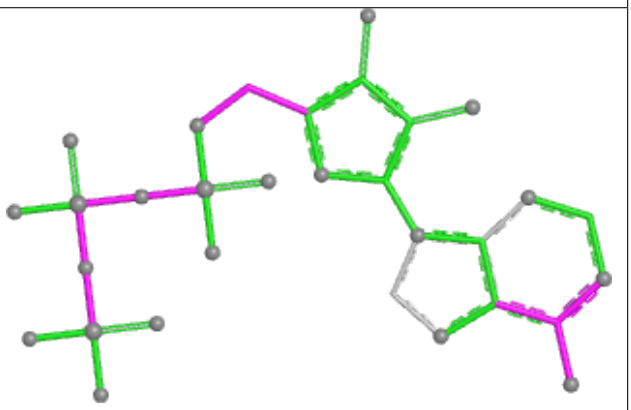
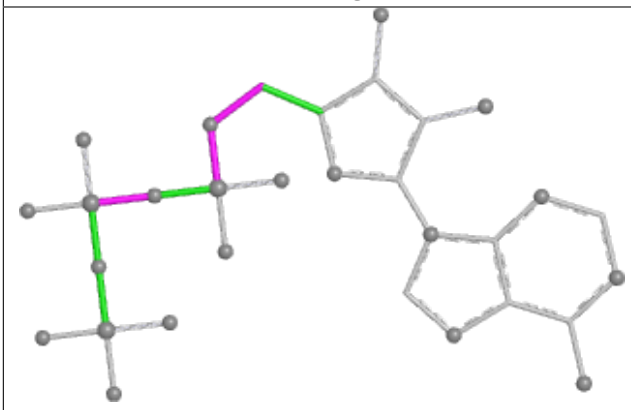
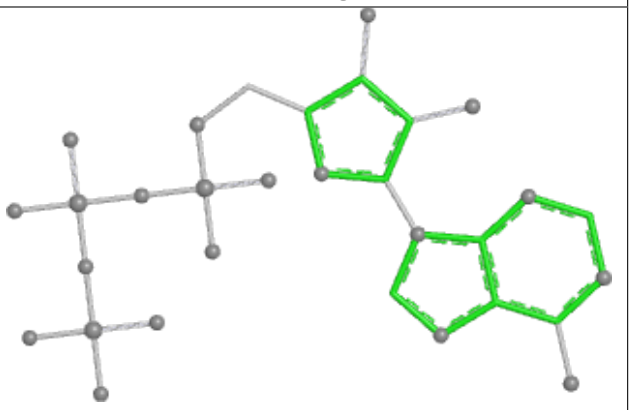
Mol	Chain	Res	Type	Atoms
34	J	501	ATP	C5'-O5'-PA-O3A
36	K	501	ADP	C5'-O5'-PA-O1A
36	K	501	ADP	C5'-O5'-PA-O2A
36	L	501	ADP	C5'-O5'-PA-O1A
34	I	501	ATP	O4'-C4'-C5'-O5'
34	I	501	ATP	C3'-C4'-C5'-O5'
34	H	501	ATP	C4'-C5'-O5'-PA
34	I	501	ATP	C4'-C5'-O5'-PA
36	L	501	ADP	C5'-O5'-PA-O3A
34	M	501	ATP	PA-O3A-PB-O2B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

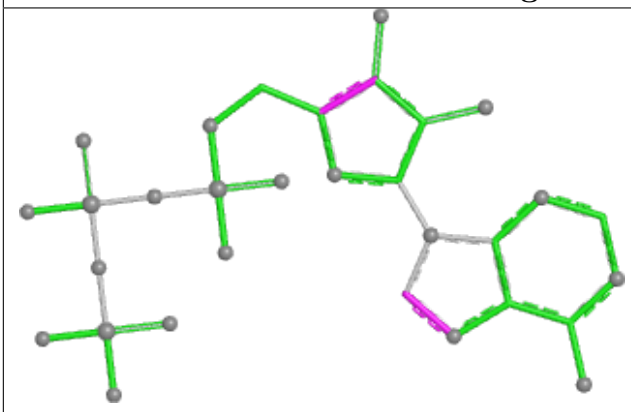
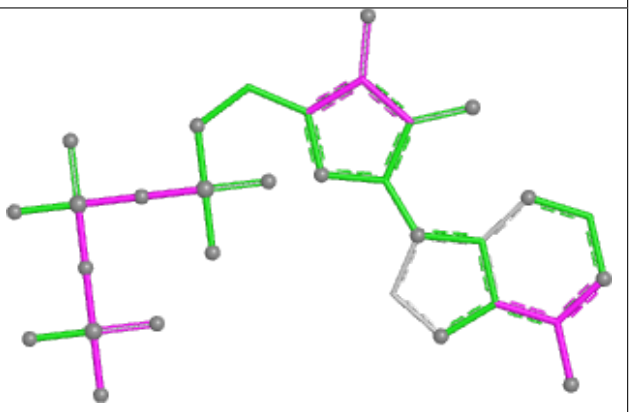
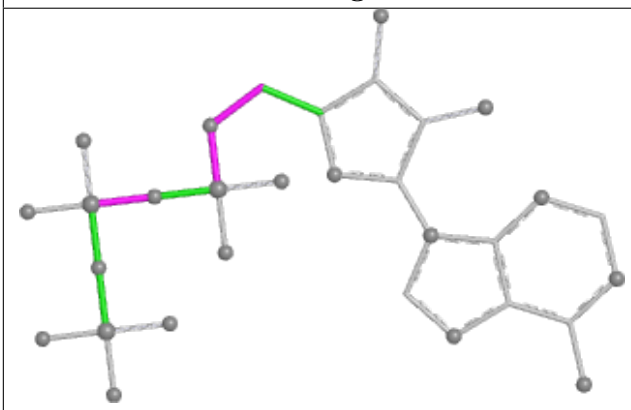
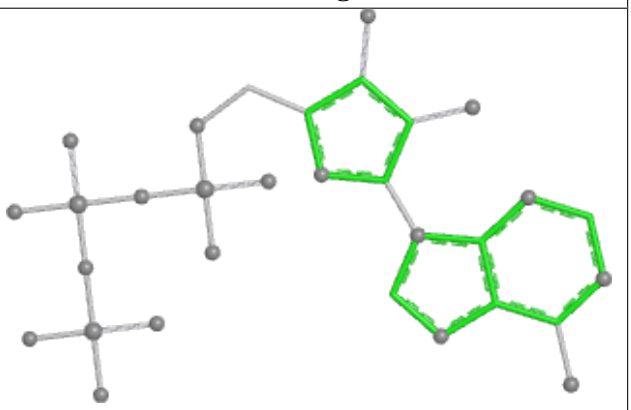
There are no ring outliers.

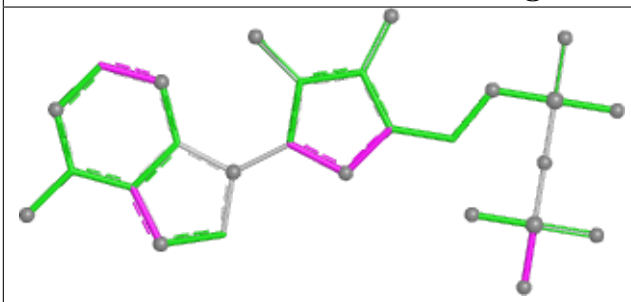
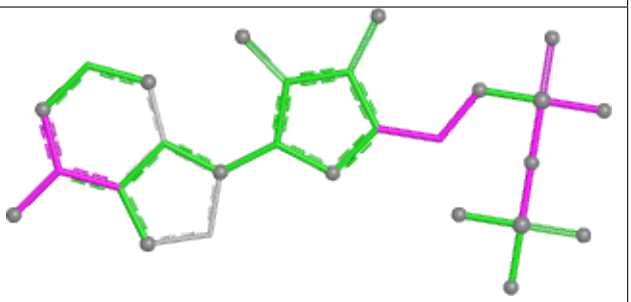
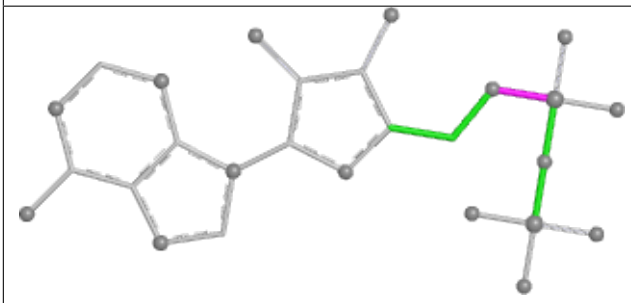
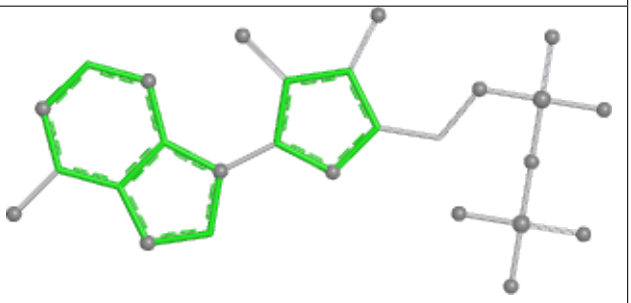
No monomer is involved in short contacts.

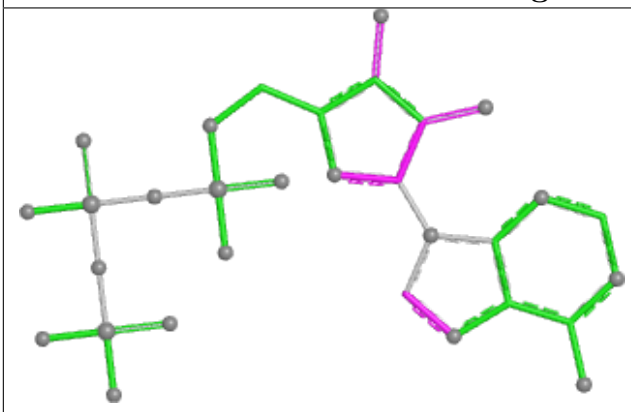
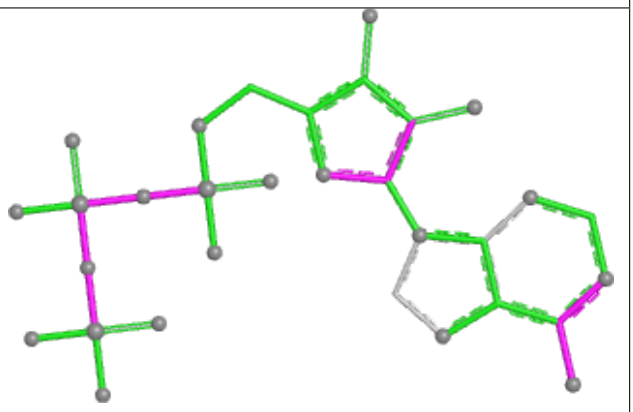
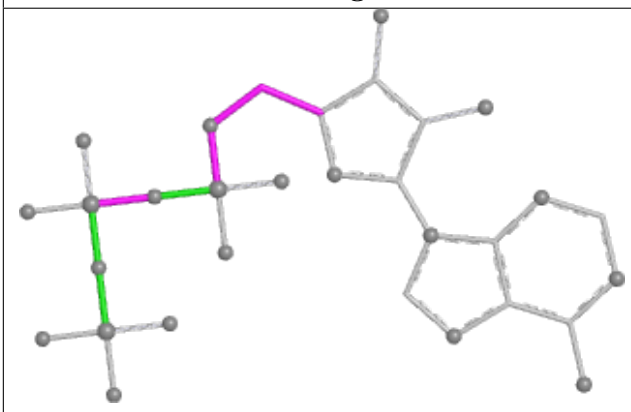
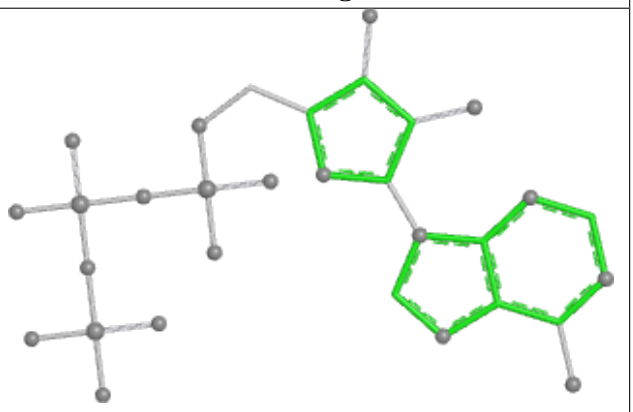
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less then 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

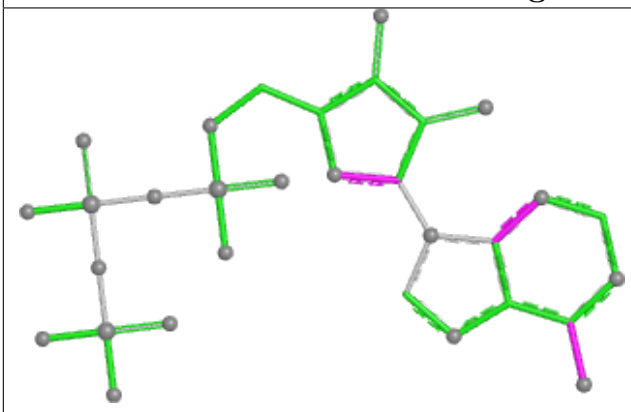
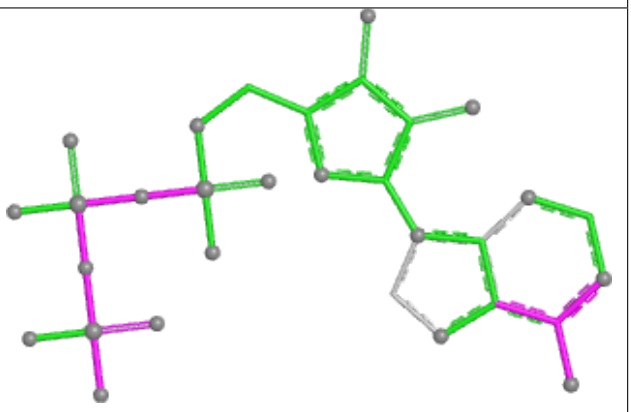
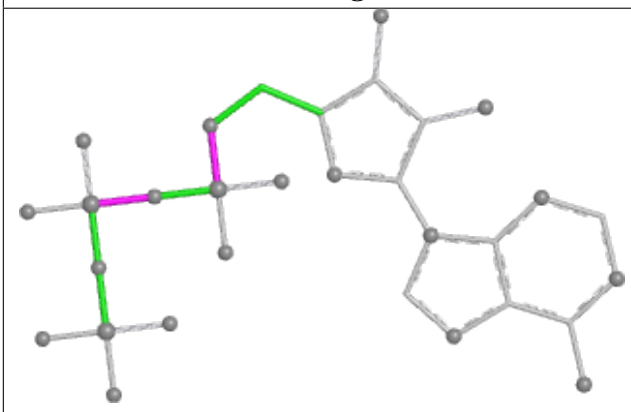
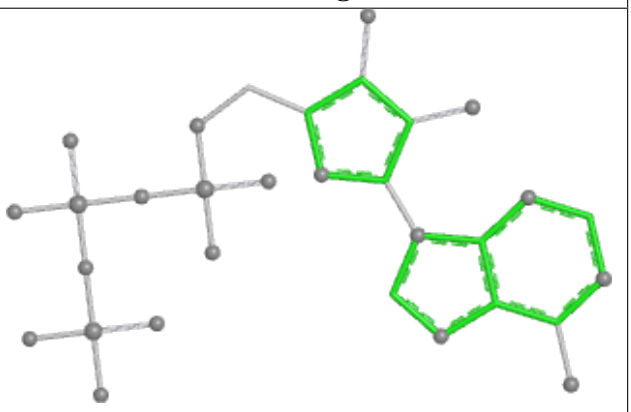
Ligand ADP K 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP H 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP L 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP I 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP J 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

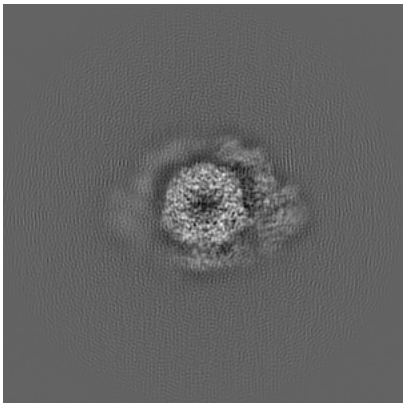
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4322. These allow visual inspection of the internal detail of the map and identification of artifacts.

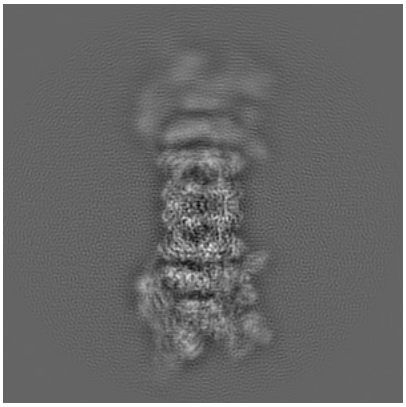
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

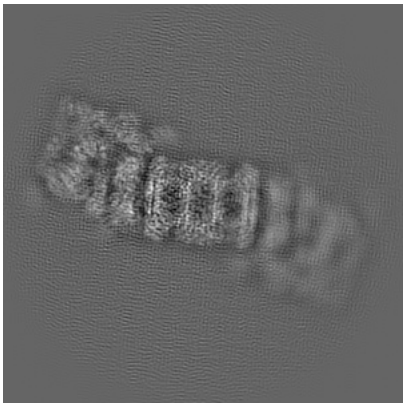
6.1.1 Primary map



X



Y

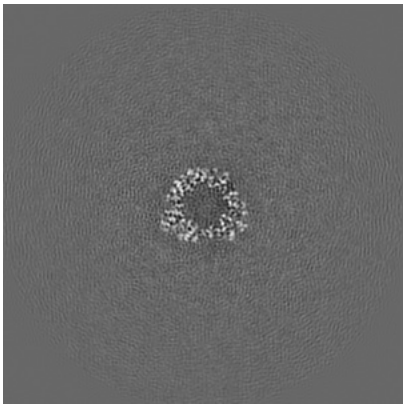


Z

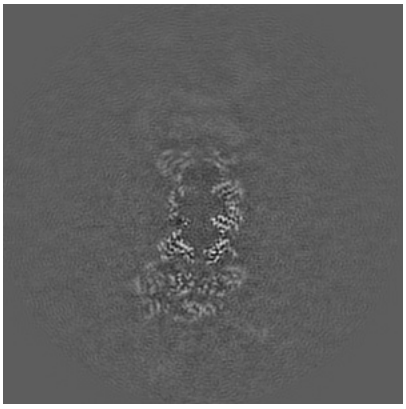
The images above show the map projected in three orthogonal directions.

6.2 Central slices

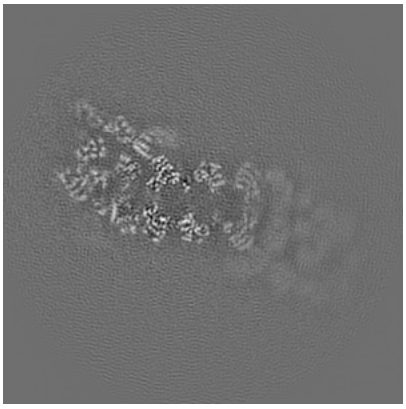
6.2.1 Primary map



X Index: 192



Y Index: 192

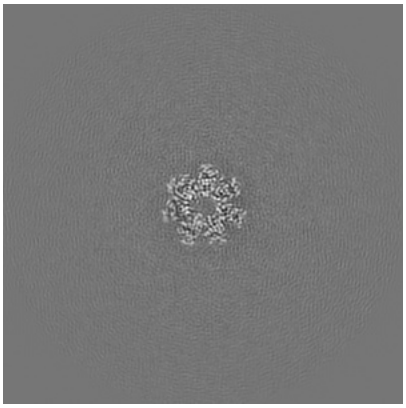


Z Index: 192

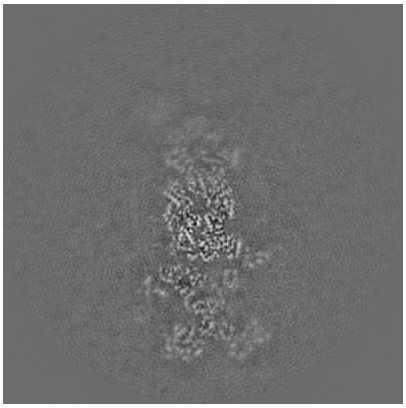
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

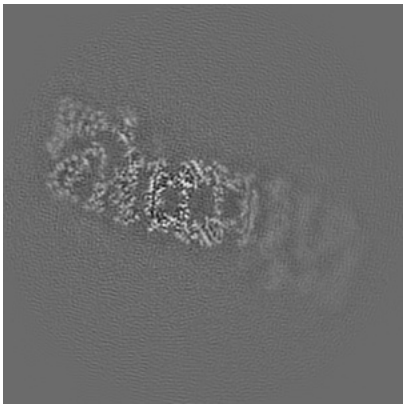
6.3.1 Primary map



X Index: 177



Y Index: 212

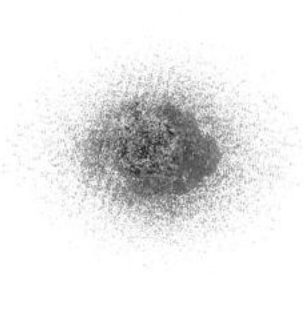


Z Index: 178

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

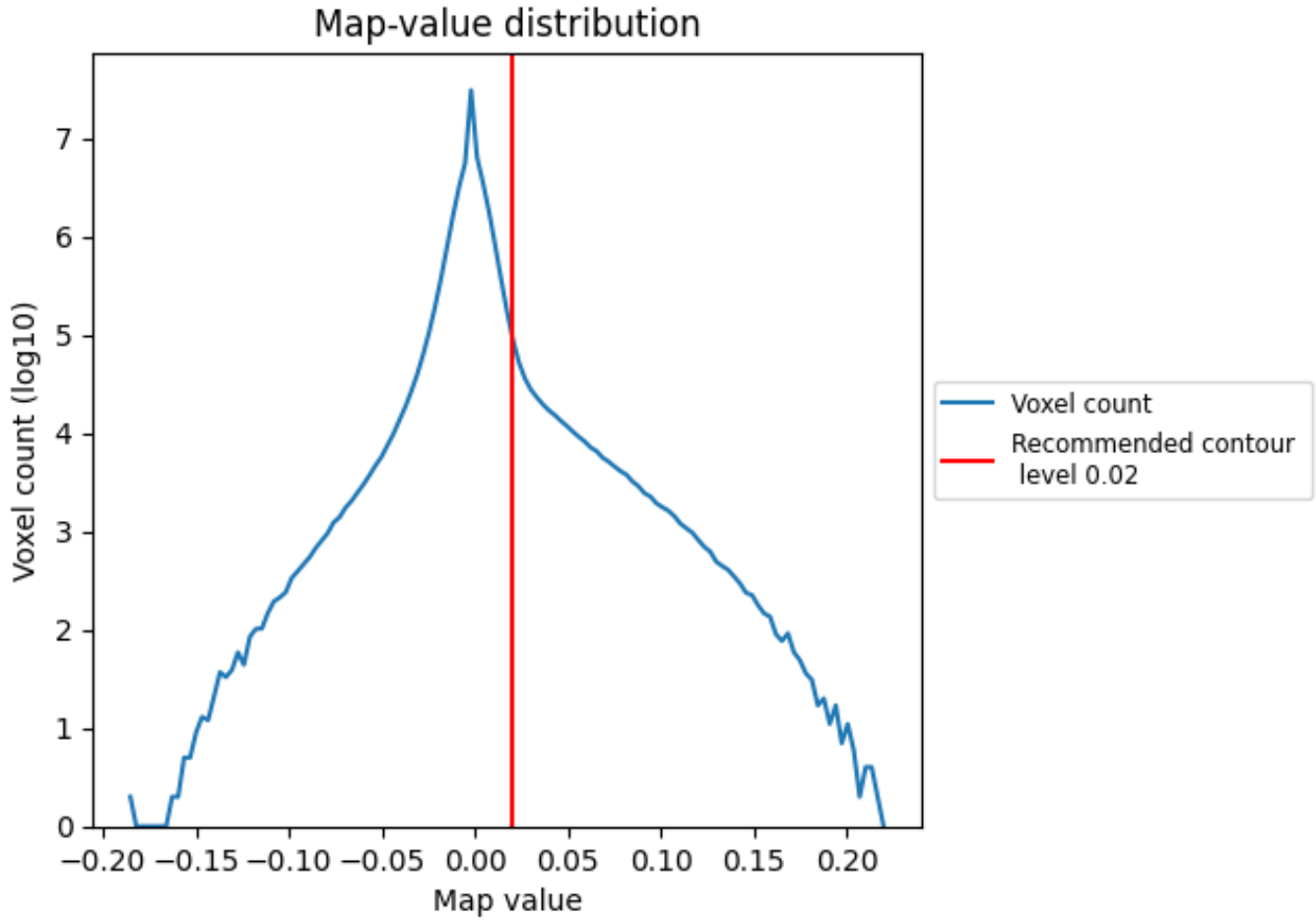
6.5 Mask visualisation (i)

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

7 Map analysis

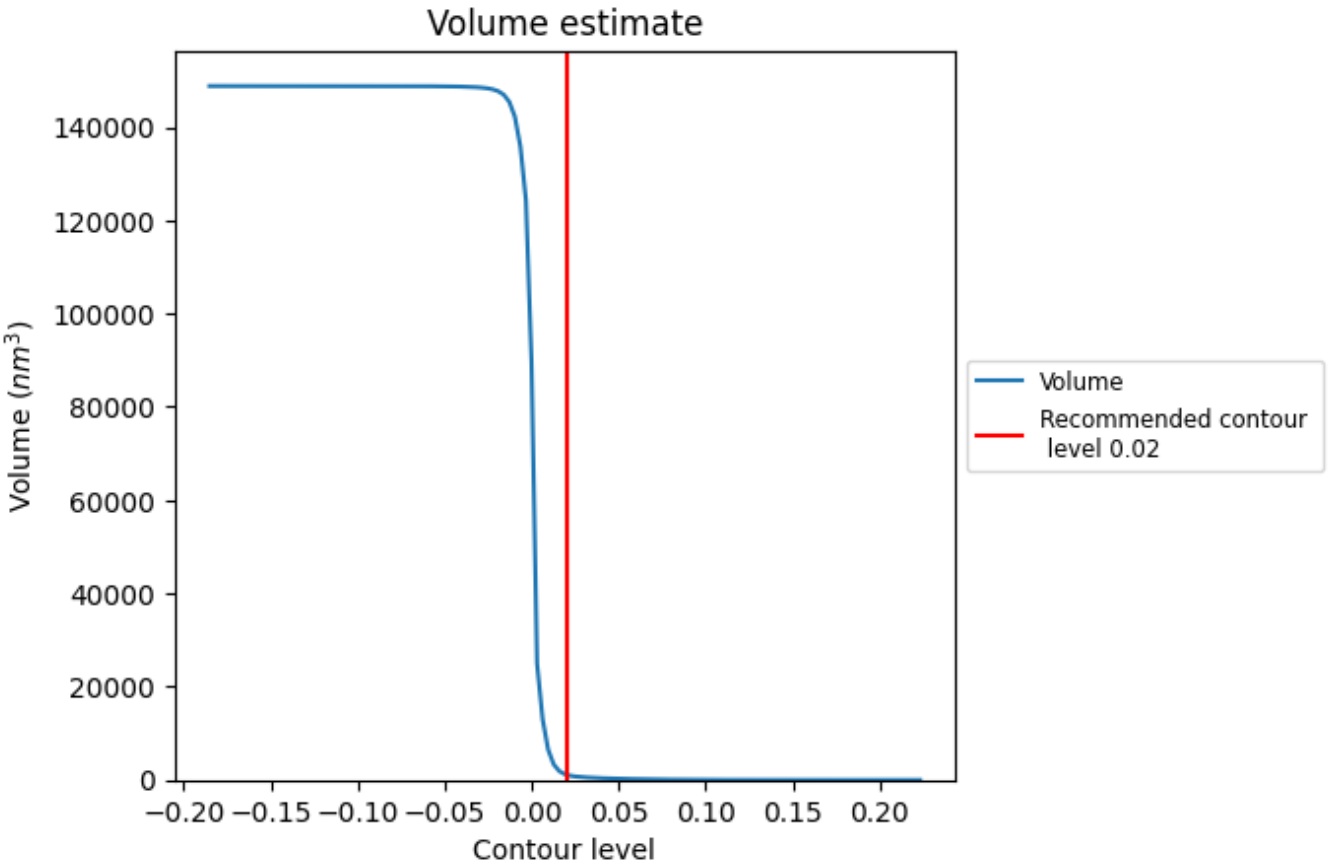
This section contains the results of statistical analysis of the map.

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.

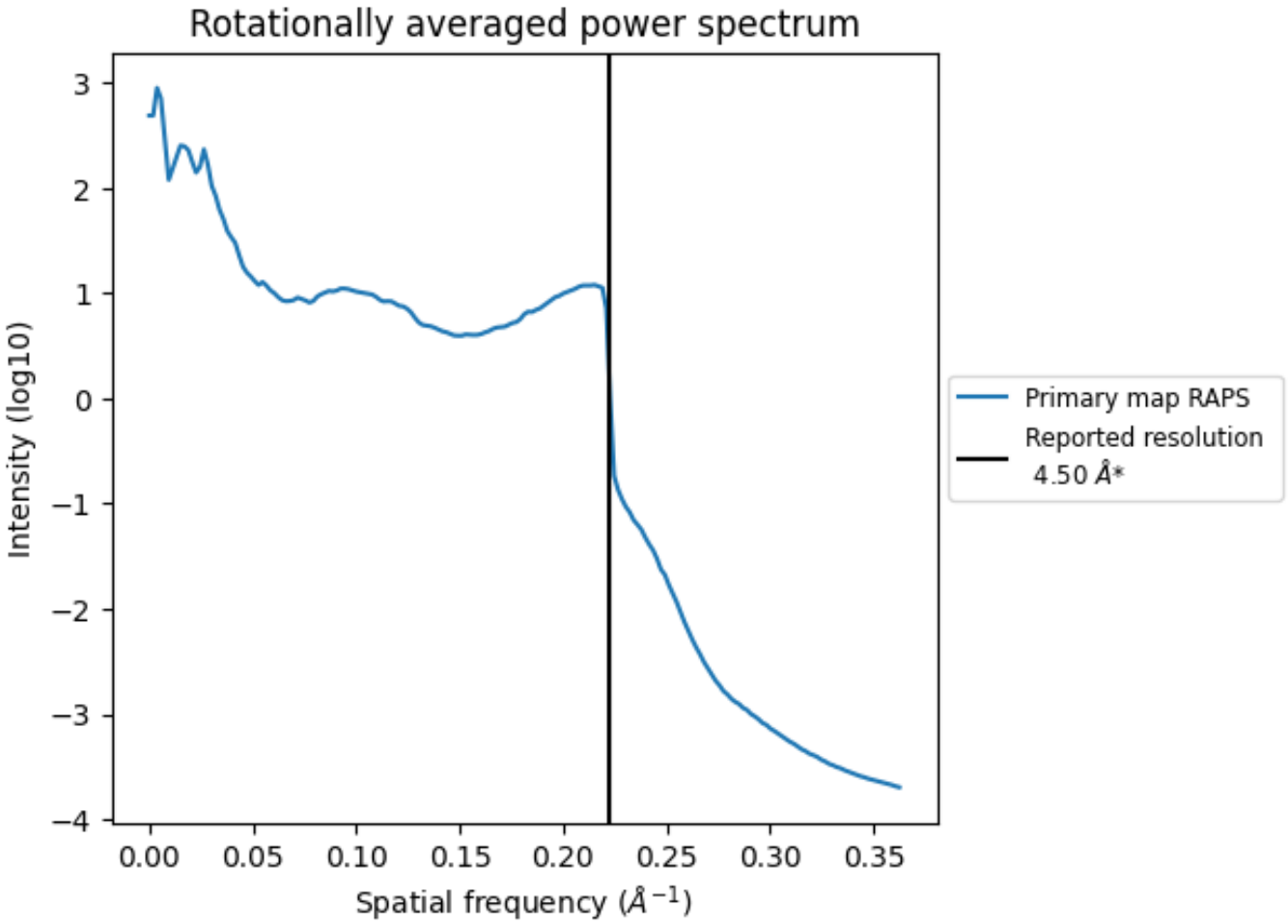
7.2 Volume estimate



The volume at the recommended contour level is 1128 nm^3; this corresponds to an approximate mass of 1019 kDa.

The volume estimate graph shows how the enclosed volume varies with the contour level. The recommended contour level is shown as a vertical line and the intersection between the line and the curve gives the volume of the enclosed surface at the given level.

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.222 Å^{-1}

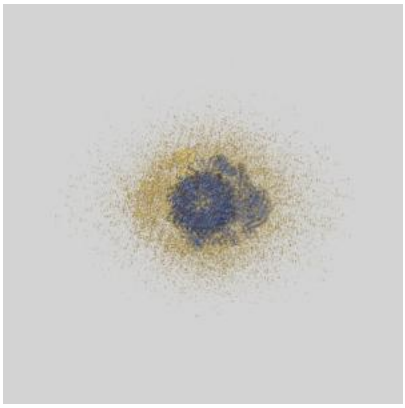
8 Fourier-Shell correlation

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

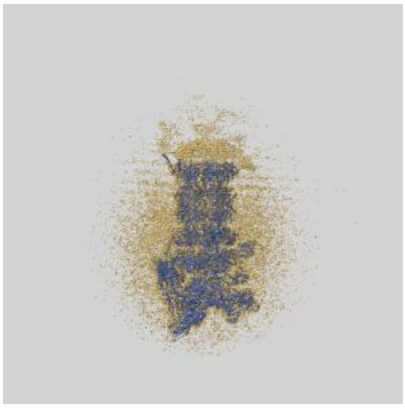
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4322 and PDB model 6FVW. Per-residue inclusion information can be found in section 3 on page 13.

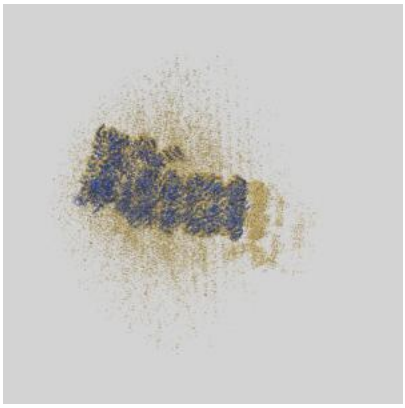
9.1 Map-model overlay



X



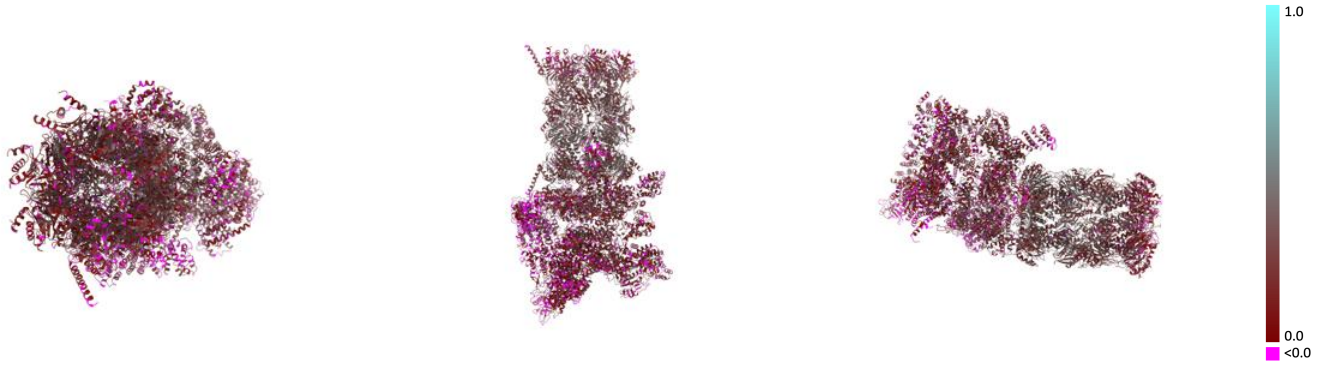
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.02 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

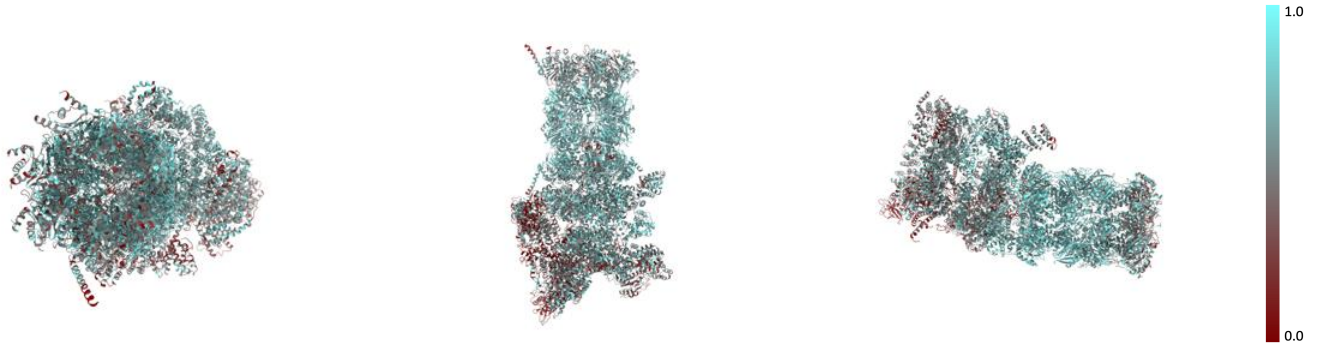
9.2 Q-score mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

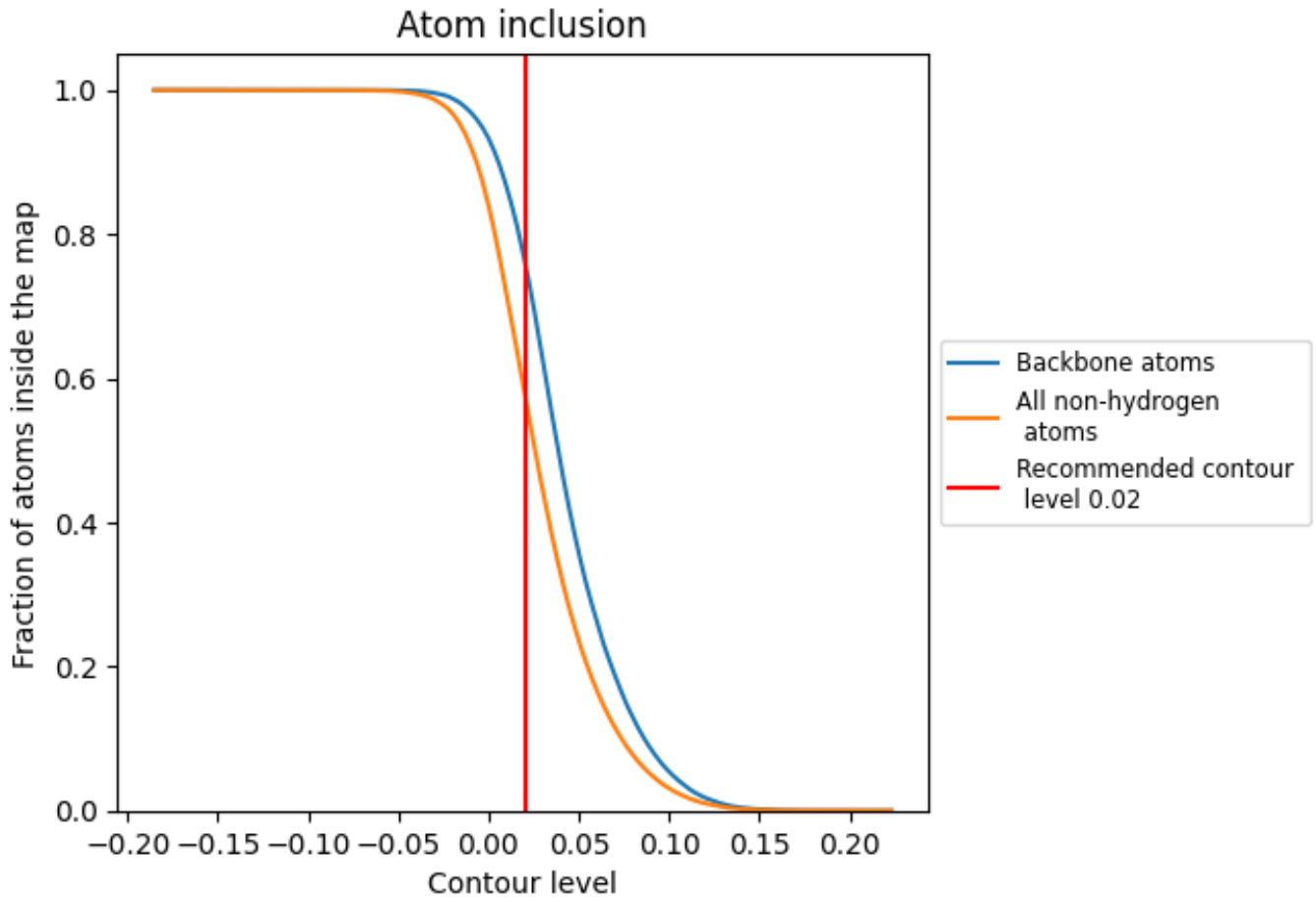
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.02).

9.4 Atom inclusion (i)



At the recommended contour level, 76% of all backbone atoms, 58% 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 (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5780	0.2040
1	0.7749	0.3320
2	0.7528	0.3300
3	0.7352	0.3300
4	0.7338	0.3070
5	0.7651	0.3140
6	0.7625	0.3240
7	0.7707	0.3240
A	0.7389	0.3050
B	0.7390	0.3200
C	0.7317	0.2950
D	0.7052	0.2880
E	0.7296	0.3120
F	0.7597	0.3260
G	0.7568	0.3100
H	0.5545	0.2050
I	0.6050	0.2220
J	0.5739	0.2010
K	0.6091	0.2080
L	0.4770	0.1500
M	0.5230	0.1880
N	0.4838	0.1380
O	0.4989	0.1400
P	0.6249	0.1740
Q	0.5863	0.1670
R	0.6086	0.1790
S	0.4385	0.1320
T	0.3997	0.0990
U	0.5504	0.1900
V	0.5841	0.2010
W	0.4052	0.1250
X	0.0385	0.0180
Y	0.3154	0.0850
Z	0.3415	0.0390
a	0.5302	0.1750

Continued on next page...

Continued from previous page...

Chain	Atom inclusion	Q-score
b	0.5134	0.1790
c	0.5409	0.1860
d	0.4877	0.1540
e	0.4957	0.1560
f	0.5526	0.1980
g	0.5536	0.1860
h	0.7062	0.2840
i	0.6973	0.2820
j	0.6787	0.2750
k	0.6893	0.2680
l	0.7035	0.2790
m	0.6934	0.2770
n	0.7201	0.3030