



Full wwPDB EM Validation Report ⓘ

Jul 12, 2022 – 10:46 pm BST

PDB ID : 7QO5
EMDB ID : EMD-14084
Title : 26S proteasome Rpt1-RK -Ubp6-UbVS complex in the si state
Authors : Hung, K.Y.S.; Klumpe, S.; Eisele, M.R.; Elsasser, S.; Geng, T.T.; Cheng, T.C.; Joshi, T.; Rudack, T.; Sakata, E.; Finley, D.
Deposited on : 2021-12-23
Resolution : 6.00 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:

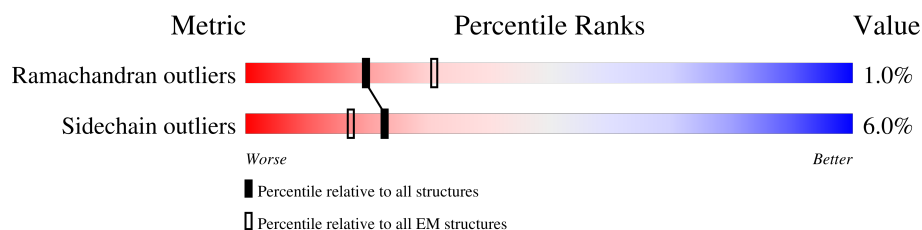
EMDB validation analysis : 0.0.1.dev8
Mogul : 1.8.4, CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.29

1 Overall quality at a glance

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

The reported resolution of this entry is 6.00 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 $\leq 5\%$. The upper red bar (where present) indicates the fraction of residues that have poor fit to the EM map (all-atom inclusion $< 40\%$). The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	252	<div> <div>11%</div> <div>80%</div> <div>12%</div> <div>• •</div> </div>
1	a	252	<div> <div>66%</div> <div>81%</div> <div>12%</div> <div>• •</div> </div>
2	B	250	<div> <div>20%</div> <div>82%</div> <div>13%</div> <div>•</div> </div>
2	b	250	<div> <div>80%</div> <div>82%</div> <div>13%</div> <div>•</div> </div>
3	C	258	<div> <div>17%</div> <div>81%</div> <div>12%</div> <div>• 5%</div> </div>
3	c	258	<div> <div>64%</div> <div>81%</div> <div>12%</div> <div>• 5%</div> </div>
4	D	254	<div> <div>9%</div> <div>86%</div> <div>• •</div> <div>7%</div> </div>
4	d	254	<div> <div>54%</div> <div>86%</div> <div>5%</div> <div>• 7%</div> </div>
5	E	260	<div> <div>13%</div> <div>74%</div> <div>18%</div> <div>• 6%</div> </div>

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
5	e	260	
6	F	234	
6	f	234	
7	G	288	
7	g	288	
8	1	215	
8	h	215	
9	2	261	
9	i	261	
10	3	205	
10	j	205	
11	4	198	
11	k	198	
12	5	287	
12	l	287	
13	6	241	
13	m	241	
14	7	266	
14	n	266	
15	W	268	
16	V	306	
17	T	274	
18	X	156	
19	Y	89	
20	Z	993	

Continued on next page...

Continued from previous page...

Mol	Chain	Length	Quality of chain
21	N	945	
22	S	523	
23	P	445	
24	Q	434	
25	R	429	
26	U	338	
27	O	393	
28	H	467	
29	I	437	
30	K	428	
31	L	437	
32	M	434	
33	J	405	
34	8	499	
35	9	128	

2 Entry composition

There are 38 unique types of molecules in this entry. The entry contains 112834 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the AltConf column contains the number of residues with at least one atom in alternate conformation and the Trace column contains the number of residues modelled with at most 2 atoms.

- Molecule 1 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		
1	A	241	Total	C	N	O	S	0	0
			1907	1214	320	365	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		
3	C	244	Total	C	N	O	S	0	0
			1904	1201	321	379	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		
4	D	236	Total	C	N	O	S	0	0
			1850	1158	323	365	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	244	Total	C	N	O	S	0	0
			1882	1176	316	383	7		
5	E	244	Total	C	N	O	S	0	0
			1882	1176	316	383	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		
7	G	242	Total	C	N	O	S	0	0
			1885	1199	328	354	4		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	i	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		
9	2	226	Total	C	N	O	S	0	0
			1719	1082	298	332	7		

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

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

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
			1561	992	264	299	6		
11	4	195	Total	C	N	O	S	0	0
			1561	992	264	299	6		

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
14	n	229	Total	C	N	O	S	0	0
			1790	1133	306	344	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
			1534	962	269	300	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
			2192	1405	349	432	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
			1032	664	169	195	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	832	Total	C	N	O	S	0	0
			6418	4078	1077	1238	25		

- 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
			3894	2488	653	738	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
			3608	2297	604	697	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
			3258	2077	535	636	10		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	U	290	Total	C	N	O	S	0	0
			2306	1454	392	453	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	391	Total	C	N	O	S	0	0
			3064	1927	551	569	17		

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	164	ARG	SER	variant	UNP P33299
H	166	LYS	THR	variant	UNP P33299

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

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

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

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

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

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

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

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

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

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

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

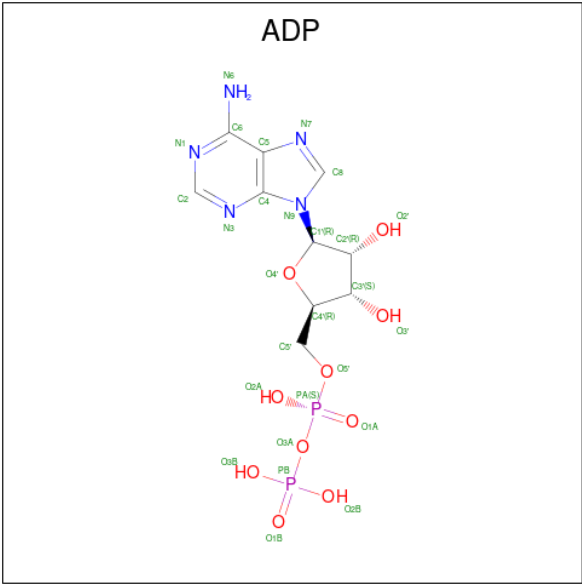
Mol	Chain	Residues	Atoms					AltConf	Trace
34	8	372	Total	C	N	O	S	0	0
			3034	1918	521	583	12		

- Molecule 35 is a protein called Ubiquitin vinyl sulfone.

Mol	Chain	Residues	Atoms					AltConf	Trace
35	9	76	Total	C	N	O	S	0	0
			601	378	105	117	1		

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).

C₁₀H₁₅N₅O₁₀P₂).

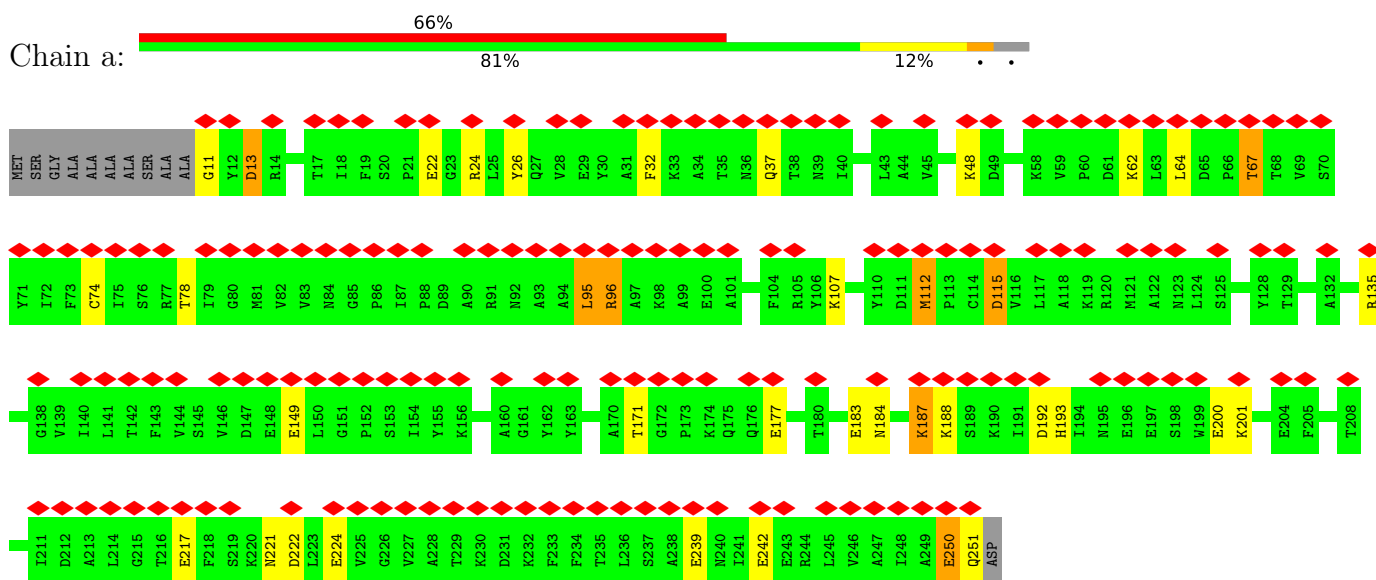


Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
38	J	1	27	10	5	10	2	0

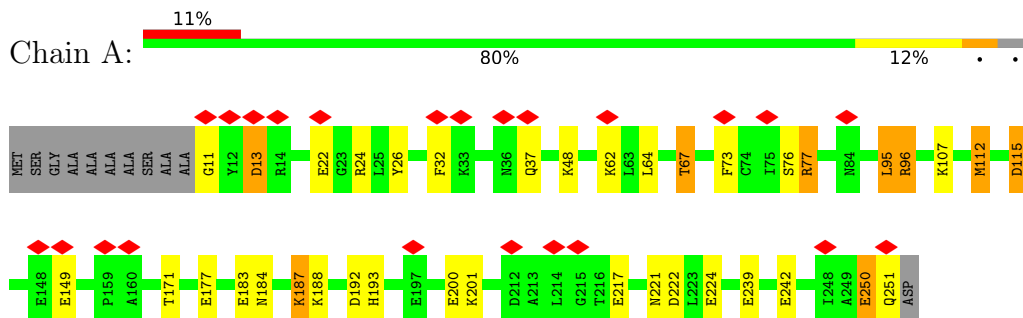
3 Residue-property plots

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

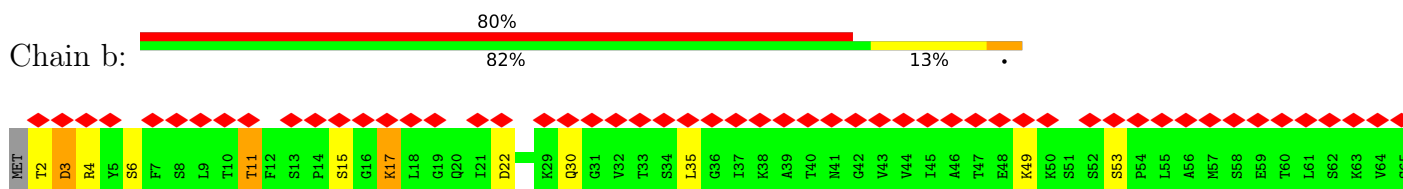
• Molecule 1: Proteasome subunit alpha type-1

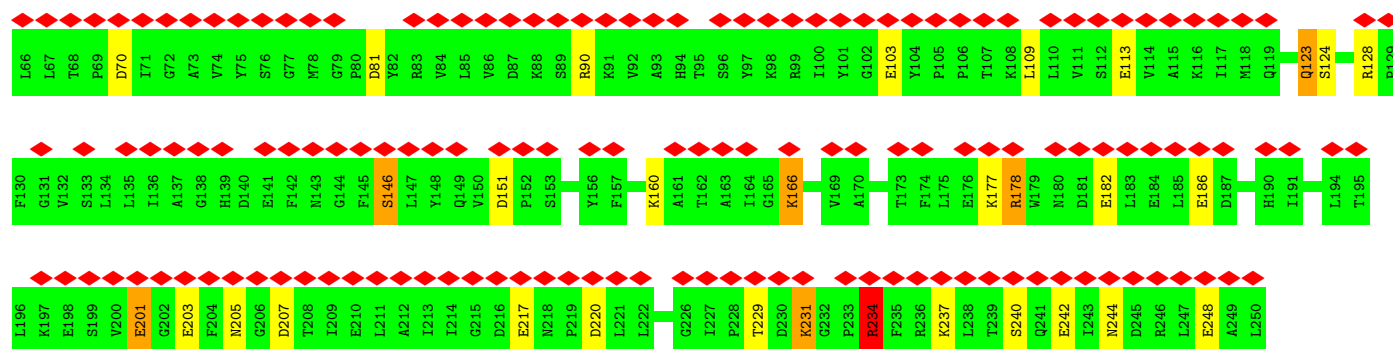


• Molecule 1: Proteasome subunit alpha type-1

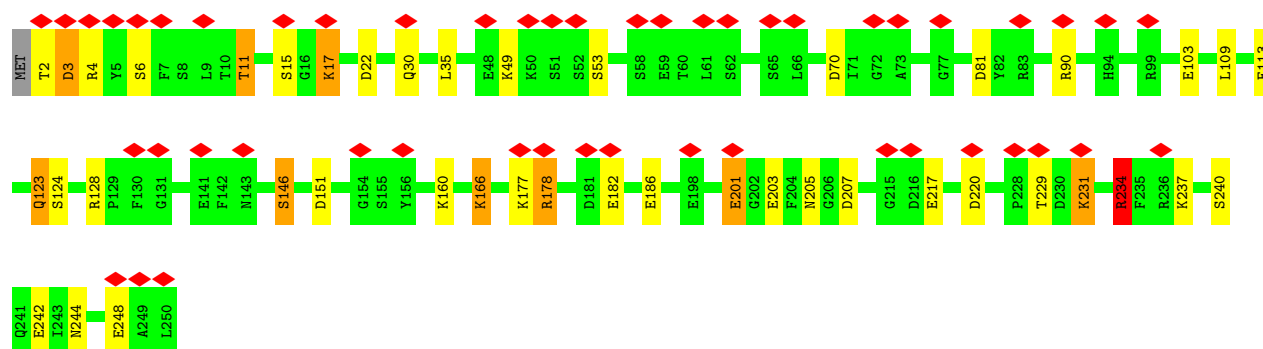
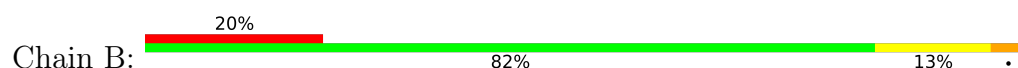


• Molecule 2: Proteasome subunit alpha type-2

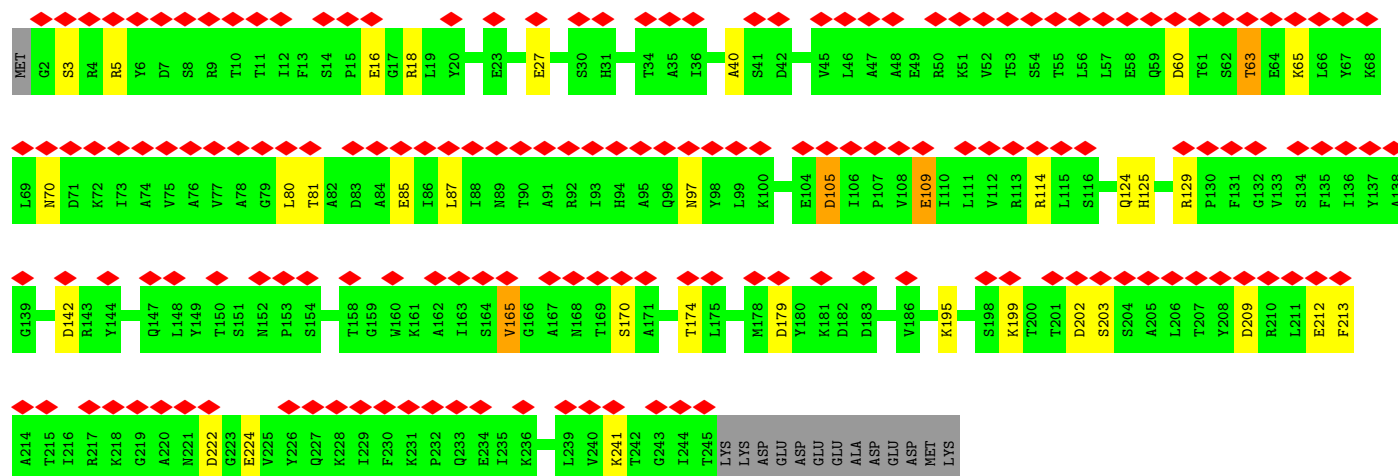
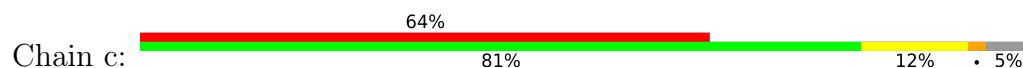




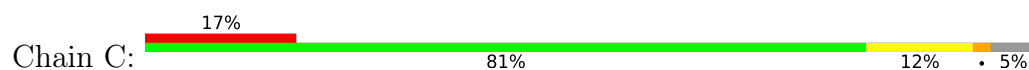
• Molecule 2: Proteasome subunit alpha type-2

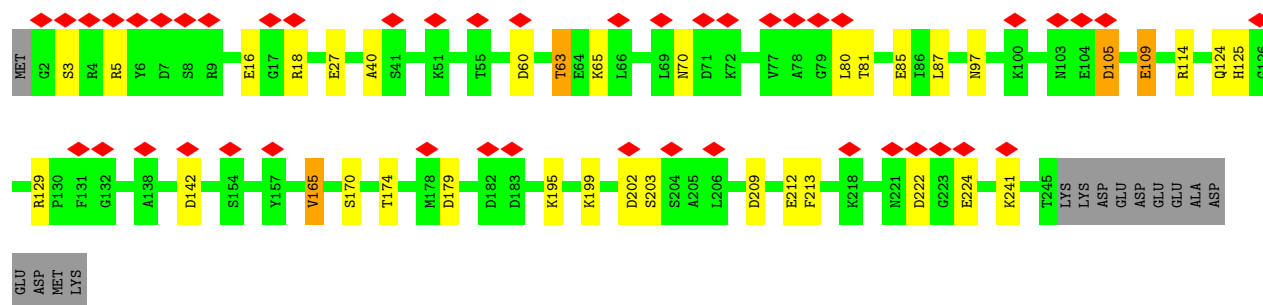


• Molecule 3: Proteasome subunit alpha type-3

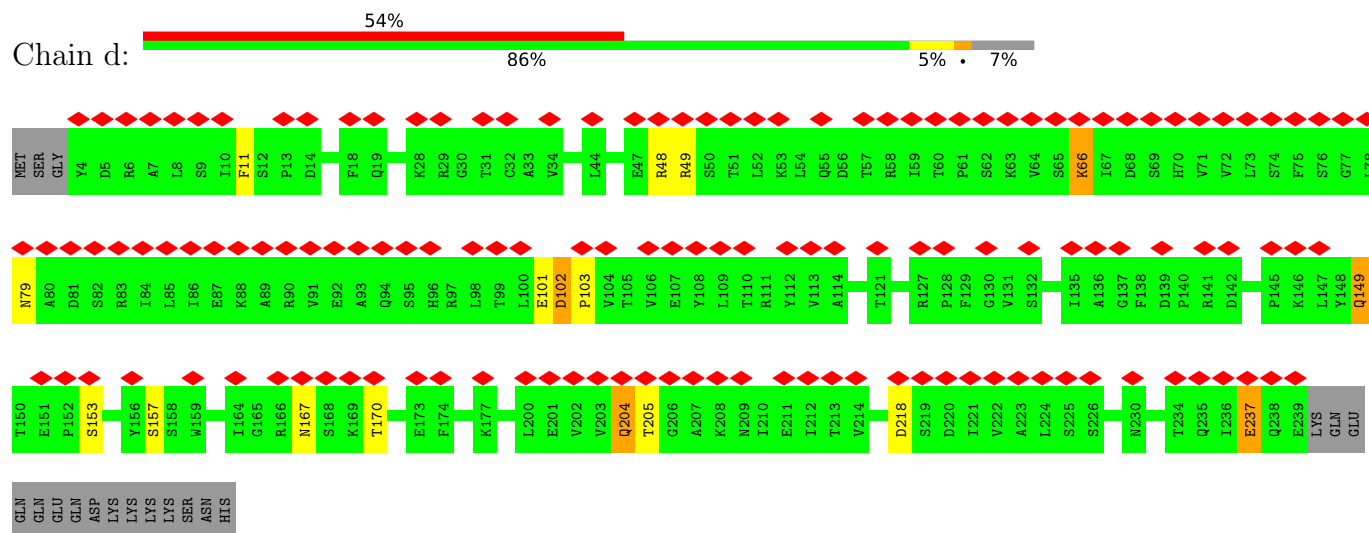


• Molecule 3: Proteasome subunit alpha type-3

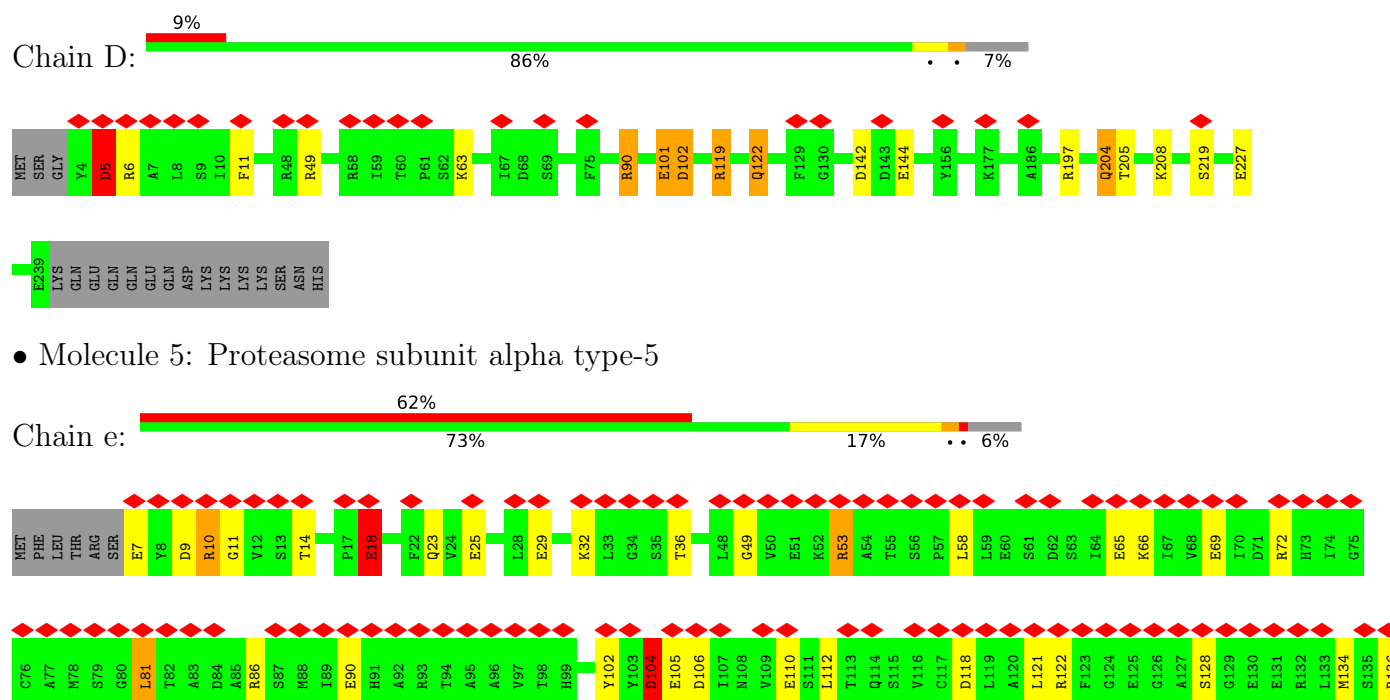




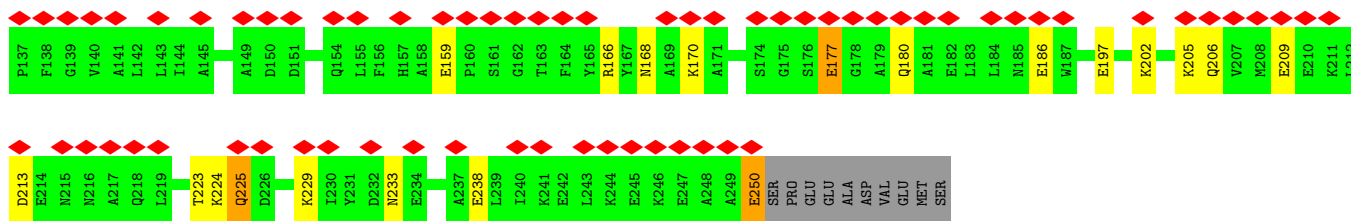
• Molecule 4: Proteasome subunit alpha type-4



• Molecule 4: Proteasome subunit alpha type-4

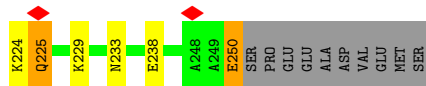
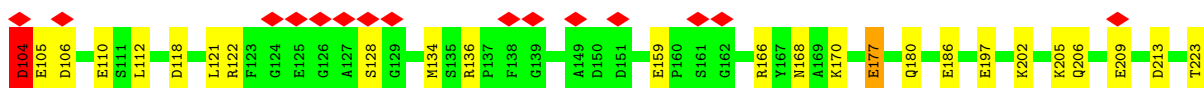


• Molecule 5: Proteasome subunit alpha type-5



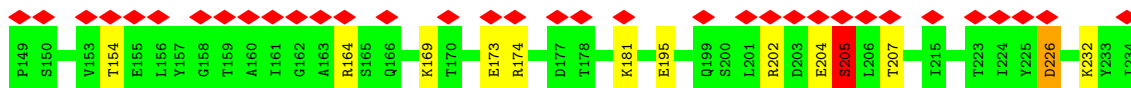
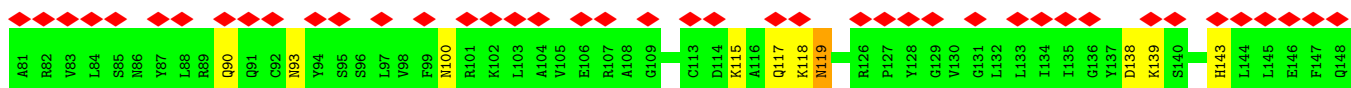
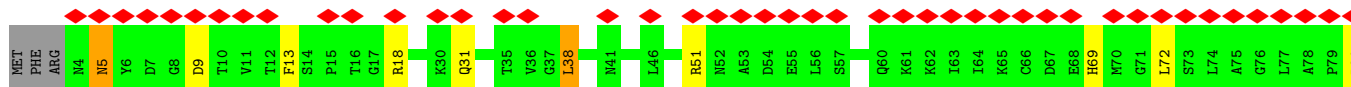
• Molecule 5: Proteasome subunit alpha type-5

Chain E: 13% 74% 18% 6%



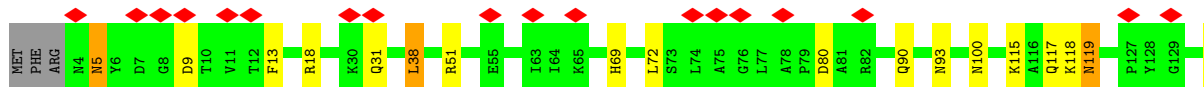
• Molecule 6: Proteasome subunit alpha type-6

Chain f: 52% 85% 12% 2%



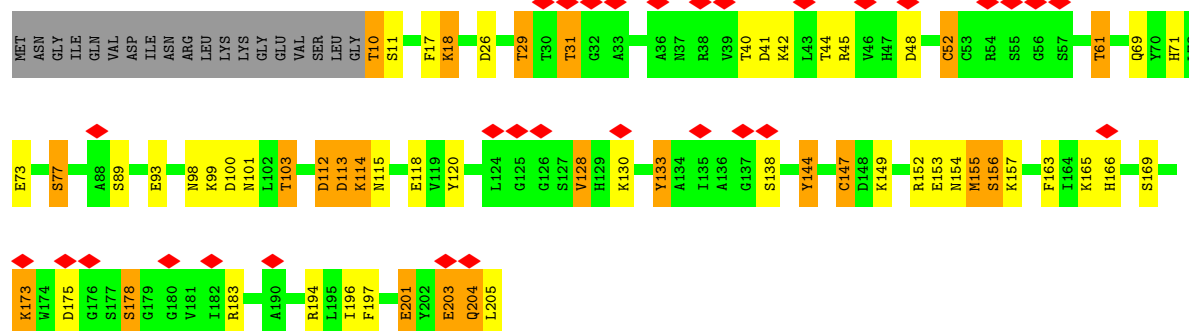
• Molecule 6: Proteasome subunit alpha type-6

Chain F: 11% 85% 12% 2%

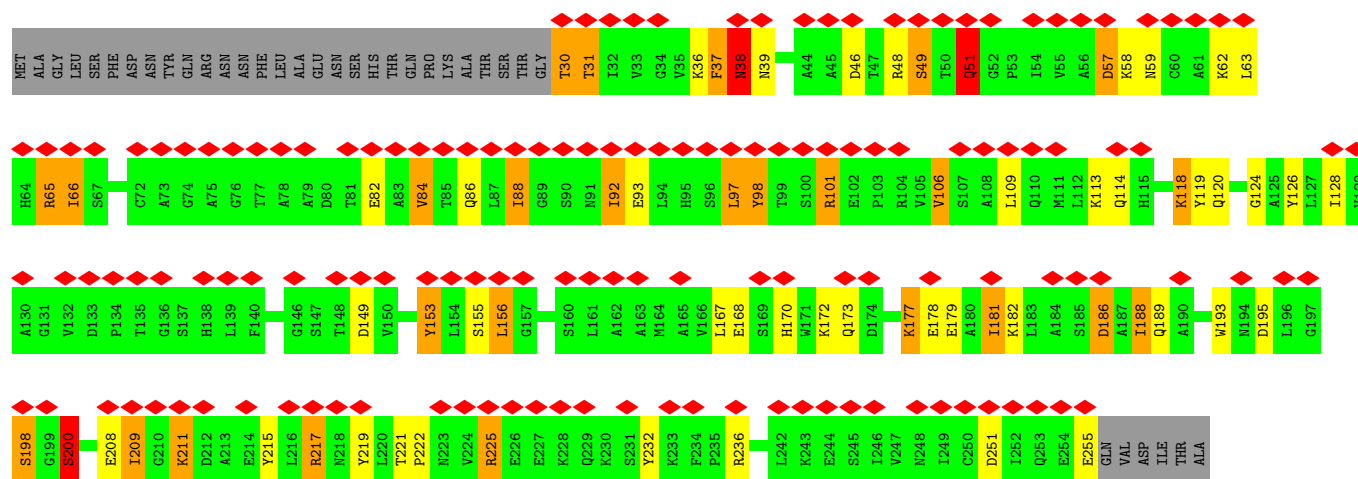


• Molecule 7: Probable proteasome subunit alpha type-7

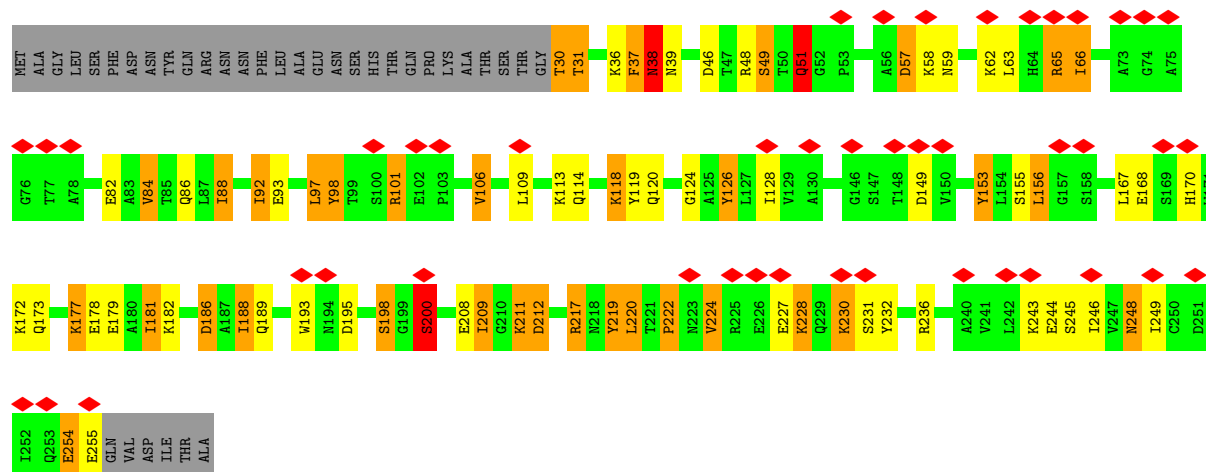




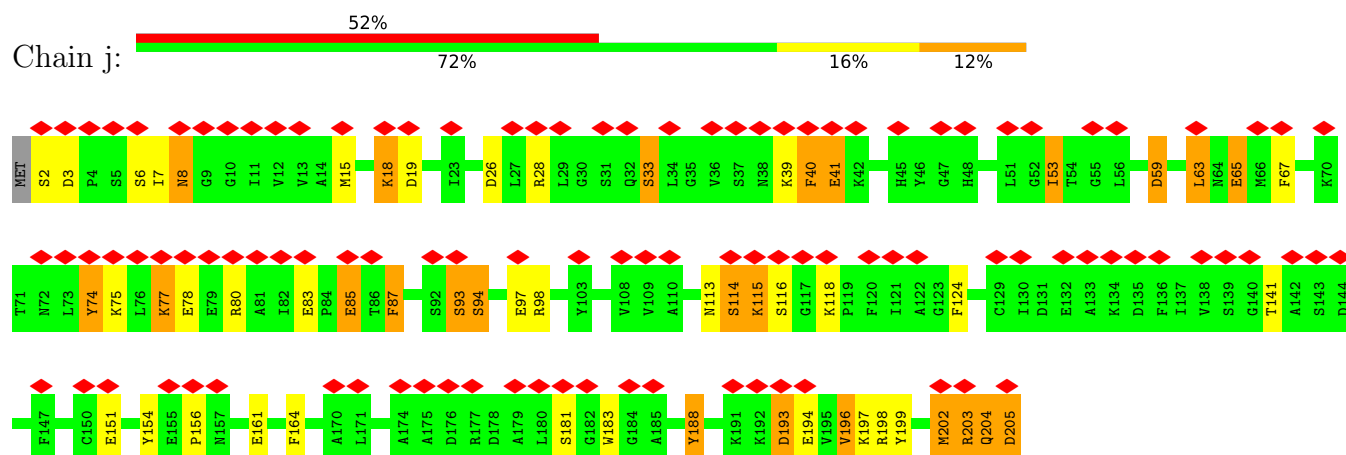
• Molecule 9: Proteasome subunit beta type-2



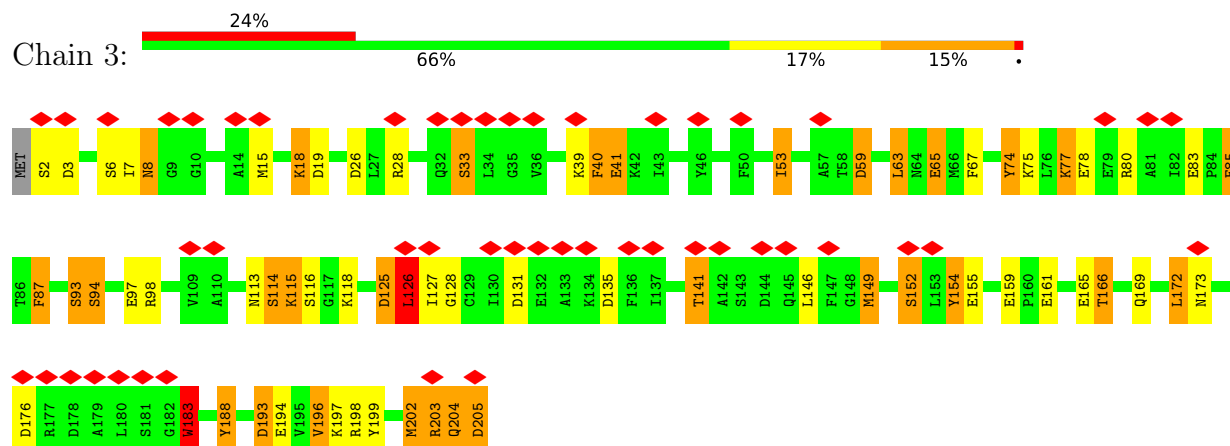
• Molecule 9: Proteasome subunit beta type-2



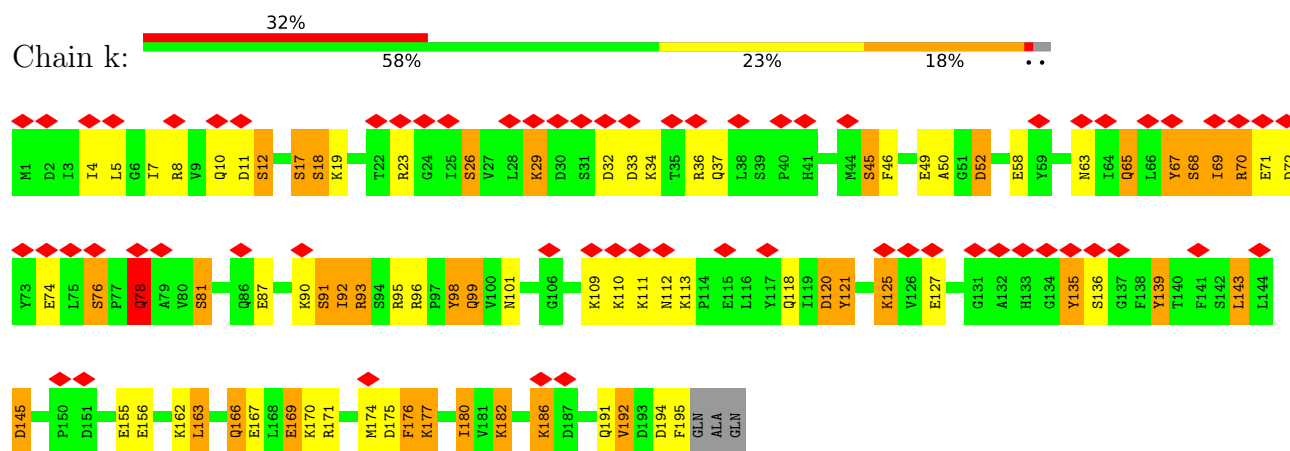
- Molecule 10: Proteasome subunit beta type-3



- Molecule 10: Proteasome subunit beta type-3

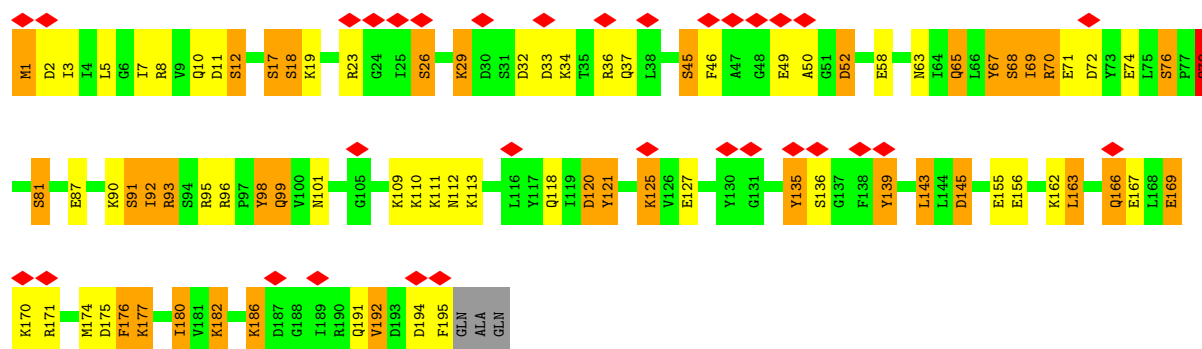


- Molecule 11: Proteasome subunit beta type-4

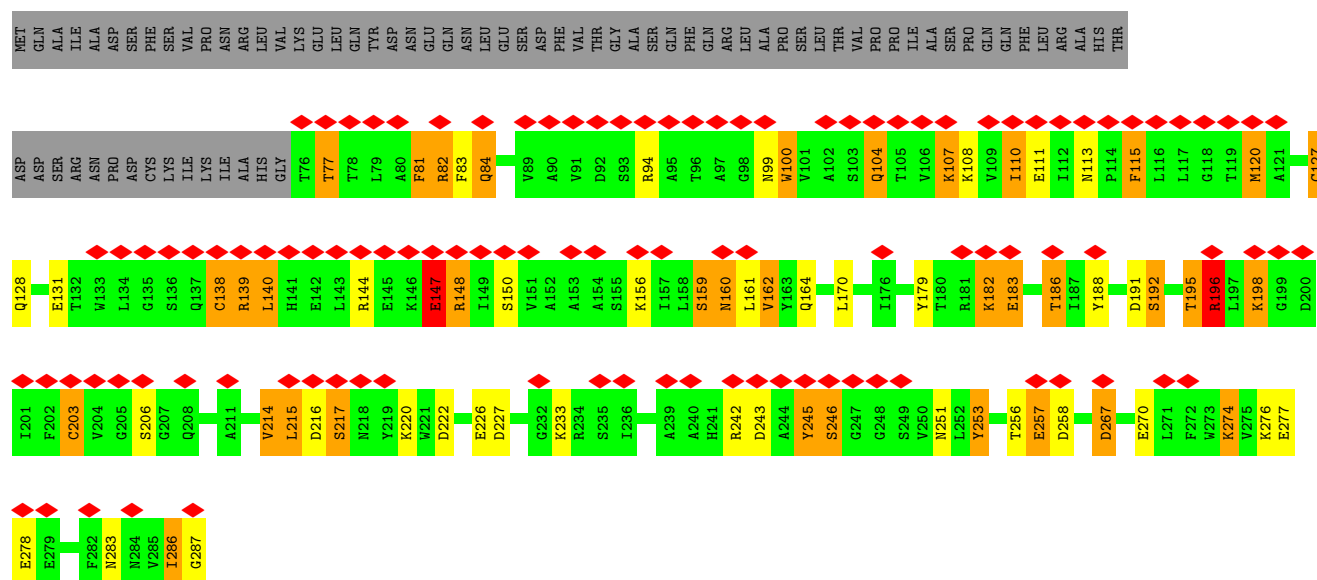


- Molecule 11: Proteasome subunit beta type-4

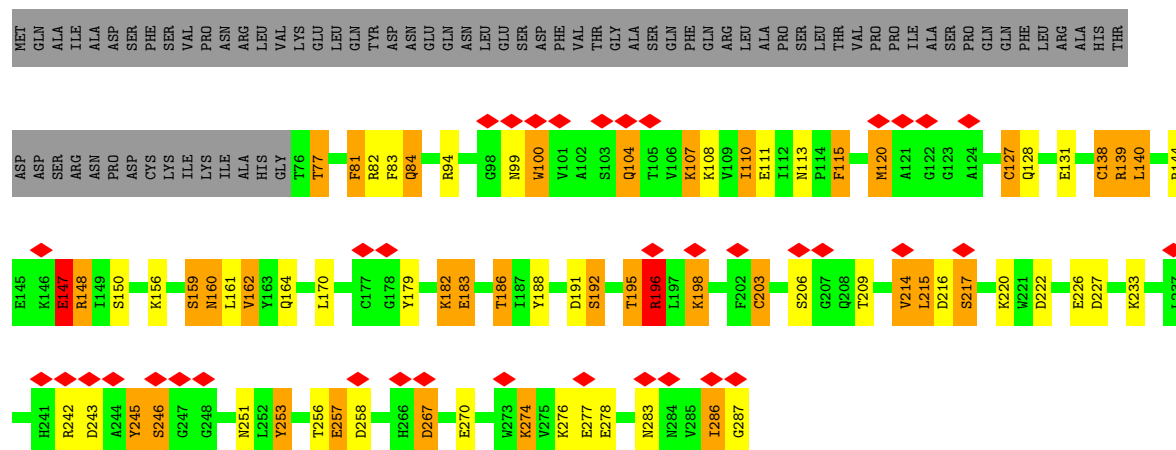




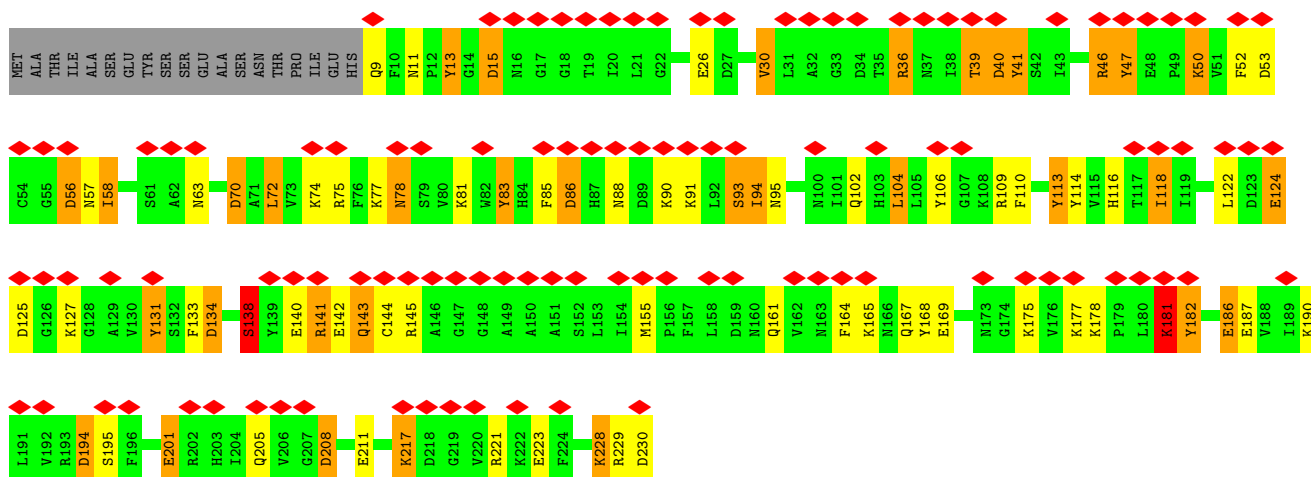
• Molecule 12: Proteasome subunit beta type-5



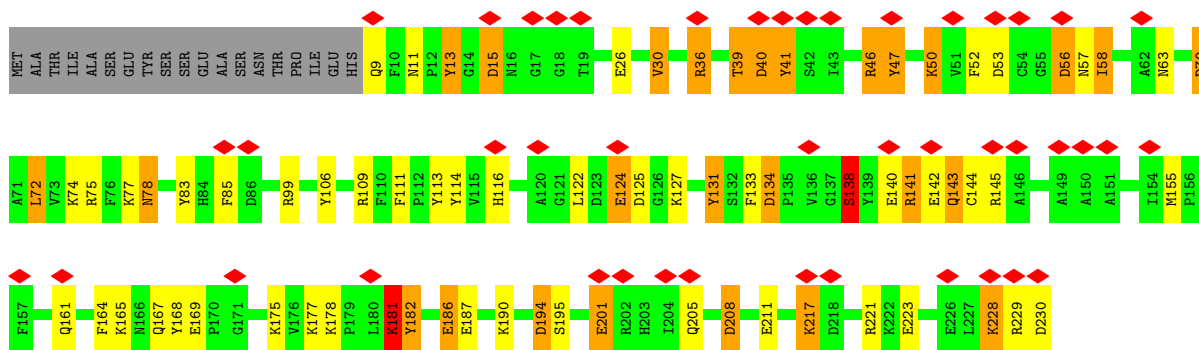
• Molecule 12: Proteasome subunit beta type-5



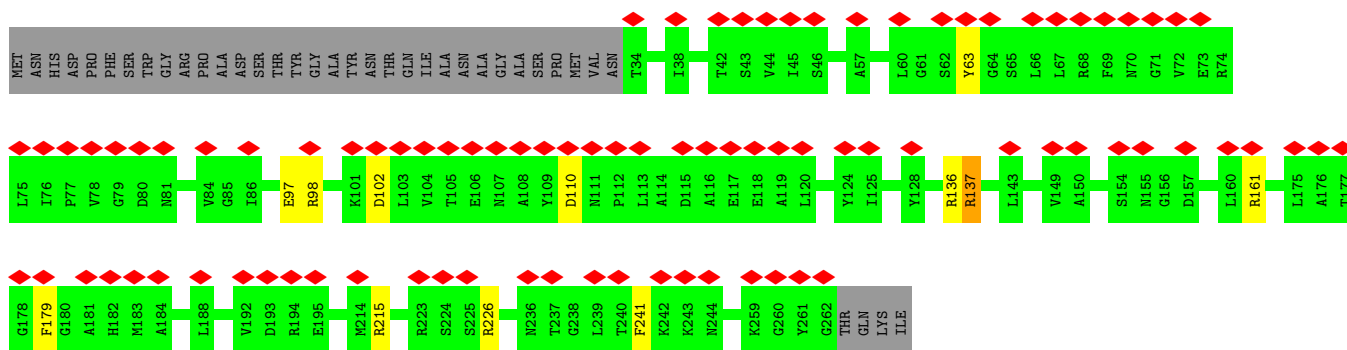
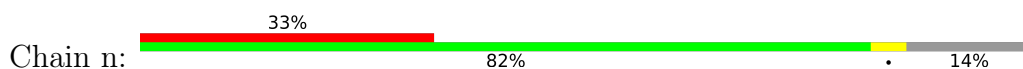
• Molecule 13: Proteasome subunit beta type-6



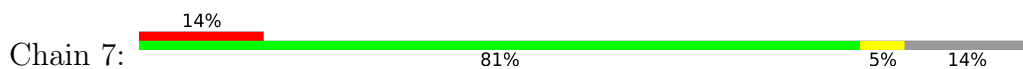
• Molecule 13: Proteasome subunit beta type-6

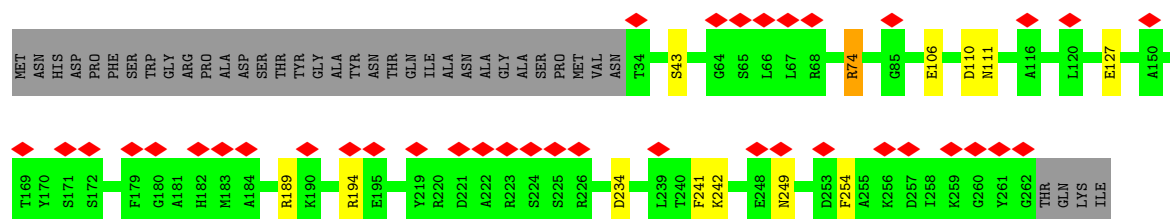


• Molecule 14: Proteasome subunit beta type-7



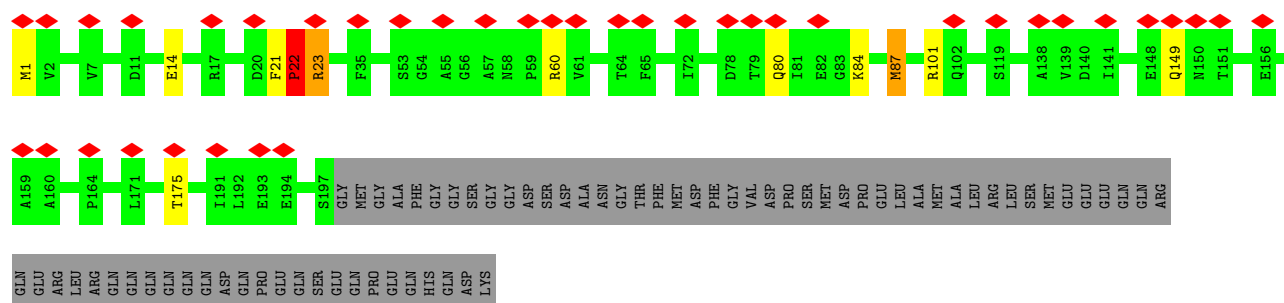
• Molecule 14: Proteasome subunit beta type-7





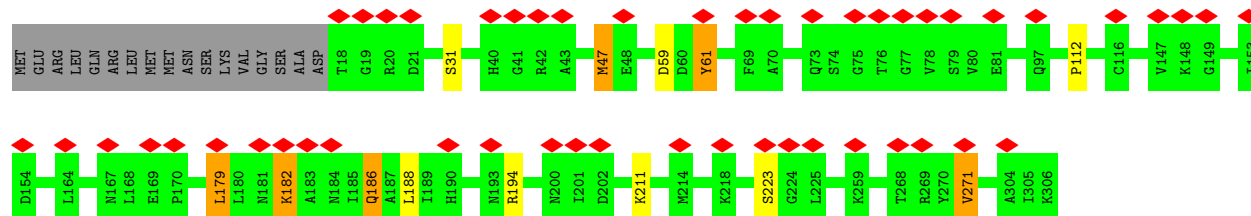
- Molecule 15: 26S proteasome regulatory subunit RPN10

Chain W:



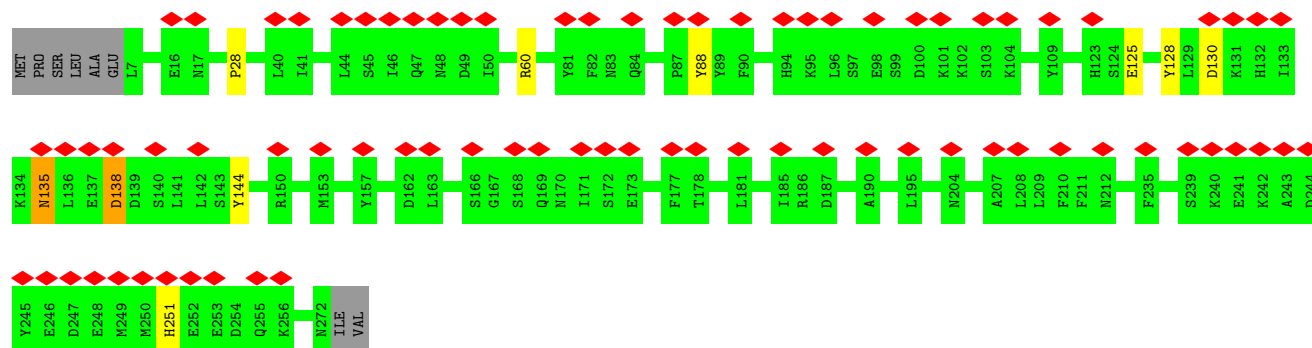
- Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:



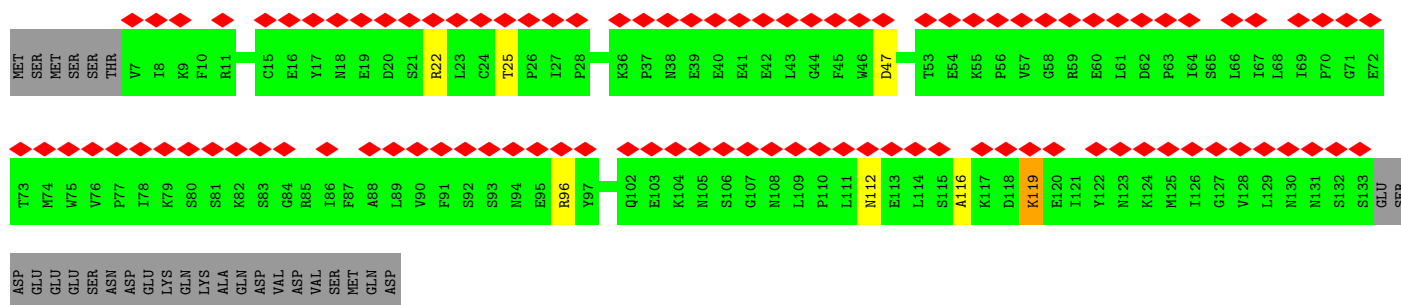
- Molecule 17: 26S proteasome regulatory subunit RPN12

Chain T:

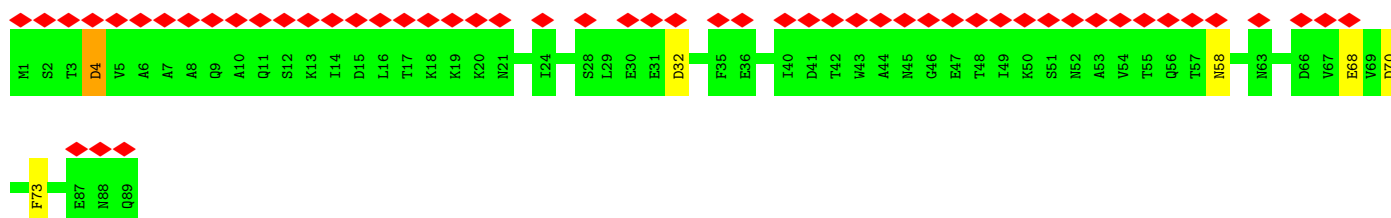
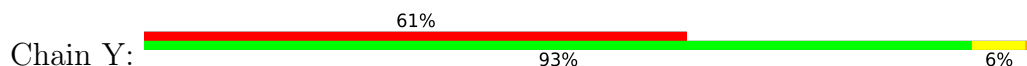


- Molecule 18: 26S proteasome regulatory subunit RPN13

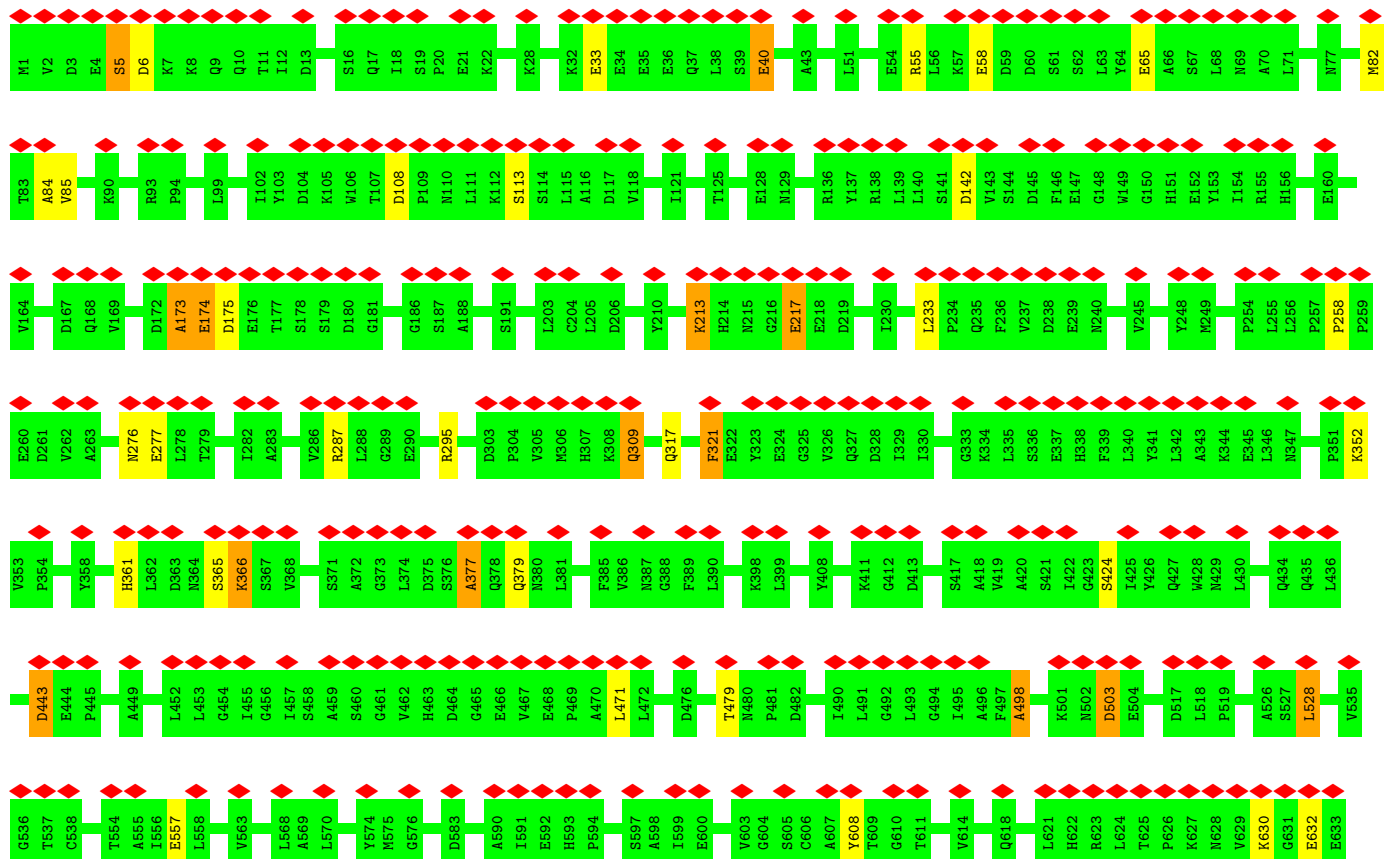
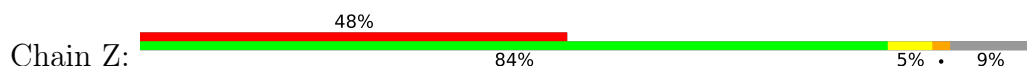
Chain X:



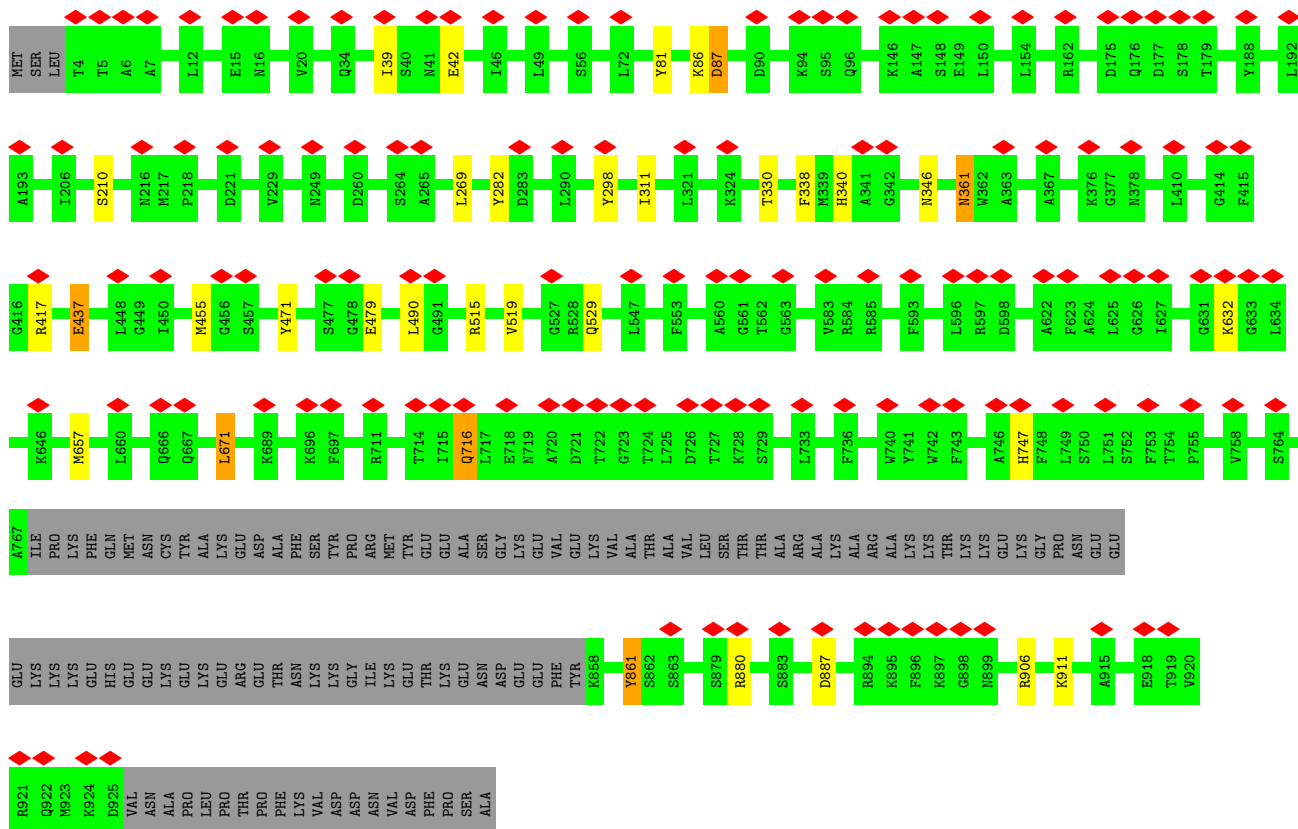
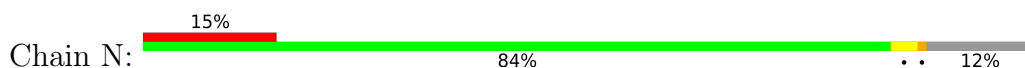
• Molecule 19: 26S proteasome complex subunit SEM1



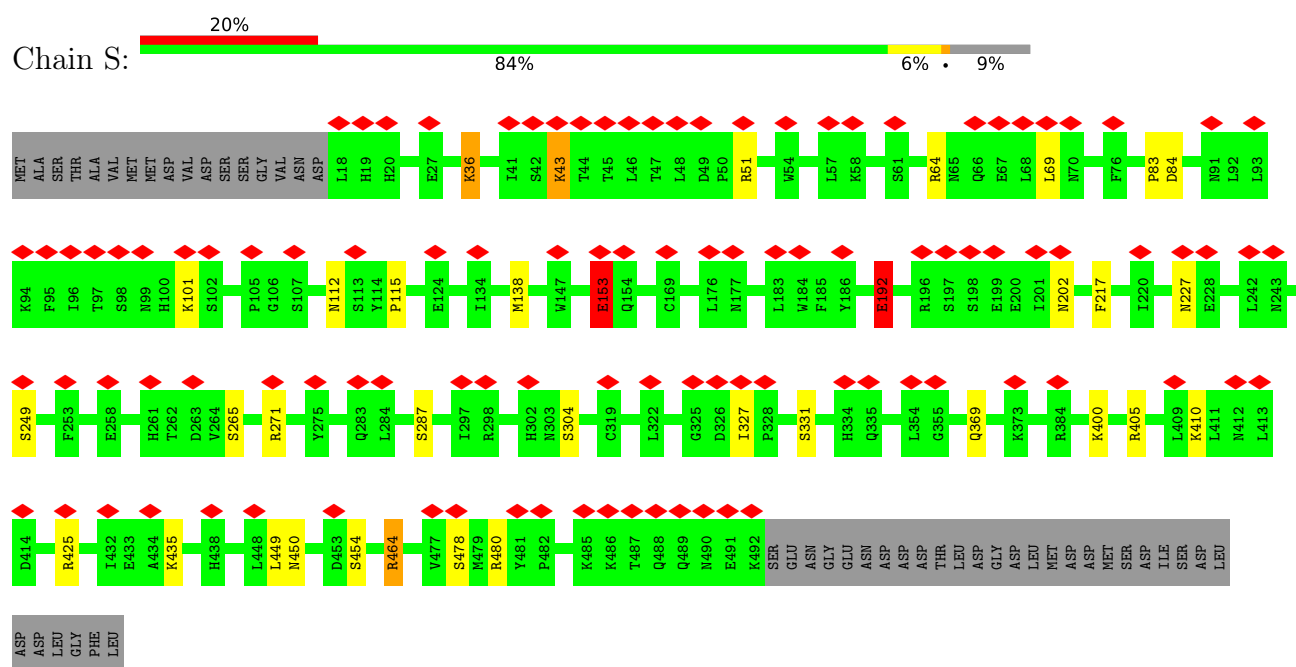
• Molecule 20: 26S proteasome regulatory subunit RPN1



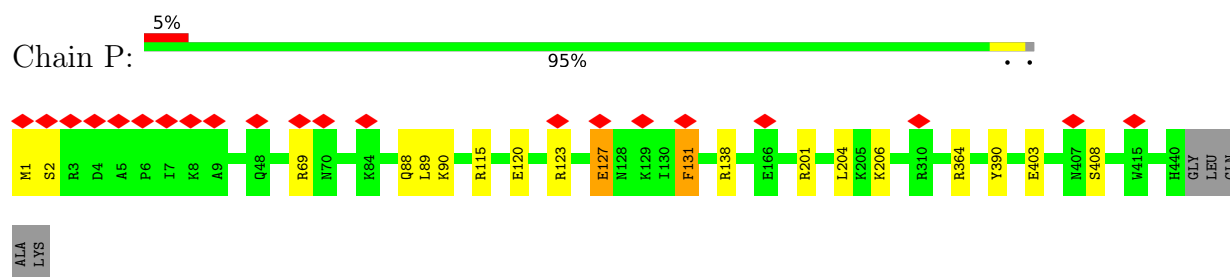
- Molecule 21: 26S proteasome regulatory subunit RPN2



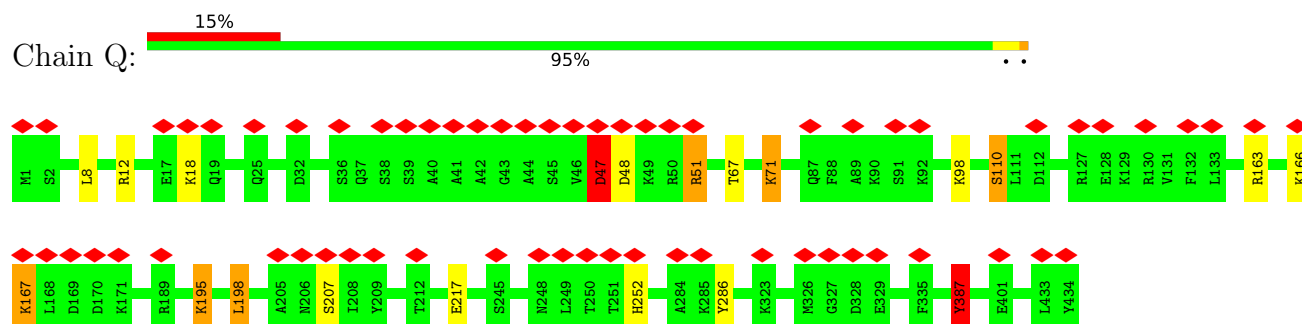
- Molecule 22: 26S proteasome regulatory subunit RPN3



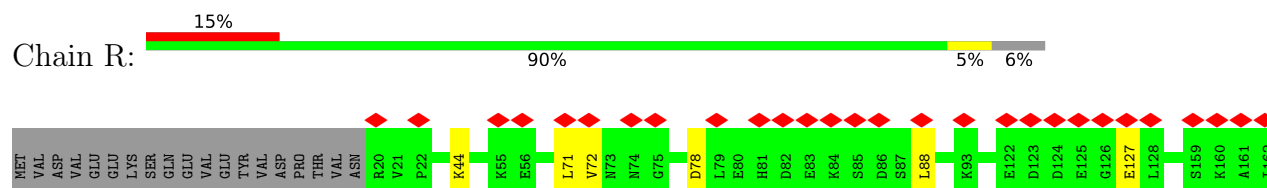
- Molecule 23: 26S proteasome regulatory subunit RPN5

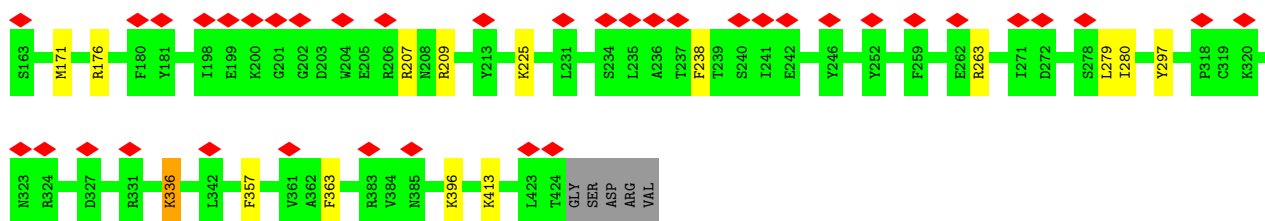


- Molecule 24: 26S proteasome regulatory subunit RPN6

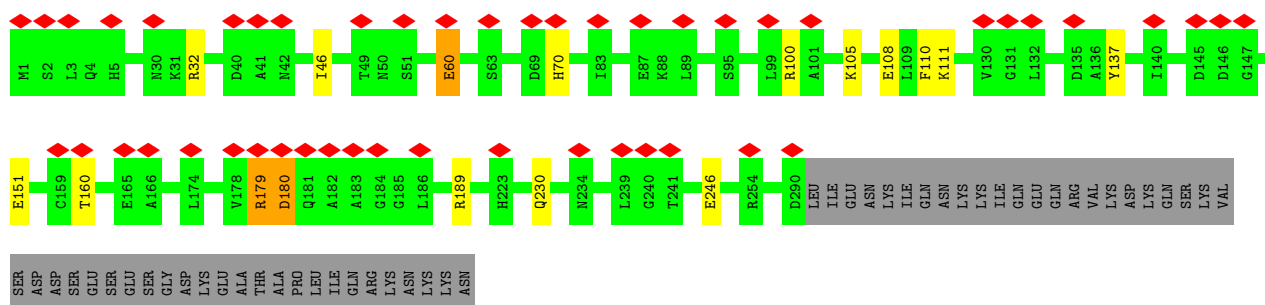
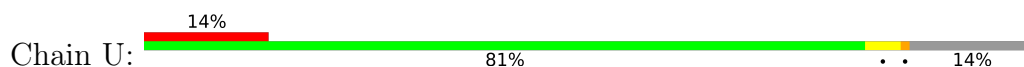


- Molecule 25: 26S proteasome regulatory subunit RPN7

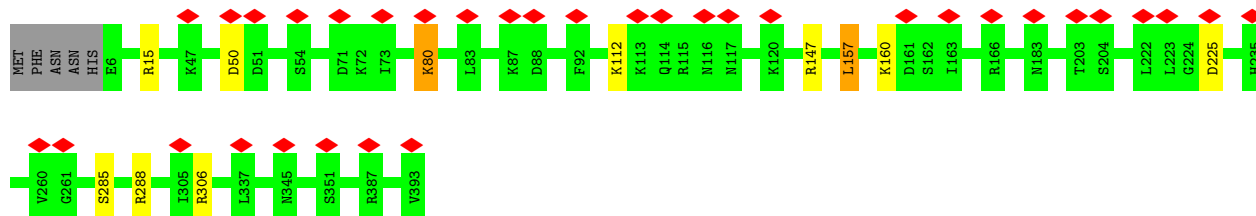




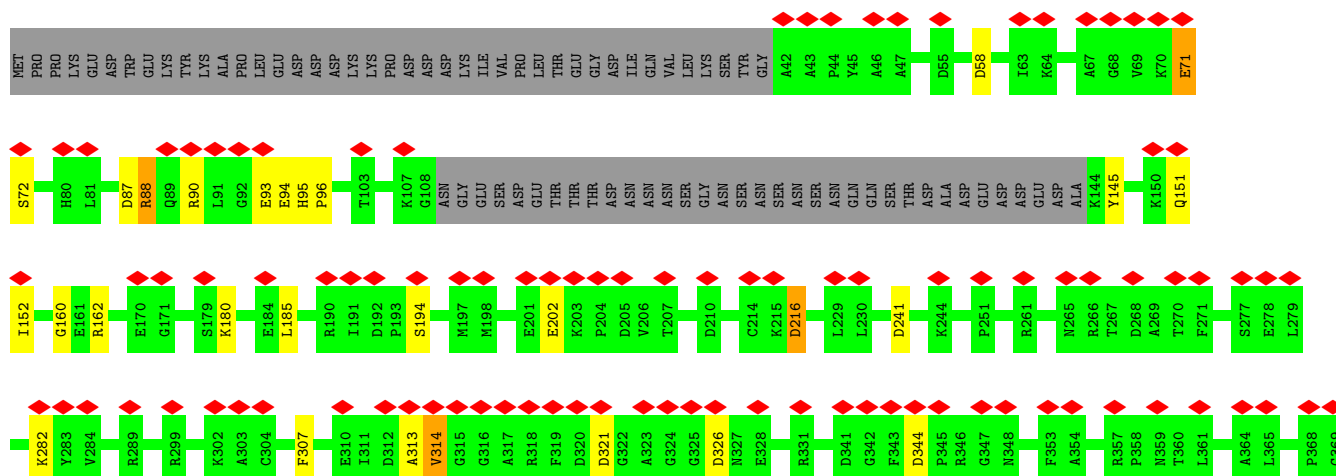
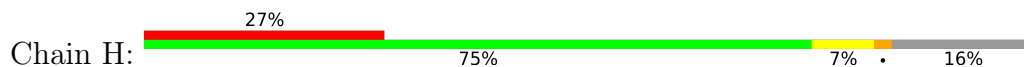
- Molecule 26: 26S proteasome regulatory subunit RPN8

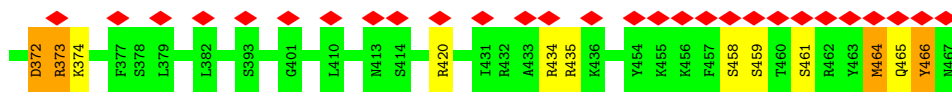


- Molecule 27: 26S proteasome regulatory subunit RPN9



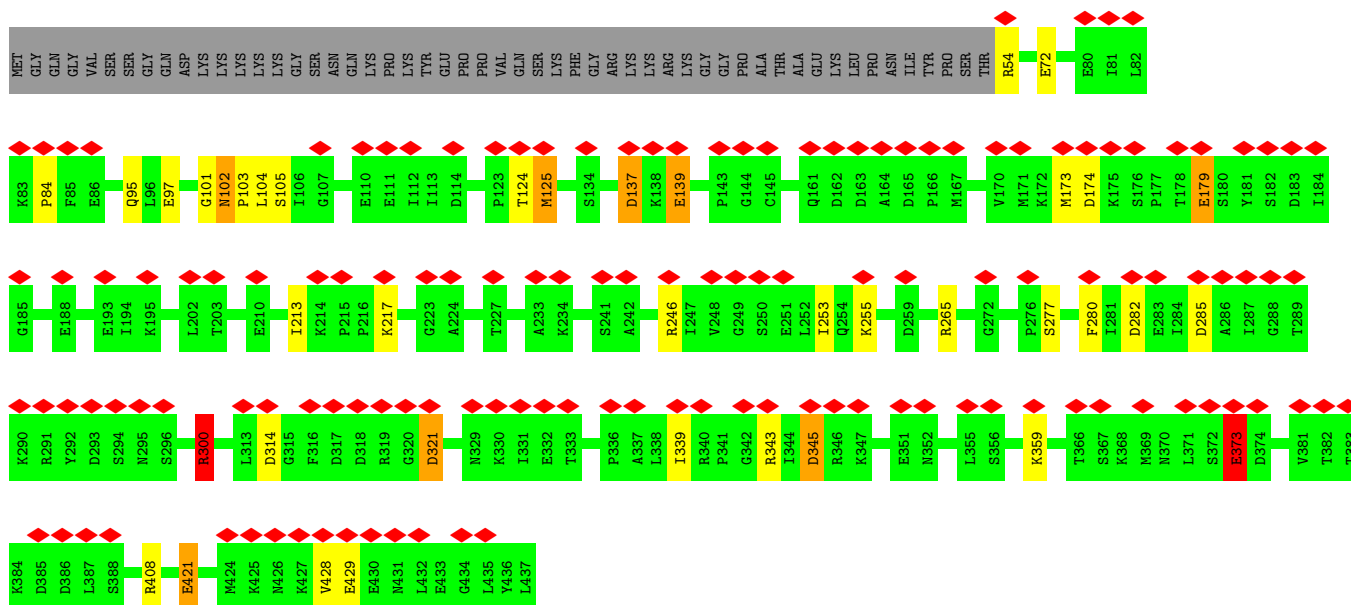
- Molecule 28: 26S proteasome regulatory subunit 7 homolog





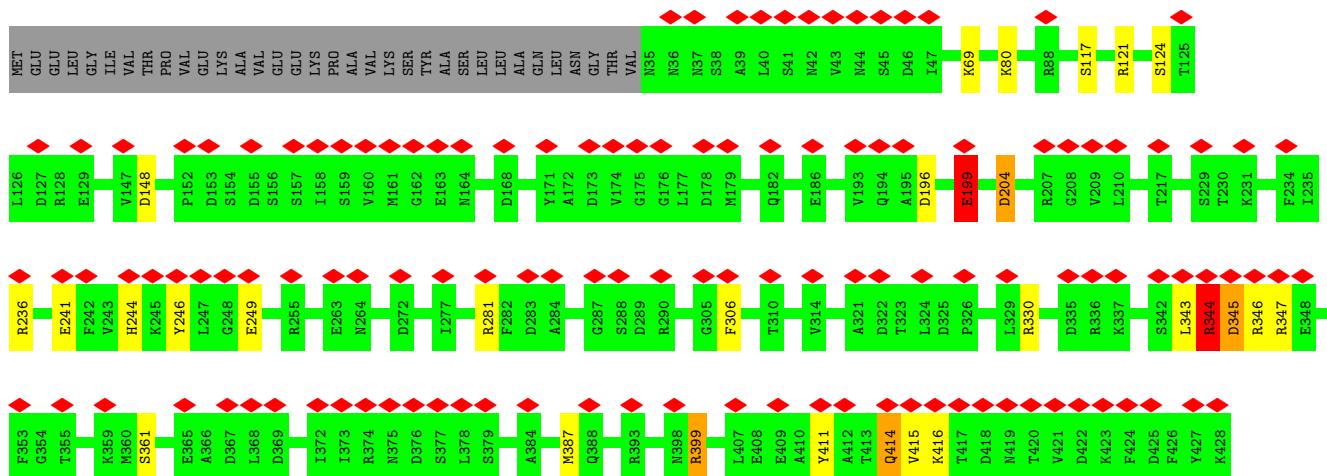
- Molecule 29: 26S proteasome regulatory subunit 4 homolog

Chain I: 31% 79% 7% 12%



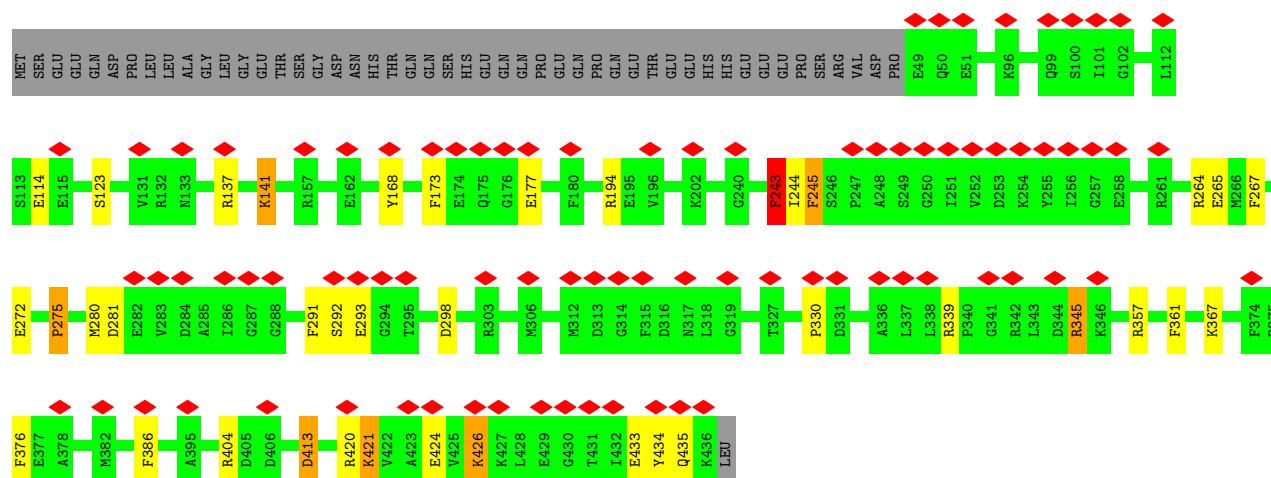
- Molecule 30: 26S proteasome regulatory subunit 6B homolog

Chain K: 29% 85% 5% 8%



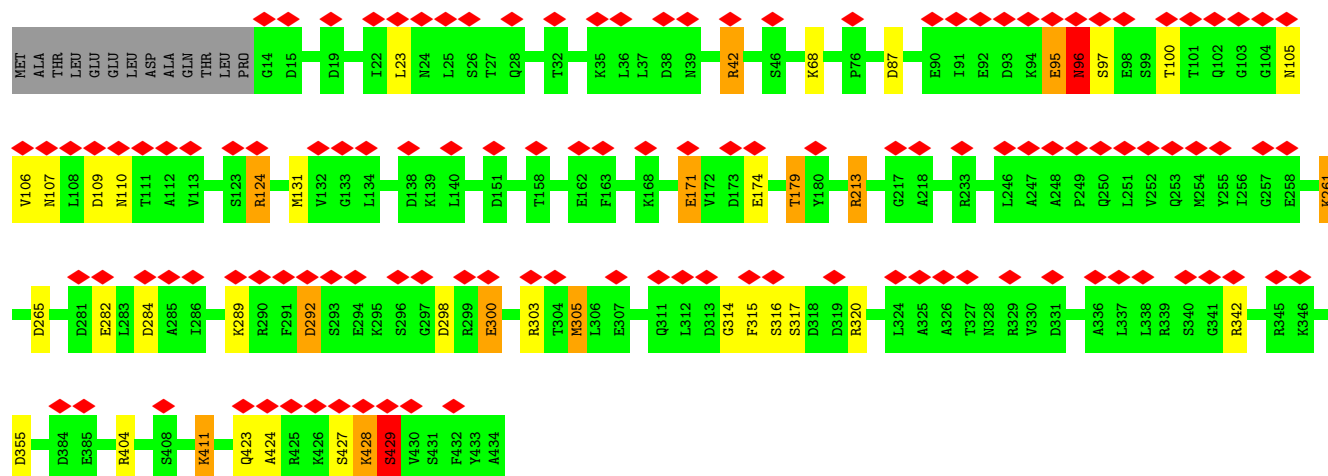
- Molecule 31: 26S proteasome subunit RPT4

Chain L: 19% 80% 7% 11%



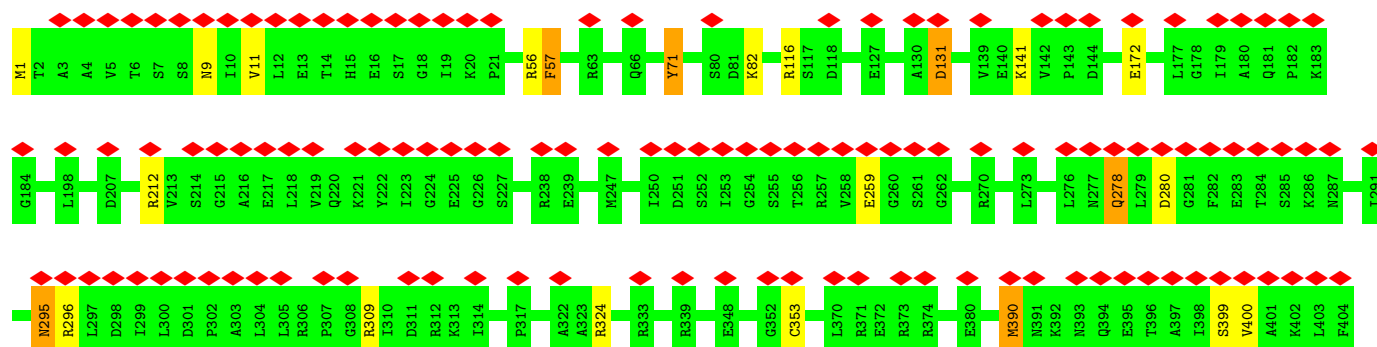
• Molecule 32: 26S proteasome regulatory subunit 6A

Chain M: 28% 87% 7%



• Molecule 33: 26S proteasome regulatory subunit 8 homolog

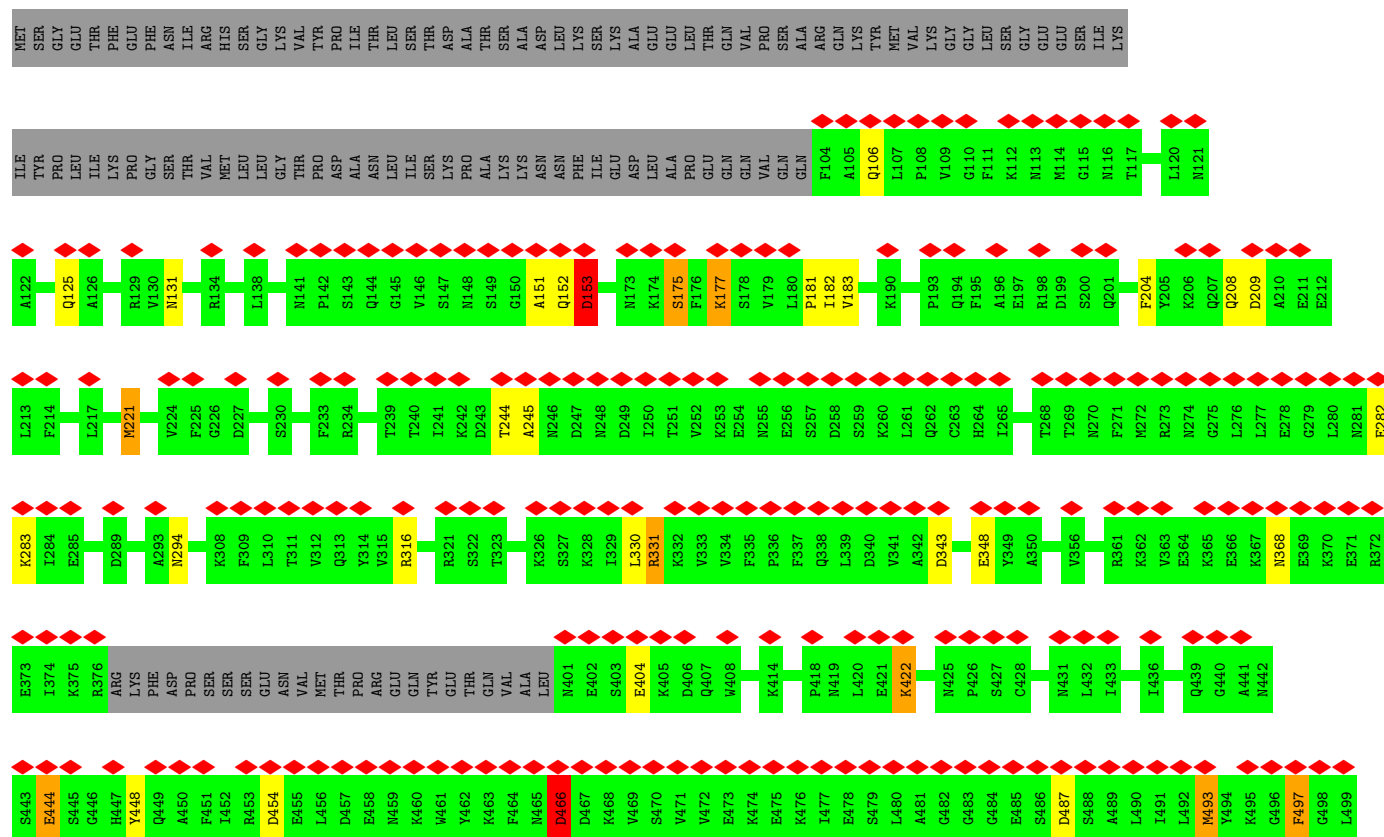
Chain J: 32% 94% 7%




◆
K405

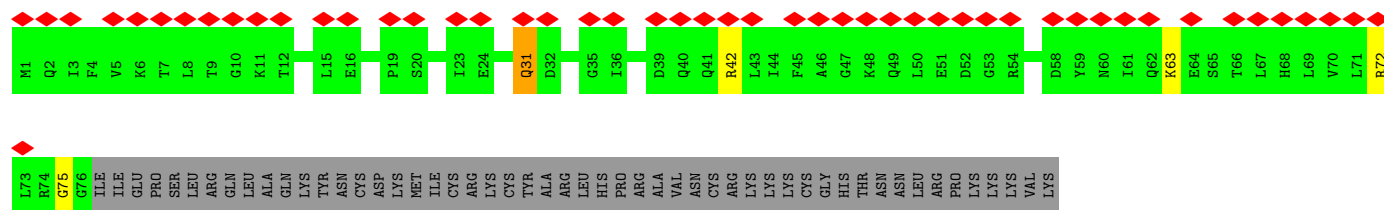
• Molecule 34: Ubiquitin carboxyl-terminal hydrolase 6

Chain 8: 



• Molecule 35: Ubiquitin vinyl sulfone

Chain 9: 



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	64766	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 ($e^-/\text{\AA}^2$)	35	Depositor
Minimum defocus (nm)	1800	Depositor
Maximum defocus (nm)	3000	Depositor
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	25.895	Depositor
Minimum map value	-17.249	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.920	Depositor
Recommended contour level	4.8	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 ⓘ

5.1 Standard geometry ⓘ

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

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	1.61	51/1945 (2.6%)	1.60	41/2634 (1.6%)
1	a	1.60	52/1945 (2.7%)	1.57	36/2634 (1.4%)
2	B	1.57	40/1944 (2.1%)	1.55	38/2632 (1.4%)
2	b	1.57	40/1944 (2.1%)	1.55	38/2632 (1.4%)
3	C	1.45	35/1934 (1.8%)	1.59	42/2618 (1.6%)
3	c	1.45	34/1934 (1.8%)	1.59	42/2618 (1.6%)
4	D	0.63	1/1879 (0.1%)	1.07	10/2546 (0.4%)
4	d	0.65	1/1879 (0.1%)	1.01	4/2546 (0.2%)
5	E	1.67	50/1908 (2.6%)	1.76	51/2571 (2.0%)
5	e	1.79	57/1908 (3.0%)	1.68	57/2571 (2.2%)
6	F	1.16	18/1800 (1.0%)	1.23	24/2433 (1.0%)
6	f	1.16	18/1800 (1.0%)	1.23	24/2433 (1.0%)
7	G	1.35	14/1925 (0.7%)	1.48	31/2599 (1.2%)
7	g	1.50	34/1925 (1.8%)	1.40	34/2599 (1.3%)
8	1	2.97	92/1541 (6.0%)	2.44	80/2087 (3.8%)
8	h	2.84	78/1541 (5.1%)	2.42	82/2087 (3.9%)
9	2	3.77	132/1750 (7.5%)	3.04	125/2373 (5.3%)
9	i	3.28	101/1750 (5.8%)	2.83	100/2373 (4.2%)
10	3	3.58	113/1611 (7.0%)	2.51	113/2174 (5.2%)
10	j	3.12	86/1611 (5.3%)	2.44	93/2174 (4.3%)
11	4	4.18	154/1589 (9.7%)	2.88	121/2142 (5.6%)
11	k	4.18	153/1589 (9.6%)	2.88	121/2142 (5.6%)
12	5	3.47	108/1681 (6.4%)	2.48	106/2274 (4.7%)
12	l	3.47	109/1681 (6.5%)	2.48	106/2274 (4.7%)
13	6	3.87	140/1795 (7.8%)	2.80	139/2420 (5.7%)
13	m	4.15	164/1795 (9.1%)	2.83	150/2420 (6.2%)
14	7	0.58	0/1821	1.03	6/2470 (0.2%)
14	n	0.67	2/1821 (0.1%)	1.08	11/2470 (0.4%)
15	W	0.68	0/1557	1.21	12/2111 (0.6%)
16	V	0.60	0/2309	1.09	12/3115 (0.4%)
17	T	0.64	2/2235 (0.1%)	1.08	6/3017 (0.2%)
18	X	0.61	0/1058	1.10	4/1432 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
19	Y	0.58	0/741	1.00	2/1000 (0.2%)
20	Z	0.62	7/7122 (0.1%)	1.10	44/9645 (0.5%)
21	N	0.61	2/6521 (0.0%)	0.96	22/8824 (0.2%)
22	S	0.59	1/3966 (0.0%)	1.09	20/5355 (0.4%)
23	P	0.59	0/3663	0.95	12/4940 (0.2%)
24	Q	0.59	0/3556	1.08	15/4787 (0.3%)
25	R	0.64	1/3313 (0.0%)	1.10	20/4469 (0.4%)
26	U	0.64	1/2340 (0.0%)	1.08	14/3168 (0.4%)
27	O	0.57	0/3247	0.97	12/4380 (0.3%)
28	H	0.64	1/3113 (0.0%)	1.12	18/4187 (0.4%)
29	I	0.69	3/3054 (0.1%)	1.34	27/4111 (0.7%)
30	K	0.66	2/3156 (0.1%)	1.16	24/4261 (0.6%)
31	L	0.68	3/3128 (0.1%)	1.33	33/4204 (0.8%)
32	M	0.70	3/3323 (0.1%)	1.35	28/4478 (0.6%)
33	J	0.61	0/3212	1.08	13/4316 (0.3%)
34	8	0.69	0/3089	1.16	21/4144 (0.5%)
35	9	0.55	0/603	1.12	5/811 (0.6%)
All	All	1.72	1903/114552 (1.7%)	1.58	2189/154701 (1.4%)

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

Continued on next page...

Continued from previous page...

Mol	Chain	#Chirality outliers	#Planarity outliers
9	i	0	7
10	3	0	2
10	j	0	1
11	4	0	1
11	k	0	1
12	5	0	3
12	l	0	3
13	6	0	5
13	m	0	8
14	7	0	2
15	W	0	4
16	V	0	1
17	T	0	3
19	Y	0	3
20	Z	0	22
21	N	0	5
22	S	0	5
23	P	0	2
24	Q	0	6
25	R	0	2
26	U	0	5
27	O	0	2
28	H	0	9
29	I	0	15
30	K	0	7
31	L	0	10
32	M	0	20
33	J	0	7
34	8	0	15
35	9	0	1
All	All	0	230

All (1903) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	153	TYR	CD1-CE1	-33.59	0.89	1.39
9	i	153	TYR	CD1-CE1	-33.55	0.89	1.39
11	k	67	TYR	CE1-CZ	-31.35	0.97	1.38
9	2	232	TYR	CE2-CZ	-31.34	0.97	1.38
11	4	67	TYR	CE1-CZ	-31.33	0.97	1.38
8	h	133	TYR	CE2-CZ	-30.37	0.99	1.38
8	1	133	TYR	CE2-CZ	-30.34	0.99	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	119	TYR	CE2-CZ	-30.15	0.99	1.38
9	2	119	TYR	CE2-CZ	-30.14	0.99	1.38
10	3	154	TYR	CE1-CZ	-29.83	0.99	1.38
9	i	126	TYR	CE1-CZ	-29.79	0.99	1.38
9	2	126	TYR	CE1-CZ	-29.74	0.99	1.38
13	m	131	TYR	CE1-CZ	-28.71	1.01	1.38
13	6	131	TYR	CE1-CZ	-28.65	1.01	1.38
12	l	115	PHE	CE2-CZ	-28.46	0.83	1.37
12	5	115	PHE	CE2-CZ	-28.46	0.83	1.37
11	4	135	TYR	CG-CD1	-28.03	1.02	1.39
11	k	135	TYR	CG-CD1	-27.99	1.02	1.39
9	2	119	TYR	CG-CD1	-27.93	1.02	1.39
9	i	119	TYR	CG-CD1	-27.88	1.02	1.39
11	k	135	TYR	CE2-CZ	-27.69	1.02	1.38
11	4	135	TYR	CE2-CZ	-27.66	1.02	1.38
11	4	49	GLU	CG-CD	-27.61	1.10	1.51
11	k	49	GLU	CG-CD	-27.60	1.10	1.51
11	k	121	TYR	CE1-CZ	-27.37	1.02	1.38
11	4	121	TYR	CE1-CZ	-27.35	1.02	1.38
9	2	232	TYR	CG-CD1	-27.34	1.03	1.39
11	4	67	TYR	CG-CD2	-27.18	1.03	1.39
11	k	67	TYR	CG-CD2	-27.17	1.03	1.39
11	k	121	TYR	CE2-CZ	-27.15	1.03	1.38
11	4	121	TYR	CE2-CZ	-27.14	1.03	1.38
13	6	47	TYR	CE1-CZ	-27.03	1.03	1.38
11	k	176	PHE	CE2-CZ	-27.02	0.86	1.37
9	2	153	TYR	CD2-CE2	-27.01	0.98	1.39
9	i	153	TYR	CD2-CE2	-27.00	0.98	1.39
13	m	47	TYR	CE1-CZ	-26.97	1.03	1.38
11	4	176	PHE	CE2-CZ	-26.96	0.86	1.37
8	1	120	TYR	CE2-CZ	-26.88	1.03	1.38
8	h	120	TYR	CE2-CZ	-26.86	1.03	1.38
13	m	182	TYR	CE2-CZ	-26.42	1.04	1.38
12	l	245	TYR	CE1-CZ	-26.41	1.04	1.38
13	6	182	TYR	CE2-CZ	-26.38	1.04	1.38
12	5	245	TYR	CE1-CZ	-26.37	1.04	1.38
11	k	139	TYR	CE1-CZ	-26.35	1.04	1.38
11	4	139	TYR	CE1-CZ	-26.32	1.04	1.38
12	5	81	PHE	CE2-CZ	-26.30	0.87	1.37
12	l	81	PHE	CE2-CZ	-26.29	0.87	1.37
12	5	188	TYR	CE1-CZ	-26.20	1.04	1.38
12	l	188	TYR	CE1-CZ	-26.16	1.04	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	74	TYR	CE2-CZ	-26.06	1.04	1.38
10	3	74	TYR	CE2-CZ	-26.06	1.04	1.38
9	2	126	TYR	CG-CD2	-25.78	1.05	1.39
13	6	181	LYS	CB-CG	-25.78	0.82	1.52
13	m	181	LYS	CB-CG	-25.75	0.83	1.52
9	i	126	TYR	CG-CD2	-25.75	1.05	1.39
8	1	133	TYR	CE1-CZ	-25.74	1.05	1.38
8	h	133	TYR	CE1-CZ	-25.69	1.05	1.38
8	1	133	TYR	CG-CD1	-25.54	1.05	1.39
8	h	133	TYR	CG-CD1	-25.52	1.05	1.39
10	3	154	TYR	CE2-CZ	-25.49	1.05	1.38
9	i	126	TYR	CE2-CZ	-25.42	1.05	1.38
9	2	126	TYR	CE2-CZ	-25.39	1.05	1.38
10	3	40	PHE	CE1-CZ	-25.36	0.89	1.37
10	j	40	PHE	CE1-CZ	-25.32	0.89	1.37
13	6	131	TYR	CG-CD2	-25.05	1.06	1.39
11	4	67	TYR	CE2-CZ	-25.00	1.06	1.38
11	k	67	TYR	CE2-CZ	-25.00	1.06	1.38
10	3	154	TYR	CG-CD2	-24.95	1.06	1.39
13	m	131	TYR	CG-CD2	-24.95	1.06	1.39
10	j	40	PHE	CG-CD2	-24.94	1.01	1.38
10	3	40	PHE	CG-CD2	-24.91	1.01	1.38
11	k	176	PHE	CG-CD1	-24.79	1.01	1.38
11	4	176	PHE	CG-CD1	-24.76	1.01	1.38
13	6	182	TYR	CD1-CE1	-24.64	1.02	1.39
13	m	182	TYR	CD1-CE1	-24.61	1.02	1.39
12	l	115	PHE	CG-CD1	-24.47	1.02	1.38
12	5	115	PHE	CG-CD1	-24.43	1.02	1.38
13	m	133	PHE	CE2-CZ	-24.31	0.91	1.37
13	6	133	PHE	CE2-CZ	-24.30	0.91	1.37
13	m	47	TYR	CE2-CZ	-24.25	1.07	1.38
13	6	47	TYR	CE2-CZ	-24.19	1.07	1.38
13	m	131	TYR	CE2-CZ	-24.11	1.07	1.38
13	6	131	TYR	CE2-CZ	-24.10	1.07	1.38
12	l	188	TYR	CG-CD2	-24.04	1.07	1.39
12	5	188	TYR	CG-CD2	-23.98	1.07	1.39
10	3	199	TYR	CE1-CZ	-23.90	1.07	1.38
10	j	199	TYR	CE1-CZ	-23.88	1.07	1.38
12	l	245	TYR	CE2-CZ	-23.84	1.07	1.38
12	5	245	TYR	CE2-CZ	-23.84	1.07	1.38
10	j	74	TYR	CG-CD1	-23.77	1.08	1.39
10	3	74	TYR	CG-CD1	-23.77	1.08	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	119	TYR	CE1-CZ	-23.75	1.07	1.38
11	k	139	TYR	CE2-CZ	-23.75	1.07	1.38
11	4	139	TYR	CE2-CZ	-23.73	1.07	1.38
9	2	119	TYR	CE1-CZ	-23.70	1.07	1.38
11	k	121	TYR	CG-CD2	-23.65	1.08	1.39
11	4	121	TYR	CG-CD2	-23.64	1.08	1.39
8	1	120	TYR	CE1-CZ	-23.63	1.07	1.38
8	h	120	TYR	CE1-CZ	-23.59	1.07	1.38
8	1	120	TYR	CG-CD1	-23.49	1.08	1.39
8	h	120	TYR	CG-CD1	-23.45	1.08	1.39
13	m	83	TYR	CE1-CZ	-23.43	1.08	1.38
11	4	121	TYR	CG-CD1	-23.11	1.09	1.39
11	k	121	TYR	CG-CD1	-23.07	1.09	1.39
11	k	139	TYR	CG-CD2	-23.07	1.09	1.39
11	4	139	TYR	CG-CD2	-23.02	1.09	1.39
13	m	83	TYR	CE2-CZ	-22.98	1.08	1.38
11	k	98	TYR	CE1-CZ	-22.45	1.09	1.38
11	4	98	TYR	CE1-CZ	-22.45	1.09	1.38
12	1	245	TYR	CG-CD2	-22.45	1.09	1.39
12	5	245	TYR	CG-CD2	-22.43	1.09	1.39
12	5	81	PHE	CE1-CZ	-22.28	0.95	1.37
12	1	81	PHE	CE1-CZ	-22.28	0.95	1.37
9	i	126	TYR	CG-CD1	-22.18	1.10	1.39
9	2	126	TYR	CG-CD1	-22.16	1.10	1.39
8	h	133	TYR	CG-CD2	-22.12	1.10	1.39
8	1	133	TYR	CG-CD2	-22.10	1.10	1.39
10	j	67	PHE	CE2-CZ	-22.08	0.95	1.37
13	6	168	TYR	CG-CD1	-22.06	1.10	1.39
10	3	67	PHE	CE2-CZ	-22.06	0.95	1.37
13	m	168	TYR	CG-CD1	-22.04	1.10	1.39
13	6	47	TYR	CG-CD1	-22.00	1.10	1.39
13	m	47	TYR	CG-CD1	-21.98	1.10	1.39
13	m	41	TYR	CE1-CZ	-21.87	1.10	1.38
13	6	41	TYR	CE1-CZ	-21.82	1.10	1.38
12	1	81	PHE	CG-CD1	-21.75	1.06	1.38
13	6	47	TYR	CG-CD2	-21.74	1.10	1.39
13	m	47	TYR	CG-CD2	-21.73	1.10	1.39
12	5	81	PHE	CG-CD1	-21.69	1.06	1.38
9	2	153	TYR	CB-CG	-21.68	1.19	1.51
9	i	153	TYR	CB-CG	-21.63	1.19	1.51
12	5	115	PHE	CE1-CZ	-21.54	0.96	1.37
12	1	115	PHE	CE1-CZ	-21.49	0.96	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	154	TYR	CG-CD1	-21.48	1.11	1.39
12	5	245	TYR	CG-CD1	-21.47	1.11	1.39
13	m	85	PHE	CE2-CZ	-21.45	0.96	1.37
12	l	245	TYR	CG-CD1	-21.36	1.11	1.39
13	m	85	PHE	CE1-CZ	-21.36	0.96	1.37
9	i	153	TYR	CG-CD1	-21.34	1.11	1.39
13	m	168	TYR	CE2-CZ	-21.32	1.10	1.38
12	5	253	TYR	CE2-CZ	-21.31	1.10	1.38
12	l	253	TYR	CE2-CZ	-21.31	1.10	1.38
13	6	168	TYR	CE2-CZ	-21.31	1.10	1.38
9	2	153	TYR	CG-CD1	-21.31	1.11	1.39
11	k	70	ARG	CZ-NH2	-21.29	1.05	1.33
11	4	70	ARG	CZ-NH2	-21.27	1.05	1.33
13	m	131	TYR	CG-CD1	-21.23	1.11	1.39
13	6	131	TYR	CG-CD1	-21.11	1.11	1.39
12	l	253	TYR	CE1-CZ	-20.93	1.11	1.38
12	5	253	TYR	CE1-CZ	-20.90	1.11	1.38
13	6	141	ARG	CZ-NH1	-20.87	1.05	1.33
13	m	141	ARG	CZ-NH1	-20.84	1.05	1.33
10	3	118	LYS	CD-CE	-20.78	0.99	1.51
10	j	118	LYS	CD-CE	-20.77	0.99	1.51
11	4	139	TYR	CG-CD1	-20.75	1.12	1.39
13	6	133	PHE	CG-CD1	-20.74	1.07	1.38
11	k	139	TYR	CG-CD1	-20.71	1.12	1.39
13	m	133	PHE	CG-CD1	-20.69	1.07	1.38
11	k	67	TYR	CG-CD1	-20.67	1.12	1.39
11	4	67	TYR	CG-CD1	-20.66	1.12	1.39
13	m	182	TYR	CD2-CE2	-20.66	1.08	1.39
9	i	153	TYR	CE2-CZ	-20.64	1.11	1.38
13	6	182	TYR	CD2-CE2	-20.63	1.08	1.39
9	2	153	TYR	CE2-CZ	-20.61	1.11	1.38
10	j	87	PHE	CE1-CZ	-20.61	0.98	1.37
10	3	87	PHE	CE1-CZ	-20.61	0.98	1.37
9	2	232	TYR	CE1-CZ	-20.58	1.11	1.38
13	m	83	TYR	CG-CD2	-20.20	1.12	1.39
9	i	65	ARG	CZ-NH1	-20.11	1.06	1.33
10	3	199	TYR	CG-CD2	-20.05	1.13	1.39
9	2	65	ARG	CZ-NH1	-20.01	1.07	1.33
10	j	199	TYR	CG-CD2	-19.98	1.13	1.39
12	5	253	TYR	CG-CD1	-19.84	1.13	1.39
12	l	253	TYR	CG-CD1	-19.80	1.13	1.39
11	k	98	TYR	CG-CD2	-19.80	1.13	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	201	GLU	CG-CD	-19.79	1.22	1.51
10	3	161	GLU	CG-CD	-19.79	1.22	1.51
8	h	120	TYR	CG-CD2	-19.76	1.13	1.39
11	4	98	TYR	CG-CD2	-19.75	1.13	1.39
8	1	120	TYR	CG-CD2	-19.73	1.13	1.39
13	m	133	PHE	CE1-CZ	-19.70	0.99	1.37
13	6	133	PHE	CE1-CZ	-19.66	0.99	1.37
10	3	199	TYR	CE2-CZ	-19.64	1.13	1.38
10	j	199	TYR	CE2-CZ	-19.61	1.13	1.38
13	m	83	TYR	CG-CD1	-19.61	1.13	1.39
8	1	153	GLU	CB-CG	-19.60	1.15	1.52
8	h	153	GLU	CB-CG	-19.59	1.15	1.52
13	m	13	TYR	CE2-CZ	-19.15	1.13	1.38
13	6	13	TYR	CE2-CZ	-19.13	1.13	1.38
13	m	142	GLU	CG-CD	-19.09	1.23	1.51
13	6	142	GLU	CG-CD	-19.08	1.23	1.51
9	2	219	TYR	CE2-CZ	-19.07	1.13	1.38
9	2	217	ARG	CZ-NH1	-19.06	1.08	1.33
10	3	87	PHE	CE2-CZ	-19.05	1.01	1.37
11	k	96	ARG	CG-CD	-19.04	1.04	1.51
13	m	187	GLU	CB-CG	-19.04	1.16	1.52
10	j	87	PHE	CE2-CZ	-19.01	1.01	1.37
9	2	119	TYR	CG-CD2	-19.01	1.14	1.39
9	i	119	TYR	CG-CD2	-19.01	1.14	1.39
13	6	187	GLU	CB-CG	-19.00	1.16	1.52
11	4	96	ARG	CG-CD	-19.00	1.04	1.51
10	3	74	TYR	CE1-CZ	-18.89	1.14	1.38
10	j	74	TYR	CE1-CZ	-18.86	1.14	1.38
13	m	85	PHE	CG-CD2	-18.81	1.10	1.38
11	4	70	ARG	CZ-NH1	-18.63	1.08	1.33
11	k	70	ARG	CZ-NH1	-18.57	1.08	1.33
13	m	46	ARG	CZ-NH2	-18.47	1.09	1.33
13	6	46	ARG	CZ-NH2	-18.44	1.09	1.33
10	j	199	TYR	CG-CD1	-18.43	1.15	1.39
10	3	199	TYR	CG-CD1	-18.42	1.15	1.39
12	1	188	TYR	CE2-CZ	-18.40	1.14	1.38
12	5	188	TYR	CE2-CZ	-18.38	1.14	1.38
10	j	67	PHE	CG-CD1	-18.35	1.11	1.38
11	k	8	ARG	CZ-NH1	-18.35	1.09	1.33
11	4	8	ARG	CZ-NH1	-18.34	1.09	1.33
10	3	159	GLU	CG-CD	-18.34	1.24	1.51
10	3	67	PHE	CG-CD1	-18.33	1.11	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	226	GLU	CB-CG	-18.23	1.17	1.52
12	l	226	GLU	CB-CG	-18.18	1.17	1.52
11	4	182	LYS	CD-CE	-18.06	1.06	1.51
11	k	182	LYS	CD-CE	-18.06	1.06	1.51
11	4	182	LYS	CE-NZ	-17.92	1.04	1.49
11	k	182	LYS	CE-NZ	-17.91	1.04	1.49
11	k	99	GLN	CB-CG	-17.87	1.04	1.52
11	4	78	GLN	CG-CD	-17.87	1.09	1.51
11	4	99	GLN	CB-CG	-17.85	1.04	1.52
11	k	78	GLN	CG-CD	-17.83	1.10	1.51
9	2	232	TYR	CG-CD2	-17.65	1.16	1.39
9	2	227	GLU	CB-CG	-17.59	1.18	1.52
8	h	26	ASP	CB-CG	-17.59	1.14	1.51
9	2	219	TYR	CE1-CZ	-17.59	1.15	1.38
8	1	26	ASP	CB-CG	-17.55	1.14	1.51
11	4	46	PHE	CE1-CZ	-17.48	1.04	1.37
13	m	41	TYR	CE2-CZ	-17.46	1.15	1.38
9	i	101	ARG	CZ-NH2	-17.44	1.10	1.33
13	6	41	TYR	CE2-CZ	-17.44	1.15	1.38
11	k	46	PHE	CE1-CZ	-17.42	1.04	1.37
9	2	101	ARG	CZ-NH2	-17.41	1.10	1.33
13	6	13	TYR	CE1-CZ	-17.34	1.16	1.38
13	m	85	PHE	CG-CD1	-17.34	1.12	1.38
13	m	41	TYR	CG-CD2	-17.33	1.16	1.39
11	4	46	PHE	CG-CD2	-17.32	1.12	1.38
13	m	145	ARG	CZ-NH2	-17.31	1.10	1.33
13	6	145	ARG	CZ-NH2	-17.30	1.10	1.33
11	k	176	PHE	CE1-CZ	-17.30	1.04	1.37
13	m	13	TYR	CE1-CZ	-17.29	1.16	1.38
11	k	46	PHE	CG-CD2	-17.29	1.12	1.38
13	6	41	TYR	CG-CD2	-17.28	1.16	1.39
11	4	176	PHE	CE1-CZ	-17.28	1.04	1.37
2	B	234	ARG	CZ-NH1	-17.27	1.10	1.33
2	b	234	ARG	CZ-NH1	-17.26	1.10	1.33
12	5	81	PHE	CG-CD2	-17.17	1.12	1.38
12	5	115	PHE	CG-CD2	-17.11	1.13	1.38
12	l	81	PHE	CG-CD2	-17.08	1.13	1.38
7	g	175	GLU	CG-CD	-17.08	1.26	1.51
12	l	115	PHE	CG-CD2	-17.03	1.13	1.38
11	4	49	GLU	CB-CG	-16.97	1.20	1.52
11	k	49	GLU	CB-CG	-16.96	1.20	1.52
11	k	96	ARG	CZ-NH2	-16.95	1.11	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	113	LYS	CE-NZ	-16.95	1.06	1.49
11	4	96	ARG	CZ-NH2	-16.95	1.11	1.33
12	5	188	TYR	CG-CD1	-16.94	1.17	1.39
11	k	113	LYS	CE-NZ	-16.93	1.06	1.49
9	2	219	TYR	CG-CD1	-16.90	1.17	1.39
13	6	201	GLU	CG-CD	-16.88	1.26	1.51
9	i	37	PHE	CG-CD2	-16.88	1.13	1.38
12	l	188	TYR	CG-CD1	-16.88	1.17	1.39
9	2	37	PHE	CG-CD2	-16.88	1.13	1.38
12	l	170	LEU	CG-CD2	-16.85	0.89	1.51
12	5	170	LEU	CG-CD2	-16.85	0.89	1.51
13	m	201	GLU	CG-CD	-16.83	1.26	1.51
10	j	87	PHE	CG-CD2	-16.74	1.13	1.38
10	3	87	PHE	CG-CD2	-16.71	1.13	1.38
11	k	93	ARG	CZ-NH2	-16.60	1.11	1.33
12	l	164	GLN	CB-CG	-16.59	1.07	1.52
11	4	93	ARG	CZ-NH2	-16.57	1.11	1.33
10	3	87	PHE	CG-CD1	-16.55	1.14	1.38
12	5	164	GLN	CB-CG	-16.55	1.07	1.52
10	j	87	PHE	CG-CD1	-16.55	1.14	1.38
9	2	219	TYR	CG-CD2	-16.52	1.17	1.39
12	5	226	GLU	CD-OE2	-16.51	1.07	1.25
12	l	226	GLU	CD-OE2	-16.39	1.07	1.25
13	m	181	LYS	CG-CD	-16.24	0.97	1.52
13	6	181	LYS	CG-CD	-16.22	0.97	1.52
13	6	182	TYR	CG-CD1	-16.19	1.18	1.39
13	m	182	TYR	CG-CD1	-16.15	1.18	1.39
12	5	274	LYS	CE-NZ	-15.98	1.09	1.49
12	l	274	LYS	CE-NZ	-15.97	1.09	1.49
13	m	182	TYR	CB-CG	-15.95	1.27	1.51
9	2	37	PHE	CE1-CZ	-15.94	1.07	1.37
13	6	133	PHE	CG-CD2	-15.92	1.14	1.38
13	m	133	PHE	CG-CD2	-15.92	1.14	1.38
9	i	37	PHE	CE1-CZ	-15.90	1.07	1.37
13	6	182	TYR	CB-CG	-15.89	1.27	1.51
11	4	10	GLN	CG-CD	-15.80	1.14	1.51
9	i	101	ARG	CD-NE	-15.77	1.19	1.46
11	k	10	GLN	CG-CD	-15.77	1.14	1.51
13	6	41	TYR	CG-CD1	-15.77	1.18	1.39
9	2	101	ARG	CD-NE	-15.75	1.19	1.46
13	m	41	TYR	CG-CD1	-15.71	1.18	1.39
11	4	135	TYR	CD1-CE1	-15.69	1.15	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	135	TYR	CD1-CE1	-15.67	1.15	1.39
13	6	13	TYR	CG-CD2	-15.66	1.18	1.39
13	m	13	TYR	CG-CD2	-15.65	1.18	1.39
10	3	67	PHE	CE1-CZ	-15.60	1.07	1.37
10	j	67	PHE	CE1-CZ	-15.59	1.07	1.37
10	j	204	GLN	CB-CG	-15.55	1.10	1.52
10	3	204	GLN	CB-CG	-15.54	1.10	1.52
9	2	230	LYS	CE-NZ	-15.47	1.10	1.49
9	i	98	TYR	CD1-CE1	-15.40	1.16	1.39
2	B	231	LYS	CE-NZ	-15.38	1.10	1.49
2	b	231	LYS	CE-NZ	-15.36	1.10	1.49
9	2	98	TYR	CD1-CE1	-15.34	1.16	1.39
10	j	40	PHE	CE2-CZ	-15.31	1.08	1.37
13	m	13	TYR	CG-CD1	-15.29	1.19	1.39
10	3	40	PHE	CE2-CZ	-15.28	1.08	1.37
13	6	13	TYR	CG-CD1	-15.25	1.19	1.39
3	c	165	VAL	CB-CG2	-15.20	1.21	1.52
5	e	10	ARG	CZ-NH1	-15.20	1.13	1.33
12	l	108	LYS	CE-NZ	-15.20	1.11	1.49
12	5	108	LYS	CE-NZ	-15.15	1.11	1.49
3	C	165	VAL	CB-CG2	-15.15	1.21	1.52
11	k	127	GLU	CD-OE1	-15.07	1.09	1.25
8	1	153	GLU	CG-CD	-15.07	1.29	1.51
11	4	127	GLU	CD-OE1	-15.06	1.09	1.25
8	h	10	THR	CB-CG2	-15.04	1.02	1.52
6	f	169	LYS	CE-NZ	-15.03	1.11	1.49
8	h	153	GLU	CG-CD	-15.03	1.29	1.51
8	1	10	THR	CB-CG2	-15.02	1.02	1.52
13	6	217	LYS	CB-CG	-15.01	1.12	1.52
6	F	169	LYS	CE-NZ	-14.99	1.11	1.49
13	m	217	LYS	CB-CG	-14.98	1.12	1.52
13	6	168	TYR	CE1-CZ	-14.97	1.19	1.38
2	B	237	LYS	CE-NZ	-14.93	1.11	1.49
2	b	237	LYS	CE-NZ	-14.93	1.11	1.49
12	l	138	CYS	CB-SG	-14.93	1.56	1.82
13	m	168	TYR	CE1-CZ	-14.92	1.19	1.38
9	2	84	VAL	CB-CG1	-14.91	1.21	1.52
12	5	138	CYS	CB-SG	-14.90	1.56	1.82
9	i	84	VAL	CB-CG1	-14.87	1.21	1.52
9	i	106	VAL	CB-CG2	-14.86	1.21	1.52
9	2	106	VAL	CB-CG2	-14.86	1.21	1.52
13	m	186	GLU	CB-CG	-14.85	1.24	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	186	GLU	CB-CG	-14.83	1.24	1.52
5	E	53	ARG	CZ-NH1	-14.73	1.13	1.33
2	B	201	GLU	CD-OE1	-14.73	1.09	1.25
2	b	201	GLU	CD-OE1	-14.67	1.09	1.25
12	5	203	CYS	CB-SG	-14.61	1.57	1.82
13	6	46	ARG	CD-NE	-14.56	1.21	1.46
12	l	156	LYS	CE-NZ	-14.56	1.12	1.49
13	m	46	ARG	CD-NE	-14.56	1.21	1.46
12	l	203	CYS	CB-SG	-14.55	1.57	1.82
12	5	156	LYS	CE-NZ	-14.55	1.12	1.49
9	2	168	GLU	CG-CD	-14.53	1.30	1.51
10	3	118	LYS	CG-CD	-14.51	1.03	1.52
9	i	168	GLU	CG-CD	-14.49	1.30	1.51
10	j	118	LYS	CG-CD	-14.49	1.03	1.52
12	5	270	GLU	CG-CD	-14.46	1.30	1.51
12	l	270	GLU	CG-CD	-14.43	1.30	1.51
10	3	159	GLU	CD-OE1	-14.42	1.09	1.25
13	6	144	CYS	CB-SG	-14.42	1.57	1.82
13	m	144	CYS	CB-SG	-14.38	1.57	1.82
9	2	248	ASN	CB-CG	-14.35	1.18	1.51
11	4	49	GLU	CD-OE1	-14.34	1.09	1.25
11	k	49	GLU	CD-OE1	-14.33	1.09	1.25
11	4	96	ARG	CD-NE	-14.30	1.22	1.46
11	k	96	ARG	CD-NE	-14.25	1.22	1.46
9	2	228	LYS	CE-NZ	-14.12	1.13	1.49
8	1	130	LYS	CE-NZ	-14.11	1.13	1.49
1	a	96	ARG	CZ-NH1	-14.11	1.14	1.33
1	A	96	ARG	CZ-NH1	-14.09	1.14	1.33
13	m	190	LYS	CE-NZ	-14.07	1.13	1.49
13	6	190	LYS	CE-NZ	-14.07	1.13	1.49
8	h	130	LYS	CE-NZ	-14.07	1.13	1.49
3	C	241	LYS	CD-CE	-14.06	1.16	1.51
3	c	241	LYS	CD-CE	-14.04	1.16	1.51
5	e	7	GLU	CG-CD	-14.03	1.30	1.51
11	k	135	TYR	CB-CG	-14.01	1.30	1.51
11	4	135	TYR	CB-CG	-14.00	1.30	1.51
5	E	159	GLU	CD-OE1	-14.00	1.10	1.25
5	e	159	GLU	CD-OE1	-13.99	1.10	1.25
7	g	209	GLU	CG-CD	-13.98	1.30	1.51
13	m	221	ARG	CG-CD	-13.95	1.17	1.51
13	m	124	GLU	CD-OE1	-13.93	1.10	1.25
13	6	221	ARG	CG-CD	-13.93	1.17	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	250	GLU	CD-OE2	-13.92	1.10	1.25
12	5	77	THR	CB-CG2	-13.91	1.06	1.52
12	l	77	THR	CB-CG2	-13.90	1.06	1.52
13	6	124	GLU	CD-OE1	-13.89	1.10	1.25
12	l	278	GLU	CB-CG	-13.87	1.25	1.52
1	a	250	GLU	CD-OE2	-13.87	1.10	1.25
12	5	278	GLU	CB-CG	-13.87	1.25	1.52
32	M	96	ASN	CG-OD1	-13.86	0.93	1.24
10	3	97	GLU	CG-CD	-13.86	1.31	1.51
2	B	186	GLU	CG-CD	-13.84	1.31	1.51
10	j	97	GLU	CG-CD	-13.81	1.31	1.51
7	g	209	GLU	CD-OE1	-13.79	1.10	1.25
2	b	186	GLU	CG-CD	-13.79	1.31	1.51
3	C	109	GLU	CG-CD	-13.72	1.31	1.51
11	4	176	PHE	CG-CD2	-13.72	1.18	1.38
11	k	176	PHE	CG-CD2	-13.68	1.18	1.38
9	2	36	LYS	CD-CE	-13.67	1.17	1.51
13	6	201	GLU	CD-OE1	-13.66	1.10	1.25
3	c	109	GLU	CG-CD	-13.65	1.31	1.51
9	i	36	LYS	CD-CE	-13.65	1.17	1.51
11	k	110	LYS	CG-CD	-13.64	1.06	1.52
8	h	45	ARG	CZ-NH2	-13.63	1.15	1.33
10	3	127	ILE	C-N	13.63	1.57	1.33
11	4	110	LYS	CG-CD	-13.63	1.06	1.52
9	i	98	TYR	CD2-CE2	-13.60	1.19	1.39
8	1	45	ARG	CZ-NH2	-13.60	1.15	1.33
9	2	98	TYR	CD2-CE2	-13.58	1.19	1.39
11	k	71	GLU	CG-CD	-13.58	1.31	1.51
13	m	201	GLU	CD-OE1	-13.58	1.10	1.25
8	1	128	VAL	CB-CG1	-13.54	1.24	1.52
11	4	71	GLU	CG-CD	-13.54	1.31	1.51
10	3	113	ASN	CB-CG	-13.51	1.20	1.51
8	h	128	VAL	CB-CG1	-13.48	1.24	1.52
5	e	177	GLU	CB-CG	-13.47	1.26	1.52
10	j	113	ASN	CB-CG	-13.46	1.20	1.51
5	E	177	GLU	CB-CG	-13.42	1.26	1.52
13	6	143	GLN	CG-CD	-13.40	1.20	1.51
12	5	182	LYS	CB-CG	-13.40	1.16	1.52
13	m	143	GLN	CG-CD	-13.39	1.20	1.51
8	h	128	VAL	CB-CG2	-13.38	1.24	1.52
10	j	75	LYS	CB-CG	-13.38	1.16	1.52
8	1	128	VAL	CB-CG2	-13.39	1.24	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	182	LYS	CB-CG	-13.38	1.16	1.52
5	e	7	GLU	CD-OE2	-13.38	1.10	1.25
10	3	159	GLU	CD-OE2	-13.38	1.10	1.25
10	3	75	LYS	CB-CG	-13.37	1.16	1.52
13	m	187	GLU	CG-CD	-13.34	1.31	1.51
8	1	183	ARG	CZ-NH2	-13.34	1.15	1.33
10	3	74	TYR	CG-CD2	-13.33	1.21	1.39
12	5	82	ARG	CZ-NH2	-13.33	1.15	1.33
10	j	74	TYR	CG-CD2	-13.33	1.21	1.39
9	2	227	GLU	CG-CD	-13.33	1.31	1.51
13	6	187	GLU	CG-CD	-13.32	1.31	1.51
5	E	90	GLU	CG-CD	-13.31	1.31	1.51
8	h	183	ARG	CZ-NH2	-13.31	1.15	1.33
12	l	82	ARG	CZ-NH2	-13.31	1.15	1.33
8	1	194	ARG	CZ-NH1	-13.28	1.15	1.33
1	a	62	LYS	CE-NZ	-13.26	1.16	1.49
5	e	90	GLU	CG-CD	-13.26	1.32	1.51
1	A	62	LYS	CE-NZ	-13.26	1.16	1.49
8	1	52	CYS	CB-SG	-13.26	1.59	1.82
8	h	52	CYS	CB-SG	-13.22	1.59	1.82
8	1	45	ARG	CD-NE	-13.18	1.24	1.46
8	h	45	ARG	CD-NE	-13.17	1.24	1.46
1	A	217	GLU	CD-OE1	-13.12	1.11	1.25
9	i	84	VAL	CB-CG2	-13.11	1.25	1.52
1	a	217	GLU	CD-OE1	-13.10	1.11	1.25
9	2	84	VAL	CB-CG2	-13.10	1.25	1.52
9	i	98	TYR	CB-CG	-13.04	1.32	1.51
9	2	98	TYR	CB-CG	-13.03	1.32	1.51
12	l	139	ARG	CD-NE	-12.97	1.24	1.46
12	l	257	GLU	CG-CD	-12.96	1.32	1.51
12	5	139	ARG	CD-NE	-12.95	1.24	1.46
12	5	257	GLU	CG-CD	-12.92	1.32	1.51
9	2	82	GLU	CB-CG	-12.92	1.27	1.52
6	F	169	LYS	CD-CE	-12.91	1.19	1.51
12	5	100	TRP	CB-CG	-12.90	1.27	1.50
9	i	82	GLU	CB-CG	-12.90	1.27	1.52
12	5	253	TYR	CG-CD2	-12.90	1.22	1.39
6	f	169	LYS	CD-CE	-12.89	1.19	1.51
9	i	37	PHE	CE2-CZ	-12.89	1.12	1.37
12	l	253	TYR	CG-CD2	-12.88	1.22	1.39
12	l	100	TRP	CB-CG	-12.88	1.27	1.50
9	2	37	PHE	CE2-CZ	-12.88	1.12	1.37

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	99	GLN	CG-CD	-12.87	1.21	1.51
11	4	99	GLN	CG-CD	-12.86	1.21	1.51
13	m	221	ARG	CZ-NH1	-12.84	1.16	1.33
11	k	93	ARG	CZ-NH1	-12.81	1.16	1.33
11	4	93	ARG	CZ-NH1	-12.80	1.16	1.33
13	6	221	ARG	CZ-NH1	-12.79	1.16	1.33
8	1	152	ARG	CG-CD	-12.78	1.20	1.51
8	h	152	ARG	CG-CD	-12.77	1.20	1.51
10	j	80	ARG	CZ-NH1	-12.77	1.16	1.33
9	i	93	GLU	CG-CD	-12.73	1.32	1.51
3	c	213	PHE	CE2-CZ	-12.73	1.13	1.37
3	C	213	PHE	CE2-CZ	-12.73	1.13	1.37
10	3	80	ARG	CZ-NH1	-12.71	1.16	1.33
8	1	203	GLU	CB-CG	-12.68	1.28	1.52
9	2	93	GLU	CG-CD	-12.65	1.32	1.51
11	k	46	PHE	CE2-CZ	-12.64	1.13	1.37
11	4	46	PHE	CE2-CZ	-12.63	1.13	1.37
10	3	161	GLU	CD-OE2	-12.56	1.11	1.25
10	3	118	LYS	CB-CG	-12.52	1.18	1.52
10	j	118	LYS	CB-CG	-12.51	1.18	1.52
12	l	162	VAL	CB-CG1	-12.47	1.26	1.52
12	5	162	VAL	CB-CG1	-12.47	1.26	1.52
13	m	36	ARG	CZ-NH2	-12.46	1.16	1.33
8	h	114	LYS	CE-NZ	-12.45	1.18	1.49
8	1	114	LYS	CE-NZ	-12.42	1.18	1.49
10	3	67	PHE	CG-CD2	-12.42	1.20	1.38
13	6	36	ARG	CZ-NH2	-12.42	1.17	1.33
10	j	67	PHE	CG-CD2	-12.40	1.20	1.38
13	m	211	GLU	CG-CD	-12.39	1.33	1.51
7	g	175	GLU	CB-CG	-12.37	1.28	1.52
13	6	77	LYS	CD-CE	-12.35	1.20	1.51
13	m	77	LYS	CD-CE	-12.34	1.20	1.51
13	6	211	GLU	CG-CD	-12.34	1.33	1.51
3	C	213	PHE	CG-CD1	-12.28	1.20	1.38
3	c	213	PHE	CG-CD1	-12.26	1.20	1.38
9	2	243	LYS	CE-NZ	-12.22	1.18	1.49
12	l	139	ARG	CZ-NH2	-12.22	1.17	1.33
10	3	155	GLU	CB-CG	-12.18	1.29	1.52
12	5	139	ARG	CZ-NH2	-12.15	1.17	1.33
5	e	10	ARG	CZ-NH2	-12.14	1.17	1.33
12	l	147	GLU	CB-CG	-12.12	1.29	1.52
10	j	75	LYS	CE-NZ	-12.11	1.18	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	147	GLU	CB-CG	-12.11	1.29	1.52
5	E	186	GLU	CD-OE1	-12.10	1.12	1.25
5	e	186	GLU	CD-OE1	-12.09	1.12	1.25
10	3	75	LYS	CE-NZ	-12.07	1.18	1.49
13	6	145	ARG	CD-NE	-12.06	1.25	1.46
9	2	255	GLU	C-O	-12.06	1.00	1.23
3	c	16	GLU	CD-OE1	-12.03	1.12	1.25
3	C	16	GLU	CD-OE1	-12.03	1.12	1.25
10	3	41	GLU	CB-CG	-12.03	1.29	1.52
13	m	145	ARG	CD-NE	-12.02	1.26	1.46
10	j	41	GLU	CB-CG	-12.01	1.29	1.52
11	k	96	ARG	CB-CG	-12.00	1.20	1.52
11	4	96	ARG	CB-CG	-12.00	1.20	1.52
2	B	242	GLU	CD-OE1	-11.99	1.12	1.25
13	6	30	VAL	CB-CG1	-11.99	1.27	1.52
13	m	30	VAL	CB-CG1	-11.96	1.27	1.52
3	C	224	GLU	CD-OE2	-11.96	1.12	1.25
13	m	114	TYR	CE2-CZ	-11.94	1.23	1.38
2	b	242	GLU	CD-OE1	-11.93	1.12	1.25
10	3	75	LYS	CD-CE	-11.93	1.21	1.51
3	c	224	GLU	CD-OE2	-11.91	1.12	1.25
13	m	221	ARG	CZ-NH2	-11.91	1.17	1.33
13	m	46	ARG	CG-CD	-11.89	1.22	1.51
13	6	221	ARG	CZ-NH2	-11.89	1.17	1.33
10	j	75	LYS	CD-CE	-11.88	1.21	1.51
3	C	165	VAL	CB-CG1	-11.88	1.27	1.52
3	c	165	VAL	CB-CG1	-11.88	1.27	1.52
13	6	46	ARG	CG-CD	-11.88	1.22	1.51
11	k	70	ARG	CD-NE	-11.87	1.26	1.46
11	4	70	ARG	CD-NE	-11.86	1.26	1.46
8	h	18	LYS	CD-CE	-11.83	1.21	1.51
12	l	162	VAL	CB-CG2	-11.83	1.28	1.52
12	5	162	VAL	CB-CG2	-11.82	1.28	1.52
8	1	18	LYS	CD-CE	-11.82	1.21	1.51
7	g	209	GLU	CD-OE2	-11.72	1.12	1.25
8	1	204	GLN	CB-CG	-11.69	1.21	1.52
9	i	208	GLU	CD-OE1	-11.64	1.12	1.25
5	e	229	LYS	CD-CE	-11.61	1.22	1.51
13	m	30	VAL	CB-CG2	-11.61	1.28	1.52
9	2	208	GLU	CD-OE1	-11.61	1.12	1.25
5	E	229	LYS	CD-CE	-11.60	1.22	1.51
13	6	142	GLU	CD-OE1	-11.58	1.12	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	30	VAL	CB-CG2	-11.58	1.28	1.52
10	3	161	GLU	CD-OE1	-11.57	1.12	1.25
13	m	58	ILE	CB-CG2	-11.56	1.17	1.52
9	2	101	ARG	CB-CG	-11.56	1.21	1.52
10	3	65	GLU	CB-CG	-11.56	1.30	1.52
13	6	58	ILE	CB-CG2	-11.56	1.17	1.52
9	i	101	ARG	CB-CG	-11.56	1.21	1.52
7	g	207	ASN	CG-ND2	-11.54	1.03	1.32
10	j	65	GLU	CB-CG	-11.54	1.30	1.52
13	6	145	ARG	NE-CZ	-11.54	1.18	1.33
13	m	142	GLU	CD-OE1	-11.53	1.12	1.25
13	m	90	LYS	CE-NZ	-11.53	1.20	1.49
1	a	188	LYS	CE-NZ	-11.51	1.20	1.49
13	m	145	ARG	NE-CZ	-11.51	1.18	1.33
13	m	36	ARG	CZ-NH1	-11.49	1.18	1.33
1	A	188	LYS	CE-NZ	-11.48	1.20	1.49
11	4	111	LYS	CE-NZ	-11.48	1.20	1.49
2	b	160	LYS	CE-NZ	-11.48	1.20	1.49
13	6	36	ARG	CZ-NH1	-11.47	1.18	1.33
11	4	98	TYR	CE2-CZ	-11.47	1.23	1.38
10	3	125	ASP	CB-CG	-11.47	1.27	1.51
11	k	111	LYS	CE-NZ	-11.46	1.20	1.49
12	l	233	LYS	CD-CE	-11.46	1.22	1.51
12	5	233	LYS	CD-CE	-11.46	1.22	1.51
1	a	107	LYS	CE-NZ	-11.46	1.20	1.49
2	B	160	LYS	CE-NZ	-11.46	1.20	1.49
10	3	75	LYS	CG-CD	-11.45	1.13	1.52
10	j	75	LYS	CG-CD	-11.44	1.13	1.52
1	A	107	LYS	CE-NZ	-11.44	1.20	1.49
13	6	228	LYS	CE-NZ	-11.44	1.20	1.49
11	k	98	TYR	CE2-CZ	-11.44	1.23	1.38
2	B	182	GLU	CD-OE2	-11.43	1.13	1.25
10	3	77	LYS	CE-NZ	-11.43	1.20	1.49
10	3	115	LYS	CD-CE	-11.43	1.22	1.51
10	j	77	LYS	CE-NZ	-11.43	1.20	1.49
13	m	228	LYS	CE-NZ	-11.43	1.20	1.49
12	5	82	ARG	CZ-NH1	-11.42	1.18	1.33
1	a	239	GLU	CD-OE2	-11.42	1.13	1.25
10	j	115	LYS	CD-CE	-11.42	1.22	1.51
1	A	239	GLU	CD-OE2	-11.41	1.13	1.25
11	4	87	GLU	CD-OE1	-11.41	1.13	1.25
13	m	168	TYR	CG-CD2	-11.39	1.24	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	182	GLU	CD-OE2	-11.39	1.13	1.25
12	l	82	ARG	CZ-NH1	-11.38	1.18	1.33
11	k	87	GLU	CD-OE1	-11.38	1.13	1.25
13	6	168	TYR	CG-CD2	-11.35	1.24	1.39
11	4	36	ARG	CZ-NH1	-11.32	1.18	1.33
11	k	36	ARG	CZ-NH1	-11.32	1.18	1.33
2	b	231	LYS	CB-CG	-11.29	1.22	1.52
2	B	231	LYS	CB-CG	-11.29	1.22	1.52
13	m	169	GLU	CD-OE1	-11.25	1.13	1.25
9	2	254	GLU	CD-OE1	-11.23	1.13	1.25
10	j	40	PHE	CG-CD1	-11.21	1.22	1.38
10	3	40	PHE	CG-CD1	-11.21	1.22	1.38
11	k	135	TYR	CD2-CE2	-11.19	1.22	1.39
11	4	135	TYR	CD2-CE2	-11.19	1.22	1.39
13	6	169	GLU	CD-OE1	-11.17	1.13	1.25
7	G	100	LYS	CB-CG	-11.17	1.22	1.52
8	1	194	ARG	CG-CD	-11.16	1.24	1.51
7	g	100	LYS	CB-CG	-11.15	1.22	1.52
9	i	168	GLU	CD-OE1	-11.15	1.13	1.25
11	4	163	LEU	CG-CD1	-11.14	1.10	1.51
11	k	163	LEU	CG-CD1	-11.13	1.10	1.51
8	1	194	ARG	CZ-NH2	-11.13	1.18	1.33
1	A	201	LYS	CD-CE	-11.08	1.23	1.51
1	a	201	LYS	CD-CE	-11.05	1.23	1.51
9	2	168	GLU	CD-OE1	-11.04	1.13	1.25
8	h	118	GLU	CG-CD	-11.04	1.35	1.51
1	a	149	GLU	CD-OE1	-11.03	1.13	1.25
1	A	149	GLU	CD-OE1	-11.03	1.13	1.25
8	1	118	GLU	CG-CD	-11.03	1.35	1.51
8	h	73	GLU	CG-CD	-10.97	1.35	1.51
10	3	146	LEU	C-N	10.96	1.59	1.34
10	j	78	GLU	CG-CD	-10.96	1.35	1.51
10	3	78	GLU	CG-CD	-10.96	1.35	1.51
13	6	161	GLN	CD-NE2	-10.96	1.05	1.32
8	1	42	LYS	CE-NZ	-10.95	1.21	1.49
13	m	161	GLN	CD-NE2	-10.94	1.05	1.32
1	A	250	GLU	CG-CD	-10.93	1.35	1.51
12	l	226	GLU	CG-CD	-10.93	1.35	1.51
8	h	42	LYS	CE-NZ	-10.93	1.21	1.49
8	1	73	GLU	CG-CD	-10.92	1.35	1.51
1	a	250	GLU	CG-CD	-10.92	1.35	1.51
1	a	48	LYS	CE-NZ	-10.92	1.21	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	106	VAL	CB-CG1	-10.91	1.29	1.52
1	A	48	LYS	CE-NZ	-10.90	1.21	1.49
9	2	208	GLU	CG-CD	-10.89	1.35	1.51
9	2	106	VAL	CB-CG1	-10.88	1.29	1.52
12	5	226	GLU	CG-CD	-10.87	1.35	1.51
13	6	208	ASP	CB-CG	-10.86	1.28	1.51
13	m	208	ASP	CB-CG	-10.86	1.28	1.51
8	h	178	SER	CB-OG	-10.84	1.28	1.42
8	1	178	SER	CB-OG	-10.82	1.28	1.42
9	i	208	GLU	CG-CD	-10.82	1.35	1.51
5	E	32	LYS	CE-NZ	-10.78	1.22	1.49
2	B	103	GLU	CD-OE1	-10.74	1.13	1.25
9	2	230	LYS	CD-CE	-10.73	1.24	1.51
21	N	282	TYR	CD2-CE2	-10.73	1.23	1.39
5	e	32	LYS	CE-NZ	-10.73	1.22	1.49
9	2	211	LYS	CB-CG	-10.70	1.23	1.52
2	b	103	GLU	CD-OE1	-10.69	1.13	1.25
13	m	50	LYS	CG-CD	-10.69	1.16	1.52
13	6	50	LYS	CG-CD	-10.69	1.16	1.52
9	i	211	LYS	CB-CG	-10.69	1.23	1.52
2	B	217	GLU	CD-OE2	-10.66	1.14	1.25
2	b	248	GLU	CD-OE1	-10.66	1.14	1.25
10	j	98	ARG	CZ-NH2	-10.62	1.19	1.33
9	i	178	GLU	CG-CD	-10.62	1.36	1.51
2	B	248	GLU	CD-OE1	-10.61	1.14	1.25
2	b	217	GLU	CD-OE2	-10.59	1.14	1.25
9	2	178	GLU	CG-CD	-10.58	1.36	1.51
10	3	98	ARG	CZ-NH2	-10.57	1.19	1.33
10	j	83	GLU	CD-OE2	-10.55	1.14	1.25
11	4	192	VAL	CB-CG1	-10.55	1.30	1.52
11	k	192	VAL	CB-CG1	-10.54	1.30	1.52
10	3	83	GLU	CD-OE2	-10.54	1.14	1.25
8	h	48	ASP	C-N	10.53	1.58	1.34
9	2	220	LEU	CG-CD2	-10.52	1.12	1.51
9	2	101	ARG	NE-CZ	-10.50	1.19	1.33
9	i	177	LYS	CE-NZ	-10.49	1.22	1.49
12	l	192	SER	CB-OG	-10.49	1.28	1.42
9	2	177	LYS	CE-NZ	-10.47	1.22	1.49
12	5	192	SER	CB-OG	-10.47	1.28	1.42
9	i	101	ARG	NE-CZ	-10.44	1.19	1.33
13	m	141	ARG	CG-CD	-10.44	1.25	1.51
5	E	102	TYR	CE1-CZ	-10.44	1.25	1.38

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	278	GLU	CD-OE2	-10.43	1.14	1.25
9	i	37	PHE	CG-CD1	-10.42	1.23	1.38
5	e	102	TYR	CE1-CZ	-10.42	1.25	1.38
13	6	141	ARG	CG-CD	-10.41	1.25	1.51
13	6	182	TYR	CE1-CZ	-10.40	1.25	1.38
13	m	182	TYR	CE1-CZ	-10.39	1.25	1.38
12	l	278	GLU	CD-OE2	-10.39	1.14	1.25
9	i	51	GLN	CB-CG	-10.39	1.24	1.52
12	l	274	LYS	CB-CG	-10.39	1.24	1.52
9	i	58	LYS	CD-CE	-10.38	1.25	1.51
9	2	58	LYS	CD-CE	-10.38	1.25	1.51
13	m	9	GLN	CD-NE2	-10.38	1.06	1.32
13	m	167	GLN	CD-NE2	-10.37	1.06	1.32
12	5	274	LYS	CB-CG	-10.37	1.24	1.52
13	6	167	GLN	CD-NE2	-10.37	1.06	1.32
13	6	9	GLN	CD-NE2	-10.37	1.06	1.32
9	2	37	PHE	CG-CD1	-10.37	1.23	1.38
9	2	51	GLN	CB-CG	-10.37	1.24	1.52
12	5	286	ILE	CB-CG2	-10.36	1.20	1.52
11	4	74	GLU	CB-CG	-10.35	1.32	1.52
12	l	286	ILE	CB-CG2	-10.33	1.20	1.52
12	l	277	GLU	CD-OE1	-10.33	1.14	1.25
10	j	8	ASN	CB-CG	-10.32	1.27	1.51
11	4	143	LEU	CG-CD1	-10.31	1.13	1.51
11	k	74	GLU	CB-CG	-10.31	1.32	1.52
5	E	102	TYR	CG-CD2	-10.31	1.25	1.39
10	j	53	ILE	CB-CG2	-10.30	1.21	1.52
10	3	8	ASN	CB-CG	-10.30	1.27	1.51
10	3	165	GLU	CD-OE2	-10.29	1.14	1.25
12	5	277	GLU	CD-OE1	-10.29	1.14	1.25
11	k	143	LEU	CG-CD1	-10.29	1.13	1.51
10	3	53	ILE	CB-CG2	-10.28	1.21	1.52
12	5	214	VAL	CB-CG2	-10.28	1.31	1.52
2	b	231	LYS	CD-CE	-10.28	1.25	1.51
5	e	102	TYR	CG-CD2	-10.27	1.25	1.39
2	B	231	LYS	CD-CE	-10.27	1.25	1.51
11	4	93	ARG	CD-NE	-10.26	1.29	1.46
12	5	82	ARG	CD-NE	-10.25	1.29	1.46
12	l	287	GLY	C-O	-10.24	1.07	1.23
12	5	287	GLY	C-O	-10.24	1.07	1.23
11	k	93	ARG	CD-NE	-10.24	1.29	1.46
12	l	214	VAL	CB-CG2	-10.24	1.31	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	189	GLN	CG-CD	-10.24	1.27	1.51
8	h	183	ARG	CD-NE	-10.23	1.29	1.46
13	m	94	ILE	CB-CG2	-10.23	1.21	1.52
12	l	82	ARG	CD-NE	-10.21	1.29	1.46
9	i	189	GLN	CG-CD	-10.21	1.27	1.51
8	1	183	ARG	CD-NE	-10.20	1.29	1.46
13	6	134	ASP	CB-CG	-10.19	1.30	1.51
13	m	134	ASP	CB-CG	-10.18	1.30	1.51
5	E	105	GLU	CD-OE1	-10.17	1.14	1.25
5	e	105	GLU	CD-OE1	-10.16	1.14	1.25
9	2	172	LYS	CE-NZ	-10.16	1.23	1.49
5	E	53	ARG	NE-CZ	-10.15	1.19	1.33
1	a	24	ARG	CG-CD	-10.15	1.26	1.51
9	i	172	LYS	CE-NZ	-10.15	1.23	1.49
29	I	139	GLU	CB-CG	-10.15	1.32	1.52
1	A	24	ARG	CG-CD	-10.14	1.26	1.51
7	g	223	GLU	CD-OE2	-10.14	1.14	1.25
1	a	22	GLU	CD-OE1	-10.07	1.14	1.25
13	m	169	GLU	CD-OE2	-10.06	1.14	1.25
13	6	169	GLU	CD-OE2	-10.06	1.14	1.25
1	A	22	GLU	CD-OE1	-10.04	1.14	1.25
1	a	184	ASN	CG-ND2	-10.04	1.07	1.32
9	2	178	GLU	CD-OE2	-10.02	1.14	1.25
1	A	184	ASN	CG-ND2	-10.01	1.07	1.32
2	B	113	GLU	CD-OE1	-10.01	1.14	1.25
2	b	113	GLU	CD-OE1	-10.00	1.14	1.25
3	c	109	GLU	CD-OE2	-9.99	1.14	1.25
3	c	109	GLU	CD-OE1	-9.98	1.14	1.25
5	e	238	GLU	CB-CG	-9.97	1.33	1.52
9	i	178	GLU	CD-OE2	-9.97	1.14	1.25
8	1	112	ASP	CB-CG	-9.96	1.30	1.51
13	6	70	ASP	CB-CG	-9.96	1.30	1.51
8	h	112	ASP	CB-CG	-9.95	1.30	1.51
3	C	109	GLU	CD-OE1	-9.94	1.14	1.25
12	l	217	SER	CB-OG	-9.94	1.29	1.42
12	5	217	SER	CB-OG	-9.94	1.29	1.42
2	b	234	ARG	CZ-NH2	-9.94	1.20	1.33
7	g	100	LYS	CD-CE	-9.93	1.26	1.51
10	j	80	ARG	CZ-NH2	-9.93	1.20	1.33
2	B	234	ARG	CZ-NH2	-9.93	1.20	1.33
13	m	114	TYR	CE1-CZ	-9.92	1.25	1.38
13	m	70	ASP	CB-CG	-9.91	1.30	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	80	ARG	CZ-NH2	-9.91	1.20	1.33
5	E	238	GLU	CB-CG	-9.91	1.33	1.52
7	G	100	LYS	CD-CE	-9.90	1.26	1.51
3	C	109	GLU	CD-OE2	-9.90	1.14	1.25
8	1	93	GLU	CD-OE2	-9.89	1.14	1.25
5	E	229	LYS	CE-NZ	-9.88	1.24	1.49
5	e	229	LYS	CE-NZ	-9.87	1.24	1.49
10	3	155	GLU	CD-OE1	-9.81	1.14	1.25
13	6	75	ARG	CZ-NH2	-9.80	1.20	1.33
8	h	93	GLU	CD-OE2	-9.80	1.14	1.25
11	k	111	LYS	CB-CG	-9.79	1.26	1.52
7	g	238	GLU	CD-OE2	-9.78	1.14	1.25
10	j	205	ASP	CB-CG	-9.78	1.31	1.51
11	4	111	LYS	CB-CG	-9.78	1.26	1.52
10	3	205	ASP	CB-CG	-9.78	1.31	1.51
11	k	170	LYS	CB-CG	-9.77	1.26	1.52
11	4	170	LYS	CB-CG	-9.77	1.26	1.52
13	m	75	ARG	CZ-NH2	-9.73	1.20	1.33
1	a	13	ASP	CB-CG	-9.71	1.31	1.51
5	e	11	GLY	C-N	9.71	1.56	1.34
1	A	13	ASP	CB-CG	-9.70	1.31	1.51
8	h	93	GLU	CD-OE1	-9.70	1.15	1.25
12	5	127	CYS	CB-SG	-9.70	1.65	1.82
8	1	93	GLU	CD-OE1	-9.69	1.15	1.25
12	l	127	CYS	CB-SG	-9.69	1.65	1.82
12	l	267	ASP	CB-CG	-9.68	1.31	1.51
11	4	155	GLU	CD-OE1	-9.68	1.15	1.25
12	5	267	ASP	CB-CG	-9.68	1.31	1.51
7	g	223	GLU	CD-OE1	-9.67	1.15	1.25
9	i	86	GLN	CD-NE2	-9.66	1.08	1.32
11	k	155	GLU	CD-OE1	-9.66	1.15	1.25
13	6	50	LYS	CE-NZ	-9.66	1.25	1.49
12	l	100	TRP	CE2-CZ2	-9.65	1.23	1.39
9	2	224	VAL	CB-CG2	-9.64	1.32	1.52
9	2	86	GLN	CD-NE2	-9.63	1.08	1.32
13	m	50	LYS	CE-NZ	-9.63	1.25	1.49
11	k	74	GLU	CD-OE2	-9.62	1.15	1.25
3	c	27	GLU	CD-OE2	-9.61	1.15	1.25
11	4	74	GLU	CD-OE2	-9.59	1.15	1.25
6	F	181	LYS	CE-NZ	-9.59	1.25	1.49
12	5	100	TRP	CE2-CZ2	-9.59	1.23	1.39
6	f	181	LYS	CE-NZ	-9.58	1.25	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	109	LEU	CG-CD1	-9.57	1.16	1.51
11	4	113	LYS	CD-CE	-9.57	1.27	1.51
9	i	109	LEU	CG-CD1	-9.57	1.16	1.51
11	k	113	LYS	CD-CE	-9.56	1.27	1.51
11	4	171	ARG	CZ-NH2	-9.55	1.20	1.33
10	3	80	ARG	NE-CZ	-9.55	1.20	1.33
1	A	239	GLU	CD-OE1	-9.55	1.15	1.25
10	j	80	ARG	NE-CZ	-9.53	1.20	1.33
11	k	171	ARG	CZ-NH2	-9.53	1.20	1.33
1	a	239	GLU	CD-OE1	-9.52	1.15	1.25
1	A	22	GLU	CG-CD	-9.52	1.37	1.51
3	C	27	GLU	CD-OE2	-9.52	1.15	1.25
12	5	196	ARG	CD-NE	-9.49	1.30	1.46
9	i	59	ASN	CB-CG	-9.49	1.29	1.51
9	2	59	ASN	CB-CG	-9.48	1.29	1.51
11	k	96	ARG	NE-CZ	-9.47	1.20	1.33
13	m	114	TYR	CG-CD2	-9.47	1.26	1.39
12	l	196	ARG	CD-NE	-9.45	1.30	1.46
11	4	95	ARG	CD-NE	-9.45	1.30	1.46
11	4	96	ARG	NE-CZ	-9.45	1.20	1.33
1	a	22	GLU	CG-CD	-9.44	1.37	1.51
7	G	33	ASN	CG-ND2	-9.44	1.09	1.32
7	g	248	ASN	CG-ND2	-9.43	1.09	1.32
11	k	95	ARG	CD-NE	-9.42	1.30	1.46
1	a	217	GLU	CD-OE2	-9.42	1.15	1.25
7	g	33	ASN	CG-ND2	-9.42	1.09	1.32
8	h	103	THR	CB-CG2	-9.42	1.21	1.52
11	4	95	ARG	CZ-NH2	-9.41	1.20	1.33
11	k	95	ARG	CZ-NH2	-9.40	1.20	1.33
1	A	217	GLU	CD-OE2	-9.40	1.15	1.25
8	1	103	THR	CB-CG2	-9.39	1.21	1.52
1	A	217	GLU	CB-CG	-9.38	1.34	1.52
8	1	149	LYS	CE-NZ	-9.37	1.25	1.49
9	2	182	LYS	CE-NZ	-9.36	1.25	1.49
12	5	257	GLU	CD-OE1	-9.35	1.15	1.25
1	a	217	GLU	CB-CG	-9.34	1.34	1.52
8	h	149	LYS	CE-NZ	-9.34	1.25	1.49
10	j	63	LEU	CG-CD2	-9.34	1.17	1.51
5	E	110	GLU	CD-OE1	-9.34	1.15	1.25
1	A	200	GLU	CD-OE2	-9.34	1.15	1.25
10	3	63	LEU	CG-CD2	-9.33	1.17	1.51
9	i	182	LYS	CE-NZ	-9.32	1.25	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	180	ILE	CB-CG2	-9.32	1.24	1.52
5	e	110	GLU	CD-OE1	-9.31	1.15	1.25
12	l	257	GLU	CD-OE1	-9.30	1.15	1.25
9	i	101	ARG	CG-CD	-9.30	1.28	1.51
11	k	180	ILE	CB-CG2	-9.30	1.24	1.52
9	i	153	TYR	CZ-OH	-9.29	1.22	1.37
9	2	101	ARG	CG-CD	-9.29	1.28	1.51
5	E	110	GLU	CD-OE2	-9.29	1.15	1.25
9	2	153	TYR	CZ-OH	-9.28	1.22	1.37
10	3	169	GLN	CG-CD	-9.28	1.29	1.51
6	F	119	ASN	CG-ND2	-9.27	1.09	1.32
2	b	103	GLU	CD-OE2	-9.27	1.15	1.25
2	B	103	GLU	CD-OE2	-9.27	1.15	1.25
5	e	110	GLU	CD-OE2	-9.27	1.15	1.25
13	6	181	LYS	CA-CB	-9.27	1.33	1.53
1	a	200	GLU	CD-OE2	-9.26	1.15	1.25
9	2	211	LYS	CD-CE	-9.26	1.28	1.51
6	f	119	ASN	CG-ND2	-9.25	1.09	1.32
13	6	205	GLN	CG-CD	-9.25	1.29	1.51
9	i	211	LYS	CD-CE	-9.24	1.28	1.51
1	A	183	GLU	CD-OE2	-9.24	1.15	1.25
13	m	181	LYS	CA-CB	-9.23	1.33	1.53
13	m	205	GLN	CG-CD	-9.22	1.29	1.51
13	m	221	ARG	CD-NE	-9.22	1.30	1.46
12	5	148	ARG	CB-CG	-9.21	1.27	1.52
12	l	148	ARG	CB-CG	-9.21	1.27	1.52
13	6	221	ARG	CD-NE	-9.21	1.30	1.46
13	m	181	LYS	CD-CE	-9.17	1.28	1.51
13	6	181	LYS	CD-CE	-9.17	1.28	1.51
13	6	182	TYR	CG-CD2	-9.16	1.27	1.39
9	i	98	TYR	CE2-CZ	-9.14	1.26	1.38
1	a	183	GLU	CD-OE2	-9.14	1.15	1.25
13	m	182	TYR	CG-CD2	-9.12	1.27	1.39
12	l	183	GLU	CB-CG	-9.11	1.34	1.52
12	5	183	GLU	CB-CG	-9.10	1.34	1.52
12	l	84	GLN	CB-CG	-9.09	1.28	1.52
12	5	84	GLN	CB-CG	-9.08	1.28	1.52
9	i	39	ASN	CG-ND2	-9.07	1.10	1.32
1	A	177	GLU	CD-OE1	-9.07	1.15	1.25
9	2	39	ASN	CG-ND2	-9.06	1.10	1.32
1	a	177	GLU	CD-OE1	-9.05	1.15	1.25
11	k	125	LYS	CB-CG	-9.04	1.28	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	98	TYR	CE2-CZ	-9.04	1.26	1.38
11	4	125	LYS	CB-CG	-9.05	1.28	1.52
10	j	65	GLU	CD-OE1	-9.02	1.15	1.25
12	l	198	LYS	CB-CG	-9.01	1.28	1.52
11	k	8	ARG	CZ-NH2	-9.01	1.21	1.33
12	5	198	LYS	CB-CG	-9.00	1.28	1.52
2	B	248	GLU	CD-OE2	-8.99	1.15	1.25
11	4	8	ARG	CZ-NH2	-8.98	1.21	1.33
12	5	100	TRP	CZ2-CH2	-8.98	1.20	1.37
2	b	248	GLU	CD-OE2	-8.98	1.15	1.25
11	k	69	ILE	CB-CG2	-8.97	1.25	1.52
12	l	100	TRP	CZ2-CH2	-8.97	1.20	1.37
7	g	215	GLU	CD-OE1	-8.96	1.15	1.25
13	m	177	LYS	C-N	8.96	1.54	1.34
10	3	6	SER	CB-OG	-8.96	1.30	1.42
13	6	177	LYS	C-N	8.96	1.54	1.34
12	l	100	TRP	CD2-CE3	-8.96	1.26	1.40
11	4	69	ILE	CB-CG2	-8.96	1.25	1.52
9	2	224	VAL	CB-CG1	-8.94	1.34	1.52
13	m	114	TYR	CG-CD1	-8.94	1.27	1.39
10	3	65	GLU	CD-OE1	-8.93	1.15	1.25
12	5	100	TRP	CD2-CE3	-8.93	1.26	1.40
7	G	104	LYS	CE-NZ	-8.93	1.26	1.49
10	j	6	SER	CB-OG	-8.93	1.30	1.42
12	5	100	TRP	CE3-CZ3	-8.91	1.23	1.38
7	g	104	LYS	CE-NZ	-8.90	1.26	1.49
1	A	95	LEU	CG-CD2	-8.88	1.19	1.51
2	B	242	GLU	CD-OE2	-8.88	1.15	1.25
11	4	127	GLU	CG-CD	-8.87	1.38	1.51
12	l	100	TRP	CE3-CZ3	-8.87	1.23	1.38
1	a	95	LEU	CG-CD2	-8.86	1.19	1.51
12	l	107	LYS	CE-NZ	-8.85	1.26	1.49
9	2	173	GLN	CB-CG	-8.85	1.28	1.52
12	5	107	LYS	CE-NZ	-8.85	1.26	1.49
9	i	173	GLN	CB-CG	-8.85	1.28	1.52
6	F	173	GLU	CD-OE1	-8.84	1.16	1.25
11	k	155	GLU	CD-OE2	-8.83	1.16	1.25
6	f	173	GLU	CD-OE1	-8.83	1.16	1.25
13	m	124	GLU	CG-CD	-8.82	1.38	1.51
11	4	155	GLU	CD-OE2	-8.81	1.16	1.25
13	6	124	GLU	CG-CD	-8.81	1.38	1.51
3	c	114	ARG	NE-CZ	-8.80	1.21	1.33

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	127	GLU	CG-CD	-8.79	1.38	1.51
13	m	201	GLU	CB-CG	-8.78	1.35	1.52
3	C	65	LYS	CE-NZ	-8.78	1.27	1.49
2	b	242	GLU	CD-OE2	-8.77	1.16	1.25
9	2	167	LEU	CG-CD1	-8.77	1.19	1.51
3	c	65	LYS	CE-NZ	-8.76	1.27	1.49
3	C	114	ARG	NE-CZ	-8.76	1.21	1.33
3	c	212	GLU	CD-OE1	-8.74	1.16	1.25
9	i	167	LEU	CG-CD1	-8.74	1.19	1.51
13	6	201	GLU	CB-CG	-8.74	1.35	1.52
3	C	212	GLU	CD-OE1	-8.73	1.16	1.25
9	2	98	TYR	CG-CD1	-8.72	1.27	1.39
9	2	62	LYS	CG-CD	-8.71	1.22	1.52
9	i	98	TYR	CG-CD1	-8.70	1.27	1.39
9	i	62	LYS	CG-CD	-8.70	1.22	1.52
9	2	178	GLU	CD-OE1	-8.69	1.16	1.25
12	l	222	ASP	CB-CG	-8.69	1.33	1.51
10	3	114	SER	CB-OG	-8.69	1.30	1.42
11	k	46	PHE	CG-CD1	-8.69	1.25	1.38
10	j	114	SER	CB-OG	-8.68	1.30	1.42
1	A	135	ARG	CZ-NH1	-8.67	1.21	1.33
10	3	28	ARG	CZ-NH1	-8.67	1.21	1.33
11	4	46	PHE	CG-CD1	-8.67	1.25	1.38
10	j	115	LYS	CB-CG	-8.66	1.29	1.52
12	5	148	ARG	CZ-NH2	-8.66	1.21	1.33
10	3	115	LYS	CB-CG	-8.65	1.29	1.52
7	g	57	LYS	CE-NZ	-8.65	1.27	1.49
10	j	28	ARG	CZ-NH1	-8.65	1.21	1.33
12	l	99	ASN	CB-CG	-8.64	1.31	1.51
9	i	178	GLU	CD-OE1	-8.64	1.16	1.25
12	l	148	ARG	CZ-NH2	-8.64	1.21	1.33
12	5	99	ASN	CB-CG	-8.64	1.31	1.51
12	5	222	ASP	CB-CG	-8.63	1.33	1.51
5	E	209	GLU	CD-OE1	-8.63	1.16	1.25
7	G	57	LYS	CE-NZ	-8.63	1.27	1.49
5	e	209	GLU	CD-OE1	-8.60	1.16	1.25
1	a	135	ARG	CZ-NH1	-8.59	1.21	1.33
12	5	84	GLN	CG-CD	-8.59	1.31	1.51
13	6	127	LYS	CE-NZ	-8.58	1.27	1.49
5	e	168	ASN	CG-ND2	-8.57	1.11	1.32
5	E	168	ASN	CG-ND2	-8.57	1.11	1.32
9	2	156	LEU	CG-CD2	-8.56	1.20	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	175	LYS	CB-CG	-8.56	1.29	1.52
13	6	175	LYS	CB-CG	-8.56	1.29	1.52
9	i	156	LEU	CG-CD2	-8.55	1.20	1.51
12	l	84	GLN	CG-CD	-8.55	1.31	1.51
11	k	109	LYS	CD-CE	-8.53	1.29	1.51
13	m	127	LYS	CE-NZ	-8.52	1.27	1.49
5	E	25	GLU	CB-CG	-8.52	1.35	1.52
11	k	186	LYS	CE-NZ	-8.52	1.27	1.49
11	4	186	LYS	CE-NZ	-8.52	1.27	1.49
12	5	104	GLN	CG-CD	-8.50	1.31	1.51
11	4	109	LYS	CD-CE	-8.50	1.30	1.51
5	E	205	LYS	CE-NZ	-8.49	1.27	1.49
12	l	140	LEU	CG-CD2	-8.49	1.20	1.51
5	e	205	LYS	CE-NZ	-8.48	1.27	1.49
10	3	165	GLU	CD-OE1	-8.48	1.16	1.25
13	6	177	LYS	CE-NZ	-8.48	1.27	1.49
12	l	104	GLN	CG-CD	-8.48	1.31	1.51
12	5	140	LEU	CG-CD2	-8.48	1.20	1.51
5	e	25	GLU	CB-CG	-8.47	1.36	1.52
3	C	124	GLN	CD-NE2	-8.47	1.11	1.32
13	m	177	LYS	CE-NZ	-8.47	1.27	1.49
9	2	155	SER	CB-OG	-8.47	1.31	1.42
13	6	155	MET	CG-SD	-8.47	1.59	1.81
3	c	124	GLN	CD-NE2	-8.46	1.11	1.32
10	j	78	GLU	CD-OE1	-8.44	1.16	1.25
10	3	98	ARG	CD-NE	-8.43	1.32	1.46
13	6	194	ASP	CB-CG	-8.43	1.34	1.51
13	m	155	MET	CG-SD	-8.43	1.59	1.81
5	e	102	TYR	CE2-CZ	-8.43	1.27	1.38
9	i	155	SER	CB-OG	-8.42	1.31	1.42
1	a	95	LEU	CG-CD1	-8.42	1.20	1.51
1	A	95	LEU	CG-CD1	-8.42	1.20	1.51
13	m	194	ASP	CB-CG	-8.41	1.34	1.51
13	m	63	ASN	CG-ND2	-8.40	1.11	1.32
5	E	209	GLU	CD-OE2	-8.40	1.16	1.25
11	4	93	ARG	CB-CG	-8.39	1.29	1.52
10	3	78	GLU	CD-OE1	-8.39	1.16	1.25
13	6	63	ASN	CG-ND2	-8.38	1.11	1.32
5	e	209	GLU	CD-OE2	-8.37	1.16	1.25
5	E	102	TYR	CE2-CZ	-8.37	1.27	1.38
10	3	115	LYS	CE-NZ	-8.37	1.28	1.49
10	j	98	ARG	CD-NE	-8.37	1.32	1.46

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	115	LYS	CE-NZ	-8.35	1.28	1.49
11	k	93	ARG	CB-CG	-8.35	1.30	1.52
8	h	69	GLN	CG-CD	-8.34	1.31	1.51
8	1	69	GLN	CG-CD	-8.32	1.31	1.51
13	m	78	ASN	CG-ND2	-8.31	1.12	1.32
13	6	78	ASN	CG-ND2	-8.31	1.12	1.32
9	i	113	LYS	CD-CE	-8.29	1.30	1.51
9	2	113	LYS	CD-CE	-8.29	1.30	1.51
13	6	75	ARG	CD-NE	-8.29	1.32	1.46
8	1	99	LYS	CE-NZ	-8.28	1.28	1.49
8	h	99	LYS	CE-NZ	-8.27	1.28	1.49
12	5	100	TRP	CG-CD1	-8.27	1.25	1.36
7	g	175	GLU	CD-OE1	-8.26	1.16	1.25
12	l	100	TRP	CG-CD1	-8.25	1.25	1.36
13	m	75	ARG	CD-NE	-8.25	1.32	1.46
8	h	147	CYS	CB-SG	-8.25	1.68	1.82
8	1	147	CYS	CB-SG	-8.24	1.68	1.82
11	4	63	ASN	CG-ND2	-8.24	1.12	1.32
11	k	167	GLU	CD-OE2	-8.24	1.16	1.25
11	4	195	PHE	CB-CG	-8.23	1.37	1.51
11	4	167	GLU	CD-OE2	-8.22	1.16	1.25
11	k	195	PHE	CB-CG	-8.22	1.37	1.51
13	m	102	GLN	CD-OE1	-8.21	1.05	1.24
7	g	245	LYS	CE-NZ	-8.21	1.28	1.49
11	k	63	ASN	CG-ND2	-8.21	1.12	1.32
3	c	241	LYS	CE-NZ	-8.19	1.28	1.49
9	i	182	LYS	CB-CG	-8.19	1.30	1.52
11	k	182	LYS	CG-CD	-8.19	1.24	1.52
13	6	228	LYS	CG-CD	-8.18	1.24	1.52
13	m	228	LYS	CG-CD	-8.17	1.24	1.52
9	2	182	LYS	CB-CG	-8.17	1.30	1.52
11	4	182	LYS	CG-CD	-8.17	1.24	1.52
3	C	241	LYS	CE-NZ	-8.16	1.28	1.49
11	k	49	GLU	CD-OE2	-8.16	1.16	1.25
8	1	113	ASP	CB-CG	-8.16	1.34	1.51
12	5	164	GLN	CG-CD	-8.15	1.32	1.51
10	3	155	GLU	CD-OE2	-8.15	1.16	1.25
17	T	130	ASP	CG-OD1	-8.15	1.06	1.25
8	1	101	ASN	CB-CG	-8.15	1.32	1.51
8	h	101	ASN	CB-CG	-8.14	1.32	1.51
8	h	113	ASP	CB-CG	-8.14	1.34	1.51
12	l	164	GLN	CG-CD	-8.13	1.32	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	165	LYS	CD-CE	-8.12	1.30	1.51
5	e	25	GLU	CD-OE2	-8.12	1.16	1.25
13	m	91	LYS	CG-CD	-8.12	1.24	1.52
11	4	49	GLU	CD-OE2	-8.10	1.16	1.25
8	1	165	LYS	CD-CE	-8.09	1.31	1.51
10	3	205	ASP	C-OXT	-8.09	1.07	1.23
5	E	25	GLU	CD-OE2	-8.09	1.16	1.25
13	m	26	GLU	CD-OE2	-8.06	1.16	1.25
7	g	41	LYS	CE-NZ	-8.06	1.28	1.49
10	j	205	ASP	C-OXT	-8.05	1.08	1.23
7	G	41	LYS	CE-NZ	-8.03	1.28	1.49
1	A	149	GLU	CD-OE2	-8.03	1.16	1.25
12	5	139	ARG	NE-CZ	-8.03	1.22	1.33
11	4	110	LYS	CB-CG	-8.02	1.30	1.52
6	f	195	GLU	CD-OE1	-8.02	1.16	1.25
11	k	110	LYS	CB-CG	-8.02	1.30	1.52
11	4	90	LYS	CE-NZ	-8.02	1.29	1.49
11	k	90	LYS	CE-NZ	-8.01	1.29	1.49
12	l	139	ARG	NE-CZ	-8.01	1.22	1.33
13	6	26	GLU	CD-OE2	-8.01	1.16	1.25
6	F	195	GLU	CD-OE1	-8.00	1.16	1.25
1	a	149	GLU	CD-OE2	-8.00	1.16	1.25
13	6	230	ASP	C-O	-8.00	1.08	1.23
8	h	98	ASN	CG-ND2	-7.99	1.12	1.32
11	k	166	GLN	CB-CG	-7.99	1.30	1.52
8	1	98	ASN	CG-ND2	-7.99	1.12	1.32
11	4	166	GLN	CB-CG	-7.99	1.30	1.52
5	E	104	ASP	CB-CG	-7.98	1.34	1.51
11	k	95	ARG	NE-CZ	-7.98	1.22	1.33
13	m	230	ASP	C-O	-7.98	1.08	1.23
2	b	2	THR	C-O	-7.97	1.08	1.23
2	B	2	THR	C-O	-7.97	1.08	1.23
2	b	49	LYS	CE-NZ	-7.96	1.29	1.49
2	B	49	LYS	CE-NZ	-7.96	1.29	1.49
11	4	95	ARG	NE-CZ	-7.96	1.22	1.33
5	e	104	ASP	CB-CG	-7.96	1.35	1.51
11	k	156	GLU	CD-OE2	-7.95	1.17	1.25
11	k	145	ASP	CB-CG	-7.94	1.35	1.51
11	4	156	GLU	CD-OE2	-7.93	1.17	1.25
11	4	72	ASP	CB-CG	-7.93	1.35	1.51
11	4	91	SER	CB-OG	-7.92	1.31	1.42
30	K	241	GLU	CD-OE1	-7.92	1.17	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	72	ASP	CB-CG	-7.92	1.35	1.51
20	Z	40	GLU	CB-CG	-7.91	1.37	1.52
11	k	169	GLU	CB-CG	-7.91	1.37	1.52
10	3	196	VAL	CB-CG1	-7.91	1.36	1.52
10	j	197	LYS	CD-CE	-7.91	1.31	1.51
11	4	145	ASP	CB-CG	-7.90	1.35	1.51
11	k	91	SER	CB-OG	-7.89	1.31	1.42
10	3	197	LYS	CD-CE	-7.88	1.31	1.51
13	m	95	ASN	CB-CG	-7.87	1.32	1.51
11	4	10	GLN	CB-CG	-7.87	1.31	1.52
11	4	169	GLU	CB-CG	-7.87	1.37	1.52
10	j	196	VAL	CB-CG1	-7.87	1.36	1.52
11	k	10	GLN	CB-CG	-7.85	1.31	1.52
7	g	191	GLU	CD-OE1	-7.84	1.17	1.25
2	b	217	GLU	CD-OE1	-7.84	1.17	1.25
13	6	134	ASP	CG-OD1	-7.83	1.07	1.25
10	3	65	GLU	CD-OE2	-7.83	1.17	1.25
1	a	200	GLU	CD-OE1	-7.82	1.17	1.25
13	m	134	ASP	CG-OD1	-7.82	1.07	1.25
13	6	57	ASN	CG-ND2	-7.81	1.13	1.32
1	A	200	GLU	CD-OE1	-7.79	1.17	1.25
5	e	90	GLU	CD-OE1	-7.79	1.17	1.25
13	m	143	GLN	CB-CG	-7.79	1.31	1.52
2	B	244	ASN	CB-CG	-7.79	1.33	1.51
6	f	173	GLU	CD-OE2	-7.78	1.17	1.25
20	Z	632	GLU	CG-CD	-7.78	1.40	1.51
9	i	120	GLN	CG-CD	-7.78	1.33	1.51
5	E	159	GLU	CG-CD	-7.78	1.40	1.51
13	m	57	ASN	CG-ND2	-7.77	1.13	1.32
9	2	120	GLN	CG-CD	-7.77	1.33	1.51
5	e	159	GLU	CG-CD	-7.77	1.40	1.51
11	k	192	VAL	CB-CG2	-7.77	1.36	1.52
2	b	244	ASN	CB-CG	-7.76	1.33	1.51
12	l	104	GLN	CD-OE1	-7.76	1.06	1.24
13	6	143	GLN	CB-CG	-7.76	1.31	1.52
6	F	173	GLU	CD-OE2	-7.75	1.17	1.25
6	f	204	GLU	CD-OE2	-7.75	1.17	1.25
13	6	142	GLU	CD-OE2	-7.74	1.17	1.25
13	m	142	GLU	CD-OE2	-7.74	1.17	1.25
12	5	104	GLN	CD-OE1	-7.73	1.06	1.24
5	E	90	GLU	CD-OE1	-7.73	1.17	1.25
11	4	192	VAL	CB-CG2	-7.73	1.36	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	217	GLU	CD-OE1	-7.73	1.17	1.25
12	5	251	ASN	CG-OD1	-7.72	1.06	1.24
10	j	77	LYS	CG-CD	-7.71	1.26	1.52
6	F	204	GLU	CD-OE2	-7.70	1.17	1.25
10	3	77	LYS	CG-CD	-7.70	1.26	1.52
10	j	65	GLU	CD-OE2	-7.69	1.17	1.25
12	l	160	ASN	CG-ND2	-7.69	1.13	1.32
6	F	5	ASN	CG-ND2	-7.69	1.13	1.32
12	l	251	ASN	CG-OD1	-7.69	1.07	1.24
6	f	5	ASN	CG-ND2	-7.68	1.13	1.32
12	5	160	ASN	CG-ND2	-7.68	1.13	1.32
13	m	58	ILE	CB-CG1	-7.66	1.32	1.54
13	6	58	ILE	CB-CG1	-7.65	1.32	1.54
13	m	118	ILE	CB-CG2	-7.64	1.29	1.52
12	5	128	GLN	CG-CD	-7.64	1.33	1.51
12	l	128	GLN	CG-CD	-7.62	1.33	1.51
10	3	193	ASP	CB-CG	-7.62	1.35	1.51
13	m	81	LYS	CD-CE	-7.62	1.32	1.51
13	6	145	ARG	CG-CD	-7.61	1.32	1.51
13	m	88	ASN	CG-ND2	-7.61	1.13	1.32
10	j	193	ASP	CB-CG	-7.61	1.35	1.51
13	m	145	ARG	CG-CD	-7.60	1.32	1.51
12	l	214	VAL	CB-CG1	-7.60	1.36	1.52
9	i	209	ILE	CB-CG2	-7.57	1.29	1.52
11	4	191	GLN	CB-CG	-7.57	1.32	1.52
12	5	214	VAL	CB-CG1	-7.57	1.36	1.52
12	l	246	SER	CB-OG	-7.57	1.32	1.42
11	k	191	GLN	CB-CG	-7.56	1.32	1.52
13	m	56	ASP	CB-CG	-7.56	1.35	1.51
9	2	209	ILE	CB-CG2	-7.56	1.29	1.52
11	k	7	ILE	CB-CG2	-7.55	1.29	1.52
12	5	246	SER	CB-OG	-7.55	1.32	1.42
8	1	203	GLU	CD-OE1	-7.54	1.17	1.25
12	l	159	SER	CB-OG	-7.54	1.32	1.42
11	4	7	ILE	CB-CG2	-7.54	1.29	1.52
13	6	56	ASP	CB-CG	-7.53	1.35	1.51
9	2	179	GLU	CB-CG	-7.52	1.37	1.52
11	4	112	ASN	CG-ND2	-7.52	1.14	1.32
12	5	128	GLN	CD-OE1	-7.51	1.07	1.24
12	l	128	GLN	CD-OE1	-7.51	1.07	1.24
7	g	191	GLU	CD-OE2	-7.51	1.17	1.25
8	1	203	GLU	CG-CD	-7.50	1.40	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	j	94	SER	CB-OG	-7.50	1.32	1.42
11	k	112	ASN	CG-ND2	-7.50	1.14	1.32
12	5	159	SER	CB-OG	-7.50	1.32	1.42
9	i	179	GLU	CB-CG	-7.49	1.38	1.52
20	Z	632	GLU	CD-OE1	-7.49	1.17	1.25
12	5	226	GLU	CD-OE1	-7.48	1.17	1.25
11	k	186	LYS	CB-CG	-7.47	1.32	1.52
1	a	74	CYS	C-N	7.46	1.51	1.34
5	e	23	GLN	CD-NE2	-7.46	1.14	1.32
11	4	186	LYS	CB-CG	-7.46	1.32	1.52
9	i	173	GLN	CD-NE2	-7.45	1.14	1.32
11	k	34	LYS	CG-CD	-7.45	1.27	1.52
5	E	23	GLN	CD-NE2	-7.45	1.14	1.32
7	g	57	LYS	CG-CD	-7.45	1.27	1.52
10	3	94	SER	CB-OG	-7.45	1.32	1.42
12	l	226	GLU	CD-OE1	-7.44	1.17	1.25
5	e	180	GLN	CD-OE1	-7.44	1.07	1.24
9	i	65	ARG	NE-CZ	-7.44	1.23	1.33
11	4	74	GLU	CG-CD	-7.44	1.40	1.51
7	G	57	LYS	CG-CD	-7.43	1.27	1.52
9	2	173	GLN	CD-NE2	-7.43	1.14	1.32
5	E	180	GLN	CD-OE1	-7.42	1.07	1.24
11	4	34	LYS	CG-CD	-7.42	1.27	1.52
1	A	64	LEU	CG-CD1	-7.42	1.24	1.51
12	5	195	THR	CB-CG2	-7.42	1.27	1.52
7	g	33	ASN	CG-OD1	-7.42	1.07	1.24
7	G	33	ASN	CG-OD1	-7.41	1.07	1.24
11	k	12	SER	CB-OG	-7.41	1.32	1.42
11	k	74	GLU	CG-CD	-7.41	1.40	1.51
13	6	26	GLU	CG-CD	-7.41	1.40	1.51
12	l	195	THR	CB-CG2	-7.41	1.27	1.52
1	a	64	LEU	CG-CD1	-7.41	1.24	1.51
11	k	98	TYR	CG-CD1	-7.39	1.29	1.39
17	T	130	ASP	CG-OD2	-7.39	1.08	1.25
13	m	26	GLU	CG-CD	-7.39	1.40	1.51
12	l	100	TRP	CG-CD2	-7.38	1.31	1.43
9	2	65	ARG	NE-CZ	-7.38	1.23	1.33
12	5	100	TRP	CG-CD2	-7.37	1.31	1.43
11	4	12	SER	CB-OG	-7.37	1.32	1.42
10	3	173	ASN	CG-OD1	-7.36	1.07	1.24
11	4	29	LYS	CB-CG	-7.36	1.32	1.52
11	k	29	LYS	CB-CG	-7.35	1.32	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	98	TYR	CG-CD1	-7.35	1.29	1.39
9	2	230	LYS	CB-CG	-7.34	1.32	1.52
8	1	115	ASN	CG-OD1	-7.34	1.07	1.24
5	E	86	ARG	CG-CD	-7.34	1.33	1.51
5	e	86	ARG	CG-CD	-7.33	1.33	1.51
13	6	228	LYS	CB-CG	-7.32	1.32	1.52
13	m	228	LYS	CB-CG	-7.31	1.32	1.52
5	e	225	GLN	CD-NE2	-7.31	1.14	1.32
8	h	115	ASN	CG-OD1	-7.31	1.07	1.24
10	j	193	ASP	CG-OD1	-7.30	1.08	1.25
13	m	15	ASP	CB-CG	-7.30	1.36	1.51
5	E	225	GLN	CD-NE2	-7.30	1.14	1.32
11	k	19	LYS	CE-NZ	-7.30	1.30	1.49
11	4	19	LYS	CE-NZ	-7.29	1.30	1.49
7	g	51	GLU	CD-OE2	-7.29	1.17	1.25
7	g	202	LEU	CG-CD1	-7.29	1.24	1.51
13	6	15	ASP	CB-CG	-7.28	1.36	1.51
12	l	148	ARG	CD-NE	-7.28	1.34	1.46
10	3	193	ASP	CG-OD1	-7.27	1.08	1.25
8	h	49	LYS	C-N	7.27	1.50	1.34
8	h	183	ARG	CZ-NH1	-7.27	1.23	1.33
13	m	168	TYR	CD2-CE2	7.27	1.50	1.39
13	m	175	LYS	CD-CE	-7.27	1.33	1.51
11	k	171	ARG	CZ-NH1	-7.27	1.23	1.33
13	6	168	TYR	CD2-CE2	7.26	1.50	1.39
13	6	175	LYS	CD-CE	-7.26	1.33	1.51
11	k	166	GLN	CD-OE1	-7.26	1.07	1.24
11	4	166	GLN	CD-OE1	-7.26	1.07	1.24
12	5	148	ARG	CD-NE	-7.25	1.34	1.46
6	F	31	GLN	CD-NE2	-7.25	1.14	1.32
5	E	224	LYS	CD-CE	-7.25	1.33	1.51
6	f	31	GLN	CD-NE2	-7.25	1.14	1.32
8	1	183	ARG	CZ-NH1	-7.24	1.23	1.33
7	G	51	GLU	CD-OE2	-7.24	1.17	1.25
11	4	171	ARG	CZ-NH1	-7.24	1.23	1.33
9	2	65	ARG	CB-CG	-7.23	1.33	1.52
5	e	224	LYS	CD-CE	-7.23	1.33	1.51
9	i	65	ARG	CB-CG	-7.22	1.33	1.52
8	1	144	TYR	CD2-CE2	-7.22	1.28	1.39
9	2	254	GLU	CB-CG	-7.22	1.38	1.52
10	j	198	ARG	CZ-NH1	-7.21	1.23	1.33
11	4	36	ARG	CG-CD	-7.21	1.33	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	36	ARG	CG-CD	-7.21	1.33	1.51
3	C	97	ASN	CG-OD1	-7.21	1.08	1.24
3	c	97	ASN	CG-OD1	-7.20	1.08	1.24
10	3	166	THR	CB-CG2	-7.20	1.28	1.52
10	j	41	GLU	CG-CD	-7.20	1.41	1.51
8	h	144	TYR	CD2-CE2	-7.19	1.28	1.39
5	e	7	GLU	CB-CG	-7.18	1.38	1.52
11	4	163	LEU	CB-CG	-7.18	1.31	1.52
10	3	198	ARG	CZ-NH1	-7.17	1.23	1.33
10	3	41	GLU	CG-CD	-7.17	1.41	1.51
11	k	163	LEU	CB-CG	-7.16	1.31	1.52
2	B	205	ASN	CG-OD1	-7.16	1.08	1.24
11	4	118	GLN	CD-NE2	-7.16	1.15	1.32
13	6	177	LYS	CG-CD	-7.15	1.28	1.52
5	e	202	LYS	CE-NZ	-7.15	1.31	1.49
10	3	183	TRP	CB-CG	-7.15	1.37	1.50
2	b	205	ASN	CG-OD1	-7.14	1.08	1.24
5	E	202	LYS	CE-NZ	-7.14	1.31	1.49
9	i	88	ILE	CG1-CD1	-7.14	1.01	1.50
3	c	97	ASN	CG-ND2	-7.14	1.15	1.32
7	G	51	GLU	CD-OE1	-7.14	1.17	1.25
11	k	118	GLN	CD-NE2	-7.14	1.15	1.32
9	2	88	ILE	CG1-CD1	-7.14	1.01	1.50
13	m	177	LYS	CG-CD	-7.13	1.28	1.52
10	3	18	LYS	CD-CE	-7.13	1.33	1.51
10	j	85	GLU	CD-OE1	-7.13	1.17	1.25
3	C	97	ASN	CG-ND2	-7.12	1.15	1.32
8	h	114	LYS	CB-CG	-7.11	1.33	1.52
8	1	45	ARG	CG-CD	-7.11	1.34	1.51
10	j	18	LYS	CD-CE	-7.11	1.33	1.51
7	g	51	GLU	CD-OE1	-7.11	1.17	1.25
10	3	85	GLU	CD-OE1	-7.10	1.17	1.25
8	h	45	ARG	CG-CD	-7.09	1.34	1.51
8	1	114	LYS	CB-CG	-7.09	1.33	1.52
10	j	113	ASN	CG-OD1	-7.09	1.08	1.24
3	C	212	GLU	CD-OE2	-7.08	1.17	1.25
8	1	201	GLU	CD-OE2	-7.08	1.17	1.25
12	l	100	TRP	CD2-CE2	-7.07	1.32	1.41
12	l	83	PHE	C-N	7.06	1.50	1.34
10	3	113	ASN	CG-OD1	-7.05	1.08	1.24
13	6	74	LYS	CE-NZ	-7.05	1.31	1.49
1	a	251	GLN	C-O	-7.05	1.09	1.23

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	74	LYS	CE-NZ	-7.04	1.31	1.49
1	A	251	GLN	C-O	-7.04	1.09	1.23
12	5	100	TRP	CD2-CE2	-7.02	1.32	1.41
2	b	201	GLU	CD-OE2	-7.01	1.18	1.25
3	c	212	GLU	CD-OE2	-7.01	1.18	1.25
2	b	205	ASN	CG-ND2	-7.00	1.15	1.32
8	h	114	LYS	CD-CE	-7.00	1.33	1.51
11	k	174	MET	CB-CG	-6.99	1.28	1.51
5	E	105	GLU	CD-OE2	-6.99	1.18	1.25
9	2	49	SER	CB-OG	-6.98	1.33	1.42
2	B	201	GLU	CD-OE2	-6.98	1.18	1.25
10	3	173	ASN	CG-ND2	-6.98	1.15	1.32
8	1	114	LYS	CD-CE	-6.98	1.33	1.51
11	4	174	MET	CB-CG	-6.97	1.29	1.51
5	E	51	GLU	CD-OE1	-6.97	1.18	1.25
9	i	49	SER	CB-OG	-6.96	1.33	1.42
10	3	196	VAL	CB-CG2	-6.96	1.38	1.52
10	j	196	VAL	CB-CG2	-6.96	1.38	1.52
2	B	205	ASN	CG-ND2	-6.95	1.15	1.32
8	h	77	SER	CB-OG	-6.95	1.33	1.42
9	i	38	ASN	CG-ND2	-6.94	1.15	1.32
5	e	105	GLU	CD-OE2	-6.93	1.18	1.25
11	k	163	LEU	CG-CD2	-6.93	1.26	1.51
8	1	77	SER	CB-OG	-6.92	1.33	1.42
9	2	38	ASN	CG-ND2	-6.92	1.15	1.32
11	k	120	ASP	CB-CG	-6.92	1.37	1.51
8	1	144	TYR	CD1-CE1	-6.91	1.28	1.39
29	I	139	GLU	CG-CD	-6.90	1.41	1.51
11	4	163	LEU	CG-CD2	-6.90	1.26	1.51
11	4	120	ASP	CB-CG	-6.89	1.37	1.51
8	h	154	ASN	CG-OD1	-6.89	1.08	1.24
2	b	30	GLN	CD-NE2	-6.89	1.15	1.32
2	B	30	GLN	CD-NE2	-6.89	1.15	1.32
3	c	27	GLU	CD-OE1	-6.89	1.18	1.25
13	m	167	GLN	CG-CD	-6.88	1.35	1.51
13	6	167	GLN	CG-CD	-6.88	1.35	1.51
8	h	144	TYR	CD1-CE1	-6.87	1.29	1.39
5	e	69	GLU	CD-OE2	-6.87	1.18	1.25
8	1	154	ASN	CG-OD1	-6.86	1.08	1.24
2	B	17	LYS	CB-CG	6.85	1.71	1.52
11	k	33	ASP	CB-CG	-6.85	1.37	1.51
3	c	16	GLU	CD-OE2	-6.84	1.18	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	227	GLU	CD-OE2	-6.84	1.18	1.25
11	4	33	ASP	CB-CG	-6.84	1.37	1.51
9	2	254	GLU	CD-OE2	-6.83	1.18	1.25
10	j	83	GLU	CD-OE1	-6.83	1.18	1.25
3	C	27	GLU	CD-OE1	-6.82	1.18	1.25
8	h	152	ARG	CD-NE	-6.82	1.34	1.46
5	E	69	GLU	CD-OE2	-6.82	1.18	1.25
2	b	17	LYS	CB-CG	6.82	1.71	1.52
11	4	111	LYS	CD-CE	-6.82	1.34	1.51
10	3	83	GLU	CD-OE1	-6.81	1.18	1.25
1	a	242	GLU	CD-OE1	-6.81	1.18	1.25
1	A	242	GLU	CD-OE1	-6.81	1.18	1.25
6	f	226	ASP	CB-CG	-6.80	1.37	1.51
8	1	152	ARG	CD-NE	-6.80	1.34	1.46
3	C	213	PHE	CE1-CZ	-6.79	1.24	1.37
11	k	76	SER	CB-OG	-6.79	1.33	1.42
9	2	177	LYS	CB-CG	-6.79	1.34	1.52
3	c	70	ASN	CG-ND2	-6.79	1.15	1.32
11	4	76	SER	CB-OG	-6.78	1.33	1.42
3	c	70	ASN	CG-OD1	-6.78	1.09	1.24
3	C	70	ASN	CG-ND2	-6.78	1.16	1.32
11	k	111	LYS	CD-CE	-6.78	1.34	1.51
3	c	213	PHE	CE1-CZ	-6.77	1.24	1.37
9	2	97	LEU	CG-CD1	-6.77	1.26	1.51
3	C	70	ASN	CG-OD1	-6.77	1.09	1.24
9	i	97	LEU	CG-CD1	-6.76	1.26	1.51
11	4	195	PHE	CE2-CZ	-6.76	1.24	1.37
9	i	177	LYS	CB-CG	-6.75	1.34	1.52
11	k	195	PHE	CE2-CZ	-6.75	1.24	1.37
3	C	16	GLU	CD-OE2	-6.75	1.18	1.25
13	6	230	ASP	CA-C	-6.74	1.35	1.52
6	F	226	ASP	CB-CG	-6.74	1.37	1.51
10	j	205	ASP	CG-OD1	-6.73	1.09	1.25
11	4	87	GLU	CD-OE2	-6.73	1.18	1.25
13	m	182	TYR	CZ-OH	-6.72	1.26	1.37
7	G	104	LYS	CD-CE	-6.72	1.34	1.51
2	B	203	GLU	CD-OE1	-6.72	1.18	1.25
13	m	230	ASP	CA-C	-6.71	1.35	1.52
10	3	205	ASP	CG-OD1	-6.71	1.09	1.25
11	k	87	GLU	CD-OE2	-6.71	1.18	1.25
12	l	144	ARG	CZ-NH2	-6.70	1.24	1.33
7	g	104	LYS	CD-CE	-6.70	1.34	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	63	ASN	CG-OD1	-6.69	1.09	1.24
11	k	118	GLN	CD-OE1	-6.69	1.09	1.24
13	6	63	ASN	CG-OD1	-6.69	1.09	1.24
11	4	118	GLN	CD-OE1	-6.68	1.09	1.24
13	6	182	TYR	CZ-OH	-6.67	1.26	1.37
1	a	224	GLU	CD-OE1	-6.67	1.18	1.25
12	5	139	ARG	CG-CD	-6.66	1.35	1.51
32	M	96	ASN	CG-ND2	-6.66	1.16	1.32
8	h	101	ASN	CG-OD1	-6.66	1.09	1.24
12	5	144	ARG	CZ-NH2	-6.66	1.24	1.33
8	1	101	ASN	CG-OD1	-6.65	1.09	1.24
10	3	77	LYS	CB-CG	-6.65	1.34	1.52
13	6	138	SER	CB-OG	-6.65	1.33	1.42
2	b	203	GLU	CD-OE1	-6.65	1.18	1.25
8	h	153	GLU	CD-OE1	-6.64	1.18	1.25
12	l	139	ARG	CG-CD	-6.64	1.35	1.51
2	b	6	SER	CB-OG	-6.63	1.33	1.42
5	e	7	GLU	CA-CB	-6.63	1.39	1.53
1	A	224	GLU	CD-OE1	-6.63	1.18	1.25
10	j	77	LYS	CB-CG	-6.63	1.34	1.52
9	2	82	GLU	CD-OE1	-6.62	1.18	1.25
10	j	98	ARG	CG-CD	-6.61	1.35	1.51
7	g	175	GLU	CD-OE2	-6.61	1.18	1.25
9	i	82	GLU	CD-OE1	-6.61	1.18	1.25
10	3	98	ARG	CG-CD	-6.61	1.35	1.51
11	4	5	LEU	C-N	6.60	1.45	1.33
11	4	112	ASN	CG-OD1	-6.60	1.09	1.24
11	k	112	ASN	CG-OD1	-6.59	1.09	1.24
7	g	215	GLU	CD-OE2	-6.58	1.18	1.25
13	m	138	SER	CB-OG	-6.58	1.33	1.42
11	k	127	GLU	CD-OE2	-6.58	1.18	1.25
13	m	106	TYR	CE1-CZ	6.57	1.47	1.38
5	e	10	ARG	CD-NE	-6.57	1.35	1.46
8	1	153	GLU	CD-OE1	-6.57	1.18	1.25
8	h	113	ASP	CG-OD2	-6.56	1.10	1.25
11	4	37	GLN	CB-CG	-6.55	1.34	1.52
5	E	225	GLN	CG-CD	-6.55	1.35	1.51
3	c	114	ARG	CZ-NH1	-6.55	1.24	1.33
5	e	225	GLN	CG-CD	-6.54	1.35	1.51
11	k	63	ASN	CG-OD1	-6.54	1.09	1.24
8	1	113	ASP	CG-OD2	-6.54	1.10	1.25
11	k	37	GLN	CB-CG	-6.54	1.34	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	e	102	TYR	CG-CD1	-6.54	1.30	1.39
11	4	34	LYS	CE-NZ	-6.54	1.32	1.49
10	3	202	MET	CB-CG	-6.53	1.30	1.51
9	i	173	GLN	CD-OE1	-6.52	1.09	1.24
7	G	57	LYS	CD-CE	-6.52	1.34	1.51
11	4	127	GLU	CD-OE2	-6.52	1.18	1.25
2	B	6	SER	CB-OG	-6.52	1.33	1.42
10	j	202	MET	CB-CG	-6.52	1.30	1.51
11	k	34	LYS	CE-NZ	-6.51	1.32	1.49
26	U	108	GLU	CB-CG	-6.51	1.39	1.52
30	K	241	GLU	CD-OE2	-6.51	1.18	1.25
10	3	33	SER	CB-OG	-6.50	1.33	1.42
2	b	49	LYS	CD-CE	-6.50	1.34	1.51
5	E	102	TYR	CG-CD1	-6.50	1.30	1.39
9	2	173	GLN	CD-OE1	-6.49	1.09	1.24
7	g	57	LYS	CD-CE	-6.49	1.35	1.51
3	C	114	ARG	CZ-NH1	-6.49	1.24	1.33
13	m	88	ASN	CG-OD1	-6.48	1.09	1.24
11	4	63	ASN	CG-OD1	-6.48	1.09	1.24
11	4	92	ILE	CB-CG2	-6.48	1.32	1.52
5	e	197	GLU	CB-CG	-6.47	1.39	1.52
2	B	49	LYS	CD-CE	-6.47	1.35	1.51
5	E	197	GLU	CB-CG	-6.47	1.39	1.52
8	h	154	ASN	CG-ND2	-6.46	1.16	1.32
11	k	92	ILE	CB-CG2	-6.46	1.32	1.52
2	B	123	GLN	CB-CG	-6.46	1.35	1.52
10	j	33	SER	CB-OG	-6.46	1.33	1.42
7	g	173	LYS	CD-CE	-6.45	1.35	1.51
9	i	156	LEU	CG-CD1	-6.45	1.27	1.51
9	2	156	LEU	CG-CD1	-6.45	1.28	1.51
13	m	90	LYS	CG-CD	-6.44	1.30	1.52
8	1	196	ILE	C-N	6.44	1.48	1.34
12	5	251	ASN	CG-ND2	-6.44	1.16	1.32
5	E	25	GLU	CD-OE1	-6.44	1.18	1.25
2	b	123	GLN	CB-CG	-6.44	1.35	1.52
3	c	199	LYS	CG-CD	-6.43	1.30	1.52
8	1	154	ASN	CG-ND2	-6.43	1.16	1.32
9	2	109	LEU	CG-CD2	-6.43	1.28	1.51
9	i	109	LEU	CG-CD2	-6.42	1.28	1.51
10	j	80	ARG	CD-NE	-6.42	1.35	1.46
5	E	159	GLU	CD-OE2	-6.42	1.18	1.25
5	e	25	GLU	CD-OE1	-6.41	1.18	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	l	251	ASN	CG-ND2	-6.41	1.16	1.32
5	e	159	GLU	CD-OE2	-6.41	1.18	1.25
2	B	234	ARG	CG-CD	-6.41	1.35	1.51
10	3	80	ARG	CD-NE	-6.40	1.35	1.46
11	k	46	PHE	CD1-CE1	6.40	1.52	1.39
2	b	234	ARG	CG-CD	-6.40	1.35	1.51
13	m	187	GLU	CD-OE1	-6.40	1.18	1.25
3	C	199	LYS	CG-CD	-6.40	1.30	1.52
11	4	46	PHE	CD1-CE1	6.40	1.52	1.39
13	m	125	ASP	CG-OD1	-6.38	1.10	1.25
13	6	187	GLU	CD-OE1	-6.36	1.18	1.25
11	k	68	SER	CB-OG	-6.36	1.33	1.42
11	4	18	SER	CB-OG	-6.36	1.33	1.42
13	6	125	ASP	CG-OD1	-6.36	1.10	1.25
5	e	69	GLU	CD-OE1	-6.36	1.18	1.25
12	5	111	GLU	CG-CD	-6.36	1.42	1.51
13	6	164	PHE	CD2-CE2	-6.36	1.26	1.39
5	e	104	ASP	CG-OD2	-6.35	1.10	1.25
8	h	115	ASN	CG-ND2	-6.35	1.17	1.32
5	e	29	GLU	CD-OE1	-6.34	1.18	1.25
5	E	69	GLU	CD-OE1	-6.34	1.18	1.25
11	4	90	LYS	CB-CG	-6.34	1.35	1.52
13	m	11	ASN	CG-ND2	-6.34	1.17	1.32
11	k	90	LYS	CB-CG	-6.33	1.35	1.52
12	l	111	GLU	CG-CD	-6.33	1.42	1.51
11	k	18	SER	CB-OG	-6.33	1.34	1.42
13	m	164	PHE	CD2-CE2	-6.33	1.26	1.39
13	6	11	ASN	CG-ND2	-6.33	1.17	1.32
9	2	186	ASP	CB-CG	-6.32	1.38	1.51
8	1	115	ASN	CG-ND2	-6.32	1.17	1.32
9	i	51	GLN	CD-OE1	-6.32	1.10	1.24
5	E	29	GLU	CD-OE1	-6.32	1.18	1.25
5	E	104	ASP	CG-OD2	-6.32	1.10	1.25
9	2	51	GLN	CD-OE1	-6.31	1.10	1.24
9	i	186	ASP	CB-CG	-6.30	1.38	1.51
13	6	114	TYR	CE2-CZ	6.30	1.46	1.38
11	4	68	SER	CB-OG	-6.29	1.34	1.42
5	E	186	GLU	CG-CD	-6.29	1.42	1.51
7	g	238	GLU	CD-OE1	-6.28	1.18	1.25
5	e	186	GLU	CG-CD	-6.28	1.42	1.51
13	m	13	TYR	CD1-CE1	6.28	1.48	1.39
9	2	58	LYS	CE-NZ	-6.27	1.33	1.49

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	58	LYS	CE-NZ	-6.26	1.33	1.49
3	c	18	ARG	CG-CD	-6.26	1.36	1.51
13	m	40	ASP	CG-OD1	-6.25	1.10	1.25
3	C	18	ARG	CG-CD	-6.25	1.36	1.51
8	h	11	SER	CB-OG	-6.25	1.34	1.42
11	4	109	LYS	CE-NZ	-6.24	1.33	1.49
3	C	124	GLN	CD-OE1	-6.24	1.10	1.24
9	i	92	ILE	CB-CG2	-6.23	1.33	1.52
13	6	40	ASP	CG-OD1	-6.23	1.11	1.25
3	c	124	GLN	CD-OE1	-6.23	1.10	1.24
13	6	13	TYR	CD1-CE1	6.23	1.48	1.39
8	1	11	SER	CB-OG	-6.22	1.34	1.42
10	j	113	ASN	CG-ND2	-6.22	1.17	1.32
10	3	113	ASN	CG-ND2	-6.22	1.17	1.32
1	A	32	PHE	CE1-CZ	-6.22	1.25	1.37
9	2	249	ILE	CA-CB	-6.22	1.40	1.54
1	a	32	PHE	CE1-CZ	-6.22	1.25	1.37
9	i	153	TYR	CA-CB	-6.22	1.40	1.53
11	k	109	LYS	CE-NZ	-6.22	1.33	1.49
9	2	92	ILE	CB-CG2	-6.21	1.33	1.52
12	5	150	SER	CB-OG	-6.21	1.34	1.42
8	1	205	LEU	N-CA	6.21	1.58	1.46
11	4	71	GLU	CD-OE2	-6.20	1.18	1.25
12	5	215	LEU	CG-CD1	-6.20	1.28	1.51
9	2	153	TYR	CA-CB	-6.20	1.40	1.53
12	l	215	LEU	CG-CD1	-6.20	1.28	1.51
2	B	182	GLU	CD-OE1	-6.19	1.18	1.25
12	l	150	SER	CB-OG	-6.19	1.34	1.42
5	e	29	GLU	CD-OE2	-6.18	1.18	1.25
8	1	69	GLN	CD-NE2	-6.18	1.17	1.32
13	6	165	LYS	CE-NZ	-6.18	1.33	1.49
2	b	182	GLU	CD-OE1	-6.17	1.18	1.25
9	i	118	LYS	CB-CG	-6.16	1.35	1.52
8	h	69	GLN	CD-NE2	-6.16	1.17	1.32
1	A	183	GLU	CD-OE1	-6.15	1.18	1.25
5	E	170	LYS	CE-NZ	-6.15	1.33	1.49
9	2	118	LYS	CB-CG	-6.15	1.35	1.52
5	E	29	GLU	CD-OE2	-6.15	1.18	1.25
11	k	110	LYS	CD-CE	-6.14	1.35	1.51
11	k	71	GLU	CD-OE2	-6.14	1.18	1.25
13	m	165	LYS	CE-NZ	-6.13	1.33	1.49
32	M	261	LYS	CG-CD	-6.13	1.31	1.52

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	110	LYS	CD-CE	-6.13	1.35	1.51
1	a	183	GLU	CD-OE1	-6.12	1.19	1.25
8	1	73	GLU	CD-OE2	-6.12	1.19	1.25
5	e	170	LYS	CE-NZ	-6.12	1.33	1.49
13	6	113	TYR	CE2-CZ	6.12	1.46	1.38
6	f	118	LYS	CE-NZ	-6.11	1.33	1.49
6	F	118	LYS	CE-NZ	-6.11	1.33	1.49
8	1	194	ARG	CD-NE	-6.10	1.36	1.46
3	c	195	LYS	CG-CD	-6.10	1.31	1.52
10	j	63	LEU	CG-CD1	-6.10	1.29	1.51
3	C	195	LYS	CG-CD	-6.09	1.31	1.52
10	3	63	LEU	CG-CD1	-6.09	1.29	1.51
1	a	188	LYS	CD-CE	-6.08	1.36	1.51
9	i	198	SER	CB-OG	-6.07	1.34	1.42
1	A	13	ASP	CG-OD1	-6.07	1.11	1.25
12	5	277	GLU	CD-OE2	-6.07	1.19	1.25
8	h	73	GLU	CD-OE2	-6.07	1.19	1.25
1	A	188	LYS	CD-CE	-6.07	1.36	1.51
1	a	13	ASP	CG-OD1	-6.06	1.11	1.25
8	h	152	ARG	CB-CG	-6.06	1.36	1.52
8	1	118	GLU	CD-OE1	-6.06	1.19	1.25
8	1	144	TYR	CB-CG	-6.06	1.42	1.51
6	F	31	GLN	CD-OE1	-6.06	1.10	1.24
8	1	152	ARG	CB-CG	-6.06	1.36	1.52
8	h	144	TYR	CB-CG	-6.05	1.42	1.51
1	A	32	PHE	CG-CD2	-6.04	1.29	1.38
9	2	198	SER	CB-OG	-6.04	1.34	1.42
8	h	118	GLU	CD-OE1	-6.03	1.19	1.25
2	B	4	ARG	CZ-NH1	-6.02	1.25	1.33
9	2	82	GLU	CD-OE2	-6.02	1.19	1.25
6	f	31	GLN	CD-OE1	-6.02	1.10	1.24
10	j	198	ARG	CZ-NH2	-6.02	1.25	1.33
12	5	216	ASP	CB-CG	-6.02	1.39	1.51
8	1	29	THR	CB-CG2	-6.02	1.32	1.52
1	a	32	PHE	CG-CD2	-6.01	1.29	1.38
11	4	81	SER	CB-OG	-6.01	1.34	1.42
9	i	88	ILE	CB-CG2	-6.01	1.34	1.52
8	h	29	THR	CB-CG2	-6.00	1.32	1.52
9	i	82	GLU	CD-OE2	-6.00	1.19	1.25
1	A	242	GLU	CD-OE2	-6.00	1.19	1.25
9	2	51	GLN	CG-CD	-6.00	1.37	1.51
12	l	216	ASP	CB-CG	-6.00	1.39	1.51

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	242	GLU	CD-OE2	-6.00	1.19	1.25
9	2	88	ILE	CB-CG2	-6.00	1.34	1.52
12	l	277	GLU	CD-OE2	-5.99	1.19	1.25
1	a	177	GLU	CD-OE2	-5.99	1.19	1.25
1	A	177	GLU	CD-OE2	-5.98	1.19	1.25
6	F	100	ASN	CG-ND2	-5.97	1.18	1.32
9	2	220	LEU	CB-CG	-5.97	1.35	1.52
9	i	51	GLN	CG-CD	-5.97	1.37	1.51
2	b	4	ARG	CZ-NH1	-5.96	1.25	1.33
12	5	100	TRP	CZ3-CH2	-5.96	1.30	1.40
20	Z	361	HIS	CE1-NE2	-5.96	1.19	1.32
11	k	81	SER	CB-OG	-5.96	1.34	1.42
8	h	16	THR	C-N	5.96	1.47	1.34
9	2	98	TYR	CZ-OH	-5.96	1.27	1.37
10	3	198	ARG	CZ-NH2	-5.95	1.25	1.33
6	f	100	ASN	CG-ND2	-5.94	1.18	1.32
12	l	100	TRP	CZ3-CH2	-5.94	1.30	1.40
2	b	4	ARG	CZ-NH2	-5.93	1.25	1.33
7	g	225	ASN	CG-ND2	-5.92	1.18	1.32
12	5	220	LYS	CB-CG	-5.92	1.36	1.52
9	i	98	TYR	CZ-OH	-5.92	1.27	1.37
2	B	4	ARG	CZ-NH2	-5.92	1.25	1.33
11	k	177	LYS	CG-CD	-5.91	1.32	1.52
11	4	177	LYS	CG-CD	-5.91	1.32	1.52
12	l	220	LYS	CB-CG	-5.90	1.36	1.52
2	b	186	GLU	CD-OE2	-5.88	1.19	1.25
4	D	119	ARG	CB-CG	-5.87	1.36	1.52
1	A	11	GLY	C-O	-5.86	1.14	1.23
1	A	112	MET	CG-SD	-5.86	1.66	1.81
8	1	17	PHE	C-N	5.85	1.47	1.34
13	m	86	ASP	CG-OD1	-5.85	1.11	1.25
13	6	57	ASN	CG-OD1	-5.84	1.11	1.24
13	m	57	ASN	CG-OD1	-5.84	1.11	1.24
13	m	229	ARG	CB-CG	-5.84	1.36	1.52
1	a	11	GLY	C-O	-5.83	1.14	1.23
2	B	186	GLU	CD-OE2	-5.83	1.19	1.25
13	m	223	GLU	CG-CD	-5.82	1.43	1.51
1	a	112	MET	CG-SD	-5.82	1.66	1.81
13	m	15	ASP	CG-OD1	-5.82	1.11	1.25
13	6	15	ASP	CG-OD1	-5.81	1.11	1.25
11	4	195	PHE	CD1-CE1	-5.80	1.27	1.39
11	k	195	PHE	CD1-CE1	-5.80	1.27	1.39

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	137	ARG	CG-CD	-5.80	1.37	1.51
13	6	223	GLU	CG-CD	-5.80	1.43	1.51
6	F	93	ASN	CG-ND2	-5.79	1.18	1.32
13	m	93	SER	CB-OG	-5.79	1.34	1.42
13	6	229	ARG	CB-CG	-5.79	1.36	1.52
11	k	125	LYS	CE-NZ	-5.79	1.34	1.49
6	f	93	ASN	CG-ND2	-5.78	1.18	1.32
12	l	131	GLU	CD-OE2	-5.77	1.19	1.25
13	m	167	GLN	CB-CG	-5.76	1.36	1.52
11	4	125	LYS	CE-NZ	-5.76	1.34	1.49
11	4	45	SER	CB-OG	-5.76	1.34	1.42
11	k	45	SER	CB-OG	-5.76	1.34	1.42
12	5	131	GLU	CD-OE2	-5.76	1.19	1.25
13	6	167	GLN	CB-CG	-5.76	1.36	1.52
13	6	187	GLU	CD-OE2	-5.76	1.19	1.25
9	i	114	GLN	CD-OE1	-5.75	1.11	1.24
8	1	61	THR	CB-CG2	-5.75	1.33	1.52
8	h	61	THR	CB-CG2	-5.75	1.33	1.52
13	6	211	GLU	CD-OE1	-5.75	1.19	1.25
9	i	31	THR	CB-CG2	-5.75	1.33	1.52
12	l	144	ARG	CD-NE	-5.73	1.36	1.46
9	2	31	THR	CB-CG2	-5.73	1.33	1.52
22	S	43	LYS	CB-CG	-5.72	1.37	1.52
9	2	114	GLN	CD-OE1	-5.71	1.11	1.24
2	B	113	GLU	CD-OE2	-5.71	1.19	1.25
13	m	187	GLU	CD-OE2	-5.71	1.19	1.25
13	m	78	ASN	CB-CG	-5.71	1.38	1.51
2	b	113	GLU	CD-OE2	-5.71	1.19	1.25
1	a	187	LYS	CB-CG	-5.71	1.37	1.52
11	4	195	PHE	CD2-CE2	-5.70	1.27	1.39
12	5	144	ARG	CD-NE	-5.69	1.36	1.46
13	6	78	ASN	CB-CG	-5.69	1.38	1.51
29	I	373	GLU	CG-CD	-5.68	1.43	1.51
2	B	11	THR	CB-CG2	-5.67	1.33	1.52
1	A	187	LYS	CB-CG	-5.67	1.37	1.52
9	2	193	TRP	CB-CG	-5.67	1.40	1.50
11	4	71	GLU	CD-OE1	-5.67	1.19	1.25
12	l	215	LEU	CG-CD2	-5.66	1.30	1.51
31	L	421	LYS	CD-CE	-5.66	1.37	1.51
9	i	30	THR	CB-CG2	-5.66	1.33	1.52
12	5	215	LEU	CG-CD2	-5.66	1.30	1.51
11	k	71	GLU	CD-OE1	-5.66	1.19	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	195	PHE	CD2-CE2	-5.65	1.27	1.39
13	m	211	GLU	CD-OE1	-5.65	1.19	1.25
9	i	193	TRP	CB-CG	-5.64	1.40	1.50
2	b	11	THR	CB-CG2	-5.63	1.33	1.52
9	2	30	THR	CB-CG2	-5.63	1.33	1.52
9	2	114	GLN	CG-CD	-5.63	1.38	1.51
9	i	114	GLN	CG-CD	-5.63	1.38	1.51
9	2	228	LYS	CB-CG	-5.62	1.37	1.52
10	j	205	ASP	CA-CB	-5.62	1.41	1.53
6	f	5	ASN	CB-CG	-5.61	1.38	1.51
11	k	166	GLN	CD-NE2	-5.61	1.18	1.32
8	h	153	GLU	CD-OE2	-5.61	1.19	1.25
8	1	153	GLU	CD-OE2	-5.60	1.19	1.25
9	2	39	ASN	CG-OD1	-5.60	1.11	1.24
11	4	166	GLN	CD-NE2	-5.60	1.18	1.32
10	3	205	ASP	CA-CB	-5.60	1.41	1.53
9	i	39	ASN	CG-OD1	-5.58	1.11	1.24
6	F	5	ASN	CB-CG	-5.58	1.38	1.51
9	i	86	GLN	CD-OE1	-5.58	1.11	1.24
9	2	86	GLN	CD-OE1	-5.58	1.11	1.24
14	n	241	PHE	CD2-CE2	-5.56	1.28	1.39
5	e	186	GLU	CD-OE2	-5.56	1.19	1.25
5	e	66	LYS	CD-CE	-5.55	1.37	1.51
5	E	66	LYS	CD-CE	-5.55	1.37	1.51
5	E	186	GLU	CD-OE2	-5.54	1.19	1.25
9	2	254	GLU	CA-CB	-5.54	1.41	1.53
12	5	186	THR	CB-CG2	-5.54	1.34	1.52
3	c	85	GLU	CD-OE2	-5.54	1.19	1.25
1	A	250	GLU	CD-OE1	-5.53	1.19	1.25
10	3	131	ASP	C-N	5.53	1.46	1.34
13	m	145	ARG	CZ-NH1	-5.52	1.25	1.33
20	Z	361	HIS	CG-CD2	-5.52	1.26	1.35
1	a	250	GLU	CD-OE1	-5.52	1.19	1.25
12	l	186	THR	CB-CG2	-5.51	1.34	1.52
8	1	156	SER	CB-OG	-5.51	1.35	1.42
8	h	144	TYR	CE2-CZ	-5.50	1.31	1.38
3	c	3	SER	C-N	5.50	1.46	1.34
10	j	203	ARG	CB-CG	-5.50	1.37	1.52
9	i	195	ASP	CG-OD1	-5.50	1.12	1.25
1	A	221	ASN	CG-ND2	-5.49	1.19	1.32
11	k	171	ARG	CD-NE	-5.49	1.37	1.46
3	C	3	SER	C-N	5.49	1.46	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	156	SER	CB-OG	-5.49	1.35	1.42
9	i	38	ASN	CG-OD1	-5.49	1.11	1.24
1	a	221	ASN	CG-ND2	-5.48	1.19	1.32
11	k	180	ILE	CB-CG1	-5.48	1.38	1.54
11	4	180	ILE	CB-CG1	-5.48	1.38	1.54
13	6	145	ARG	CZ-NH1	-5.48	1.25	1.33
3	C	85	GLU	CD-OE2	-5.48	1.19	1.25
9	2	195	ASP	CG-OD1	-5.48	1.12	1.25
9	i	181	ILE	CB-CG2	-5.48	1.35	1.52
9	2	181	ILE	CB-CG2	-5.47	1.35	1.52
8	h	31	THR	CB-CG2	-5.47	1.34	1.52
9	2	38	ASN	CG-OD1	-5.47	1.11	1.24
2	b	146	SER	CB-OG	-5.46	1.35	1.42
10	3	203	ARG	CB-CG	-5.46	1.37	1.52
1	a	37	GLN	CD-NE2	-5.46	1.19	1.32
8	1	201	GLU	CB-CG	-5.46	1.41	1.52
20	Z	632	GLU	CB-CG	-5.46	1.41	1.52
8	1	31	THR	CB-CG2	-5.45	1.34	1.52
1	A	37	GLN	CD-NE2	-5.45	1.19	1.32
13	6	106	TYR	CG-CD1	5.45	1.46	1.39
2	b	234	ARG	CD-NE	-5.44	1.37	1.46
8	h	42	LYS	CD-CE	-5.44	1.37	1.51
2	B	146	SER	CB-OG	-5.44	1.35	1.42
8	h	173	LYS	CE-NZ	-5.43	1.35	1.49
8	1	42	LYS	CD-CE	-5.43	1.37	1.51
8	1	48	ASP	C-N	-5.43	1.21	1.34
8	1	173	LYS	CE-NZ	-5.43	1.35	1.49
10	3	131	ASP	CG-OD1	-5.43	1.12	1.25
2	B	234	ARG	CD-NE	-5.42	1.37	1.46
11	4	171	ARG	CD-NE	-5.42	1.37	1.46
8	1	98	ASN	CG-OD1	-5.42	1.12	1.24
8	1	144	TYR	CE2-CZ	-5.42	1.31	1.38
12	5	258	ASP	CG-OD1	-5.41	1.12	1.25
11	4	109	LYS	CG-CD	-5.40	1.34	1.52
12	5	100	TRP	NE1-CE2	-5.40	1.30	1.37
31	L	421	LYS	CE-NZ	5.40	1.62	1.49
10	3	128	GLY	C-O	-5.40	1.15	1.23
8	h	98	ASN	CG-OD1	-5.40	1.12	1.24
3	C	202	ASP	CG-OD2	-5.40	1.12	1.25
12	l	258	ASP	CG-OD1	-5.39	1.12	1.25
13	6	195	SER	CB-OG	-5.39	1.35	1.42
3	c	202	ASP	CG-OD2	-5.39	1.12	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	72	LEU	CG-CD2	-5.39	1.31	1.51
13	6	72	LEU	CG-CD2	-5.38	1.31	1.51
10	3	183	TRP	CG-CD1	-5.38	1.29	1.36
11	k	109	LYS	CG-CD	-5.37	1.34	1.52
9	i	46	ASP	CG-OD2	-5.37	1.13	1.25
12	l	100	TRP	NE1-CE2	-5.37	1.30	1.37
8	1	18	LYS	CE-NZ	-5.37	1.35	1.49
10	3	85	GLU	CG-CD	-5.36	1.44	1.51
8	h	18	LYS	CE-NZ	-5.36	1.35	1.49
13	m	195	SER	CB-OG	-5.36	1.35	1.42
7	G	215	GLU	CB-CG	5.36	1.62	1.52
10	3	172	LEU	CG-CD1	-5.36	1.32	1.51
9	2	46	ASP	CG-OD2	-5.36	1.13	1.25
28	H	145	TYR	CE2-CZ	-5.35	1.31	1.38
10	j	98	ARG	NE-CZ	-5.34	1.26	1.33
3	c	129	ARG	CG-CD	-5.34	1.38	1.51
3	C	129	ARG	CG-CD	-5.34	1.38	1.51
11	k	52	ASP	CB-CG	-5.33	1.40	1.51
1	a	67	THR	CB-CG2	-5.33	1.34	1.52
8	1	204	GLN	C-N	5.33	1.46	1.34
10	3	98	ARG	NE-CZ	-5.33	1.26	1.33
1	A	184	ASN	CG-OD1	-5.32	1.12	1.24
11	k	10	GLN	CD-NE2	-5.32	1.19	1.32
11	4	52	ASP	CB-CG	-5.32	1.40	1.51
1	A	222	ASP	CG-OD2	-5.32	1.13	1.25
1	a	184	ASN	CG-OD1	-5.32	1.12	1.24
5	e	65	GLU	CD-OE1	-5.31	1.19	1.25
1	A	67	THR	CB-CG2	-5.31	1.34	1.52
11	4	10	GLN	CD-NE2	-5.30	1.19	1.32
8	1	130	LYS	CG-CD	-5.30	1.34	1.52
1	a	222	ASP	CG-OD2	-5.30	1.13	1.25
11	4	170	LYS	CD-CE	-5.30	1.38	1.51
1	a	32	PHE	CE2-CZ	-5.29	1.27	1.37
8	h	130	LYS	CG-CD	-5.29	1.34	1.52
13	m	72	LEU	CG-CD1	-5.29	1.32	1.51
5	E	65	GLU	CD-OE1	-5.29	1.19	1.25
9	2	246	ILE	CG1-CD1	-5.28	1.14	1.50
5	e	18	GLU	C-N	5.28	1.42	1.33
11	k	170	LYS	CD-CE	-5.28	1.38	1.51
10	j	85	GLU	CG-CD	-5.27	1.44	1.51
13	6	72	LEU	CG-CD1	-5.27	1.32	1.51
13	m	113	TYR	C-N	-5.25	1.22	1.34

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	58	GLU	CD-OE1	-5.25	1.19	1.25
11	4	74	GLU	CD-OE1	-5.25	1.19	1.25
11	k	169	GLU	CD-OE1	-5.25	1.19	1.25
8	1	152	ARG	NE-CZ	-5.24	1.26	1.33
3	C	224	GLU	CD-OE1	-5.24	1.19	1.25
3	c	224	GLU	CD-OE1	-5.23	1.19	1.25
10	j	19	ASP	CG-OD1	-5.23	1.13	1.25
11	4	169	GLU	CD-OE1	-5.23	1.19	1.25
8	h	155	MET	CB-CG	-5.23	1.34	1.51
7	g	202	LEU	CG-CD2	-5.22	1.32	1.51
6	f	93	ASN	CG-OD1	-5.22	1.12	1.24
8	h	112	ASP	CG-OD1	-5.22	1.13	1.25
11	k	74	GLU	CD-OE1	-5.22	1.20	1.25
8	1	155	MET	CB-CG	-5.22	1.34	1.51
1	A	32	PHE	CE2-CZ	-5.21	1.27	1.37
5	e	104	ASP	CG-OD1	-5.21	1.13	1.25
8	h	152	ARG	NE-CZ	-5.21	1.26	1.33
6	F	93	ASN	CG-OD1	-5.21	1.12	1.24
5	E	104	ASP	CG-OD1	-5.21	1.13	1.25
8	1	112	ASP	CG-OD1	-5.21	1.13	1.25
13	m	118	ILE	CB-CG1	-5.20	1.39	1.54
6	f	90	GLN	CD-NE2	-5.20	1.19	1.32
10	3	19	ASP	CG-OD1	-5.20	1.13	1.25
13	m	110	PHE	CG-CD2	5.20	1.46	1.38
13	m	205	GLN	CD-OE1	-5.20	1.12	1.24
13	6	56	ASP	CG-OD1	-5.20	1.13	1.25
13	6	205	GLN	CD-OE1	-5.20	1.12	1.24
8	1	100	ASP	CG-OD1	-5.19	1.13	1.25
11	k	143	LEU	CG-CD2	-5.18	1.32	1.51
11	4	143	LEU	CG-CD2	-5.18	1.32	1.51
12	5	160	ASN	CG-OD1	-5.18	1.12	1.24
6	F	90	GLN	CD-NE2	-5.18	1.20	1.32
1	A	192	ASP	CG-OD1	-5.17	1.13	1.25
12	l	104	GLN	CB-CG	-5.17	1.38	1.52
20	Z	632	GLU	CD-OE2	5.17	1.31	1.25
13	m	56	ASP	CG-OD1	-5.17	1.13	1.25
12	5	148	ARG	CG-CD	-5.16	1.39	1.51
12	l	148	ARG	CG-CD	-5.16	1.39	1.51
8	h	100	ASP	CG-OD1	-5.15	1.13	1.25
11	k	58	GLU	CD-OE2	-5.15	1.20	1.25
12	5	104	GLN	CB-CG	-5.15	1.38	1.52
1	a	192	ASP	CG-OD1	-5.14	1.13	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	26	SER	CB-OG	-5.14	1.35	1.42
31	L	367	LYS	CE-NZ	5.14	1.61	1.49
10	j	15	MET	CB-CG	-5.14	1.34	1.51
9	i	37	PHE	CD2-CE2	5.14	1.49	1.39
10	j	161	GLU	CB-CG	5.14	1.61	1.52
5	e	233	ASN	CG-OD1	-5.14	1.12	1.24
10	3	15	MET	CB-CG	-5.13	1.34	1.51
11	k	58	GLU	CD-OE1	-5.13	1.20	1.25
11	k	65	GLN	CB-CG	-5.13	1.38	1.52
10	3	93	SER	CB-OG	-5.13	1.35	1.42
1	A	222	ASP	CG-OD1	-5.12	1.13	1.25
12	l	160	ASN	CG-OD1	-5.12	1.12	1.24
25	R	225	LYS	CE-NZ	5.12	1.61	1.49
1	a	222	ASP	CG-OD1	-5.12	1.13	1.25
13	m	178	LYS	CB-CG	5.12	1.66	1.52
10	j	93	SER	CB-OG	-5.11	1.35	1.42
11	k	69	ILE	CB-CG1	-5.11	1.39	1.54
13	m	39	THR	CB-CG2	-5.11	1.35	1.52
5	E	233	ASN	CG-OD1	-5.11	1.12	1.24
11	4	167	GLU	CD-OE1	-5.11	1.20	1.25
11	4	26	SER	CB-OG	-5.10	1.35	1.42
13	6	39	THR	CB-CG2	-5.09	1.35	1.52
11	4	69	ILE	CB-CG1	-5.09	1.39	1.54
9	2	37	PHE	CD2-CE2	5.09	1.49	1.39
11	4	65	GLN	CB-CG	-5.08	1.38	1.52
13	6	178	LYS	CB-CG	5.08	1.66	1.52
1	A	26	TYR	CG-CD2	-5.08	1.32	1.39
13	m	122	LEU	CG-CD2	-5.08	1.33	1.51
13	6	122	LEU	CG-CD2	-5.08	1.33	1.51
21	N	282	TYR	CB-CG	-5.08	1.44	1.51
7	G	177	GLU	CD-OE2	5.07	1.31	1.25
10	3	152	SER	CB-OG	-5.06	1.35	1.42
1	a	26	TYR	CG-CD2	-5.06	1.32	1.39
9	2	254	GLU	N-CA	-5.06	1.36	1.46
9	i	93	GLU	CD-OE2	-5.06	1.20	1.25
11	k	167	GLU	CD-OE1	-5.05	1.20	1.25
10	3	188	TYR	CE2-CZ	-5.05	1.31	1.38
11	4	58	GLU	CD-OE2	-5.03	1.20	1.25
12	5	191	ASP	CG-OD2	-5.03	1.13	1.25
5	e	177	GLU	CD-OE1	-5.03	1.20	1.25
10	j	151	GLU	CD-OE1	-5.03	1.20	1.25
12	l	191	ASP	CG-OD2	-5.02	1.13	1.25

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	93	GLU	CD-OE2	-5.02	1.20	1.25
10	j	188	TYR	CE2-CZ	-5.01	1.32	1.38
4	d	66	LYS	CD-CE	-5.01	1.38	1.51
3	C	142	ASP	CG-OD2	-5.01	1.13	1.25
13	6	15	ASP	CG-OD2	-5.00	1.13	1.25
8	1	152	ARG	CZ-NH2	-5.00	1.26	1.33

All (2189) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	65	ARG	NE-CZ-NH1	-46.33	97.13	120.30
9	2	65	ARG	NE-CZ-NH1	-46.27	97.17	120.30
9	i	65	ARG	NE-CZ-NH2	43.31	141.96	120.30
9	2	65	ARG	NE-CZ-NH2	43.26	141.93	120.30
11	4	70	ARG	NE-CZ-NH1	38.29	139.45	120.30
11	k	70	ARG	NE-CZ-NH1	38.20	139.40	120.30
5	E	53	ARG	NE-CZ-NH1	-36.92	101.84	120.30
8	h	183	ARG	NE-CZ-NH1	34.56	137.58	120.30
8	1	183	ARG	NE-CZ-NH1	34.55	137.57	120.30
9	i	153	TYR	CB-CG-CD1	-33.08	101.16	121.00
9	2	153	TYR	CB-CG-CD1	-33.02	101.19	121.00
9	2	101	ARG	NE-CZ-NH2	-31.85	104.38	120.30
9	i	101	ARG	NE-CZ-NH2	-31.80	104.40	120.30
13	m	46	ARG	NE-CZ-NH1	30.94	135.77	120.30
13	6	46	ARG	NE-CZ-NH1	30.87	135.74	120.30
9	2	220	LEU	CB-CG-CD2	30.84	163.43	111.00
11	k	93	ARG	NE-CZ-NH1	28.02	134.31	120.30
11	4	93	ARG	NE-CZ-NH1	27.86	134.23	120.30
12	5	139	ARG	NE-CZ-NH2	-27.21	106.69	120.30
3	C	114	ARG	NE-CZ-NH1	-27.16	106.72	120.30
3	c	114	ARG	NE-CZ-NH1	-27.15	106.73	120.30
12	l	139	ARG	NE-CZ-NH2	-27.11	106.75	120.30
13	m	46	ARG	NE-CZ-NH2	-26.81	106.90	120.30
29	I	373	GLU	OE1-CD-OE2	-26.67	91.30	123.30
13	6	46	ARG	NE-CZ-NH2	-26.62	106.99	120.30
8	h	45	ARG	NE-CZ-NH1	26.53	133.56	120.30
8	1	45	ARG	NE-CZ-NH1	26.53	133.56	120.30
9	2	217	ARG	NE-CZ-NH2	26.50	133.55	120.30
13	m	141	ARG	NE-CZ-NH2	26.29	133.45	120.30
10	j	98	ARG	NE-CZ-NH1	26.21	133.41	120.30
13	6	141	ARG	NE-CZ-NH2	26.18	133.39	120.30
10	3	98	ARG	NE-CZ-NH1	26.15	133.38	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	141	ARG	NE-CZ-NH1	-25.78	107.41	120.30
13	6	141	ARG	NE-CZ-NH1	-25.70	107.45	120.30
10	3	98	ARG	NE-CZ-NH2	-25.49	107.56	120.30
10	j	98	ARG	NE-CZ-NH2	-25.47	107.56	120.30
12	l	82	ARG	NE-CZ-NH1	22.94	131.77	120.30
12	5	82	ARG	NE-CZ-NH1	22.93	131.76	120.30
31	L	367	LYS	CB-CG-CD	22.57	170.28	111.60
9	2	153	TYR	CB-CG-CD2	22.26	134.36	121.00
9	i	153	TYR	CB-CG-CD2	22.14	134.29	121.00
8	1	130	LYS	CD-CE-NZ	21.98	162.25	111.70
8	h	130	LYS	CD-CE-NZ	21.94	162.17	111.70
12	5	220	LYS	CD-CE-NZ	-21.48	62.30	111.70
12	l	220	LYS	CD-CE-NZ	-21.47	62.31	111.70
11	k	93	ARG	NH1-CZ-NH2	-21.36	95.90	119.40
11	4	93	ARG	NH1-CZ-NH2	-21.35	95.92	119.40
3	c	241	LYS	CD-CE-NZ	21.13	160.31	111.70
3	C	241	LYS	CD-CE-NZ	21.12	160.28	111.70
22	S	43	LYS	CB-CG-CD	21.02	166.25	111.60
32	M	261	LYS	CA-CB-CG	20.85	159.27	113.40
13	6	36	ARG	NE-CZ-NH1	20.56	130.58	120.30
13	m	36	ARG	NE-CZ-NH1	20.54	130.57	120.30
5	e	10	ARG	NE-CZ-NH1	20.35	130.47	120.30
12	5	170	LEU	CB-CG-CD1	20.34	145.58	111.00
12	l	170	LEU	CB-CG-CD1	20.30	145.50	111.00
13	6	181	LYS	CD-CE-NZ	-20.29	65.03	111.70
13	m	181	LYS	CD-CE-NZ	-20.28	65.06	111.70
8	1	114	LYS	CD-CE-NZ	-20.25	65.13	111.70
8	h	114	LYS	CD-CE-NZ	-20.23	65.17	111.70
2	B	49	LYS	CD-CE-NZ	20.20	158.15	111.70
2	b	49	LYS	CD-CE-NZ	20.18	158.13	111.70
9	2	101	ARG	NE-CZ-NH1	20.18	130.39	120.30
31	L	421	LYS	CG-CD-CE	20.13	172.30	111.90
9	i	101	ARG	NE-CZ-NH1	20.07	130.33	120.30
5	E	53	ARG	NE-CZ-NH2	20.05	130.33	120.30
11	4	174	MET	CG-SD-CE	-20.05	68.13	100.20
11	k	174	MET	CG-SD-CE	-20.04	68.14	100.20
11	4	96	ARG	NE-CZ-NH2	-19.95	110.33	120.30
11	k	96	ARG	NE-CZ-NH2	-19.91	110.34	120.30
8	1	113	ASP	CB-CG-OD1	19.80	136.12	118.30
8	h	113	ASP	CB-CG-OD1	19.73	136.06	118.30
10	3	40	PHE	CB-CG-CD1	19.64	134.54	120.80
10	j	40	PHE	CB-CG-CD1	19.63	134.54	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	M	68	LYS	CG-CD-CE	19.40	170.09	111.90
8	1	113	ASP	CB-CG-OD2	-19.28	100.95	118.30
8	h	113	ASP	CB-CG-OD2	-19.27	100.95	118.30
10	j	39	LYS	CB-CG-CD	19.23	161.60	111.60
10	3	39	LYS	CB-CG-CD	19.21	161.55	111.60
9	i	51	GLN	CA-CB-CG	19.04	155.29	113.40
32	M	171	GLU	OE1-CD-OE2	-19.02	100.47	123.30
9	2	51	GLN	CA-CB-CG	19.02	155.24	113.40
11	k	36	ARG	NE-CZ-NH2	18.98	129.79	120.30
8	h	183	ARG	NE-CZ-NH2	-18.97	110.81	120.30
11	4	176	PHE	CB-CG-CD2	18.96	134.07	120.80
11	4	36	ARG	NE-CZ-NH2	18.93	129.77	120.30
8	1	183	ARG	NE-CZ-NH2	-18.93	110.84	120.30
11	k	176	PHE	CB-CG-CD2	18.89	134.02	120.80
9	i	211	LYS	CB-CG-CD	18.86	160.63	111.60
9	2	211	LYS	CB-CG-CD	18.82	160.54	111.60
15	W	87	MET	CB-CG-SD	18.80	168.79	112.40
13	m	75	ARG	NE-CZ-NH2	-18.67	110.97	120.30
13	6	75	ARG	NE-CZ-NH2	-18.62	110.99	120.30
13	6	228	LYS	CD-CE-NZ	-18.48	69.19	111.70
13	m	228	LYS	CD-CE-NZ	-18.48	69.21	111.70
1	A	96	ARG	NE-CZ-NH2	18.37	129.49	120.30
32	M	42	ARG	NE-CZ-NH2	-18.37	111.11	120.30
9	2	220	LEU	CD1-CG-CD2	-18.36	55.41	110.50
10	3	205	ASP	CB-CG-OD2	18.35	134.82	118.30
10	j	205	ASP	CB-CG-OD2	18.32	134.79	118.30
1	a	96	ARG	NE-CZ-NH2	18.32	129.46	120.30
8	h	45	ARG	NE-CZ-NH2	-18.23	111.18	120.30
12	l	156	LYS	CD-CE-NZ	18.21	153.59	111.70
12	5	156	LYS	CD-CE-NZ	18.21	153.59	111.70
11	k	70	ARG	NH1-CZ-NH2	-18.20	99.38	119.40
12	l	82	ARG	NH1-CZ-NH2	-18.14	99.44	119.40
13	m	182	TYR	CB-CG-CD1	-18.14	110.12	121.00
12	5	82	ARG	NH1-CZ-NH2	-18.14	99.45	119.40
29	I	373	GLU	CG-CD-OE1	18.12	154.54	118.30
11	4	70	ARG	NH1-CZ-NH2	-18.12	99.47	119.40
8	1	45	ARG	NE-CZ-NH2	-18.10	111.25	120.30
11	4	171	ARG	NE-CZ-NH1	18.07	129.34	120.30
13	6	182	TYR	CB-CG-CD1	-18.02	110.19	121.00
11	k	171	ARG	NE-CZ-NH1	18.02	129.31	120.30
29	I	139	GLU	CA-CB-CG	17.93	152.84	113.40
12	5	161	LEU	CB-CG-CD2	-17.90	80.57	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	161	LEU	CB-CG-CD2	-17.89	80.59	111.00
25	R	225	LYS	CG-CD-CE	17.85	165.46	111.90
11	k	8	ARG	NE-CZ-NH2	17.65	129.12	120.30
8	1	42	LYS	CD-CE-NZ	17.62	152.23	111.70
8	h	42	LYS	CD-CE-NZ	17.61	152.20	111.70
2	b	234	ARG	NE-CZ-NH2	17.59	129.09	120.30
11	4	8	ARG	NE-CZ-NH2	17.57	129.09	120.30
2	B	234	ARG	NE-CZ-NH2	17.56	129.08	120.30
24	Q	166	LYS	CB-CG-CD	17.42	156.88	111.60
1	A	135	ARG	NE-CZ-NH1	-17.28	111.66	120.30
1	a	135	ARG	NE-CZ-NH1	-17.28	111.66	120.30
9	2	230	LYS	CD-CE-NZ	17.20	151.27	111.70
24	Q	166	LYS	CA-CB-CG	17.15	151.13	113.40
17	T	130	ASP	CB-CG-OD1	16.94	133.55	118.30
11	k	143	LEU	CB-CG-CD2	16.83	139.62	111.00
11	4	143	LEU	CB-CG-CD2	16.82	139.59	111.00
11	k	36	ARG	NE-CZ-NH1	-16.74	111.93	120.30
10	j	205	ASP	CB-CG-OD1	-16.73	103.25	118.30
10	3	205	ASP	CB-CG-OD1	-16.72	103.25	118.30
11	4	36	ARG	NE-CZ-NH1	-16.70	111.95	120.30
12	5	82	ARG	NE-CZ-NH2	16.62	128.61	120.30
12	l	82	ARG	NE-CZ-NH2	16.62	128.61	120.30
9	i	167	LEU	CB-CG-CD1	-16.58	82.81	111.00
9	2	167	LEU	CB-CG-CD1	-16.58	82.82	111.00
10	j	41	GLU	CA-CB-CG	16.53	149.77	113.40
10	3	41	GLU	CA-CB-CG	16.52	149.75	113.40
11	4	170	LYS	CB-CG-CD	16.48	154.44	111.60
11	k	170	LYS	CB-CG-CD	16.47	154.41	111.60
2	B	234	ARG	NH1-CZ-NH2	-16.46	101.30	119.40
2	b	234	ARG	NH1-CZ-NH2	-16.45	101.30	119.40
12	5	81	PHE	CB-CG-CD2	16.36	132.25	120.80
10	3	63	LEU	CB-CG-CD1	16.33	138.76	111.00
10	j	63	LEU	CB-CG-CD1	16.31	138.73	111.00
12	l	81	PHE	CB-CG-CD2	16.29	132.21	120.80
17	T	130	ASP	OD1-CG-OD2	-16.26	92.41	123.30
13	6	134	ASP	CB-CG-OD1	-16.21	103.71	118.30
13	m	134	ASP	CB-CG-OD1	-16.16	103.76	118.30
11	k	135	TYR	CB-CG-CD1	-16.12	111.33	121.00
11	4	135	TYR	CB-CG-CD1	-15.99	111.41	121.00
10	3	19	ASP	CB-CG-OD2	15.80	132.52	118.30
10	j	19	ASP	CB-CG-OD2	15.79	132.51	118.30
12	5	115	PHE	CB-CG-CD2	15.78	131.85	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	115	PHE	CB-CG-CD2	15.73	131.81	120.80
9	2	51	GLN	CB-CG-CD	15.66	152.32	111.60
9	i	51	GLN	CB-CG-CD	15.62	152.22	111.60
11	k	110	LYS	CD-CE-NZ	-15.57	75.90	111.70
11	4	110	LYS	CD-CE-NZ	-15.55	75.93	111.70
1	a	135	ARG	NE-CZ-NH2	15.48	128.04	120.30
29	I	373	GLU	CG-CD-OE2	-15.45	87.41	118.30
10	j	74	TYR	CB-CG-CD2	15.42	130.25	121.00
9	2	156	LEU	CB-CG-CD1	15.42	137.21	111.00
9	i	156	LEU	CB-CG-CD1	15.41	137.19	111.00
17	T	130	ASP	CB-CG-OD2	15.39	132.16	118.30
10	3	74	TYR	CB-CG-CD2	15.38	130.23	121.00
8	1	194	ARG	NH1-CZ-NH2	-15.35	102.51	119.40
1	A	135	ARG	NE-CZ-NH2	15.34	127.97	120.30
10	j	124	PHE	O-C-N	15.31	147.20	122.70
11	4	67	TYR	CB-CG-CD1	15.18	130.11	121.00
11	k	67	TYR	CB-CG-CD1	15.11	130.07	121.00
13	6	125	ASP	CB-CG-OD2	14.90	131.71	118.30
13	m	145	ARG	NE-CZ-NH2	-14.88	112.86	120.30
13	m	125	ASP	CB-CG-OD2	14.85	131.66	118.30
13	6	145	ARG	NE-CZ-NH2	-14.80	112.90	120.30
3	C	114	ARG	NE-CZ-NH2	14.63	127.61	120.30
11	4	96	ARG	NE-CZ-NH1	14.59	127.59	120.30
13	m	104	LEU	O-C-N	-14.57	99.38	122.70
3	c	114	ARG	NE-CZ-NH2	14.57	127.58	120.30
11	k	96	ARG	NE-CZ-NH1	14.53	127.56	120.30
7	g	245	LYS	CD-CE-NZ	-14.44	78.50	111.70
10	3	77	LYS	CD-CE-NZ	-14.34	78.73	111.70
22	S	43	LYS	CA-CB-CG	14.34	144.94	113.40
10	j	77	LYS	CD-CE-NZ	-14.31	78.78	111.70
2	b	242	GLU	OE1-CD-OE2	-14.25	106.20	123.30
2	B	242	GLU	OE1-CD-OE2	-14.20	106.25	123.30
7	G	57	LYS	CB-CG-CD	14.17	148.44	111.60
7	g	57	LYS	CB-CG-CD	14.16	148.43	111.60
11	k	135	TYR	CB-CG-CD2	14.15	129.49	121.00
6	F	51	ARG	NE-CZ-NH2	14.06	127.33	120.30
11	4	135	TYR	CB-CG-CD2	14.04	129.42	121.00
9	i	156	LEU	CD1-CG-CD2	-13.96	68.62	110.50
8	1	26	ASP	CB-CG-OD2	-13.96	105.74	118.30
9	2	156	LEU	CD1-CG-CD2	-13.96	68.62	110.50
6	f	51	ARG	NE-CZ-NH2	13.95	127.27	120.30
13	6	36	ARG	NH1-CZ-NH2	-13.94	104.06	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	26	ASP	CB-CG-OD2	-13.93	105.76	118.30
9	i	84	VAL	CG1-CB-CG2	-13.92	88.62	110.90
13	m	75	ARG	NE-CZ-NH1	13.91	127.26	120.30
13	m	36	ARG	NH1-CZ-NH2	-13.91	104.10	119.40
9	2	84	VAL	CG1-CB-CG2	-13.90	88.66	110.90
9	2	211	LYS	CA-CB-CG	13.90	143.97	113.40
9	i	211	LYS	CA-CB-CG	13.88	143.93	113.40
11	4	113	LYS	CD-CE-NZ	13.86	143.57	111.70
11	k	113	LYS	CD-CE-NZ	13.84	143.53	111.70
13	6	75	ARG	NE-CZ-NH1	13.83	127.22	120.30
25	R	225	LYS	CD-CE-NZ	-13.76	80.06	111.70
13	6	109	ARG	NE-CZ-NH2	-13.75	113.42	120.30
12	5	107	LYS	CD-CE-NZ	13.75	143.32	111.70
12	l	107	LYS	CD-CE-NZ	13.72	143.25	111.70
24	Q	51	ARG	NE-CZ-NH1	13.70	127.15	120.30
5	E	229	LYS	CD-CE-NZ	13.68	143.16	111.70
9	i	119	TYR	CB-CG-CD2	13.67	129.20	121.00
29	I	139	GLU	CB-CG-CD	13.66	151.10	114.20
5	e	229	LYS	CD-CE-NZ	13.65	143.11	111.70
11	k	7	ILE	CG1-CB-CG2	-13.65	81.38	111.40
11	4	7	ILE	CG1-CB-CG2	-13.64	81.40	111.40
13	6	40	ASP	CB-CG-OD2	13.63	130.57	118.30
13	m	40	ASP	CB-CG-OD2	13.62	130.56	118.30
13	m	169	GLU	OE1-CD-OE2	-13.61	106.97	123.30
13	6	169	GLU	OE1-CD-OE2	-13.60	106.98	123.30
11	4	109	LYS	CD-CE-NZ	13.59	142.95	111.70
9	2	119	TYR	CB-CG-CD2	13.58	129.15	121.00
11	k	109	LYS	CD-CE-NZ	13.57	142.91	111.70
11	4	163	LEU	CA-CB-CG	13.54	146.45	115.30
11	k	163	LEU	CA-CB-CG	13.53	146.42	115.30
13	m	133	PHE	CB-CG-CD2	13.52	130.27	120.80
13	6	133	PHE	CB-CG-CD2	13.52	130.26	120.80
13	m	145	ARG	CD-NE-CZ	-13.52	104.68	123.60
5	E	20	ARG	NE-CZ-NH2	-13.52	113.54	120.30
32	M	261	LYS	CB-CG-CD	13.49	146.68	111.60
13	6	145	ARG	CD-NE-CZ	-13.49	104.72	123.60
8	1	194	ARG	NE-CZ-NH2	13.46	127.03	120.30
9	2	30	THR	OG1-CB-CG2	-13.46	79.05	110.00
9	i	30	THR	OG1-CB-CG2	-13.45	79.06	110.00
11	k	163	LEU	CB-CG-CD2	13.44	133.84	111.00
5	e	18	GLU	CA-C-N	-13.43	89.34	116.20
11	4	163	LEU	CB-CG-CD2	13.43	133.82	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Q	166	LYS	CG-CD-CE	13.42	152.15	111.90
9	2	232	TYR	CD1-CE1-CZ	13.31	131.78	119.80
30	K	241	GLU	OE1-CD-OE2	-13.30	107.34	123.30
9	2	156	LEU	CB-CG-CD2	13.19	133.43	111.00
9	i	156	LEU	CB-CG-CD2	13.18	133.40	111.00
13	m	208	ASP	CB-CG-OD2	-13.11	106.50	118.30
13	6	168	TYR	CD1-CE1-CZ	13.09	131.58	119.80
9	2	119	TYR	CD1-CE1-CZ	13.06	131.55	119.80
12	5	139	ARG	NE-CZ-NH1	13.05	126.83	120.30
13	m	168	TYR	CD1-CE1-CZ	13.04	131.54	119.80
13	6	208	ASP	CB-CG-OD2	-13.03	106.57	118.30
10	3	155	GLU	OE1-CD-OE2	-13.03	107.67	123.30
12	l	139	ARG	NE-CZ-NH1	13.03	126.81	120.30
13	m	131	TYR	CB-CG-CD1	13.00	128.80	121.00
11	4	163	LEU	CD1-CG-CD2	-13.00	71.51	110.50
9	i	119	TYR	CD1-CE1-CZ	12.99	131.50	119.80
3	c	202	ASP	CB-CG-OD1	12.98	129.98	118.30
11	k	163	LEU	CD1-CG-CD2	-12.98	71.57	110.50
13	m	134	ASP	CB-CG-OD2	12.96	129.97	118.30
12	l	144	ARG	CG-CD-NE	-12.96	84.58	111.80
12	5	144	ARG	CG-CD-NE	-12.96	84.58	111.80
13	m	104	LEU	C-N-CA	12.95	154.08	121.70
1	A	192	ASP	CB-CG-OD2	12.94	129.94	118.30
1	a	192	ASP	CB-CG-OD2	12.93	129.94	118.30
1	a	250	GLU	CG-CD-OE1	12.92	144.15	118.30
1	A	250	GLU	CG-CD-OE1	12.92	144.14	118.30
3	C	202	ASP	CB-CG-OD1	12.92	129.93	118.30
13	6	134	ASP	CB-CG-OD2	12.91	129.92	118.30
2	b	237	LYS	CD-CE-NZ	12.89	141.36	111.70
2	B	237	LYS	CD-CE-NZ	12.89	141.34	111.70
11	4	8	ARG	NH1-CZ-NH2	-12.89	105.22	119.40
8	1	152	ARG	CG-CD-NE	-12.88	84.75	111.80
13	6	131	TYR	CB-CG-CD1	12.87	128.72	121.00
11	k	8	ARG	NH1-CZ-NH2	-12.86	105.25	119.40
8	h	152	ARG	CG-CD-NE	-12.85	84.82	111.80
11	4	143	LEU	CD1-CG-CD2	-12.84	71.98	110.50
13	m	221	ARG	NH1-CZ-NH2	-12.83	105.29	119.40
13	6	221	ARG	NH1-CZ-NH2	-12.83	105.29	119.40
11	k	143	LEU	CD1-CG-CD2	-12.82	72.03	110.50
12	5	188	TYR	CB-CG-CD1	12.82	128.69	121.00
20	Z	632	GLU	CB-CG-CD	12.81	148.78	114.20
20	Z	632	GLU	CA-CB-CG	-12.80	85.23	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	67	TYR	CZ-CE2-CD2	12.76	131.29	119.80
11	k	67	TYR	CZ-CE2-CD2	12.75	131.28	119.80
12	l	188	TYR	CB-CG-CD1	12.75	128.65	121.00
1	a	217	GLU	OE1-CD-OE2	-12.74	108.01	123.30
2	B	234	ARG	CG-CD-NE	12.69	138.44	111.80
1	A	217	GLU	OE1-CD-OE2	-12.68	108.08	123.30
32	M	171	GLU	CG-CD-OE2	-12.68	92.94	118.30
10	j	80	ARG	NE-CZ-NH2	12.65	126.63	120.30
2	b	234	ARG	CG-CD-NE	12.64	138.35	111.80
31	L	367	LYS	CG-CD-CE	12.64	149.83	111.90
10	3	80	ARG	NE-CZ-NH2	12.63	126.61	120.30
32	M	96	ASN	CB-CG-OD1	-12.63	96.35	121.60
11	4	98	TYR	CB-CG-CD1	12.59	128.56	121.00
32	M	171	GLU	CG-CD-OE1	12.54	143.39	118.30
12	5	140	LEU	CB-CG-CD1	12.53	132.30	111.00
11	k	98	TYR	CB-CG-CD1	12.53	128.52	121.00
8	1	10	THR	OG1-CB-CG2	-12.53	81.18	110.00
12	l	140	LEU	CB-CG-CD1	12.53	132.29	111.00
9	i	195	ASP	CB-CG-OD2	12.52	129.57	118.30
8	h	10	THR	OG1-CB-CG2	-12.51	81.22	110.00
9	2	195	ASP	CB-CG-OD2	12.50	129.55	118.30
1	a	239	GLU	OE1-CD-OE2	-12.48	108.32	123.30
26	U	100	ARG	NE-CZ-NH2	-12.47	114.07	120.30
1	A	239	GLU	OE1-CD-OE2	-12.46	108.35	123.30
10	3	126	LEU	O-C-N	-12.43	102.81	122.70
5	e	18	GLU	O-C-N	12.37	144.22	123.20
2	B	103	GLU	OE1-CD-OE2	-12.32	108.51	123.30
9	2	232	TYR	CB-CG-CD2	12.30	128.38	121.00
8	h	194	ARG	NE-CZ-NH2	-12.28	114.16	120.30
2	b	103	GLU	OE1-CD-OE2	-12.27	108.58	123.30
8	h	152	ARG	NE-CZ-NH1	12.23	126.42	120.30
12	l	226	GLU	CG-CD-OE1	12.21	142.72	118.30
11	4	93	ARG	NE-CZ-NH2	12.21	126.41	120.30
12	5	226	GLU	CG-CD-OE1	12.21	142.72	118.30
8	1	10	THR	CA-CB-CG2	12.19	129.47	112.40
8	h	10	THR	CA-CB-CG2	12.19	129.47	112.40
12	5	162	VAL	CG1-CB-CG2	-12.19	91.40	110.90
8	1	152	ARG	NE-CZ-NH1	12.18	126.39	120.30
11	k	93	ARG	NE-CZ-NH2	12.17	126.38	120.30
12	l	162	VAL	CG1-CB-CG2	-12.16	91.44	110.90
12	l	104	GLN	CA-CB-CG	12.12	140.06	113.40
12	5	104	GLN	CA-CB-CG	12.12	140.05	113.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	18	LYS	CD-CE-NZ	12.11	139.55	111.70
8	l	18	LYS	CD-CE-NZ	12.11	139.54	111.70
12	l	196	ARG	NE-CZ-NH1	-12.09	114.25	120.30
3	c	142	ASP	CB-CG-OD2	12.08	129.17	118.30
3	C	142	ASP	CB-CG-OD2	12.08	129.17	118.30
28	H	464	MET	CB-CG-SD	12.07	148.63	112.40
12	5	196	ARG	NE-CZ-NH1	-12.03	114.28	120.30
5	E	213	ASP	CB-CG-OD2	12.01	129.11	118.30
5	e	110	GLU	OE1-CD-OE2	-12.01	108.89	123.30
5	e	10	ARG	NH1-CZ-NH2	-11.96	106.24	119.40
1	A	250	GLU	CG-CD-OE2	-11.96	94.39	118.30
5	E	110	GLU	OE1-CD-OE2	-11.95	108.96	123.30
1	a	250	GLU	CG-CD-OE2	-11.95	94.41	118.30
5	e	213	ASP	CB-CG-OD2	11.94	129.05	118.30
1	A	96	ARG	NE-CZ-NH1	-11.88	114.36	120.30
1	a	96	ARG	NE-CZ-NH1	-11.81	114.40	120.30
9	2	88	ILE	CB-CG1-CD1	-11.79	80.88	113.90
10	3	193	ASP	CB-CG-OD2	11.79	128.91	118.30
2	B	248	GLU	OE1-CD-OE2	-11.78	109.16	123.30
9	i	88	ILE	CB-CG1-CD1	-11.78	80.92	113.90
2	b	248	GLU	OE1-CD-OE2	-11.77	109.17	123.30
13	m	168	TYR	CB-CG-CD2	11.77	128.06	121.00
10	3	39	LYS	CA-CB-CG	11.74	139.24	113.40
10	j	39	LYS	CA-CB-CG	11.74	139.22	113.40
10	j	193	ASP	CB-CG-OD2	11.73	128.86	118.30
10	3	74	TYR	CD1-CE1-CZ	11.69	130.32	119.80
13	6	168	TYR	CB-CG-CD2	11.68	128.01	121.00
10	j	74	TYR	CD1-CE1-CZ	11.62	130.26	119.80
10	j	98	ARG	CG-CD-NE	-11.61	87.41	111.80
1	a	64	LEU	CB-CG-CD2	11.61	130.73	111.00
10	j	205	ASP	CA-C-O	11.60	144.46	120.10
2	b	201	GLU	OE1-CD-OE2	-11.59	109.39	123.30
13	m	47	TYR	CB-CG-CD2	11.59	127.95	121.00
1	a	13	ASP	CB-CG-OD1	-11.59	107.87	118.30
1	A	13	ASP	CB-CG-OD1	-11.59	107.87	118.30
10	3	205	ASP	CA-C-O	11.59	144.43	120.10
10	3	98	ARG	CG-CD-NE	-11.58	87.48	111.80
12	5	196	ARG	CD-NE-CZ	11.58	139.81	123.60
1	A	64	LEU	CB-CG-CD2	11.58	130.68	111.00
13	6	47	TYR	CB-CG-CD2	11.57	127.94	121.00
3	C	16	GLU	OE1-CD-OE2	-11.55	109.44	123.30
12	l	196	ARG	CD-NE-CZ	11.55	139.77	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	149	GLU	OE1-CD-OE2	-11.55	109.44	123.30
2	B	201	GLU	OE1-CD-OE2	-11.55	109.44	123.30
9	2	37	PHE	CB-CG-CD1	11.53	128.87	120.80
1	a	149	GLU	OE1-CD-OE2	-11.52	109.47	123.30
3	c	16	GLU	OE1-CD-OE2	-11.52	109.48	123.30
9	i	37	PHE	CB-CG-CD1	11.50	128.85	120.80
10	3	165	GLU	OE1-CD-OE2	-11.50	109.50	123.30
11	4	11	ASP	CB-CG-OD1	11.48	128.64	118.30
11	k	11	ASP	CB-CG-OD1	11.46	128.61	118.30
9	i	109	LEU	CD1-CG-CD2	-11.45	76.14	110.50
9	2	109	LEU	CD1-CG-CD2	-11.45	76.16	110.50
13	m	230	ASP	CA-C-O	-11.44	96.08	120.10
13	6	177	LYS	CD-CE-NZ	11.43	137.99	111.70
13	6	230	ASP	CA-C-O	-11.42	96.11	120.10
10	j	124	PHE	CA-C-N	-11.42	92.08	117.20
9	2	153	TYR	OH-CZ-CE2	-11.41	89.28	120.10
9	i	46	ASP	CB-CG-OD1	11.40	128.56	118.30
13	m	177	LYS	CD-CE-NZ	11.40	137.92	111.70
1	a	115	ASP	CB-CG-OD1	11.38	128.55	118.30
1	A	115	ASP	CB-CG-OD1	11.38	128.55	118.30
9	i	153	TYR	OH-CZ-CE2	-11.36	89.42	120.10
9	2	46	ASP	CB-CG-OD1	11.35	128.51	118.30
10	3	154	TYR	CB-CG-CD1	11.33	127.80	121.00
31	L	421	LYS	CB-CG-CD	11.30	140.99	111.60
13	6	111	PHE	CB-CG-CD1	-11.25	112.92	120.80
8	1	197	PHE	CB-CG-CD2	-11.21	112.95	120.80
31	L	367	LYS	CD-CE-NZ	-11.16	86.04	111.70
2	B	217	GLU	OE1-CD-OE2	-11.15	109.92	123.30
8	h	128	VAL	CG1-CB-CG2	-11.14	93.08	110.90
10	3	131	ASP	CB-CG-OD2	11.13	128.31	118.30
2	b	217	GLU	OE1-CD-OE2	-11.12	109.95	123.30
8	1	128	VAL	CG1-CB-CG2	-11.12	93.12	110.90
3	c	209	ASP	CB-CG-OD1	11.11	128.30	118.30
11	4	121	TYR	CB-CG-CD1	11.11	127.67	121.00
3	C	209	ASP	CB-CG-OD1	11.10	128.29	118.30
24	Q	51	ARG	N-CA-CB	-11.09	90.64	110.60
12	5	108	LYS	CD-CE-NZ	11.09	137.20	111.70
11	k	121	TYR	CB-CG-CD1	11.08	127.65	121.00
12	l	108	LYS	CD-CE-NZ	11.07	137.17	111.70
32	M	261	LYS	CG-CD-CE	11.05	145.05	111.90
7	g	223	GLU	OE1-CD-OE2	-11.05	110.04	123.30
8	h	93	GLU	OE1-CD-OE2	-11.04	110.05	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	133	TYR	CD1-CE1-CZ	11.04	129.73	119.80
12	l	253	TYR	CD1-CE1-CZ	11.04	129.73	119.80
8	1	133	TYR	CD1-CE1-CZ	11.03	129.72	119.80
10	j	53	ILE	CG1-CB-CG2	-11.02	87.16	111.40
8	1	93	GLU	OE1-CD-OE2	-11.02	110.08	123.30
13	6	131	TYR	CZ-CE2-CD2	11.02	129.71	119.80
10	3	53	ILE	CG1-CB-CG2	-11.01	87.17	111.40
10	3	154	TYR	CZ-CE2-CD2	11.01	129.71	119.80
13	m	221	ARG	CB-CG-CD	11.00	140.19	111.60
13	6	221	ARG	CB-CG-CD	10.99	140.18	111.60
13	6	221	ARG	NE-CZ-NH1	10.99	125.80	120.30
1	A	64	LEU	CB-CG-CD1	-10.98	92.33	111.00
12	5	253	TYR	CD1-CE1-CZ	10.98	129.68	119.80
13	m	131	TYR	CZ-CE2-CD2	10.98	129.68	119.80
1	a	64	LEU	CB-CG-CD1	-10.97	92.34	111.00
12	l	144	ARG	NE-CZ-NH2	-10.94	114.83	120.30
13	m	221	ARG	NE-CZ-NH1	10.94	125.77	120.30
5	e	209	GLU	OE1-CD-OE2	-10.91	110.20	123.30
5	E	209	GLU	OE1-CD-OE2	-10.90	110.22	123.30
11	4	155	GLU	OE1-CD-OE2	-10.88	110.24	123.30
12	5	144	ARG	NE-CZ-NH2	-10.88	114.86	120.30
11	k	155	GLU	OE1-CD-OE2	-10.85	110.28	123.30
11	4	121	TYR	CZ-CE2-CD2	10.84	129.56	119.80
2	B	220	ASP	CB-CG-OD2	10.84	128.06	118.30
6	f	9	ASP	CB-CG-OD1	10.80	128.02	118.30
16	V	194	ARG	CG-CD-NE	10.80	134.48	111.80
6	F	9	ASP	CB-CG-OD1	10.80	128.02	118.30
11	k	121	TYR	CZ-CE2-CD2	10.79	129.51	119.80
5	e	9	ASP	CB-CG-OD2	10.78	128.00	118.30
2	b	220	ASP	CB-CG-OD2	10.77	127.99	118.30
12	5	242	ARG	NE-CZ-NH2	10.76	125.68	120.30
10	j	75	LYS	CD-CE-NZ	10.74	136.40	111.70
12	l	242	ARG	NE-CZ-NH2	10.73	125.67	120.30
10	3	75	LYS	CD-CE-NZ	10.72	136.36	111.70
13	m	53	ASP	CB-CG-OD2	10.69	127.92	118.30
5	E	105	GLU	OE1-CD-OE2	-10.69	110.47	123.30
11	4	145	ASP	CB-CG-OD1	-10.69	108.68	118.30
13	6	53	ASP	CB-CG-OD2	10.69	127.92	118.30
5	e	105	GLU	OE1-CD-OE2	-10.68	110.48	123.30
11	k	145	ASP	CB-CG-OD1	-10.68	108.69	118.30
9	2	228	LYS	CD-CE-NZ	10.67	136.23	111.70
1	A	95	LEU	CB-CG-CD2	10.65	129.11	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	a	95	LEU	CB-CG-CD2	10.65	129.11	111.00
9	i	172	LYS	CD-CE-NZ	10.62	136.11	111.70
11	k	170	LYS	CA-CB-CG	10.61	136.74	113.40
20	Z	774	ARG	NE-CZ-NH2	-10.61	115.00	120.30
8	1	120	TYR	CD1-CE1-CZ	10.60	129.34	119.80
11	4	170	LYS	CA-CB-CG	10.60	136.72	113.40
9	2	172	LYS	CD-CE-NZ	10.60	136.07	111.70
9	2	98	TYR	CB-CG-CD1	-10.59	114.65	121.00
9	2	126	TYR	CZ-CE2-CD2	10.58	129.32	119.80
9	i	126	TYR	CZ-CE2-CD2	10.57	129.31	119.80
8	h	120	TYR	CD1-CE1-CZ	10.55	129.30	119.80
9	i	98	TYR	CB-CG-CD1	-10.51	114.69	121.00
13	m	50	LYS	CB-CG-CD	10.50	138.91	111.60
8	1	133	TYR	CB-CG-CD2	10.50	127.30	121.00
12	l	191	ASP	CB-CG-OD1	10.49	127.74	118.30
13	6	50	LYS	CB-CG-CD	10.49	138.86	111.60
24	Q	166	LYS	CD-CE-NZ	-10.48	87.58	111.70
8	1	133	TYR	CD1-CG-CD2	-10.48	106.37	117.90
31	L	243	PHE	CB-CG-CD2	-10.48	113.46	120.80
8	h	133	TYR	CD1-CG-CD2	-10.46	106.39	117.90
8	1	194	ARG	NE-CZ-NH1	10.46	125.53	120.30
12	5	191	ASP	CB-CG-OD1	10.45	127.70	118.30
12	l	81	PHE	CD1-CG-CD2	-10.44	104.73	118.30
12	l	188	TYR	CZ-CE2-CD2	10.44	129.20	119.80
12	5	81	PHE	CD1-CG-CD2	-10.40	104.78	118.30
5	E	118	ASP	CB-CG-OD1	10.40	127.66	118.30
5	e	118	ASP	CB-CG-OD1	10.39	127.66	118.30
8	h	133	TYR	CB-CG-CD2	10.38	127.23	121.00
12	5	188	TYR	CZ-CE2-CD2	10.38	129.14	119.80
6	F	173	GLU	OE1-CD-OE2	-10.36	110.86	123.30
5	e	205	LYS	CD-CE-NZ	10.36	135.53	111.70
5	E	205	LYS	CD-CE-NZ	10.36	135.53	111.70
13	m	86	ASP	OD1-CG-OD2	-10.36	103.62	123.30
6	f	173	GLU	OE1-CD-OE2	-10.35	110.88	123.30
13	m	46	ARG	CD-NE-CZ	-10.35	109.11	123.60
13	6	46	ARG	CD-NE-CZ	-10.32	109.15	123.60
8	h	100	ASP	CB-CG-OD2	10.30	127.57	118.30
8	1	100	ASP	CB-CG-OD2	10.28	127.55	118.30
7	g	202	LEU	CB-CG-CD2	10.28	128.47	111.00
9	2	36	LYS	CD-CE-NZ	10.24	135.25	111.70
12	5	226	GLU	CA-CB-CG	10.22	135.89	113.40
13	m	113	TYR	CB-CG-CD2	-10.22	114.87	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	36	LYS	CD-CE-NZ	10.21	135.18	111.70
12	l	139	ARG	CD-NE-CZ	-10.21	109.31	123.60
5	e	7	GLU	CG-CD-OE2	-10.20	97.89	118.30
12	l	226	GLU	CA-CB-CG	10.18	135.80	113.40
12	5	139	ARG	CD-NE-CZ	-10.18	109.34	123.60
15	W	87	MET	CG-SD-CE	10.17	116.48	100.20
11	k	121	TYR	CD1-CE1-CZ	10.15	128.93	119.80
13	m	182	TYR	CB-CG-CD2	10.14	127.08	121.00
6	F	169	LYS	CD-CE-NZ	-10.13	88.39	111.70
13	m	13	TYR	CZ-CE2-CD2	10.13	128.92	119.80
13	6	13	TYR	CZ-CE2-CD2	10.13	128.92	119.80
6	f	169	LYS	CD-CE-NZ	-10.13	88.41	111.70
13	6	47	TYR	CD1-CE1-CZ	10.12	128.91	119.80
25	R	225	LYS	CB-CG-CD	10.12	137.90	111.60
10	3	67	PHE	CB-CG-CD2	10.10	127.87	120.80
13	6	182	TYR	CB-CG-CD2	10.10	127.06	121.00
11	4	121	TYR	CD1-CE1-CZ	10.10	128.89	119.80
13	m	47	TYR	CD1-CE1-CZ	10.07	128.86	119.80
10	3	154	TYR	CD1-CG-CD2	-10.06	106.83	117.90
10	3	193	ASP	CB-CG-OD1	-10.04	109.27	118.30
11	4	121	TYR	CD1-CG-CD2	-10.03	106.87	117.90
11	k	121	TYR	CD1-CG-CD2	-10.02	106.88	117.90
13	m	194	ASP	CB-CG-OD1	-10.01	109.29	118.30
11	4	111	LYS	CD-CE-NZ	10.01	134.72	111.70
30	K	199	GLU	OE1-CD-OE2	-10.00	111.30	123.30
10	j	193	ASP	CB-CG-OD1	-9.99	109.30	118.30
13	6	194	ASP	CB-CG-OD1	-9.97	109.33	118.30
31	L	367	LYS	CA-CB-CG	9.97	135.34	113.40
10	j	67	PHE	CB-CG-CD2	9.97	127.78	120.80
22	S	192	GLU	OE1-CD-OE2	-9.97	111.34	123.30
15	W	21	PHE	CB-CG-CD2	9.96	127.78	120.80
11	k	111	LYS	CD-CE-NZ	9.96	134.60	111.70
11	k	46	PHE	CB-CG-CD1	9.94	127.76	120.80
11	4	46	PHE	CB-CG-CD1	9.94	127.76	120.80
12	5	258	ASP	CB-CG-OD2	9.93	127.24	118.30
13	6	177	LYS	CB-CG-CD	9.93	137.42	111.60
31	L	421	LYS	CD-CE-NZ	-9.92	88.88	111.70
13	m	177	LYS	CB-CG-CD	9.92	137.39	111.60
10	j	118	LYS	CB-CG-CD	9.88	137.30	111.60
10	3	118	LYS	CB-CG-CD	9.88	137.27	111.60
11	4	67	TYR	CD1-CG-CD2	-9.87	107.05	117.90
12	l	258	ASP	CB-CG-OD2	9.86	127.18	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	47	TYR	CD1-CG-CD2	-9.86	107.05	117.90
8	h	133	TYR	CZ-CE2-CD2	9.86	128.67	119.80
9	i	101	ARG	CD-NE-CZ	-9.85	109.81	123.60
11	k	67	TYR	CD1-CG-CD2	-9.85	107.06	117.90
12	l	115	PHE	CD1-CG-CD2	-9.85	105.49	118.30
12	5	115	PHE	CD1-CG-CD2	-9.85	105.50	118.30
9	2	101	ARG	CD-NE-CZ	-9.85	109.81	123.60
10	j	118	LYS	CD-CE-NZ	-9.84	89.06	111.70
10	3	118	LYS	CD-CE-NZ	-9.82	89.10	111.70
13	6	46	ARG	CG-CD-NE	9.81	132.40	111.80
32	M	68	LYS	CB-CG-CD	9.81	137.10	111.60
13	m	46	ARG	CG-CD-NE	9.79	132.37	111.80
10	3	154	TYR	CD1-CE1-CZ	9.78	128.60	119.80
9	2	153	TYR	CZ-CE2-CD2	-9.77	111.00	119.80
10	j	198	ARG	NE-CZ-NH1	9.77	125.19	120.30
12	l	245	TYR	CD1-CE1-CZ	9.77	128.60	119.80
13	6	47	TYR	CD1-CG-CD2	-9.77	107.15	117.90
1	A	200	GLU	OE1-CD-OE2	-9.77	111.57	123.30
8	1	133	TYR	CZ-CE2-CD2	9.77	128.59	119.80
1	a	200	GLU	OE1-CD-OE2	-9.77	111.58	123.30
1	a	112	MET	CG-SD-CE	9.76	115.82	100.20
1	A	112	MET	CG-SD-CE	9.76	115.82	100.20
9	i	126	TYR	CB-CG-CD1	9.76	126.86	121.00
12	l	214	VAL	CG1-CB-CG2	-9.76	95.29	110.90
9	i	153	TYR	CZ-CE2-CD2	-9.76	111.02	119.80
12	l	147	GLU	CA-CB-CG	9.75	134.85	113.40
10	3	198	ARG	NE-CZ-NH1	9.75	125.17	120.30
12	5	147	GLU	CA-CB-CG	9.75	134.85	113.40
2	b	70	ASP	CB-CG-OD1	9.74	127.06	118.30
12	5	214	VAL	CG1-CB-CG2	-9.74	95.32	110.90
8	h	41	ASP	CB-CG-OD1	9.72	127.05	118.30
8	1	120	TYR	CB-CG-CD2	9.72	126.83	121.00
8	1	41	ASP	CB-CG-OD1	9.69	127.03	118.30
5	E	20	ARG	O-C-N	-9.69	107.19	122.70
12	l	245	TYR	CB-CG-CD2	9.69	126.81	121.00
3	c	222	ASP	CB-CG-OD2	9.68	127.02	118.30
8	h	120	TYR	CB-CG-CD2	9.68	126.81	121.00
3	C	222	ASP	CB-CG-OD2	9.67	127.00	118.30
9	2	126	TYR	CB-CG-CD1	9.66	126.80	121.00
2	B	70	ASP	CB-CG-OD1	9.66	126.99	118.30
10	3	131	ASP	O-C-N	9.66	138.15	122.70
13	m	40	ASP	OD1-CG-OD2	-9.65	104.97	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	245	TYR	CD1-CE1-CZ	9.64	128.48	119.80
13	6	40	ASP	OD1-CG-OD2	-9.64	104.98	123.30
13	m	221	ARG	CG-CD-NE	9.61	131.97	111.80
13	6	221	ARG	CG-CD-NE	9.60	131.95	111.80
7	g	57	LYS	CA-CB-CG	9.59	134.51	113.40
7	G	57	LYS	CA-CB-CG	9.59	134.49	113.40
7	g	206	ASP	CB-CG-OD2	9.57	126.92	118.30
11	k	139	TYR	CZ-CE2-CD2	9.57	128.41	119.80
15	W	87	MET	CA-CB-CG	9.55	129.54	113.30
7	g	104	LYS	CD-CE-NZ	-9.55	89.74	111.70
12	5	245	TYR	CB-CG-CD2	9.55	126.73	121.00
13	6	99	ARG	NE-CZ-NH1	9.55	125.07	120.30
9	i	92	ILE	CB-CG1-CD1	9.55	140.63	113.90
9	2	92	ILE	CB-CG1-CD1	9.54	140.62	113.90
11	4	139	TYR	CZ-CE2-CD2	9.54	128.38	119.80
7	G	104	LYS	CD-CE-NZ	-9.53	89.78	111.70
28	H	314	VAL	N-CA-C	-9.53	85.27	111.00
32	M	42	ARG	CD-NE-CZ	9.53	136.94	123.60
8	1	114	LYS	CG-CD-CE	9.53	140.48	111.90
12	5	115	PHE	CD1-CE1-CZ	9.52	131.53	120.10
32	M	124	ARG	CG-CD-NE	-9.52	91.82	111.80
8	h	114	LYS	CG-CD-CE	9.51	140.44	111.90
12	l	115	PHE	CD1-CE1-CZ	9.51	131.51	120.10
13	6	182	TYR	OH-CZ-CE2	-9.48	94.51	120.10
13	m	182	TYR	OH-CZ-CE2	-9.46	94.57	120.10
11	k	139	TYR	CB-CG-CD2	9.45	126.67	121.00
9	i	126	TYR	CD1-CG-CD2	-9.43	107.52	117.90
9	i	37	PHE	CB-CG-CD2	-9.43	114.20	120.80
13	m	77	LYS	CD-CE-NZ	9.43	133.38	111.70
11	k	87	GLU	OE1-CD-OE2	-9.42	111.99	123.30
9	2	126	TYR	CD1-CG-CD2	-9.42	107.54	117.90
13	6	77	LYS	CD-CE-NZ	9.42	133.36	111.70
13	6	109	ARG	NE-CZ-NH1	9.42	125.01	120.30
11	4	139	TYR	CB-CG-CD2	9.39	126.64	121.00
7	G	114	ASP	CB-CG-OD2	9.39	126.75	118.30
11	k	176	PHE	CD1-CE1-CZ	9.39	131.37	120.10
12	5	170	LEU	CD1-CG-CD2	-9.39	82.34	110.50
12	l	170	LEU	CD1-CG-CD2	-9.38	82.38	110.50
11	4	176	PHE	CD1-CE1-CZ	9.38	131.35	120.10
1	a	115	ASP	OD1-CG-OD2	-9.37	105.49	123.30
13	m	104	LEU	CA-C-N	9.37	137.81	117.20
7	g	114	ASP	CB-CG-OD2	9.36	126.72	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	115	ASP	OD1-CG-OD2	-9.36	105.51	123.30
11	4	87	GLU	OE1-CD-OE2	-9.36	112.06	123.30
11	4	176	PHE	CD1-CG-CD2	-9.35	106.14	118.30
12	l	245	TYR	CZ-CE2-CD2	9.35	128.21	119.80
13	6	131	TYR	CD1-CG-CD2	-9.35	107.62	117.90
1	A	13	ASP	CB-CG-OD2	9.35	126.71	118.30
13	m	85	PHE	CB-CG-CD1	9.34	127.33	120.80
13	m	113	TYR	C-N-CA	-9.34	98.36	121.70
9	i	119	TYR	CD1-CG-CD2	-9.33	107.63	117.90
11	k	139	TYR	CD1-CG-CD2	-9.33	107.63	117.90
9	2	37	PHE	CB-CG-CD2	-9.33	114.27	120.80
11	4	135	TYR	CD1-CE1-CZ	9.33	128.19	119.80
11	4	139	TYR	CD1-CG-CD2	-9.32	107.64	117.90
11	k	176	PHE	CD1-CG-CD2	-9.32	106.18	118.30
2	b	81	ASP	CB-CG-OD1	9.32	126.69	118.30
5	e	224	LYS	CG-CD-CE	9.32	139.85	111.90
5	E	224	LYS	CG-CD-CE	9.32	139.85	111.90
13	m	141	ARG	CG-CD-NE	9.32	131.36	111.80
1	a	13	ASP	CB-CG-OD2	9.31	126.68	118.30
12	5	245	TYR	CZ-CE2-CD2	9.31	128.18	119.80
10	3	149	MET	CA-CB-CG	9.31	129.12	113.30
13	6	133	PHE	CD1-CG-CD2	-9.30	106.21	118.30
3	c	105	ASP	OD1-CG-OD2	-9.30	105.63	123.30
9	2	31	THR	OG1-CB-CG2	-9.29	88.62	110.00
9	2	119	TYR	CD1-CG-CD2	-9.29	107.68	117.90
13	m	133	PHE	CD1-CG-CD2	-9.29	106.22	118.30
13	6	141	ARG	CG-CD-NE	9.29	131.30	111.80
13	m	131	TYR	CD1-CG-CD2	-9.29	107.69	117.90
2	B	81	ASP	CB-CG-OD1	9.29	126.66	118.30
9	i	31	THR	OG1-CB-CG2	-9.28	88.65	110.00
28	H	420	ARG	NE-CZ-NH1	9.28	124.94	120.30
3	C	105	ASP	OD1-CG-OD2	-9.28	105.67	123.30
11	k	135	TYR	CD1-CE1-CZ	9.27	128.15	119.80
5	e	53	ARG	NE-CZ-NH1	9.27	124.93	120.30
9	i	215	TYR	CB-CG-CD1	9.24	126.55	121.00
10	3	87	PHE	CD1-CG-CD2	-9.24	106.29	118.30
22	S	43	LYS	CG-CD-CE	9.24	139.61	111.90
10	j	87	PHE	CD1-CG-CD2	-9.23	106.30	118.30
5	E	20	ARG	NE-CZ-NH1	9.23	124.91	120.30
30	K	399	ARG	CB-CG-CD	9.22	135.57	111.60
3	c	212	GLU	OE1-CD-OE2	-9.22	112.24	123.30
5	E	10	ARG	NE-CZ-NH1	-9.20	115.70	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	47	TYR	CZ-CE2-CD2	9.19	128.07	119.80
10	j	202	MET	CA-CB-CG	9.19	128.92	113.30
3	C	212	GLU	OE1-CD-OE2	-9.19	112.28	123.30
7	g	238	GLU	OE1-CD-OE2	-9.18	112.28	123.30
13	m	47	TYR	CZ-CE2-CD2	9.18	128.06	119.80
10	3	202	MET	CA-CB-CG	9.17	128.89	113.30
31	L	339	ARG	NE-CZ-NH2	-9.16	115.72	120.30
11	k	163	LEU	CB-CG-CD1	9.15	126.56	111.00
25	R	176	ARG	NE-CZ-NH2	-9.15	115.72	120.30
11	4	163	LEU	CB-CG-CD1	9.15	126.56	111.00
1	A	77	ARG	NE-CZ-NH1	9.12	124.86	120.30
3	C	27	GLU	OE1-CD-OE2	-9.11	112.36	123.30
13	m	85	PHE	CD1-CG-CD2	-9.11	106.45	118.30
9	i	84	VAL	CA-CB-CG2	9.11	124.56	110.90
26	U	100	ARG	NE-CZ-NH1	9.09	124.85	120.30
9	2	126	TYR	CD1-CE1-CZ	9.09	127.98	119.80
9	2	84	VAL	CA-CB-CG2	9.08	124.52	110.90
10	3	83	GLU	OE1-CD-OE2	-9.07	112.41	123.30
10	j	83	GLU	OE1-CD-OE2	-9.07	112.42	123.30
11	4	139	TYR	CD1-CE1-CZ	9.07	127.96	119.80
12	5	277	GLU	OE1-CD-OE2	-9.06	112.43	123.30
10	j	154	TYR	CG-CD2-CE2	-9.05	114.06	121.30
12	l	277	GLU	OE1-CD-OE2	-9.05	112.44	123.30
13	6	85	PHE	CB-CG-CD1	-9.04	114.47	120.80
3	c	27	GLU	OE1-CD-OE2	-9.04	112.45	123.30
13	6	211	GLU	CG-CD-OE1	-9.04	100.22	118.30
1	a	222	ASP	CB-CG-OD1	9.04	126.43	118.30
11	k	139	TYR	CD1-CE1-CZ	9.04	127.93	119.80
13	m	211	GLU	CG-CD-OE1	-9.03	100.24	118.30
2	B	113	GLU	OE1-CD-OE2	-9.03	112.46	123.30
2	b	113	GLU	OE1-CD-OE2	-9.03	112.47	123.30
9	i	126	TYR	CD1-CE1-CZ	9.03	127.92	119.80
1	A	222	ASP	CB-CG-OD1	9.01	126.41	118.30
5	e	250	GLU	CA-C-O	8.99	138.99	120.10
12	5	245	TYR	CD1-CG-CD2	-8.98	108.02	117.90
5	E	250	GLU	CA-C-O	8.98	138.95	120.10
5	e	229	LYS	CG-CD-CE	8.97	138.81	111.90
10	j	80	ARG	NE-CZ-NH1	-8.96	115.82	120.30
5	E	229	LYS	CG-CD-CE	8.96	138.77	111.90
8	h	202	TYR	CG-CD1-CE1	-8.95	114.14	121.30
12	l	245	TYR	CD1-CG-CD2	-8.94	108.06	117.90
13	m	83	TYR	CB-CG-CD1	8.95	126.37	121.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	80	ARG	NE-CZ-NH1	-8.94	115.83	120.30
2	B	220	ASP	OD1-CG-OD2	-8.94	106.31	123.30
10	j	40	PHE	CZ-CE2-CD2	8.93	130.82	120.10
8	1	120	TYR	CD1-CG-CD2	-8.93	108.08	117.90
10	3	63	LEU	CD1-CG-CD2	-8.93	83.72	110.50
10	j	63	LEU	CD1-CG-CD2	-8.92	83.73	110.50
2	b	220	ASP	OD1-CG-OD2	-8.91	106.37	123.30
8	h	120	TYR	CD1-CG-CD2	-8.88	108.13	117.90
10	3	40	PHE	CZ-CE2-CD2	8.88	130.76	120.10
10	j	124	PHE	C-N-CA	-8.87	99.54	121.70
20	Z	774	ARG	NE-CZ-NH1	8.87	124.73	120.30
11	k	186	LYS	CD-CE-NZ	8.86	132.08	111.70
13	m	143	GLN	CA-CB-CG	8.86	132.88	113.40
11	4	121	TYR	CE1-CZ-CE2	-8.86	105.63	119.80
11	k	8	ARG	CD-NE-CZ	8.85	136.00	123.60
9	i	57	ASP	CB-CG-OD1	8.85	126.27	118.30
12	l	226	GLU	OE1-CD-OE2	-8.85	112.68	123.30
22	S	36	LYS	CD-CE-NZ	8.84	132.04	111.70
11	k	121	TYR	CE1-CZ-CE2	-8.83	105.67	119.80
11	4	8	ARG	CD-NE-CZ	8.83	135.97	123.60
11	4	186	LYS	CB-CG-CD	8.83	134.56	111.60
11	k	186	LYS	CB-CG-CD	8.83	134.56	111.60
11	4	186	LYS	CD-CE-NZ	8.83	132.01	111.70
8	h	133	TYR	CE1-CZ-CE2	-8.83	105.68	119.80
13	6	143	GLN	CA-CB-CG	8.83	132.82	113.40
11	4	135	TYR	CA-CB-CG	8.82	130.16	113.40
9	2	57	ASP	CB-CG-OD1	8.81	126.23	118.30
13	6	144	CYS	CA-CB-SG	8.81	129.86	114.00
10	3	87	PHE	CB-CG-CD1	8.80	126.96	120.80
8	1	133	TYR	CE1-CZ-CE2	-8.79	105.73	119.80
9	2	232	TYR	CD1-CG-CD2	-8.79	108.23	117.90
13	m	144	CYS	CA-CB-SG	8.79	129.82	114.00
11	k	46	PHE	CZ-CE2-CD2	8.79	130.64	120.10
11	k	135	TYR	CA-CB-CG	8.78	130.09	113.40
23	P	138	ARG	NE-CZ-NH1	8.78	124.69	120.30
12	5	226	GLU	OE1-CD-OE2	-8.78	112.77	123.30
8	h	52	CYS	CA-CB-SG	8.77	129.79	114.00
8	1	52	CYS	CA-CB-SG	8.77	129.79	114.00
11	4	46	PHE	CZ-CE2-CD2	8.77	130.62	120.10
10	j	87	PHE	CB-CG-CD1	8.76	126.93	120.80
1	A	222	ASP	CB-CG-OD2	8.75	126.18	118.30
12	l	148	ARG	CG-CD-NE	8.75	130.17	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
14	7	74	ARG	NE-CZ-NH2	-8.74	115.93	120.30
12	5	226	GLU	CG-CD-OE2	-8.74	100.82	118.30
12	5	148	ARG	CG-CD-NE	8.73	130.14	111.80
12	1	226	GLU	CG-CD-OE2	-8.73	100.84	118.30
30	K	399	ARG	CA-CB-CG	8.71	132.55	113.40
9	2	219	TYR	CB-CG-CD2	8.70	126.22	121.00
1	a	222	ASP	CB-CG-OD2	8.69	126.12	118.30
8	h	133	TYR	CB-CG-CD1	8.69	126.21	121.00
10	3	26	ASP	CB-CG-OD1	8.67	126.11	118.30
13	m	83	TYR	CD1-CE1-CZ	8.67	127.60	119.80
18	X	22	ARG	NE-CZ-NH1	8.66	124.63	120.30
9	2	119	TYR	CE1-CZ-CE2	-8.65	105.97	119.80
5	E	213	ASP	OD1-CG-OD2	-8.63	106.89	123.30
32	M	96	ASN	CB-CG-ND2	8.62	137.40	116.70
5	e	213	ASP	OD1-CG-OD2	-8.62	106.92	123.30
8	1	133	TYR	CB-CG-CD1	8.62	126.17	121.00
10	j	26	ASP	CB-CG-OD1	8.61	126.05	118.30
34	8	221	MET	CB-CG-SD	8.62	138.25	112.40
10	3	154	TYR	CE1-CZ-CE2	-8.61	106.03	119.80
9	i	119	TYR	CE1-CZ-CE2	-8.61	106.03	119.80
20	Z	943	LYS	CA-CB-CG	8.61	132.34	113.40
10	j	28	ARG	NE-CZ-NH2	8.61	124.60	120.30
13	6	72	LEU	CB-CG-CD1	8.61	125.63	111.00
13	m	142	GLU	CB-CG-CD	8.60	137.43	114.20
30	K	347	ARG	NE-CZ-NH2	8.60	124.60	120.30
11	4	93	ARG	CG-CD-NE	8.60	129.85	111.80
13	6	142	GLU	CB-CG-CD	8.59	137.40	114.20
13	6	221	ARG	NE-CZ-NH2	8.59	124.60	120.30
13	m	72	LEU	CB-CG-CD1	8.59	125.60	111.00
10	j	141	THR	CA-CB-CG2	-8.58	100.39	112.40
13	6	131	TYR	CD1-CE1-CZ	8.58	127.52	119.80
11	k	93	ARG	CG-CD-NE	8.57	129.80	111.80
13	m	221	ARG	NE-CZ-NH2	8.57	124.58	120.30
34	8	466	ASP	N-CA-CB	-8.55	95.21	110.60
1	a	183	GLU	OE1-CD-OE2	-8.54	113.05	123.30
10	3	176	ASP	CB-CG-OD1	8.54	125.98	118.30
5	e	136	ARG	NE-CZ-NH2	-8.54	116.03	120.30
9	2	217	ARG	NE-CZ-NH1	-8.53	116.04	120.30
8	h	120	TYR	CZ-CE2-CD2	8.52	127.47	119.80
10	3	28	ARG	NE-CZ-NH2	8.51	124.56	120.30
8	1	120	TYR	CZ-CE2-CD2	8.51	127.46	119.80
1	a	177	GLU	OE1-CD-OE2	-8.50	113.11	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	131	TYR	CD1-CE1-CZ	8.50	127.45	119.80
1	A	177	GLU	OE1-CD-OE2	-8.48	113.12	123.30
9	2	37	PHE	CD1-CG-CD2	-8.48	107.27	118.30
13	m	94	ILE	CG1-CB-CG2	-8.48	92.74	111.40
1	A	183	GLU	OE1-CD-OE2	-8.47	113.13	123.30
13	6	83	TYR	CB-CG-CD1	-8.47	115.92	121.00
13	m	86	ASP	CB-CG-OD2	8.46	125.91	118.30
10	3	199	TYR	CD1-CE1-CZ	8.45	127.40	119.80
21	N	515	ARG	NE-CZ-NH2	-8.44	116.08	120.30
5	e	7	GLU	CG-CD-OE1	8.44	135.18	118.30
10	j	199	TYR	CD1-CE1-CZ	8.44	127.40	119.80
5	E	136	ARG	NE-CZ-NH2	-8.44	116.08	120.30
9	i	37	PHE	CD1-CG-CD2	-8.43	107.34	118.30
13	m	83	TYR	CD1-CG-CD2	-8.43	108.63	117.90
12	l	161	LEU	CA-CB-CG	8.41	134.65	115.30
12	5	161	LEU	CA-CB-CG	8.41	134.64	115.30
22	S	43	LYS	CD-CE-NZ	-8.41	92.36	111.70
10	j	154	TYR	CB-CG-CD2	-8.40	115.96	121.00
11	4	67	TYR	CE1-CZ-CE2	-8.40	106.36	119.80
11	k	67	TYR	CE1-CZ-CE2	-8.40	106.36	119.80
11	k	29	LYS	CA-CB-CG	8.39	131.86	113.40
11	k	23	ARG	NE-CZ-NH2	8.39	124.50	120.30
33	J	390	MET	CG-SD-CE	-8.38	86.80	100.20
7	g	215	GLU	OE1-CD-OE2	-8.37	113.25	123.30
1	A	222	ASP	OD1-CG-OD2	-8.37	107.39	123.30
11	4	23	ARG	NE-CZ-NH2	8.37	124.48	120.30
31	L	426	LYS	CD-CE-NZ	8.37	130.94	111.70
11	4	29	LYS	CA-CB-CG	8.36	131.80	113.40
1	a	222	ASP	OD1-CG-OD2	-8.36	107.42	123.30
4	D	119	ARG	CB-CG-CD	8.35	133.31	111.60
13	6	131	TYR	CE1-CZ-CE2	-8.35	106.44	119.80
5	e	9	ASP	OD1-CG-OD2	-8.35	107.44	123.30
7	G	20	ARG	NE-CZ-NH1	-8.35	116.13	120.30
9	2	230	LYS	CA-CB-CG	8.34	131.74	113.40
13	6	47	TYR	CE1-CZ-CE2	-8.34	106.46	119.80
10	3	172	LEU	CB-CG-CD2	8.33	125.16	111.00
13	m	47	TYR	CE1-CZ-CE2	-8.33	106.47	119.80
1	a	250	GLU	OE1-CD-OE2	-8.32	113.31	123.30
7	g	20	ARG	NE-CZ-NH1	-8.32	116.14	120.30
1	A	250	GLU	OE1-CD-OE2	-8.32	113.32	123.30
11	4	135	TYR	CE1-CZ-OH	8.32	142.56	120.10
7	g	93	ARG	NE-CZ-NH1	8.31	124.46	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	149	LYS	CD-CE-NZ	8.31	130.82	111.70
20	Z	321	PHE	CB-CG-CD2	-8.31	114.98	120.80
11	k	135	TYR	CE1-CZ-OH	8.31	142.54	120.10
11	4	11	ASP	OD1-CG-OD2	-8.30	107.52	123.30
7	G	93	ARG	NE-CZ-NH1	8.30	124.45	120.30
9	2	126	TYR	CE1-CZ-CE2	-8.30	106.52	119.80
3	C	105	ASP	CB-CG-OD1	8.29	125.77	118.30
8	h	149	LYS	CD-CE-NZ	8.29	130.78	111.70
11	k	11	ASP	OD1-CG-OD2	-8.29	107.56	123.30
13	m	131	TYR	CE1-CZ-CE2	-8.29	106.54	119.80
10	3	176	ASP	CB-CG-OD2	8.29	125.76	118.30
3	c	105	ASP	CB-CG-OD1	8.28	125.75	118.30
6	F	138	ASP	CB-CG-OD1	8.28	125.75	118.30
10	j	199	TYR	CZ-CE2-CD2	8.28	127.25	119.80
3	c	202	ASP	OD1-CG-OD2	-8.27	107.58	123.30
6	f	138	ASP	CB-CG-OD1	8.27	125.74	118.30
3	C	202	ASP	OD1-CG-OD2	-8.27	107.59	123.30
9	2	232	TYR	CE1-CZ-CE2	-8.26	106.58	119.80
9	i	149	ASP	CB-CG-OD2	8.26	125.73	118.30
12	5	81	PHE	CD1-CE1-CZ	8.26	130.01	120.10
9	i	126	TYR	CE1-CZ-CE2	-8.26	106.59	119.80
7	g	191	GLU	OE1-CD-OE2	-8.25	113.39	123.30
2	b	160	LYS	CD-CE-NZ	8.24	130.65	111.70
13	m	113	TYR	CA-C-N	-8.23	99.08	117.20
24	Q	167	LYS	CD-CE-NZ	8.23	130.63	111.70
10	3	176	ASP	OD1-CG-OD2	-8.23	107.67	123.30
13	6	30	VAL	CG1-CB-CG2	-8.22	97.74	110.90
30	K	80	LYS	CD-CE-NZ	-8.22	92.78	111.70
2	B	160	LYS	CD-CE-NZ	8.22	130.61	111.70
29	I	300	ARG	CB-CG-CD	8.22	132.96	111.60
9	2	217	ARG	NH1-CZ-NH2	-8.22	110.36	119.40
5	e	25	GLU	OE1-CD-OE2	-8.21	113.44	123.30
12	l	81	PHE	CD1-CE1-CZ	8.21	129.96	120.10
3	C	109	GLU	CA-CB-CG	8.21	131.47	113.40
3	c	109	GLU	CA-CB-CG	8.20	131.44	113.40
9	2	149	ASP	CB-CG-OD2	8.20	125.68	118.30
10	3	199	TYR	CZ-CE2-CD2	8.20	127.18	119.80
9	i	211	LYS	O-C-N	8.20	135.81	122.70
13	m	145	ARG	NE-CZ-NH1	8.19	124.39	120.30
13	6	127	LYS	CD-CE-NZ	8.19	130.54	111.70
13	m	127	LYS	CD-CE-NZ	8.18	130.52	111.70
13	m	30	VAL	CG1-CB-CG2	-8.18	97.81	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	83	TYR	CZ-CE2-CD2	8.18	127.16	119.80
5	E	25	GLU	OE1-CD-OE2	-8.18	113.48	123.30
10	3	67	PHE	CD1-CG-CD2	-8.18	107.67	118.30
10	j	67	PHE	CD1-CG-CD2	-8.18	107.67	118.30
9	i	58	LYS	CD-CE-NZ	-8.17	92.92	111.70
8	h	175	ASP	CB-CG-OD1	8.16	125.65	118.30
12	5	242	ARG	NE-CZ-NH1	-8.16	116.22	120.30
13	6	145	ARG	NE-CZ-NH1	8.16	124.38	120.30
9	2	58	LYS	CD-CE-NZ	-8.14	92.97	111.70
12	l	245	TYR	CE1-CZ-CE2	-8.12	106.81	119.80
8	1	175	ASP	CB-CG-OD1	8.11	125.60	118.30
13	6	72	LEU	CD1-CG-CD2	-8.11	86.17	110.50
35	9	31	GLN	CA-CB-CG	8.11	131.24	113.40
30	K	199	GLU	CG-CD-OE2	-8.11	102.08	118.30
12	l	242	ARG	NE-CZ-NH1	-8.10	116.25	120.30
2	b	201	GLU	CG-CD-OE2	8.10	134.50	118.30
9	2	254	GLU	OE1-CD-OE2	-8.10	113.58	123.30
13	m	72	LEU	CD1-CG-CD2	-8.10	86.21	110.50
2	B	201	GLU	CG-CD-OE2	8.10	134.49	118.30
10	3	40	PHE	CD1-CG-CD2	-8.09	107.78	118.30
34	8	331	ARG	NE-CZ-NH1	8.09	124.35	120.30
12	5	245	TYR	CE1-CZ-CE2	-8.09	106.85	119.80
9	i	181	ILE	CG1-CB-CG2	-8.08	93.63	111.40
7	g	114	ASP	OD1-CG-OD2	-8.07	107.96	123.30
29	I	246	ARG	NE-CZ-NH1	-8.07	116.27	120.30
9	2	181	ILE	CG1-CB-CG2	-8.07	93.65	111.40
10	j	40	PHE	CD1-CG-CD2	-8.07	107.81	118.30
7	G	114	ASP	OD1-CG-OD2	-8.06	107.98	123.30
5	e	18	GLU	N-CA-CB	8.06	125.10	110.60
15	W	60	ARG	NE-CZ-NH1	8.06	124.33	120.30
8	h	194	ARG	NE-CZ-NH1	8.05	124.33	120.30
11	4	139	TYR	CE1-CZ-CE2	-8.04	106.93	119.80
11	k	70	ARG	CD-NE-CZ	8.04	134.85	123.60
11	k	139	TYR	CE1-CZ-CE2	-8.04	106.94	119.80
8	1	201	GLU	CG-CD-OE2	-8.03	102.23	118.30
6	F	80	ASP	CB-CG-OD1	8.01	125.51	118.30
20	Z	366	LYS	CB-CG-CD	8.01	132.43	111.60
11	k	99	GLN	CB-CG-CD	8.00	132.40	111.60
11	4	70	ARG	CD-NE-CZ	8.00	134.80	123.60
11	4	99	GLN	CB-CG-CD	8.00	132.40	111.60
12	l	188	TYR	CD1-CG-CD2	-8.00	109.10	117.90
29	I	300	ARG	NE-CZ-NH2	-8.00	116.30	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	i	57	ASP	CB-CG-OD2	8.00	125.50	118.30
13	m	70	ASP	CB-CG-OD2	-7.99	111.11	118.30
20	Z	58	GLU	CA-CB-CG	-7.99	95.83	113.40
9	i	57	ASP	OD1-CG-OD2	-7.98	108.14	123.30
13	6	70	ASP	CB-CG-OD2	-7.98	111.12	118.30
12	5	188	TYR	CD1-CG-CD2	-7.98	109.12	117.90
12	5	140	LEU	CD1-CG-CD2	-7.97	86.60	110.50
29	I	321	ASP	CB-CG-OD2	-7.96	111.14	118.30
9	i	153	TYR	CA-CB-CG	7.96	128.52	113.40
9	2	57	ASP	CB-CG-OD2	7.96	125.46	118.30
12	l	77	THR	OG1-CB-CG2	-7.95	91.71	110.00
12	l	140	LEU	CD1-CG-CD2	-7.95	86.66	110.50
6	f	80	ASP	CB-CG-OD1	7.95	125.45	118.30
9	2	57	ASP	OD1-CG-OD2	-7.94	108.21	123.30
8	h	45	ARG	CD-NE-CZ	-7.94	112.48	123.60
8	1	120	TYR	CE1-CZ-CE2	-7.94	107.09	119.80
11	4	69	ILE	CB-CG1-CD1	7.94	136.13	113.90
9	i	217	ARG	NE-CZ-NH1	7.94	124.27	120.30
9	2	153	TYR	CA-CB-CG	7.93	128.48	113.40
11	k	69	ILE	CB-CG1-CD1	7.93	136.10	113.90
9	2	227	GLU	CA-CB-CG	7.93	130.84	113.40
3	c	5	ARG	NE-CZ-NH1	7.93	124.26	120.30
8	h	120	TYR	CE1-CZ-CE2	-7.92	107.12	119.80
12	5	77	THR	OG1-CB-CG2	-7.92	91.78	110.00
3	C	5	ARG	NE-CZ-NH1	7.92	124.26	120.30
5	e	81	LEU	CB-CG-CD2	7.91	124.44	111.00
12	5	276	LYS	CD-CE-NZ	7.91	129.88	111.70
20	Z	217	GLU	CA-CB-CG	7.91	130.79	113.40
5	E	81	LEU	CB-CG-CD2	7.90	124.43	111.00
12	l	276	LYS	CD-CE-NZ	7.89	129.86	111.70
8	1	45	ARG	CD-NE-CZ	-7.89	112.55	123.60
3	c	224	GLU	OE1-CD-OE2	-7.89	113.83	123.30
12	l	215	LEU	CB-CG-CD2	7.89	124.41	111.00
11	4	98	TYR	CZ-CE2-CD2	7.88	126.89	119.80
1	a	22	GLU	CG-CD-OE1	-7.88	102.54	118.30
7	g	57	LYS	CG-CD-CE	7.88	135.53	111.90
1	A	22	GLU	CG-CD-OE1	-7.88	102.55	118.30
12	5	215	LEU	CB-CG-CD2	7.87	124.39	111.00
12	5	215	LEU	CD1-CG-CD2	-7.87	86.89	110.50
12	l	215	LEU	CD1-CG-CD2	-7.87	86.89	110.50
3	C	224	GLU	OE1-CD-OE2	-7.86	113.86	123.30
7	G	57	LYS	CG-CD-CE	7.86	135.47	111.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	45	ARG	CG-CD-NE	7.85	128.28	111.80
10	3	199	TYR	CB-CG-CD2	7.85	125.71	121.00
11	k	98	TYR	CZ-CE2-CD2	7.84	126.86	119.80
8	h	128	VAL	CA-CB-CG1	7.83	122.65	110.90
7	g	20	ARG	NE-CZ-NH2	7.83	124.22	120.30
9	i	195	ASP	OD1-CG-OD2	-7.83	108.43	123.30
8	h	45	ARG	CG-CD-NE	7.82	128.22	111.80
10	j	199	TYR	CB-CG-CD2	7.81	125.69	121.00
9	2	195	ASP	OD1-CG-OD2	-7.81	108.46	123.30
8	1	128	VAL	CA-CB-CG1	7.80	122.61	110.90
4	D	90	ARG	CB-CG-CD	7.80	131.89	111.60
10	j	199	TYR	CD1-CG-CD2	-7.80	109.32	117.90
6	F	138	ASP	CB-CG-OD2	7.80	125.32	118.30
12	5	222	ASP	CB-CG-OD2	-7.80	111.28	118.30
30	K	148	ASP	CB-CG-OD1	7.79	125.31	118.30
10	3	131	ASP	OD1-CG-OD2	-7.78	108.52	123.30
12	1	222	ASP	CB-CG-OD2	-7.78	111.30	118.30
10	3	199	TYR	CD1-CG-CD2	-7.78	109.34	117.90
9	2	208	GLU	CG-CD-OE1	-7.77	102.76	118.30
7	g	114	ASP	CB-CG-OD1	7.77	125.29	118.30
9	i	208	GLU	CG-CD-OE1	-7.77	102.77	118.30
13	6	53	ASP	OD1-CG-OD2	-7.77	108.54	123.30
13	m	122	LEU	CB-CG-CD1	7.77	124.20	111.00
13	6	122	LEU	CB-CG-CD1	7.76	124.20	111.00
13	m	53	ASP	OD1-CG-OD2	-7.76	108.56	123.30
30	K	344	ARG	N-CA-CB	-7.76	96.63	110.60
7	G	20	ARG	NE-CZ-NH2	7.76	124.18	120.30
29	I	179	GLU	OE1-CD-OE2	-7.76	113.99	123.30
13	m	133	PHE	CD1-CE1-CZ	7.75	129.41	120.10
3	C	209	ASP	OD1-CG-OD2	-7.75	108.58	123.30
9	2	227	GLU	CG-CD-OE2	-7.75	102.80	118.30
15	W	23	ARG	NE-CZ-NH1	7.75	124.17	120.30
10	3	126	LEU	CA-C-N	7.75	134.24	117.20
5	E	180	GLN	CA-CB-CG	7.74	130.44	113.40
30	K	199	GLU	CG-CD-OE1	7.74	133.78	118.30
1	A	73	PHE	O-C-N	7.73	135.07	122.70
5	e	180	GLN	CA-CB-CG	7.73	130.40	113.40
20	Z	849	ARG	NE-CZ-NH2	-7.73	116.44	120.30
3	c	60	ASP	CB-CG-OD1	7.72	125.25	118.30
3	c	209	ASP	OD1-CG-OD2	-7.72	108.63	123.30
7	G	114	ASP	CB-CG-OD1	7.72	125.25	118.30
6	f	138	ASP	CB-CG-OD2	7.72	125.25	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	4	156	GLU	OE1-CD-OE2	-7.71	114.05	123.30
12	l	191	ASP	OD1-CG-OD2	-7.70	108.67	123.30
13	6	133	PHE	CD1-CE1-CZ	7.70	129.34	120.10
12	5	191	ASP	OD1-CG-OD2	-7.70	108.67	123.30
11	k	156	GLU	OE1-CD-OE2	-7.70	114.06	123.30
3	C	60	ASP	CB-CG-OD1	7.70	125.23	118.30
11	k	67	TYR	CD1-CE1-CZ	7.70	126.72	119.80
3	c	222	ASP	OD1-CG-OD2	-7.69	108.69	123.30
4	d	149	GLN	CA-CB-CG	7.69	130.31	113.40
10	j	115	LYS	CB-CG-CD	7.68	131.58	111.60
10	3	115	LYS	CB-CG-CD	7.68	131.57	111.60
3	C	222	ASP	OD1-CG-OD2	-7.67	108.72	123.30
11	4	67	TYR	CD1-CE1-CZ	7.67	126.70	119.80
7	g	201	TYR	CB-CG-CD2	-7.67	116.40	121.00
6	f	181	LYS	CD-CE-NZ	7.67	129.33	111.70
11	k	135	TYR	OH-CZ-CE2	-7.66	99.42	120.10
13	m	36	ARG	CD-NE-CZ	7.66	134.32	123.60
6	F	181	LYS	CD-CE-NZ	7.66	129.31	111.70
34	8	493	MET	CG-SD-CE	-7.66	87.95	100.20
11	4	135	TYR	OH-CZ-CE2	-7.65	99.44	120.10
9	i	209	ILE	CB-CG1-CD1	7.65	135.32	113.90
9	2	209	ILE	CB-CG1-CD1	7.65	135.32	113.90
21	N	671	LEU	CB-CG-CD2	7.64	123.99	111.00
16	V	194	ARG	NE-CZ-NH2	-7.64	116.48	120.30
13	6	36	ARG	CD-NE-CZ	7.64	134.30	123.60
6	F	138	ASP	OD1-CG-OD2	-7.64	108.79	123.30
10	3	118	LYS	CG-CD-CE	7.63	134.80	111.90
10	j	118	LYS	CG-CD-CE	7.63	134.80	111.90
9	2	243	LYS	CD-CE-NZ	7.63	129.24	111.70
27	O	306	ARG	NE-CZ-NH1	7.63	124.11	120.30
5	E	104	ASP	OD1-CG-OD2	-7.62	108.83	123.30
8	h	100	ASP	OD1-CG-OD2	-7.62	108.83	123.30
3	c	142	ASP	OD1-CG-OD2	-7.61	108.84	123.30
5	e	58	LEU	O-C-N	-7.60	110.54	122.70
8	l	100	ASP	OD1-CG-OD2	-7.60	108.86	123.30
8	l	194	ARG	CB-CG-CD	7.60	131.36	111.60
5	e	104	ASP	OD1-CG-OD2	-7.59	108.87	123.30
6	f	138	ASP	OD1-CG-OD2	-7.59	108.87	123.30
3	C	142	ASP	OD1-CG-OD2	-7.59	108.87	123.30
8	h	17	PHE	CB-CG-CD2	-7.58	115.49	120.80
12	l	233	LYS	CD-CE-NZ	-7.58	94.27	111.70
12	5	82	ARG	CG-CD-NE	7.58	127.72	111.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	J	57	PHE	CB-CG-CD2	-7.58	115.50	120.80
12	l	82	ARG	CG-CD-NE	7.57	127.70	111.80
12	5	233	LYS	CD-CE-NZ	-7.56	94.30	111.70
13	m	113	TYR	CG-CD2-CE2	-7.56	115.25	121.30
13	m	181	LYS	CG-CD-CE	-7.54	89.28	111.90
14	n	179	PHE	CB-CG-CD1	-7.54	115.52	120.80
11	4	145	ASP	CB-CG-OD2	7.54	125.09	118.30
23	P	69	ARG	NE-CZ-NH2	-7.54	116.53	120.30
8	h	175	ASP	CB-CG-OD2	7.54	125.08	118.30
13	6	181	LYS	CG-CD-CE	-7.54	89.30	111.90
28	H	434	ARG	NE-CZ-NH2	-7.53	116.53	120.30
11	k	145	ASP	CB-CG-OD2	7.53	125.08	118.30
9	2	126	TYR	CB-CG-CD2	7.53	125.52	121.00
11	4	139	TYR	CB-CG-CD1	7.53	125.52	121.00
10	j	74	TYR	CD1-CG-CD2	-7.53	109.62	117.90
13	6	182	TYR	CE1-CZ-OH	7.51	140.39	120.10
12	l	270	GLU	OE1-CD-OE2	7.50	132.30	123.30
13	m	141	ARG	CD-NE-CZ	7.50	134.10	123.60
21	N	455	MET	CB-CG-SD	7.50	134.91	112.40
11	4	109	LYS	CG-CD-CE	7.50	134.41	111.90
11	k	109	LYS	CG-CD-CE	7.50	134.39	111.90
13	m	182	TYR	CE1-CZ-OH	7.49	140.33	120.10
10	j	65	GLU	OE1-CD-OE2	-7.49	114.31	123.30
13	6	124	GLU	CG-CD-OE2	7.49	133.28	118.30
31	L	345	ARG	NE-CZ-NH1	7.49	124.04	120.30
13	m	124	GLU	CG-CD-OE2	7.49	133.27	118.30
5	E	69	GLU	OE1-CD-OE2	-7.49	114.32	123.30
10	3	74	TYR	CD1-CG-CD2	-7.48	109.67	117.90
1	A	22	GLU	CG-CD-OE2	7.48	133.25	118.30
11	k	139	TYR	CB-CG-CD1	7.47	125.48	121.00
2	B	178	ARG	NE-CZ-NH1	7.47	124.04	120.30
12	l	214	VAL	CA-CB-CG1	7.47	122.11	110.90
10	3	65	GLU	OE1-CD-OE2	-7.47	114.34	123.30
13	6	141	ARG	CD-NE-CZ	7.46	134.05	123.60
8	1	175	ASP	CB-CG-OD2	7.46	125.02	118.30
33	J	57	PHE	CB-CG-CD1	7.45	126.02	120.80
9	i	126	TYR	CB-CG-CD2	7.45	125.47	121.00
12	l	253	TYR	CZ-CE2-CD2	7.45	126.51	119.80
12	5	270	GLU	OE1-CD-OE2	7.45	132.24	123.30
12	l	188	TYR	CE1-CZ-CE2	-7.45	107.88	119.80
1	a	22	GLU	CG-CD-OE2	7.45	133.19	118.30
5	e	69	GLU	OE1-CD-OE2	-7.45	114.37	123.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	214	VAL	CA-CB-CG1	7.44	122.06	110.90
7	G	190	ARG	NE-CZ-NH1	7.43	124.02	120.30
10	3	74	TYR	CE1-CZ-CE2	-7.43	107.91	119.80
20	Z	174	GLU	N-CA-CB	-7.43	97.22	110.60
9	2	249	ILE	CA-CB-CG1	-7.42	96.90	111.00
11	k	121	TYR	CB-CG-CD2	7.42	125.45	121.00
12	5	188	TYR	CE1-CZ-CE2	-7.41	107.94	119.80
12	5	253	TYR	CZ-CE2-CD2	7.41	126.47	119.80
20	Z	366	LYS	N-CA-CB	7.41	123.93	110.60
11	4	121	TYR	CB-CG-CD2	7.40	125.44	121.00
14	n	137	ARG	NE-CZ-NH2	7.40	124.00	120.30
32	M	124	ARG	NE-CZ-NH1	-7.40	116.60	120.30
8	h	175	ASP	OD1-CG-OD2	-7.40	109.24	123.30
10	j	74	TYR	CE1-CZ-CE2	-7.39	107.97	119.80
13	6	72	LEU	CB-CG-CD2	7.39	123.57	111.00
13	m	72	LEU	CB-CG-CD2	7.39	123.56	111.00
12	l	253	TYR	CB-CG-CD2	7.39	125.43	121.00
5	e	86	ARG	CG-CD-NE	7.38	127.30	111.80
13	6	186	GLU	CA-CB-CG	7.37	129.62	113.40
13	m	186	GLU	CA-CB-CG	7.37	129.60	113.40
8	1	197	PHE	O-C-N	7.37	134.48	122.70
5	E	86	ARG	CG-CD-NE	7.36	127.26	111.80
31	L	420	ARG	NE-CZ-NH1	7.36	123.98	120.30
3	c	179	ASP	CB-CG-OD2	7.36	124.92	118.30
12	l	100	TRP	CA-CB-CG	7.35	127.67	113.70
13	m	41	TYR	CD1-CG-CD2	-7.35	109.81	117.90
31	L	420	ARG	NE-CZ-NH2	-7.35	116.62	120.30
13	m	41	TYR	CZ-CE2-CD2	7.35	126.41	119.80
13	6	41	TYR	CZ-CE2-CD2	7.34	126.41	119.80
7	G	185	GLU	C-N-CA	7.34	137.72	122.30
12	5	253	TYR	CB-CG-CD2	7.34	125.41	121.00
5	E	32	LYS	CD-CE-NZ	7.34	128.59	111.70
8	1	175	ASP	OD1-CG-OD2	-7.34	109.35	123.30
9	i	217	ARG	NE-CZ-NH2	-7.34	116.63	120.30
11	4	96	ARG	CD-NE-CZ	-7.34	113.33	123.60
3	C	179	ASP	CB-CG-OD2	7.33	124.90	118.30
12	5	100	TRP	CA-CB-CG	7.33	127.63	113.70
11	4	194	ASP	CB-CG-OD1	7.33	124.90	118.30
13	6	41	TYR	CD1-CG-CD2	-7.32	109.85	117.90
9	2	46	ASP	OD1-CG-OD2	-7.31	109.41	123.30
5	e	32	LYS	CD-CE-NZ	7.31	128.51	111.70
10	3	205	ASP	CB-CA-C	-7.31	95.78	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	96	ARG	CD-NE-CZ	-7.30	113.38	123.60
10	j	205	ASP	CB-CA-C	-7.30	95.80	110.40
11	k	5	LEU	C-N-CA	7.30	137.63	122.30
11	k	194	ASP	CB-CG-OD1	7.30	124.87	118.30
2	b	178	ARG	NE-CZ-NH1	7.30	123.95	120.30
9	i	46	ASP	OD1-CG-OD2	-7.29	109.44	123.30
9	2	153	TYR	CE1-CZ-OH	7.28	139.75	120.10
27	O	157	LEU	CB-CG-CD1	7.27	123.37	111.00
34	8	444	GLU	OE1-CD-OE2	-7.27	114.58	123.30
1	A	192	ASP	OD1-CG-OD2	-7.27	109.49	123.30
13	6	125	ASP	OD1-CG-OD2	-7.27	109.49	123.30
33	J	56	ARG	NE-CZ-NH1	7.27	123.93	120.30
9	i	48	ARG	NE-CZ-NH2	7.26	123.93	120.30
9	2	48	ARG	NE-CZ-NH2	7.25	123.93	120.30
8	h	155	MET	CA-CB-CG	7.25	125.63	113.30
9	i	153	TYR	CE1-CZ-OH	7.25	139.68	120.10
8	1	155	MET	CA-CB-CG	7.25	125.62	113.30
1	a	192	ASP	OD1-CG-OD2	-7.24	109.54	123.30
13	6	58	ILE	CB-CG1-CD1	7.24	134.18	113.90
17	T	60	ARG	NE-CZ-NH1	7.24	123.92	120.30
9	2	219	TYR	CD1-CG-CD2	-7.24	109.94	117.90
8	h	41	ASP	OD1-CG-OD2	-7.24	109.55	123.30
13	m	58	ILE	CB-CG1-CD1	7.24	134.16	113.90
13	m	125	ASP	OD1-CG-OD2	-7.24	109.55	123.30
9	2	224	VAL	CG1-CB-CG2	-7.24	99.32	110.90
2	B	2	THR	O-C-N	-7.23	111.13	122.70
12	5	233	LYS	CG-CD-CE	7.23	133.59	111.90
12	5	243	ASP	CB-CG-OD1	7.22	124.80	118.30
12	l	233	LYS	CG-CD-CE	7.22	133.56	111.90
7	G	51	GLU	OE1-CD-OE2	-7.22	114.64	123.30
8	1	41	ASP	OD1-CG-OD2	-7.22	109.59	123.30
12	l	164	GLN	CB-CG-CD	7.21	130.34	111.60
7	g	51	GLU	OE1-CD-OE2	-7.21	114.65	123.30
11	k	180	ILE	CG1-CB-CG2	-7.21	95.54	111.40
12	l	243	ASP	CB-CG-OD1	7.20	124.78	118.30
2	b	22	ASP	CB-CG-OD2	7.20	124.78	118.30
11	k	125	LYS	CB-CG-CD	7.20	130.31	111.60
6	F	164	ARG	NE-CZ-NH2	7.20	123.90	120.30
11	4	125	LYS	CB-CG-CD	7.20	130.31	111.60
2	b	2	THR	O-C-N	-7.20	111.19	122.70
9	i	119	TYR	CZ-CE2-CD2	7.19	126.27	119.80
1	A	96	ARG	CB-CG-CD	7.19	130.30	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	119	TYR	CZ-CE2-CD2	7.19	126.27	119.80
1	a	96	ARG	CB-CG-CD	7.19	130.29	111.60
2	b	182	GLU	OE1-CD-OE2	-7.19	114.67	123.30
11	4	180	ILE	CG1-CB-CG2	-7.19	95.58	111.40
13	m	85	PHE	CB-CG-CD2	7.19	125.83	120.80
2	B	182	GLU	OE1-CD-OE2	-7.19	114.67	123.30
12	5	164	GLN	CB-CG-CD	7.19	130.29	111.60
10	3	77	LYS	CG-CD-CE	7.18	133.44	111.90
14	7	189	ARG	NE-CZ-NH1	7.18	123.89	120.30
10	j	78	GLU	CG-CD-OE1	-7.18	103.94	118.30
10	j	77	LYS	CG-CD-CE	7.18	133.43	111.90
11	k	96	ARG	CB-CG-CD	7.17	130.26	111.60
10	3	78	GLU	CG-CD-OE1	-7.17	103.95	118.30
11	4	96	ARG	CB-CG-CD	7.17	130.25	111.60
10	j	199	TYR	CE1-CZ-CE2	-7.17	108.33	119.80
14	n	136	ARG	NE-CZ-NH1	7.16	123.88	120.30
10	3	67	PHE	CD1-CE1-CZ	7.16	128.69	120.10
29	I	300	ARG	CA-CB-CG	7.16	129.14	113.40
7	g	232	LYS	CD-CE-NZ	7.14	128.13	111.70
10	3	199	TYR	CE1-CZ-CE2	-7.14	108.38	119.80
5	E	134	MET	CA-CB-CG	7.13	125.43	113.30
2	B	22	ASP	CB-CG-OD2	7.13	124.71	118.30
10	3	74	TYR	CZ-CE2-CD2	7.12	126.21	119.80
11	4	19	LYS	CD-CE-NZ	-7.12	95.31	111.70
4	D	119	ARG	CA-CB-CG	7.12	129.07	113.40
8	1	17	PHE	O-C-N	-7.12	111.31	122.70
20	Z	943	LYS	CB-CG-CD	7.12	130.11	111.60
5	e	134	MET	CA-CB-CG	7.12	125.40	113.30
11	4	74	GLU	CB-CG-CD	7.12	133.41	114.20
10	j	78	GLU	CA-CB-CG	-7.11	97.75	113.40
5	E	8	TYR	CB-CG-CD2	-7.11	116.73	121.00
10	j	67	PHE	CD1-CE1-CZ	7.11	128.63	120.10
31	L	361	PHE	CB-CG-CD2	-7.11	115.83	120.80
8	1	183	ARG	NH1-CZ-NH2	-7.11	111.58	119.40
6	f	164	ARG	NE-CZ-NH2	7.10	123.85	120.30
11	k	19	LYS	CD-CE-NZ	-7.10	95.37	111.70
10	3	78	GLU	CA-CB-CG	-7.10	97.78	113.40
11	k	74	GLU	CB-CG-CD	7.10	133.36	114.20
5	E	118	ASP	OD1-CG-OD2	-7.10	109.82	123.30
5	E	8	TYR	CB-CG-CD1	7.09	125.26	121.00
8	h	183	ARG	NH1-CZ-NH2	-7.09	111.60	119.40
13	m	83	TYR	CE1-CZ-CE2	-7.08	108.48	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	36	LYS	CG-CD-CE	7.07	133.12	111.90
22	S	192	GLU	CG-CD-OE1	7.07	132.44	118.30
5	e	118	ASP	OD1-CG-OD2	-7.07	109.87	123.30
3	C	165	VAL	CG1-CB-CG2	-7.07	99.59	110.90
28	H	372	ASP	N-CA-CB	-7.07	97.88	110.60
3	c	165	VAL	CG1-CB-CG2	-7.06	99.60	110.90
5	e	81	LEU	CA-CB-CG	7.06	131.53	115.30
10	j	74	TYR	CZ-CE2-CD2	7.06	126.15	119.80
13	6	142	GLU	CG-CD-OE2	-7.06	104.19	118.30
9	i	36	LYS	CG-CD-CE	7.05	133.06	111.90
24	Q	51	ARG	NE-CZ-NH2	-7.05	116.77	120.30
4	D	49	ARG	NE-CZ-NH2	-7.05	116.78	120.30
2	b	22	ASP	CB-CG-OD1	7.04	124.64	118.30
5	E	81	LEU	CA-CB-CG	7.04	131.50	115.30
2	B	22	ASP	CB-CG-OD1	7.04	124.64	118.30
13	6	168	TYR	CE1-CZ-CE2	-7.04	108.54	119.80
12	5	245	TYR	CB-CG-CD1	7.04	125.22	121.00
13	m	181	LYS	CB-CA-C	-7.04	96.33	110.40
13	m	142	GLU	CG-CD-OE2	-7.03	104.23	118.30
13	m	168	TYR	CE1-CZ-CE2	-7.03	108.55	119.80
13	6	181	LYS	CB-CA-C	-7.03	96.33	110.40
25	R	263	ARG	NE-CZ-NH2	-7.03	116.78	120.30
11	k	110	LYS	CB-CG-CD	7.03	129.88	111.60
11	4	110	LYS	CB-CG-CD	7.03	129.87	111.60
8	1	133	TYR	CG-CD2-CE2	7.02	126.92	121.30
5	e	102	TYR	CB-CG-CD1	7.01	125.21	121.00
9	2	155	SER	CA-CB-OG	7.01	130.14	111.20
13	m	81	LYS	CD-CE-NZ	7.01	127.83	111.70
20	Z	824	ASN	CB-CG-OD1	-7.01	107.58	121.60
9	i	155	SER	CA-CB-OG	7.01	130.13	111.20
10	j	28	ARG	NE-CZ-NH1	-7.00	116.80	120.30
5	E	53	ARG	NH1-CZ-NH2	7.00	127.10	119.40
6	f	9	ASP	OD1-CG-OD2	-6.99	110.02	123.30
16	V	182	LYS	CA-CB-CG	6.98	128.76	113.40
6	F	9	ASP	OD1-CG-OD2	-6.98	110.05	123.30
6	F	226	ASP	CB-CG-OD2	-6.97	112.02	118.30
13	m	41	TYR	CB-CG-CD1	6.97	125.18	121.00
8	1	194	ARG	CG-CD-NE	6.97	126.44	111.80
2	b	22	ASP	OD1-CG-OD2	-6.96	110.07	123.30
12	l	286	ILE	CG1-CB-CG2	-6.96	96.09	111.40
10	3	28	ARG	NE-CZ-NH1	-6.96	116.82	120.30
12	5	286	ILE	CG1-CB-CG2	-6.96	96.10	111.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	13	TYR	CE1-CZ-CE2	-6.96	108.67	119.80
4	d	66	LYS	CB-CG-CD	-6.95	93.52	111.60
13	6	13	TYR	CE1-CZ-CE2	-6.95	108.68	119.80
27	O	80	LYS	CA-CB-CG	6.94	128.68	113.40
5	E	102	TYR	CB-CG-CD1	6.94	125.16	121.00
10	j	97	GLU	OE1-CD-OE2	6.94	131.62	123.30
2	B	22	ASP	OD1-CG-OD2	-6.93	110.13	123.30
6	f	226	ASP	CB-CG-OD2	-6.93	112.06	118.30
8	h	133	TYR	CG-CD2-CE2	6.93	126.84	121.30
11	4	127	GLU	CG-CD-OE2	6.93	132.16	118.30
22	S	192	GLU	CG-CD-OE2	-6.92	104.45	118.30
9	2	109	LEU	CB-CG-CD1	6.92	122.76	111.00
11	k	167	GLU	OE1-CD-OE2	-6.92	115.00	123.30
31	L	168	TYR	CB-CG-CD1	-6.92	116.85	121.00
22	S	271	ARG	NE-CZ-NH1	6.92	123.76	120.30
13	m	50	LYS	CD-CE-NZ	6.91	127.59	111.70
13	6	114	TYR	CG-CD2-CE2	6.91	126.83	121.30
10	j	2	SER	N-CA-C	-6.91	92.35	111.00
12	l	215	LEU	CB-CG-CD1	6.91	122.75	111.00
5	E	86	ARG	CB-CG-CD	6.91	129.56	111.60
11	k	127	GLU	CG-CD-OE2	6.90	132.11	118.30
5	E	9	ASP	CB-CG-OD2	6.90	124.51	118.30
5	e	86	ARG	CB-CG-CD	6.90	129.54	111.60
13	6	41	TYR	CB-CG-CD1	6.90	125.14	121.00
9	i	109	LEU	CB-CG-CD1	6.90	122.72	111.00
3	C	179	ASP	CB-CG-OD1	6.89	124.50	118.30
10	3	2	SER	N-CA-C	-6.89	92.39	111.00
1	A	48	LYS	CD-CE-NZ	6.89	127.55	111.70
12	5	215	LEU	CB-CG-CD1	6.89	122.71	111.00
10	3	97	GLU	OE1-CD-OE2	6.89	131.56	123.30
1	a	48	LYS	CD-CE-NZ	6.88	127.53	111.70
11	4	120	ASP	CB-CG-OD1	-6.88	112.11	118.30
13	6	50	LYS	CD-CE-NZ	6.88	127.53	111.70
11	4	167	GLU	OE1-CD-OE2	-6.87	115.05	123.30
11	k	120	ASP	CB-CG-OD1	-6.86	112.13	118.30
11	k	171	ARG	NH1-CZ-NH2	-6.85	111.86	119.40
31	L	280	MET	CB-CG-SD	6.84	132.92	112.40
23	P	69	ARG	NE-CZ-NH1	6.83	123.72	120.30
9	2	37	PHE	CZ-CE2-CD2	6.83	128.30	120.10
11	k	95	ARG	NE-CZ-NH1	6.83	123.72	120.30
12	l	245	TYR	CB-CG-CD1	6.83	125.10	121.00
3	C	5	ARG	NE-CZ-NH2	-6.83	116.89	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	148	ARG	CD-NE-CZ	-6.83	114.04	123.60
34	8	331	ARG	NE-CZ-NH2	-6.83	116.89	120.30
12	l	148	ARG	CD-NE-CZ	-6.82	114.05	123.60
3	c	179	ASP	CB-CG-OD1	6.82	124.44	118.30
3	C	224	GLU	CG-CD-OE1	6.82	131.93	118.30
3	c	224	GLU	CG-CD-OE1	6.81	131.93	118.30
12	5	164	GLN	CG-CD-OE1	-6.81	107.97	121.60
11	4	95	ARG	NE-CZ-NH1	6.81	123.70	120.30
11	4	171	ARG	NH1-CZ-NH2	-6.81	111.91	119.40
10	3	131	ASP	CA-C-N	-6.80	102.24	117.20
12	l	164	GLN	CG-CD-OE1	-6.79	108.01	121.60
12	l	253	TYR	CE1-CZ-CE2	-6.79	108.93	119.80
9	i	37	PHE	CZ-CE2-CD2	6.79	128.25	120.10
13	6	114	TYR	CG-CD1-CE1	-6.79	115.87	121.30
12	5	257	GLU	CB-CG-CD	6.79	132.53	114.20
9	2	211	LYS	CD-CE-NZ	6.79	127.31	111.70
9	i	211	LYS	CD-CE-NZ	6.79	127.31	111.70
12	l	220	LYS	CG-CD-CE	6.78	132.24	111.90
12	l	257	GLU	CB-CG-CD	6.78	132.51	114.20
5	E	10	ARG	NH1-CZ-NH2	6.78	126.86	119.40
20	Z	528	LEU	CB-CG-CD1	6.77	122.51	111.00
13	m	13	TYR	CD1-CG-CD2	-6.77	110.45	117.90
4	D	5	ASP	CB-CA-C	6.77	123.94	110.40
9	2	230	LYS	CG-CD-CE	6.77	132.21	111.90
29	I	343	ARG	NE-CZ-NH2	6.77	123.68	120.30
12	5	220	LYS	CG-CD-CE	6.77	132.20	111.90
12	5	253	TYR	CE1-CZ-CE2	-6.76	108.98	119.80
12	5	258	ASP	OD1-CG-OD2	-6.76	110.46	123.30
3	c	5	ARG	NE-CZ-NH2	-6.76	116.92	120.30
12	l	257	GLU	CG-CD-OE1	-6.75	104.81	118.30
3	C	179	ASP	OD1-CG-OD2	-6.75	110.48	123.30
8	1	120	TYR	CB-CG-CD1	6.74	125.04	121.00
12	5	257	GLU	CG-CD-OE1	-6.74	104.82	118.30
9	2	219	TYR	CZ-CE2-CD2	6.74	125.86	119.80
13	6	13	TYR	CD1-CG-CD2	-6.74	110.49	117.90
21	N	515	ARG	NE-CZ-NH1	6.74	123.67	120.30
12	l	258	ASP	OD1-CG-OD2	-6.73	110.51	123.30
3	c	179	ASP	OD1-CG-OD2	-6.72	110.52	123.30
10	3	205	ASP	N-CA-C	6.72	129.14	111.00
13	6	111	PHE	CB-CG-CD2	6.72	125.50	120.80
8	1	42	LYS	CG-CD-CE	6.71	132.02	111.90
13	6	41	TYR	CD1-CE1-CZ	6.70	125.83	119.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	E	29	GLU	OE1-CD-OE2	-6.70	115.26	123.30
8	h	42	LYS	CG-CD-CE	6.70	132.00	111.90
2	B	151	ASP	OD1-CG-OD2	-6.70	110.57	123.30
10	j	205	ASP	N-CA-C	6.70	129.08	111.00
8	h	120	TYR	CB-CG-CD1	6.69	125.02	121.00
2	b	151	ASP	OD1-CG-OD2	-6.69	110.58	123.30
2	b	81	ASP	OD1-CG-OD2	-6.69	110.59	123.30
5	e	29	GLU	OE1-CD-OE2	-6.69	115.27	123.30
20	Z	295	ARG	NE-CZ-NH1	6.68	123.64	120.30
3	C	16	GLU	CG-CD-OE2	6.68	131.66	118.30
14	n	215	ARG	NE-CZ-NH2	6.67	123.64	120.30
2	B	81	ASP	OD1-CG-OD2	-6.67	110.62	123.30
16	V	182	LYS	CB-CG-CD	6.67	128.96	111.60
30	K	80	LYS	CB-CG-CD	6.67	128.95	111.60
3	c	16	GLU	CG-CD-OE2	6.67	131.64	118.30
12	l	120	MET	CB-CG-SD	6.67	132.42	112.40
9	2	246	ILE	CB-CG1-CD1	6.67	132.58	113.90
1	a	62	LYS	CD-CE-NZ	6.67	127.04	111.70
13	m	83	TYR	CB-CG-CD2	6.67	125.00	121.00
11	k	135	TYR	CB-CA-C	-6.66	97.08	110.40
14	n	98	ARG	NE-CZ-NH1	6.66	123.63	120.30
11	4	135	TYR	CB-CA-C	-6.66	97.09	110.40
13	m	41	TYR	CD1-CE1-CZ	6.65	125.79	119.80
9	2	222	PRO	C-N-CA	6.65	138.32	121.70
9	2	106	VAL	CG1-CB-CG2	-6.65	100.26	110.90
12	5	120	MET	CB-CG-SD	6.65	132.34	112.40
20	Z	721	ASN	CB-CG-OD1	-6.65	108.31	121.60
1	A	62	LYS	CD-CE-NZ	6.65	126.99	111.70
9	2	168	GLU	CG-CD-OE1	-6.64	105.01	118.30
7	g	173	LYS	CD-CE-NZ	6.64	126.97	111.70
13	m	47	TYR	CB-CG-CD1	6.63	124.98	121.00
10	3	154	TYR	CB-CG-CD2	6.63	124.98	121.00
13	6	15	ASP	CB-CG-OD1	6.62	124.26	118.30
23	P	88	GLN	C-N-CA	6.62	138.25	121.70
16	V	194	ARG	CD-NE-CZ	6.62	132.87	123.60
10	j	199	TYR	CB-CG-CD1	6.62	124.97	121.00
9	i	168	GLU	CG-CD-OE1	-6.62	105.07	118.30
12	l	206	SER	CA-CB-OG	6.61	129.05	111.20
9	i	106	VAL	CG1-CB-CG2	-6.61	100.33	110.90
6	F	80	ASP	OD1-CG-OD2	-6.61	110.75	123.30
7	G	242	PHE	CB-CG-CD1	6.61	125.42	120.80
13	m	15	ASP	CB-CG-OD1	6.60	124.24	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	5	206	SER	CA-CB-OG	6.60	129.02	111.20
8	h	17	PHE	O-C-N	6.60	133.26	122.70
8	h	18	LYS	CG-CD-CE	6.60	131.70	111.90
32	M	213	ARG	NE-CZ-NH1	-6.59	117.00	120.30
1	a	95	LEU	CD1-CG-CD2	-6.59	90.73	110.50
28	H	373	ARG	NE-CZ-NH1	-6.59	117.00	120.30
3	c	60	ASP	OD1-CG-OD2	-6.58	110.79	123.30
29	I	359	LYS	CD-CE-NZ	6.58	126.83	111.70
8	1	18	LYS	CG-CD-CE	6.58	131.63	111.90
12	l	170	LEU	CA-CB-CG	-6.57	100.18	115.30
6	f	80	ASP	OD1-CG-OD2	-6.57	110.81	123.30
13	m	118	ILE	CG1-CB-CG2	-6.57	96.95	111.40
1	A	95	LEU	CD1-CG-CD2	-6.57	90.80	110.50
7	g	201	TYR	CB-CG-CD1	6.56	124.94	121.00
7	g	206	ASP	OD1-CG-OD2	-6.55	110.86	123.30
12	5	170	LEU	CA-CB-CG	-6.55	100.24	115.30
8	1	203	GLU	CA-CB-CG	-6.55	99.00	113.40
10	3	199	TYR	CB-CG-CD1	6.55	124.93	121.00
3	C	60	ASP	OD1-CG-OD2	-6.54	110.87	123.30
11	4	192	VAL	CG1-CB-CG2	-6.53	100.45	110.90
2	b	3	ASP	N-CA-CB	6.53	122.34	110.60
11	k	192	VAL	CG1-CB-CG2	-6.52	100.47	110.90
2	B	3	ASP	N-CA-CB	6.51	122.33	110.60
5	e	186	GLU	CG-CD-OE2	6.50	131.30	118.30
13	6	47	TYR	CB-CG-CD1	6.50	124.90	121.00
26	U	180	ASP	CB-CG-OD1	6.49	124.14	118.30
9	i	51	GLN	N-CA-CB	6.49	122.28	110.60
9	2	51	GLN	N-CA-CB	6.49	122.28	110.60
20	Z	909	ARG	CB-CG-CD	6.49	128.48	111.60
12	l	286	ILE	CB-CG1-CD1	-6.49	95.74	113.90
12	5	286	ILE	CB-CG1-CD1	-6.48	95.75	113.90
32	M	95	GLU	OE1-CD-OE2	-6.48	115.52	123.30
5	E	186	GLU	CG-CD-OE2	6.48	131.27	118.30
27	O	288	ARG	NE-CZ-NH2	-6.47	117.06	120.30
9	2	209	ILE	CA-CB-CG2	6.47	123.84	110.90
20	Z	632	GLU	CG-CD-OE2	-6.47	105.36	118.30
12	l	182	LYS	CA-CB-CG	6.47	127.63	113.40
10	3	135	ASP	CB-CG-OD1	-6.47	112.48	118.30
11	k	32	ASP	CB-CG-OD2	6.46	124.11	118.30
12	5	182	LYS	CA-CB-CG	6.46	127.61	113.40
32	M	300	GLU	OE1-CD-OE2	-6.46	115.55	123.30
3	c	222	ASP	CB-CG-OD1	6.45	124.11	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	232	TYR	CZ-CE2-CD2	6.45	125.60	119.80
9	2	254	GLU	CA-CB-CG	6.45	127.59	113.40
13	6	187	GLU	CB-CG-CD	6.45	131.61	114.20
9	i	209	ILE	CA-CB-CG2	6.45	123.79	110.90
13	m	187	GLU	CB-CG-CD	6.45	131.60	114.20
11	4	32	ASP	CB-CG-OD2	6.45	124.10	118.30
3	C	222	ASP	CB-CG-OD1	6.44	124.10	118.30
27	O	15	ARG	NE-CZ-NH2	-6.44	117.08	120.30
9	2	212	ASP	CB-CG-OD2	6.44	124.09	118.30
3	C	80	LEU	CB-CG-CD1	6.42	121.92	111.00
11	k	17	SER	CA-CB-OG	6.42	128.54	111.20
21	N	519	VAL	CG1-CB-CG2	6.42	121.17	110.90
23	P	127	GLU	OE1-CD-OE2	-6.42	115.59	123.30
31	L	426	LYS	CB-CG-CD	6.42	128.29	111.60
12	l	286	ILE	CA-CB-CG1	6.42	123.19	111.00
8	h	114	LYS	CB-CG-CD	6.42	128.28	111.60
9	i	106	VAL	CA-CB-CG1	6.42	120.53	110.90
26	U	180	ASP	CB-CG-OD2	-6.41	112.53	118.30
9	2	106	VAL	CA-CB-CG1	6.41	120.51	110.90
9	2	118	LYS	CA-CB-CG	6.41	127.50	113.40
9	i	118	LYS	CA-CB-CG	6.41	127.50	113.40
11	4	17	SER	CA-CB-OG	6.41	128.50	111.20
13	6	113	TYR	CB-CG-CD1	6.41	124.84	121.00
3	c	80	LEU	CB-CG-CD1	6.40	121.89	111.00
32	M	404	ARG	NE-CZ-NH2	-6.40	117.10	120.30
12	5	286	ILE	CA-CB-CG1	6.40	123.16	111.00
7	G	242	PHE	CB-CG-CD2	-6.40	116.32	120.80
22	S	464	ARG	CB-CG-CD	6.40	128.23	111.60
8	1	114	LYS	CB-CG-CD	6.40	128.23	111.60
13	6	168	TYR	CE1-CZ-OH	6.40	137.37	120.10
21	N	671	LEU	CA-CB-CG	6.40	130.01	115.30
2	B	151	ASP	CB-CG-OD1	6.39	124.06	118.30
31	L	404	ARG	NE-CZ-NH1	6.39	123.50	120.30
10	j	15	MET	CA-CB-CG	6.39	124.17	113.30
11	4	8	ARG	NE-CZ-NH1	6.39	123.50	120.30
13	m	168	TYR	CE1-CZ-OH	6.38	137.34	120.10
9	2	219	TYR	CD1-CE1-CZ	6.38	125.55	119.80
12	l	104	GLN	CG-CD-OE1	-6.38	108.83	121.60
13	6	41	TYR	CB-CG-CD2	6.38	124.83	121.00
13	m	41	TYR	CB-CG-CD2	6.38	124.83	121.00
17	T	128	TYR	CA-CB-CG	6.38	125.52	113.40
9	i	211	LYS	CA-C-N	-6.37	103.19	117.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	849	ARG	NE-CZ-NH1	6.36	123.48	120.30
10	3	15	MET	CA-CB-CG	6.36	124.11	113.30
12	5	104	GLN	CG-CD-OE1	-6.36	108.88	121.60
32	M	320	ARG	NE-CZ-NH1	6.36	123.48	120.30
6	f	202	ARG	NE-CZ-NH1	-6.35	117.12	120.30
12	l	148	ARG	NE-CZ-NH1	6.34	123.47	120.30
8	h	163	PHE	CB-CG-CD2	6.33	125.23	120.80
11	k	8	ARG	NE-CZ-NH1	6.33	123.47	120.30
12	l	188	TYR	CD1-CE1-CZ	6.33	125.50	119.80
6	F	202	ARG	NE-CZ-NH1	-6.33	117.14	120.30
20	Z	608	TYR	CB-CG-CD2	-6.33	117.20	121.00
2	b	151	ASP	CB-CG-OD1	6.32	123.99	118.30
18	X	22	ARG	NE-CZ-NH2	-6.32	117.14	120.30
12	5	188	TYR	CD1-CE1-CZ	6.32	125.48	119.80
25	R	176	ARG	NE-CZ-NH1	6.31	123.45	120.30
12	l	148	ARG	CA-CB-CG	6.31	127.28	113.40
14	n	226	ARG	NE-CZ-NH2	-6.30	117.15	120.30
13	6	124	GLU	CG-CD-OE1	-6.30	105.71	118.30
7	g	245	LYS	CG-CD-CE	6.29	130.79	111.90
12	5	148	ARG	CA-CB-CG	6.29	127.24	113.40
12	l	278	GLU	OE1-CD-OE2	-6.29	115.75	123.30
11	4	49	GLU	OE1-CD-OE2	6.29	130.84	123.30
9	i	177	LYS	CA-CB-CG	6.28	127.22	113.40
8	1	197	PHE	CB-CG-CD1	6.28	125.20	120.80
9	2	177	LYS	CA-CB-CG	6.28	127.23	113.40
8	h	202	TYR	CZ-CE2-CD2	-6.28	114.15	119.80
20	Z	213	LYS	CB-CG-CD	6.28	127.93	111.60
20	Z	498	ALA	N-CA-CB	-6.28	101.31	110.10
15	W	101	ARG	NE-CZ-NH1	6.28	123.44	120.30
32	M	303	ARG	NE-CZ-NH1	6.28	123.44	120.30
10	3	75	LYS	CB-CG-CD	6.27	127.91	111.60
11	4	99	GLN	CA-CB-CG	-6.27	99.60	113.40
13	6	167	GLN	CG-CD-OE1	6.27	134.14	121.60
9	i	225	ARG	NE-CZ-NH1	-6.27	117.17	120.30
11	k	49	GLU	OE1-CD-OE2	6.27	130.82	123.30
13	m	124	GLU	CG-CD-OE1	-6.27	105.77	118.30
13	6	187	GLU	CG-CD-OE2	-6.26	105.77	118.30
26	U	32	ARG	NE-CZ-NH1	6.26	123.43	120.30
10	j	75	LYS	CB-CG-CD	6.26	127.88	111.60
11	4	81	SER	CA-CB-OG	6.26	128.10	111.20
15	W	21	PHE	CB-CG-CD1	-6.26	116.42	120.80
8	h	31	THR	CA-CB-CG2	6.26	121.16	112.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
5	e	18	GLU	C-N-CA	-6.25	109.17	122.30
11	k	99	GLN	CA-CB-CG	-6.25	99.64	113.40
13	m	167	GLN	CG-CD-OE1	6.25	134.10	121.60
13	m	187	GLU	CG-CD-OE2	-6.25	105.80	118.30
8	l	31	THR	CA-CB-CG2	6.25	121.15	112.40
29	I	265	ARG	NE-CZ-NH1	6.25	123.42	120.30
12	5	278	GLU	OE1-CD-OE2	-6.25	115.80	123.30
11	k	81	SER	CA-CB-OG	6.25	128.06	111.20
12	5	148	ARG	NE-CZ-NH1	6.24	123.42	120.30
12	l	94	ARG	NE-CZ-NH1	-6.24	117.18	120.30
10	3	85	GLU	OE1-CD-OE2	-6.23	115.83	123.30
25	R	44	LYS	CD-CE-NZ	-6.23	97.38	111.70
11	4	95	ARG	CD-NE-CZ	-6.22	114.89	123.60
11	k	95	ARG	CD-NE-CZ	-6.22	114.89	123.60
10	3	149	MET	CB-CG-SD	6.22	131.05	112.40
22	S	36	LYS	CB-CG-CD	6.21	127.75	111.60
7	G	91	ARG	NE-CZ-NH1	6.21	123.40	120.30
12	5	94	ARG	NE-CZ-NH1	-6.21	117.20	120.30
5	e	136	ARG	CB-CG-CD	6.19	127.68	111.60
20	Z	40	GLU	CA-CB-CG	6.19	127.01	113.40
12	l	253	TYR	CD1-CG-CD2	-6.18	111.10	117.90
3	c	129	ARG	CG-CD-NE	6.18	124.78	111.80
9	2	232	TYR	CG-CD2-CE2	6.18	126.24	121.30
10	j	85	GLU	OE1-CD-OE2	-6.18	115.89	123.30
9	2	227	GLU	CB-CG-CD	6.18	130.88	114.20
5	e	10	ARG	CD-NE-CZ	6.17	132.25	123.60
6	f	118	LYS	CD-CE-NZ	6.17	125.90	111.70
3	C	129	ARG	CG-CD-NE	6.17	124.77	111.80
26	U	111	LYS	CD-CE-NZ	6.17	125.89	111.70
7	g	91	ARG	NE-CZ-NH1	6.17	123.38	120.30
4	D	197	ARG	NE-CZ-NH2	-6.17	117.22	120.30
5	E	136	ARG	CB-CG-CD	6.17	127.63	111.60
15	W	60	ARG	NE-CZ-NH2	-6.16	117.22	120.30
31	L	357	ARG	NE-CZ-NH1	6.16	123.38	120.30
6	F	118	LYS	CD-CE-NZ	6.16	125.86	111.70
12	5	198	LYS	CA-CB-CG	6.16	126.95	113.40
12	5	253	TYR	CD1-CG-CD2	-6.16	111.13	117.90
13	m	85	PHE	CZ-CE2-CD2	6.16	127.49	120.10
11	4	37	GLN	CA-CB-CG	6.15	126.92	113.40
20	Z	941	ARG	NE-CZ-NH1	6.15	123.37	120.30
21	N	437	GLU	OE1-CD-OE2	-6.14	115.93	123.30
2	b	6	SER	CA-CB-OG	6.13	127.77	111.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	L	141	LYS	CB-CG-CD	6.13	127.55	111.60
13	6	26	GLU	CG-CD-OE1	6.13	130.56	118.30
29	I	408	ARG	NE-CZ-NH2	-6.13	117.23	120.30
13	m	86	ASP	CB-CG-OD1	6.13	123.81	118.30
11	k	37	GLN	CA-CB-CG	6.12	126.87	113.40
8	l	173	LYS	CD-CE-NZ	-6.12	97.62	111.70
30	K	281	ARG	NE-CZ-NH1	6.12	123.36	120.30
12	l	198	LYS	CA-CB-CG	6.12	126.86	113.40
22	S	153	GLU	N-CA-CB	-6.12	99.59	110.60
8	h	173	LYS	CD-CE-NZ	-6.12	97.64	111.70
14	n	215	ARG	NE-CZ-NH1	-6.12	117.24	120.30
5	E	105	GLU	CG-CD-OE2	6.11	130.53	118.30
5	e	105	GLU	CG-CD-OE2	6.11	130.52	118.30
5	e	213	ASP	CB-CG-OD1	6.11	123.80	118.30
31	L	243	PHE	CB-CG-CD1	6.11	125.08	120.80
7	G	211	ASP	CB-CG-OD2	6.10	123.79	118.30
29	I	54	ARG	NE-CZ-NH1	6.10	123.35	120.30
2	B	6	SER	CA-CB-OG	6.10	127.68	111.20
18	X	119	LYS	CA-CB-CG	6.10	126.82	113.40
13	m	26	GLU	CG-CD-OE1	6.09	130.49	118.30
26	U	137	TYR	CB-CG-CD2	-6.09	117.34	121.00
1	A	76	SER	O-C-N	6.09	132.44	122.70
24	Q	195	LYS	CD-CE-NZ	-6.08	97.71	111.70
9	2	211	LYS	CG-CD-CE	6.08	130.14	111.90
10	3	198	ARG	NH1-CZ-NH2	-6.08	112.71	119.40
20	Z	40	GLU	CG-CD-OE1	6.08	130.45	118.30
5	E	213	ASP	CB-CG-OD1	6.07	123.77	118.30
28	H	216	ASP	CB-CA-C	-6.07	98.25	110.40
15	W	101	ARG	NE-CZ-NH2	-6.07	117.27	120.30
8	h	202	TYR	CB-CG-CD2	-6.06	117.36	121.00
9	i	211	LYS	CG-CD-CE	6.06	130.09	111.90
20	Z	40	GLU	CG-CD-OE2	-6.06	106.17	118.30
33	J	324	ARG	NE-CZ-NH1	6.06	123.33	120.30
21	N	338	PHE	CB-CG-CD2	-6.06	116.56	120.80
29	I	345	ASP	N-CA-CB	-6.06	99.69	110.60
26	U	60	GLU	OE1-CD-OE2	-6.05	116.03	123.30
7	g	94	GLU	OE1-CD-OE2	-6.04	116.05	123.30
25	R	363	PHE	CB-CG-CD1	6.04	125.03	120.80
9	2	208	GLU	CG-CD-OE2	6.04	130.38	118.30
13	6	26	GLU	CG-CD-OE2	-6.04	106.22	118.30
29	I	217	LYS	CD-CE-NZ	-6.04	97.82	111.70
10	j	198	ARG	NH1-CZ-NH2	-6.03	112.76	119.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	831	LEU	CB-CG-CD2	6.03	121.26	111.00
12	l	220	LYS	CA-CB-CG	6.03	126.67	113.40
14	7	74	ARG	CG-CD-NE	-6.02	99.15	111.80
1	A	73	PHE	C-N-CA	-6.02	106.65	121.70
7	G	94	GLU	OE1-CD-OE2	-6.02	116.08	123.30
6	F	80	ASP	CB-CG-OD2	6.02	123.72	118.30
9	i	208	GLU	CG-CD-OE2	6.02	130.34	118.30
9	i	221	THR	CA-CB-CG2	-6.02	103.98	112.40
13	m	26	GLU	CG-CD-OE2	-6.01	106.27	118.30
25	R	336	LYS	CB-CG-CD	6.01	127.22	111.60
1	A	149	GLU	CG-CD-OE2	6.01	130.31	118.30
6	f	80	ASP	CB-CG-OD2	6.00	123.70	118.30
3	c	109	GLU	CG-CD-OE1	-6.00	106.29	118.30
2	B	123	GLN	CA-CB-CG	6.00	126.60	113.40
8	l	73	GLU	CG-CD-OE2	-6.00	106.30	118.30
3	c	109	GLU	CG-CD-OE2	6.00	130.30	118.30
12	5	220	LYS	CA-CB-CG	6.00	126.59	113.40
8	h	73	GLU	CG-CD-OE2	-5.99	106.31	118.30
13	m	208	ASP	CB-CG-OD1	5.99	123.69	118.30
3	C	109	GLU	CG-CD-OE2	5.99	130.28	118.30
31	L	404	ARG	NE-CZ-NH2	-5.99	117.31	120.30
1	a	242	GLU	OE1-CD-OE2	-5.99	116.11	123.30
2	b	123	GLN	CA-CB-CG	5.99	126.58	113.40
1	a	149	GLU	CG-CD-OE2	5.98	130.27	118.30
12	l	120	MET	CG-SD-CE	5.98	109.77	100.20
9	2	219	TYR	CE1-CZ-CE2	-5.98	110.24	119.80
12	5	120	MET	CG-SD-CE	5.97	109.76	100.20
13	6	208	ASP	CB-CG-OD1	5.97	123.67	118.30
8	h	17	PHE	CA-C-N	-5.97	104.07	117.20
10	j	97	GLU	CG-CD-OE1	-5.97	106.36	118.30
11	4	2	ASP	CB-CG-OD2	5.97	123.67	118.30
12	5	198	LYS	CB-CG-CD	5.97	127.12	111.60
1	A	242	GLU	OE1-CD-OE2	-5.96	116.15	123.30
25	R	209	ARG	NE-CZ-NH1	5.96	123.28	120.30
10	3	97	GLU	CG-CD-OE1	-5.96	106.39	118.30
8	l	163	PHE	CB-CG-CD1	5.95	124.97	120.80
3	C	109	GLU	CG-CD-OE1	-5.95	106.40	118.30
8	h	144	TYR	CB-CG-CD1	-5.95	117.43	121.00
12	l	198	LYS	CB-CG-CD	5.95	127.06	111.60
5	e	104	ASP	CB-CG-OD1	5.94	123.65	118.30
13	m	194	ASP	CB-CG-OD2	5.94	123.65	118.30
13	6	143	GLN	CB-CA-C	-5.94	98.51	110.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	1	144	TYR	CB-CG-CD1	-5.94	117.43	121.00
25	R	396	LYS	CD-CE-NZ	-5.94	98.03	111.70
27	O	147	ARG	NE-CZ-NH1	5.94	123.27	120.30
11	k	10	GLN	CB-CG-CD	5.93	127.02	111.60
25	R	238	PHE	CB-CG-CD1	-5.93	116.65	120.80
5	E	104	ASP	CB-CG-OD1	5.93	123.63	118.30
13	m	143	GLN	CB-CA-C	-5.92	98.55	110.40
16	V	186	GLN	CB-CA-C	-5.92	98.55	110.40
25	R	171	MET	CG-SD-CE	-5.92	90.73	100.20
7	G	234	ASP	CB-CG-OD1	-5.92	112.97	118.30
9	2	186	ASP	CB-CG-OD2	5.91	123.62	118.30
11	4	10	GLN	CB-CG-CD	5.91	126.97	111.60
9	2	217	ARG	CG-CD-NE	5.91	124.21	111.80
13	6	194	ASP	CB-CG-OD2	5.91	123.62	118.30
11	4	72	ASP	CB-CG-OD1	-5.89	113.00	118.30
11	4	194	ASP	OD1-CG-OD2	-5.89	112.12	123.30
8	h	100	ASP	CB-CG-OD1	5.88	123.59	118.30
20	Z	295	ARG	NE-CZ-NH2	-5.88	117.36	120.30
13	m	230	ASP	CB-CA-C	-5.88	98.65	110.40
13	6	41	TYR	CE1-CZ-CE2	-5.88	110.40	119.80
22	S	51	ARG	NE-CZ-NH2	-5.88	117.36	120.30
8	1	100	ASP	CB-CG-OD1	5.87	123.59	118.30
20	Z	175	ASP	CB-CA-C	5.87	122.15	110.40
21	N	880	ARG	NE-CZ-NH1	5.87	123.24	120.30
4	d	48	ARG	NE-CZ-NH2	-5.87	117.36	120.30
11	k	135	TYR	CG-CD1-CE1	-5.87	116.61	121.30
8	h	155	MET	CB-CG-SD	5.87	130.00	112.40
8	1	155	MET	CB-CG-SD	5.87	130.00	112.40
12	5	191	ASP	CB-CG-OD2	5.87	123.58	118.30
29	I	125	MET	N-CA-C	5.87	126.84	111.00
6	F	174	ARG	NE-CZ-NH2	-5.86	117.37	120.30
9	2	236	ARG	NE-CZ-NH2	-5.86	117.37	120.30
21	N	455	MET	CG-SD-CE	5.86	109.58	100.20
9	2	227	GLU	CG-CD-OE1	5.86	130.01	118.30
29	I	124	THR	C-N-CA	5.86	136.34	121.70
5	e	11	GLY	O-C-N	5.85	132.06	122.70
11	4	5	LEU	O-C-N	5.85	133.15	123.20
13	m	41	TYR	CE1-CZ-CE2	-5.85	110.44	119.80
13	m	211	GLU	CB-CG-CD	5.85	130.00	114.20
11	4	11	ASP	CB-CG-OD2	5.85	123.56	118.30
11	4	135	TYR	CG-CD1-CE1	-5.85	116.62	121.30
13	6	211	GLU	CB-CG-CD	5.85	129.99	114.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	Z	173	ALA	C-N-CA	5.85	136.32	121.70
11	4	127	GLU	OE1-CD-OE2	-5.85	116.28	123.30
9	i	186	ASP	CB-CG-OD2	5.84	123.56	118.30
13	6	58	ILE	CG1-CB-CG2	-5.84	98.54	111.40
13	6	230	ASP	CB-CA-C	-5.84	98.71	110.40
20	Z	40	GLU	N-CA-CB	-5.84	100.08	110.60
3	C	63	THR	CA-CB-CG2	-5.84	104.22	112.40
25	R	88	LEU	CB-CG-CD2	5.84	120.93	111.00
13	m	58	ILE	CG1-CB-CG2	-5.84	98.55	111.40
8	1	152	ARG	CB-CG-CD	5.84	126.78	111.60
5	e	58	LEU	CA-C-N	5.84	130.04	117.20
3	c	63	THR	CA-CB-CG2	-5.83	104.23	112.40
8	h	152	ARG	CB-CG-CD	5.83	126.77	111.60
10	j	87	PHE	CB-CG-CD2	5.83	124.88	120.80
11	k	72	ASP	CB-CG-OD1	-5.83	113.05	118.30
10	3	141	THR	CA-CB-CG2	-5.83	104.23	112.40
32	M	411	LYS	CA-CB-CG	5.83	126.23	113.40
29	I	253	ILE	CG1-CB-CG2	-5.83	98.58	111.40
11	k	11	ASP	CB-CG-OD2	5.83	123.54	118.30
11	k	194	ASP	OD1-CG-OD2	-5.83	112.23	123.30
13	m	168	TYR	CD1-CG-CD2	-5.83	111.49	117.90
12	l	191	ASP	CB-CG-OD2	5.82	123.54	118.30
11	4	125	LYS	CA-CB-CG	5.82	126.21	113.40
11	k	69	ILE	CG1-CB-CG2	-5.82	98.60	111.40
11	4	69	ILE	CG1-CB-CG2	-5.82	98.59	111.40
16	V	271	VAL	N-CA-CB	-5.82	98.69	111.50
10	3	135	ASP	CB-CG-OD2	5.82	123.53	118.30
8	1	99	LYS	CD-CE-NZ	5.81	125.07	111.70
8	h	99	LYS	CD-CE-NZ	5.81	125.06	111.70
13	6	53	ASP	CB-CG-OD1	5.81	123.53	118.30
34	8	348	GLU	CG-CD-OE1	-5.81	106.68	118.30
11	k	125	LYS	CA-CB-CG	5.80	126.17	113.40
3	C	63	THR	C-N-CA	-5.80	107.19	121.70
28	H	71	GLU	CA-CB-CG	5.80	126.17	113.40
6	f	174	ARG	NE-CZ-NH2	-5.80	117.40	120.30
9	i	225	ARG	NE-CZ-NH2	5.80	123.20	120.30
13	m	211	GLU	CG-CD-OE2	5.80	129.90	118.30
22	S	36	LYS	CG-CD-CE	5.80	129.29	111.90
13	6	211	GLU	CG-CD-OE2	5.79	129.88	118.30
6	f	205	SER	N-CA-CB	5.79	119.18	110.50
13	m	53	ASP	CB-CG-OD1	5.79	123.51	118.30
9	i	66	ILE	CB-CG1-CD1	5.78	130.09	113.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	6	114	TYR	CZ-CE2-CD2	-5.78	114.59	119.80
10	3	87	PHE	CB-CG-CD2	5.78	124.84	120.80
3	c	63	THR	C-N-CA	-5.78	107.25	121.70
12	l	267	ASP	CB-CG-OD1	-5.78	113.10	118.30
6	F	205	SER	N-CA-CB	5.78	119.16	110.50
12	5	267	ASP	CB-CG-OD1	-5.78	113.10	118.30
13	6	168	TYR	CD1-CG-CD2	-5.78	111.55	117.90
11	k	127	GLU	OE1-CD-OE2	-5.77	116.37	123.30
9	2	66	ILE	CB-CG1-CD1	5.77	130.06	113.90
28	H	185	LEU	CB-CG-CD2	5.77	120.81	111.00
28	H	434	ARG	NE-CZ-NH1	5.77	123.19	120.30
13	m	85	PHE	CD1-CE1-CZ	5.77	127.02	120.10
22	S	410	LYS	CD-CE-NZ	5.76	124.96	111.70
5	E	180	GLN	CG-CD-OE1	-5.76	110.08	121.60
10	3	26	ASP	OD1-CG-OD2	-5.76	112.36	123.30
10	j	26	ASP	OD1-CG-OD2	-5.76	112.36	123.30
24	Q	198	LEU	CB-CG-CD2	5.76	120.79	111.00
7	g	22	PHE	CA-C-N	-5.76	104.53	117.20
34	8	466	ASP	CB-CG-OD1	5.76	123.48	118.30
5	e	180	GLN	CG-CD-OE1	-5.75	110.09	121.60
13	m	195	SER	CA-CB-OG	5.75	126.73	111.20
5	E	10	ARG	NE-CZ-NH2	-5.75	117.42	120.30
7	G	22	PHE	CA-C-N	-5.75	104.56	117.20
32	M	23	LEU	CB-CG-CD2	5.74	120.76	111.00
13	6	195	SER	CA-CB-OG	5.74	126.70	111.20
27	O	15	ARG	NE-CZ-NH1	5.74	123.17	120.30
10	3	78	GLU	CB-CG-CD	5.74	129.69	114.20
11	k	166	GLN	CA-CB-CG	5.73	126.01	113.40
14	n	161	ARG	NE-CZ-NH2	-5.73	117.43	120.30
10	j	78	GLU	CB-CG-CD	5.73	129.67	114.20
10	3	87	PHE	CZ-CE2-CD2	5.73	126.97	120.10
31	L	434	TYR	CB-CG-CD2	-5.73	117.56	121.00
32	M	95	GLU	C-N-CA	5.72	136.01	121.70
11	4	166	GLN	CA-CB-CG	5.72	125.97	113.40
29	I	421	GLU	OE1-CD-OE2	-5.71	116.44	123.30
7	G	206	ASP	CB-CG-OD1	5.71	123.44	118.30
11	k	110	LYS	CG-CD-CE	-5.71	94.78	111.90
1	a	107	LYS	CD-CE-NZ	5.70	124.81	111.70
8	1	178	SER	CA-CB-OG	5.70	126.58	111.20
11	4	110	LYS	CG-CD-CE	-5.70	94.80	111.90
1	A	107	LYS	CD-CE-NZ	5.70	124.80	111.70
30	K	343	LEU	CB-CG-CD1	5.69	120.68	111.00

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
8	h	197	PHE	CD1-CG-CD2	-5.69	110.90	118.30
13	m	182	TYR	CG-CD1-CE1	-5.69	116.75	121.30
31	L	137	ARG	CG-CD-NE	5.69	123.75	111.80
22	S	36	LYS	CA-CB-CG	5.69	125.92	113.40
8	h	178	SER	CA-CB-OG	5.69	126.55	111.20
4	D	63	LYS	CD-CE-NZ	-5.69	98.62	111.70
30	K	344	ARG	CB-CG-CD	5.69	126.38	111.60
16	V	47	MET	CG-SD-CE	5.68	109.29	100.20
20	Z	366	LYS	CA-CB-CG	5.67	125.88	113.40
7	g	22	PHE	O-C-N	5.67	131.77	122.70
7	G	22	PHE	O-C-N	5.67	131.77	122.70
10	j	87	PHE	CZ-CE2-CD2	5.66	126.90	120.10
12	5	139	ARG	NH1-CZ-NH2	5.66	125.62	119.40
9	2	177	LYS	CB-CG-CD	5.66	126.30	111.60
10	3	74	TYR	CE1-CZ-OH	5.66	135.37	120.10
10	j	154	TYR	CZ-CE2-CD2	5.65	124.89	119.80
5	e	9	ASP	CB-CG-OD1	5.65	123.39	118.30
10	j	74	TYR	CE1-CZ-OH	5.65	135.35	120.10
12	l	139	ARG	NH1-CZ-NH2	5.65	125.61	119.40
13	6	122	LEU	CD1-CG-CD2	-5.65	93.56	110.50
8	h	41	ASP	CB-CG-OD2	5.64	123.38	118.30
30	K	330	ARG	NE-CZ-NH1	5.64	123.12	120.30
9	i	82	GLU	OE1-CD-OE2	-5.64	116.53	123.30
11	k	191	GLN	CA-CB-CG	5.64	125.81	113.40
2	b	217	GLU	CG-CD-OE1	5.64	129.57	118.30
20	Z	287	ARG	NE-CZ-NH2	-5.63	117.48	120.30
19	Y	73	PHE	CB-CG-CD2	-5.63	116.86	120.80
9	i	177	LYS	CB-CG-CD	5.63	126.24	111.60
20	Z	813	PHE	CB-CG-CD2	-5.63	116.86	120.80
10	3	8	ASN	CB-CG-ND2	-5.63	103.19	116.70
13	6	182	TYR	CG-CD1-CE1	-5.63	116.80	121.30
26	U	137	TYR	CB-CG-CD1	5.63	124.38	121.00
3	C	195	LYS	CB-CG-CD	5.62	126.22	111.60
8	1	41	ASP	CB-CG-OD2	5.62	123.36	118.30
23	P	364	ARG	NE-CZ-NH1	5.62	123.11	120.30
13	m	122	LEU	CD1-CG-CD2	-5.62	93.64	110.50
1	A	73	PHE	CA-C-N	-5.62	104.83	117.20
10	3	118	LYS	CA-CB-CG	5.62	125.77	113.40
11	4	191	GLN	CA-CB-CG	5.62	125.77	113.40
30	K	344	ARG	NE-CZ-NH1	-5.62	117.49	120.30
10	j	8	ASN	CB-CG-ND2	-5.62	103.21	116.70
24	Q	51	ARG	CD-NE-CZ	5.62	131.47	123.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	217	GLU	CG-CD-OE1	5.62	129.53	118.30
9	2	118	LYS	CD-CE-NZ	-5.62	98.78	111.70
7	G	229	LYS	N-CA-CB	5.61	120.70	110.60
3	c	195	LYS	CB-CG-CD	5.61	126.19	111.60
9	2	82	GLU	OE1-CD-OE2	-5.61	116.57	123.30
10	j	118	LYS	CA-CB-CG	5.61	125.74	113.40
23	P	201	ARG	NE-CZ-NH1	5.61	123.10	120.30
13	6	155	MET	CG-SD-CE	-5.61	91.23	100.20
21	N	81	TYR	CA-CB-CG	-5.61	102.74	113.40
9	i	118	LYS	CD-CE-NZ	-5.61	98.81	111.70
33	J	116	ARG	NE-CZ-NH2	-5.61	117.50	120.30
13	m	155	MET	CG-SD-CE	-5.60	91.23	100.20
25	R	357	PHE	CB-CG-CD1	-5.60	116.88	120.80
24	Q	163	ARG	NE-CZ-NH2	-5.60	117.50	120.30
10	j	18	LYS	CB-CG-CD	5.60	126.15	111.60
5	e	159	GLU	OE1-CD-OE2	-5.59	116.58	123.30
10	3	18	LYS	CB-CG-CD	5.59	126.14	111.60
2	b	70	ASP	OD1-CG-OD2	-5.59	112.68	123.30
4	D	101	GLU	N-CA-CB	-5.58	100.55	110.60
13	m	113	TYR	O-C-N	5.58	131.63	122.70
11	4	91	SER	CA-CB-OG	5.58	126.27	111.20
28	H	420	ARG	NE-CZ-NH2	-5.58	117.51	120.30
27	O	147	ARG	NE-CZ-NH2	-5.58	117.51	120.30
12	5	227	ASP	CB-CG-OD2	5.57	123.32	118.30
33	J	296	ARG	NE-CZ-NH1	5.57	123.08	120.30
5	E	159	GLU	CG-CD-OE2	5.57	129.44	118.30
10	3	41	GLU	N-CA-CB	-5.57	100.58	110.60
1	a	239	GLU	CG-CD-OE1	5.56	129.43	118.30
11	k	91	SER	CA-CB-OG	5.56	126.22	111.20
1	A	239	GLU	CG-CD-OE1	5.56	129.43	118.30
5	e	159	GLU	CG-CD-OE2	5.56	129.42	118.30
10	j	41	GLU	N-CA-CB	-5.56	100.59	110.60
22	S	271	ARG	NE-CZ-NH2	-5.56	117.52	120.30
13	m	58	ILE	CA-CB-CG1	-5.56	100.44	111.00
2	B	166	LYS	CD-CE-NZ	5.55	124.48	111.70
5	E	159	GLU	OE1-CD-OE2	-5.55	116.63	123.30
2	B	70	ASP	OD1-CG-OD2	-5.55	112.75	123.30
13	6	58	ILE	CA-CB-CG1	-5.55	100.45	111.00
21	N	906	ARG	NE-CZ-NH1	5.55	123.08	120.30
8	h	17	PHE	CD1-CG-CD2	5.55	125.52	118.30
12	l	227	ASP	CB-CG-OD2	5.54	123.29	118.30
23	P	123	ARG	NE-CZ-NH2	-5.54	117.53	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	91	LYS	CD-CE-NZ	5.54	124.45	111.70
10	3	127	ILE	O-C-N	-5.54	113.78	123.20
16	V	61	TYR	CB-CG-CD2	-5.54	117.67	121.00
34	8	466	ASP	CB-CG-OD2	-5.54	113.31	118.30
10	j	78	GLU	CG-CD-OE2	5.54	129.38	118.30
25	R	238	PHE	CB-CG-CD2	5.54	124.68	120.80
16	V	188	LEU	CB-CG-CD2	5.54	120.42	111.00
6	f	169	LYS	CG-CD-CE	5.54	128.52	111.90
13	m	113	TYR	CZ-CE2-CD2	5.54	124.79	119.80
2	b	166	LYS	CD-CE-NZ	5.54	124.43	111.70
6	F	169	LYS	CG-CD-CE	5.54	128.51	111.90
16	V	179	LEU	CB-CG-CD2	-5.54	101.59	111.00
9	i	126	TYR	CG-CD1-CE1	5.53	125.73	121.30
12	5	245	TYR	CG-CD1-CE1	5.53	125.72	121.30
10	3	78	GLU	CG-CD-OE2	5.53	129.35	118.30
9	2	181	ILE	CA-CB-CG2	5.53	121.95	110.90
22	S	480	ARG	NE-CZ-NH2	5.53	123.06	120.30
8	1	205	LEU	CB-CG-CD1	5.52	120.38	111.00
13	6	13	TYR	CD1-CE1-CZ	5.51	124.76	119.80
9	i	181	ILE	CA-CB-CG2	5.51	121.93	110.90
10	j	164	PHE	CB-CG-CD2	-5.51	116.94	120.80
12	5	144	ARG	NE-CZ-NH1	5.51	123.05	120.30
13	6	182	TYR	CA-CB-CG	-5.51	102.94	113.40
2	B	2	THR	CA-C-N	5.50	129.31	117.20
5	e	238	GLU	CA-CB-CG	5.50	125.50	113.40
5	E	238	GLU	CA-CB-CG	5.50	125.50	113.40
30	K	236	ARG	NE-CZ-NH2	-5.50	117.55	120.30
13	m	182	TYR	CA-CB-CG	-5.50	102.95	113.40
9	i	198	SER	CA-CB-OG	5.50	126.04	111.20
11	k	135	TYR	CZ-CE2-CD2	-5.50	114.85	119.80
21	N	716	GLN	CA-CB-CG	5.50	125.50	113.40
31	L	275	PRO	CA-N-CD	-5.49	103.81	111.50
31	L	413	ASP	CB-CG-OD1	5.49	123.25	118.30
8	h	198	TYR	CD1-CE1-CZ	5.49	124.74	119.80
2	B	207	ASP	CB-CG-OD1	5.49	123.24	118.30
11	4	135	TYR	CZ-CE2-CD2	-5.49	114.86	119.80
33	J	324	ARG	NE-CZ-NH2	-5.49	117.56	120.30
9	2	126	TYR	CG-CD1-CE1	5.49	125.69	121.30
21	N	282	TYR	CB-CG-CD2	-5.49	117.71	121.00
9	2	198	SER	CA-CB-OG	5.48	126.00	111.20
21	N	87	ASP	N-CA-CB	5.48	120.47	110.60
35	9	31	GLN	CB-CG-CD	5.48	125.85	111.60

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	b	207	ASP	CB-CG-OD1	5.48	123.23	118.30
10	j	203	ARG	CB-CG-CD	5.48	125.84	111.60
14	n	179	PHE	CB-CG-CD2	5.48	124.64	120.80
20	Z	40	GLU	CB-CG-CD	5.48	128.99	114.20
20	Z	174	GLU	N-CA-C	5.48	125.79	111.00
7	g	86	ARG	NE-CZ-NH1	5.47	123.04	120.30
26	U	110	PHE	CB-CG-CD2	-5.47	116.97	120.80
5	e	136	ARG	NE-CZ-NH1	5.47	123.03	120.30
7	g	72	ARG	CD-NE-CZ	5.47	131.25	123.60
9	i	153	TYR	CD1-CG-CD2	5.46	123.91	117.90
2	b	2	THR	CA-C-N	5.46	129.22	117.20
10	3	203	ARG	CB-CG-CD	5.46	125.80	111.60
31	L	424	GLU	CA-CB-CG	-5.46	101.38	113.40
34	8	183	VAL	CA-CB-CG1	-5.46	102.71	110.90
9	i	188	ILE	CB-CG1-CD1	5.46	129.19	113.90
13	m	30	VAL	CA-CB-CG2	5.46	119.09	110.90
9	2	188	ILE	CB-CG1-CD1	5.46	129.18	113.90
21	N	298	TYR	CB-CG-CD2	-5.46	117.72	121.00
12	l	192	SER	CA-CB-OG	5.45	125.92	111.20
12	l	144	ARG	NE-CZ-NH1	5.45	123.02	120.30
5	E	136	ARG	NE-CZ-NH1	5.45	123.02	120.30
12	5	192	SER	CA-CB-OG	5.45	125.91	111.20
13	m	13	TYR	CD1-CE1-CZ	5.44	124.69	119.80
10	j	87	PHE	CD1-CE1-CZ	5.44	126.62	120.10
13	6	30	VAL	CA-CB-CG2	5.43	119.05	110.90
34	8	153	ASP	CB-CG-OD2	-5.43	113.41	118.30
12	5	110	ILE	CB-CG1-CD1	5.43	129.11	113.90
10	3	87	PHE	CD1-CE1-CZ	5.43	126.61	120.10
13	6	83	TYR	CG-CD1-CE1	-5.43	116.96	121.30
20	Z	55	ARG	NE-CZ-NH2	-5.43	117.58	120.30
10	3	127	ILE	CA-C-N	5.43	127.06	116.20
13	6	165	LYS	CD-CE-NZ	5.43	124.18	111.70
12	l	110	ILE	CB-CG1-CD1	5.42	129.09	113.90
9	i	211	LYS	CB-CA-C	-5.42	99.56	110.40
9	2	211	LYS	CB-CA-C	-5.42	99.56	110.40
9	2	153	TYR	CE1-CZ-CE2	5.42	128.47	119.80
11	4	49	GLU	CG-CD-OE1	-5.41	107.47	118.30
5	e	186	GLU	OE1-CD-OE2	-5.41	116.81	123.30
3	c	109	GLU	CB-CG-CD	5.41	128.80	114.20
8	h	197	PHE	CG-CD2-CE2	5.41	126.75	120.80
14	n	97	GLU	CA-CB-CG	5.41	125.29	113.40
3	C	109	GLU	CB-CG-CD	5.41	128.80	114.20

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	49	GLU	CG-CD-OE1	-5.40	107.49	118.30
13	m	165	LYS	CD-CE-NZ	5.40	124.13	111.70
3	C	87	LEU	CB-CG-CD2	5.40	120.18	111.00
8	1	204	GLN	CA-CB-CG	5.40	125.28	113.40
7	G	72	ARG	CD-NE-CZ	5.39	131.15	123.60
11	4	90	LYS	CD-CE-NZ	5.39	124.10	111.70
3	c	87	LEU	CB-CG-CD2	5.39	120.16	111.00
13	m	94	ILE	CA-CB-CG1	5.39	121.24	111.00
8	1	10	THR	CA-CB-OG1	5.38	120.31	109.00
8	h	197	PHE	CB-CG-CD1	5.38	124.57	120.80
9	i	153	TYR	CE1-CZ-CE2	5.38	128.41	119.80
3	c	60	ASP	CB-CG-OD2	5.38	123.14	118.30
8	h	10	THR	CA-CB-OG1	5.38	120.30	109.00
13	m	47	TYR	CG-CD1-CE1	5.38	125.60	121.30
5	E	186	GLU	OE1-CD-OE2	-5.38	116.85	123.30
34	8	316	ARG	NE-CZ-NH2	5.38	122.99	120.30
9	i	232	TYR	CA-CB-CG	-5.37	103.19	113.40
11	k	90	LYS	CD-CE-NZ	5.37	124.06	111.70
34	8	348	GLU	CG-CD-OE2	5.37	129.05	118.30
32	M	429	SER	N-CA-C	-5.37	96.50	111.00
9	2	153	TYR	CD1-CG-CD2	5.37	123.81	117.90
28	H	434	ARG	CD-NE-CZ	5.37	131.12	123.60
33	J	259	GLU	CG-CD-OE2	5.37	129.04	118.30
20	Z	321	PHE	CB-CG-CD1	5.37	124.56	120.80
12	l	83	PHE	CB-CG-CD1	-5.37	117.04	120.80
13	6	50	LYS	CA-CB-CG	5.37	125.20	113.40
32	M	96	ASN	N-CA-CB	-5.37	100.94	110.60
33	J	71	TYR	N-CA-C	-5.36	96.52	111.00
7	G	86	ARG	NE-CZ-NH1	5.36	122.98	120.30
9	i	219	TYR	CG-CD2-CE2	5.36	125.59	121.30
10	j	83	GLU	CG-CD-OE1	5.36	129.01	118.30
20	Z	873	LEU	CA-CB-CG	5.36	127.62	115.30
28	H	216	ASP	N-CA-CB	5.36	120.25	110.60
8	h	198	TYR	CB-CG-CD2	5.35	124.21	121.00
10	3	83	GLU	CG-CD-OE1	5.35	129.00	118.30
25	R	297	TYR	CA-CB-CG	5.35	123.57	113.40
9	i	97	LEU	CD1-CG-CD2	-5.35	94.45	110.50
12	l	245	TYR	CG-CD1-CE1	5.34	125.57	121.30
30	K	246	TYR	CA-CB-CG	-5.34	103.25	113.40
28	H	344	ASP	N-CA-CB	5.34	120.22	110.60
2	B	113	GLU	CG-CD-OE2	5.34	128.98	118.30
13	6	85	PHE	CB-CG-CD2	5.34	124.54	120.80

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
13	m	50	LYS	CA-CB-CG	5.34	125.14	113.40
26	U	179	ARG	CD-NE-CZ	5.34	131.07	123.60
28	H	58	ASP	CB-CG-OD1	5.34	123.10	118.30
2	b	113	GLU	CG-CD-OE2	5.33	128.97	118.30
21	N	39	ILE	CG1-CB-CG2	-5.33	99.66	111.40
12	l	81	PHE	CZ-CE2-CD2	5.33	126.50	120.10
3	C	209	ASP	CB-CG-OD2	5.33	123.10	118.30
9	2	97	LEU	CD1-CG-CD2	-5.33	94.50	110.50
20	Z	909	ARG	CA-CB-CG	5.33	125.13	113.40
30	K	411	TYR	CB-CG-CD1	-5.33	117.80	121.00
13	m	228	LYS	CB-CG-CD	-5.33	97.74	111.60
13	6	228	LYS	CB-CG-CD	-5.33	97.75	111.60
9	i	232	TYR	CD1-CE1-CZ	5.33	124.59	119.80
10	3	131	ASP	CB-CG-OD1	5.33	123.09	118.30
9	i	101	ARG	NH1-CZ-NH2	5.33	125.26	119.40
30	K	346	ARG	NE-CZ-NH2	-5.33	117.64	120.30
3	C	60	ASP	CB-CG-OD2	5.32	123.09	118.30
12	5	81	PHE	CZ-CE2-CD2	5.32	126.48	120.10
31	L	194	ARG	NE-CZ-NH2	-5.32	117.64	120.30
33	J	259	GLU	CG-CD-OE1	-5.32	107.66	118.30
10	3	63	LEU	CB-CG-CD2	5.32	120.04	111.00
10	3	154	TYR	CG-CD1-CE1	5.32	125.56	121.30
9	i	114	GLN	CG-CD-OE1	-5.32	110.97	121.60
9	2	254	GLU	CB-CA-C	-5.32	99.76	110.40
26	U	105	LYS	CG-CD-CE	5.32	127.85	111.90
6	f	51	ARG	NH1-CZ-NH2	-5.32	113.55	119.40
18	X	47	ASP	CB-CG-OD2	5.31	123.08	118.30
15	W	22	PRO	O-C-N	-5.31	114.20	122.70
7	G	224	THR	CA-CB-CG2	-5.31	104.97	112.40
35	9	72	ARG	NE-CZ-NH1	5.31	122.95	120.30
8	h	26	ASP	OD1-CG-OD2	5.31	133.38	123.30
9	2	114	GLN	CG-CD-OE1	-5.30	110.99	121.60
5	e	49	GLY	O-C-N	5.30	131.18	122.70
22	S	64	ARG	NE-CZ-NH2	-5.30	117.65	120.30
8	l	26	ASP	OD1-CG-OD2	5.30	133.37	123.30
10	j	63	LEU	CB-CG-CD2	5.30	120.01	111.00
2	b	124	SER	N-CA-CB	5.30	118.44	110.50
9	i	225	ARG	CD-NE-CZ	5.30	131.01	123.60
3	C	85	GLU	OE1-CD-OE2	-5.30	116.94	123.30
9	2	101	ARG	NH1-CZ-NH2	5.30	125.23	119.40
23	P	115	ARG	NE-CZ-NH2	5.30	122.95	120.30
34	8	444	GLU	CG-CD-OE1	5.30	128.89	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	255	GLU	CA-C-O	-5.29	108.98	120.10
34	8	177	LYS	CB-CG-CD	5.29	125.36	111.60
2	B	124	SER	N-CA-CB	5.29	118.43	110.50
29	I	173	MET	CA-CB-CG	5.29	122.29	113.30
9	i	236	ARG	CD-NE-CZ	5.28	131.00	123.60
6	F	51	ARG	NH1-CZ-NH2	-5.28	113.59	119.40
20	Z	55	ARG	NE-CZ-NH1	5.28	122.94	120.30
30	K	399	ARG	NE-CZ-NH1	5.28	122.94	120.30
10	j	8	ASN	CB-CG-OD1	5.28	132.15	121.60
29	I	125	MET	CB-CA-C	-5.28	99.85	110.40
29	I	300	ARG	NE-CZ-NH1	5.28	122.94	120.30
9	2	228	LYS	CA-CB-CG	5.27	125.00	113.40
21	N	861	TYR	N-CA-C	-5.27	96.76	111.00
13	6	47	TYR	CG-CD1-CE1	5.27	125.52	121.30
14	7	74	ARG	NE-CZ-NH1	5.27	122.94	120.30
3	c	85	GLU	OE1-CD-OE2	-5.27	116.98	123.30
35	9	72	ARG	NE-CZ-NH2	-5.26	117.67	120.30
2	b	220	ASP	CB-CG-OD1	5.26	123.03	118.30
32	M	305	MET	CB-CG-SD	5.25	128.16	112.40
3	c	209	ASP	CB-CG-OD2	5.25	123.03	118.30
25	R	363	PHE	CB-CG-CD2	-5.25	117.12	120.80
23	P	204	LEU	CB-CG-CD1	-5.25	102.08	111.00
2	B	220	ASP	CB-CG-OD1	5.25	123.02	118.30
11	4	169	GLU	CB-CG-CD	-5.24	100.04	114.20
28	H	88	ARG	CG-CD-NE	5.24	122.81	111.80
30	K	344	ARG	CG-CD-NE	5.24	122.81	111.80
12	l	107	LYS	CB-CG-CD	5.24	125.22	111.60
28	H	435	ARG	NE-CZ-NH2	-5.24	117.68	120.30
10	3	65	GLU	CB-CG-CD	5.23	128.33	114.20
23	P	131	PHE	CB-CG-CD1	-5.23	117.14	120.80
10	3	8	ASN	CB-CG-OD1	5.23	132.06	121.60
6	f	195	GLU	OE1-CD-OE2	-5.23	117.02	123.30
4	D	90	ARG	N-CA-CB	-5.23	101.19	110.60
6	F	195	GLU	OE1-CD-OE2	-5.23	117.02	123.30
30	K	69	LYS	CG-CD-CE	-5.23	96.21	111.90
8	1	112	ASP	CB-CA-C	-5.23	99.95	110.40
34	8	493	MET	CA-CB-CG	5.23	122.19	113.30
8	h	112	ASP	CB-CA-C	-5.22	99.95	110.40
7	g	202	LEU	CD1-CG-CD2	-5.22	94.83	110.50
10	j	33	SER	CA-CB-OG	5.22	125.30	111.20
10	j	65	GLU	CB-CG-CD	5.22	128.30	114.20
21	N	906	ARG	NE-CZ-NH2	-5.22	117.69	120.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
11	k	5	LEU	N-CA-C	-5.22	96.90	111.00
11	k	169	GLU	CB-CG-CD	-5.22	100.11	114.20
12	5	107	LYS	CB-CG-CD	5.22	125.17	111.60
10	3	33	SER	CA-CB-OG	5.22	125.28	111.20
12	5	209	THR	O-C-N	5.21	131.04	122.70
34	8	125	GLN	CA-CB-CG	5.21	124.87	113.40
14	7	234	ASP	CB-CG-OD1	5.21	122.99	118.30
5	E	180	GLN	CG-CD-NE2	5.21	129.20	116.70
11	4	139	TYR	CG-CD1-CE1	5.21	125.47	121.30
9	2	219	TYR	CG-CD1-CE1	5.21	125.47	121.30
13	m	228	LYS	CA-CB-CG	5.21	124.85	113.40
13	m	52	PHE	CB-CG-CD1	-5.20	117.16	120.80
11	4	194	ASP	CB-CG-OD2	5.20	122.98	118.30
2	b	90	ARG	NE-CZ-NH2	-5.20	117.70	120.30
13	6	228	LYS	CA-CB-CG	5.20	124.84	113.40
34	8	331	ARG	N-CA-C	-5.20	96.96	111.00
8	1	157	LYS	CD-CE-NZ	5.20	123.65	111.70
22	S	153	GLU	OE1-CD-OE2	-5.20	117.07	123.30
8	h	157	LYS	CD-CE-NZ	5.19	123.65	111.70
5	e	180	GLN	CG-CD-NE2	5.19	129.15	116.70
11	k	177	LYS	CG-CD-CE	5.19	127.47	111.90
5	e	177	GLU	CA-CB-CG	5.19	124.81	113.40
14	7	241	PHE	CB-CG-CD2	-5.19	117.17	120.80
31	L	420	ARG	CD-NE-CZ	5.19	130.86	123.60
11	k	139	TYR	CG-CD1-CE1	5.18	125.45	121.30
19	Y	73	PHE	CB-CG-CD1	5.18	124.43	120.80
10	j	181	SER	N-CA-CB	5.18	118.27	110.50
11	k	58	GLU	OE1-CD-OE2	-5.18	117.08	123.30
11	4	177	LYS	CG-CD-CE	5.18	127.44	111.90
26	U	189	ARG	NE-CZ-NH1	5.18	122.89	120.30
13	m	187	GLU	CA-CB-CG	-5.18	102.01	113.40
11	k	5	LEU	O-C-N	-5.18	114.40	123.20
8	h	153	GLU	CB-CG-CD	5.18	128.18	114.20
11	4	58	GLU	OE1-CD-OE2	-5.18	117.09	123.30
7	g	72	ARG	NE-CZ-NH1	-5.17	117.71	120.30
8	1	153	GLU	CB-CG-CD	5.17	128.17	114.20
13	6	187	GLU	CA-CB-CG	-5.17	102.02	113.40
20	Z	774	ARG	CG-CD-NE	-5.17	100.94	111.80
8	h	192	VAL	O-C-N	-5.17	114.43	122.70
31	L	245	PHE	N-CA-C	-5.17	97.03	111.00
5	E	177	GLU	CA-CB-CG	5.17	124.77	113.40
12	l	277	GLU	CG-CD-OE2	5.17	128.63	118.30

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
9	2	30	THR	CA-CB-CG2	5.17	119.63	112.40
12	5	277	GLU	CG-CD-OE2	5.16	128.63	118.30
9	i	30	THR	CA-CB-CG2	5.16	119.62	112.40
20	Z	802	ASP	N-CA-CB	-5.16	101.31	110.60
13	6	52	PHE	CB-CG-CD1	-5.16	117.19	120.80
21	N	471	TYR	CA-CB-CG	5.16	123.20	113.40
6	f	204	GLU	OE1-CD-OE2	-5.16	117.11	123.30
27	O	160	LYS	CG-CD-CE	5.16	127.37	111.90
5	E	166	ARG	NE-CZ-NH2	5.15	122.88	120.30
8	h	153	GLU	CG-CD-OE1	-5.15	107.99	118.30
10	3	74	TYR	CB-CG-CD1	-5.15	117.91	121.00
35	9	42	ARG	NE-CZ-NH2	-5.15	117.72	120.30
8	1	153	GLU	CG-CD-OE1	-5.15	108.00	118.30
27	O	80	LYS	CB-CA-C	5.15	120.70	110.40
29	I	179	GLU	CG-CD-OE2	-5.15	108.00	118.30
28	H	90	ARG	NE-CZ-NH1	5.15	122.87	120.30
31	L	264	ARG	NE-CZ-NH1	-5.14	117.73	120.30
6	f	232	LYS	CA-CB-CG	5.14	124.71	113.40
8	1	156	SER	CA-CB-OG	5.14	125.08	111.20
6	F	232	LYS	CA-CB-CG	5.14	124.71	113.40
6	F	204	GLU	OE1-CD-OE2	-5.14	117.13	123.30
10	j	196	VAL	CG1-CB-CG2	-5.13	102.69	110.90
13	m	167	GLN	CG-CD-NE2	-5.13	104.39	116.70
25	R	207	ARG	NE-CZ-NH1	5.13	122.86	120.30
5	e	166	ARG	NE-CZ-NH2	5.13	122.86	120.30
13	6	167	GLN	CG-CD-NE2	-5.13	104.39	116.70
15	W	87	MET	N-CA-CB	-5.13	101.37	110.60
8	h	156	SER	CA-CB-OG	5.12	125.04	111.20
17	T	144	TYR	CA-CB-CG	5.12	123.12	113.40
24	Q	167	LYS	CG-CD-CE	5.12	127.25	111.90
7	G	72	ARG	NE-CZ-NH1	-5.12	117.74	120.30
11	k	192	VAL	CA-CB-CG2	5.11	118.57	110.90
34	8	444	GLU	CG-CD-OE2	-5.11	108.08	118.30
10	3	196	VAL	CG1-CB-CG2	-5.11	102.72	110.90
10	j	19	ASP	OD1-CG-OD2	-5.10	113.60	123.30
11	k	194	ASP	CB-CG-OD2	5.10	122.89	118.30
33	J	278	GLN	CA-CB-CG	5.10	124.63	113.40
14	n	110	ASP	CB-CA-C	-5.10	100.20	110.40
10	3	19	ASP	OD1-CG-OD2	-5.10	113.61	123.30
21	N	338	PHE	CB-CG-CD1	5.10	124.37	120.80
10	3	172	LEU	CD1-CG-CD2	-5.09	95.22	110.50
11	4	192	VAL	CA-CB-CG2	5.09	118.54	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
10	3	126	LEU	C-N-CA	5.09	134.43	121.70
32	M	342	ARG	NE-CZ-NH1	5.09	122.85	120.30
16	V	182	LYS	N-CA-CB	-5.09	101.44	110.60
6	f	38	LEU	CB-CG-CD2	5.09	119.65	111.00
33	J	82	LYS	CD-CE-NZ	5.08	123.39	111.70
31	L	168	TYR	CB-CG-CD2	5.08	124.05	121.00
24	Q	71	LYS	CB-CG-CD	5.08	124.80	111.60
6	F	38	LEU	CB-CG-CD2	5.08	119.63	111.00
23	P	390	TYR	CB-CG-CD1	-5.07	117.96	121.00
10	j	114	SER	CA-CB-OG	5.07	124.89	111.20
32	M	300	GLU	CA-CB-CG	5.07	124.56	113.40
10	3	59	ASP	CB-CG-OD2	-5.07	113.74	118.30
34	8	283	LYS	CD-CE-NZ	5.07	123.35	111.70
7	G	245	LYS	O-C-N	-5.06	114.60	122.70
10	3	114	SER	CA-CB-OG	5.06	124.87	111.20
10	j	74	TYR	CB-CG-CD1	-5.06	117.96	121.00
2	B	90	ARG	NE-CZ-NH2	-5.06	117.77	120.30
11	4	110	LYS	CA-CB-CG	5.06	124.53	113.40
11	k	110	LYS	CA-CB-CG	5.06	124.53	113.40
30	K	241	GLU	CG-CD-OE1	5.06	128.42	118.30
7	G	100	LYS	CG-CD-CE	5.05	127.05	111.90
7	G	100	LYS	CB-CG-CD	5.05	124.73	111.60
13	6	99	ARG	CD-NE-CZ	-5.05	116.53	123.60
9	i	149	ASP	OD1-CG-OD2	-5.05	113.71	123.30
9	2	149	ASP	OD1-CG-OD2	-5.05	113.71	123.30
13	6	116	HIS	N-CA-C	-5.05	97.37	111.00
25	R	413	LYS	CD-CE-NZ	5.05	123.31	111.70
3	C	213	PHE	CD1-CG-CD2	-5.04	111.74	118.30
29	I	428	VAL	CG1-CB-CG2	-5.04	102.83	110.90
7	g	100	LYS	CG-CD-CE	5.04	127.03	111.90
11	4	1	MET	CG-SD-CE	-5.04	92.14	100.20
13	6	217	LYS	CD-CE-NZ	-5.04	100.11	111.70
13	m	138	SER	CA-CB-OG	5.04	124.81	111.20
3	c	213	PHE	CD1-CG-CD2	-5.04	111.75	118.30
7	g	100	LYS	CB-CG-CD	5.04	124.70	111.60
34	8	422	LYS	CD-CE-NZ	5.04	123.29	111.70
26	U	46	ILE	CG1-CB-CG2	-5.03	100.33	111.40
13	6	138	SER	CA-CB-OG	5.03	124.78	111.20
27	O	160	LYS	CD-CE-NZ	5.03	123.27	111.70
4	D	197	ARG	NE-CZ-NH1	5.03	122.81	120.30
13	m	217	LYS	CD-CE-NZ	-5.02	100.15	111.70
12	5	162	VAL	CA-CB-CG2	5.02	118.43	110.90

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
12	l	162	VAL	CA-CB-CG2	5.02	118.42	110.90
10	j	98	ARG	CB-CG-CD	5.01	124.64	111.60
7	G	184	PRO	N-CA-CB	5.01	109.32	103.30
8	1	153	GLU	CA-CB-CG	-5.01	102.37	113.40
10	j	59	ASP	CB-CG-OD2	-5.01	113.79	118.30
24	Q	195	LYS	CB-CG-CD	5.01	124.63	111.60
27	O	80	LYS	N-CA-CB	-5.01	101.58	110.60
21	N	657	MET	CG-SD-CE	-5.01	92.19	100.20
8	h	153	GLU	CA-CB-CG	-5.01	102.39	113.40
10	3	98	ARG	CB-CG-CD	5.01	124.62	111.60
13	6	116	HIS	CA-CB-CG	-5.01	105.09	113.60
4	d	49	ARG	NE-CZ-NH1	5.00	122.80	120.30
5	e	49	GLY	CA-C-N	-5.00	106.19	117.20
13	6	58	ILE	CA-CB-CG2	5.00	120.90	110.90
31	L	267	PHE	CB-CG-CD2	-5.00	117.30	120.80

There are no chirality outliers.

All (230) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	201	GLU	Sidechain
9	2	124	GLY	Mainchain
9	2	200	SER	Mainchain
9	2	248	ASN	Sidechain
9	2	37	PHE	Sidechain
9	2	38	ASN	Sidechain
9	2	51	GLN	Sidechain
10	3	126	LEU	Mainchain
10	3	85	GLU	Sidechain
11	4	78	GLN	Sidechain
12	5	147	GLU	Sidechain
12	5	196	ARG	Sidechain
12	5	83	PHE	Mainchain
13	6	13	TYR	Sidechain
13	6	181	LYS	Mainchain
13	6	182	TYR	Sidechain
13	6	36	ARG	Sidechain
13	6	70	ASP	Sidechain
14	7	106	GLU	Sidechain
14	7	74	ARG	Sidechain
34	8	131	ASN	Sidechain
34	8	152	GLN	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
34	8	153	ASP	Sidechain
34	8	175	SER	Peptide
34	8	181	PRO	Peptide
34	8	208	GLN	Peptide
34	8	244	THR	Peptide
34	8	282	GLU	Sidechain
34	8	330	LEU	Peptide
34	8	343	ASP	Sidechain
34	8	368	ASN	Sidechain
34	8	444	GLU	Sidechain
34	8	448	TYR	Peptide
34	8	466	ASP	Sidechain
34	8	497	PHE	Mainchain
35	9	75	GLY	Peptide
1	A	115	ASP	Sidechain
1	A	250	GLU	Sidechain
1	A	77	ARG	Sidechain
2	B	234	ARG	Sidechain
3	C	105	ASP	Sidechain
3	C	109	GLU	Sidechain
3	C	63	THR	Mainchain
4	D	102	ASP	Mainchain
4	D	122	GLN	Sidechain
4	D	204	GLN	Mainchain
4	D	5	ASP	Sidechain
5	E	104	ASP	Sidechain
5	E	106	ASP	Sidechain
5	E	17	PRO	Peptide
5	E	206	GLN	Sidechain
6	F	13	PHE	Peptide
6	F	18	ARG	Peptide
6	F	205	SER	Mainchain
7	G	13	SER	Peptide
7	G	183	HIS	Sidechain
7	G	190	ARG	Sidechain
7	G	21	ASN	Peptide
7	G	242	PHE	Sidechain
7	G	72	ARG	Sidechain
28	H	151	GLN	Peptide
28	H	160	GLY	Peptide
28	H	241	ASP	Sidechain
28	H	313	ALA	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
28	H	326	ASP	Sidechain
28	H	466	TYR	Mainchain
28	H	93	GLU	Sidechain
28	H	94	GLU	Peptide
28	H	96	PRO	Peptide
29	I	101	GLY	Peptide
29	I	104	LEU	Peptide
29	I	137	ASP	Sidechain
29	I	174	ASP	Sidechain
29	I	179	GLU	Sidechain
29	I	280	PHE	Sidechain
29	I	282	ASP	Sidechain
29	I	285	ASP	Sidechain
29	I	300	ARG	Sidechain
29	I	314	ASP	Sidechain
29	I	321	ASP	Sidechain
29	I	339	ILE	Peptide
29	I	373	GLU	Sidechain
29	I	421	GLU	Sidechain
29	I	429	GLU	Peptide
33	J	131	ASP	Sidechain
33	J	172	GLU	Sidechain
33	J	212	ARG	Sidechain
33	J	280	ASP	Sidechain
33	J	295	ASN	Sidechain
33	J	399	SER	Peptide
33	J	9	ASN	Sidechain
30	K	196	ASP	Sidechain
30	K	199	GLU	Sidechain
30	K	204	ASP	Sidechain
30	K	244	HIS	Sidechain
30	K	345	ASP	Sidechain
30	K	414	GLN	Sidechain
30	K	415	VAL	Mainchain
31	L	173	PHE	Peptide
31	L	243	PHE	Sidechain
31	L	244	ILE	Peptide
31	L	265	GLU	Sidechain
31	L	292	SER	Peptide
31	L	293	GLU	Sidechain
31	L	298	ASP	Sidechain
31	L	376	PHE	Peptide

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
31	L	386	PHE	Sidechain
31	L	433	GLU	Sidechain
32	M	105	ASN	Peptide,Sidechain
32	M	107	ASN	Sidechain
32	M	171	GLU	Sidechain
32	M	179	THR	Mainchain
32	M	265	ASP	Sidechain
32	M	282	GLU	Mainchain
32	M	284	ASP	Sidechain
32	M	292	ASP	Sidechain
32	M	298	ASP	Sidechain
32	M	300	GLU	Sidechain
32	M	314	GLY	Peptide
32	M	315	PHE	Peptide
32	M	355	ASP	Sidechain
32	M	42	ARG	Sidechain
32	M	423	GLN	Peptide
32	M	428	LYS	Mainchain,Peptide
32	M	95	GLU	Sidechain
32	M	96	ASN	Sidechain
21	N	346	ASN	Sidechain
21	N	361	ASN	Mainchain
21	N	437	GLU	Sidechain
21	N	86	LYS	Mainchain
21	N	887	ASP	Sidechain
27	O	225	ASP	Sidechain
27	O	50	ASP	Sidechain
23	P	127	GLU	Sidechain
23	P	131	PHE	Sidechain
24	Q	110	SER	Mainchain
24	Q	217	GLU	Sidechain
24	Q	387	TYR	Mainchain
24	Q	47	ASP	Mainchain
24	Q	48	ASP	Mainchain
24	Q	67	THR	Peptide
25	R	127	GLU	Sidechain
25	R	279	LEU	Peptide
22	S	153	GLU	Sidechain
22	S	192	GLU	Sidechain
22	S	217	PHE	Sidechain
22	S	227	ASN	Sidechain
22	S	369	GLN	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
17	T	135	ASN	Sidechain
17	T	138	ASP	Mainchain
17	T	251	HIS	Peptide
26	U	151	GLU	Peptide
26	U	230	GLN	Sidechain
26	U	246	GLU	Sidechain
26	U	60	GLU	Sidechain
26	U	70	HIS	Sidechain
16	V	61	TYR	Sidechain
15	W	14	GLU	Sidechain
15	W	149	GLN	Sidechain
15	W	23	ARG	Peptide
15	W	80	GLN	Sidechain
19	Y	4	ASP	Mainchain
19	Y	58	ASN	Sidechain
19	Y	70	ASP	Sidechain
20	Z	108	ASP	Sidechain
20	Z	276	ASN	Sidechain
20	Z	321	PHE	Sidechain
20	Z	33	GLU	Sidechain
20	Z	365	SER	Mainchain
20	Z	377	ALA	Mainchain
20	Z	379	GLN	Sidechain
20	Z	443	ASP	Mainchain,Sidechain
20	Z	5	SER	Peptide
20	Z	503	ASP	Sidechain
20	Z	6	ASP	Sidechain
20	Z	65	GLU	Sidechain
20	Z	721	ASN	Sidechain
20	Z	728	LYS	Mainchain
20	Z	751	ASP	Sidechain
20	Z	802	ASP	Mainchain
20	Z	807	VAL	Peptide
20	Z	824	ASN	Sidechain
20	Z	84	ALA	Peptide
20	Z	959	HIS	Sidechain
20	Z	961	GLU	Sidechain
1	a	115	ASP	Sidechain
1	a	250	GLU	Sidechain
2	b	234	ARG	Sidechain
3	c	105	ASP	Sidechain
3	c	109	GLU	Sidechain

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Group
3	c	63	THR	Mainchain
4	d	102	ASP	Mainchain
4	d	204	GLN	Mainchain
4	d	237	GLU	Sidechain
4	d	79	ASN	Sidechain
5	e	104	ASP	Sidechain
5	e	106	ASP	Sidechain
5	e	18	GLU	Mainchain
5	e	206	GLN	Sidechain
6	f	13	PHE	Peptide
6	f	18	ARG	Peptide
6	f	205	SER	Mainchain
7	g	13	SER	Peptide
7	g	184	PRO	Mainchain
7	g	21	ASN	Peptide
7	g	72	ARG	Sidechain
8	h	202	TYR	Sidechain
9	i	124	GLY	Mainchain
9	i	200	SER	Mainchain
9	i	217	ARG	Sidechain
9	i	225	ARG	Sidechain
9	i	37	PHE	Sidechain
9	i	38	ASN	Sidechain
9	i	51	GLN	Sidechain
10	j	85	GLU	Sidechain
11	k	78	GLN	Sidechain
12	l	147	GLU	Sidechain
12	l	196	ARG	Sidechain
12	l	82	ARG	Mainchain
13	m	104	LEU	Mainchain
13	m	113	TYR	Mainchain
13	m	13	TYR	Sidechain
13	m	181	LYS	Mainchain
13	m	182	TYR	Sidechain
13	m	36	ARG	Sidechain
13	m	70	ASP	Sidechain
13	m	86	ASP	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 ⓘ

5.3.1 Protein backbone ⓘ

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/252 (95%)	229 (96%)	10 (4%)	0	100	100
1	a	239/252 (95%)	228 (95%)	11 (5%)	0	100	100
2	B	247/250 (99%)	237 (96%)	8 (3%)	2 (1%)	19	60
2	b	247/250 (99%)	237 (96%)	8 (3%)	2 (1%)	19	60
3	C	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	34	72
3	c	242/258 (94%)	233 (96%)	8 (3%)	1 (0%)	34	72
4	D	234/254 (92%)	219 (94%)	10 (4%)	5 (2%)	7	36
4	d	234/254 (92%)	218 (93%)	11 (5%)	5 (2%)	7	36
5	E	242/260 (93%)	227 (94%)	14 (6%)	1 (0%)	34	72
5	e	242/260 (93%)	224 (93%)	15 (6%)	3 (1%)	13	50
6	F	229/234 (98%)	222 (97%)	6 (3%)	1 (0%)	34	72
6	f	229/234 (98%)	222 (97%)	6 (3%)	1 (0%)	34	72
7	G	240/288 (83%)	225 (94%)	14 (6%)	1 (0%)	34	72
7	g	240/288 (83%)	227 (95%)	12 (5%)	1 (0%)	34	72
8	1	194/215 (90%)	187 (96%)	7 (4%)	0	100	100
8	h	194/215 (90%)	185 (95%)	9 (5%)	0	100	100
9	2	224/261 (86%)	213 (95%)	9 (4%)	2 (1%)	17	56
9	i	224/261 (86%)	209 (93%)	12 (5%)	3 (1%)	12	48
10	3	202/205 (98%)	191 (95%)	9 (4%)	2 (1%)	15	54
10	j	202/205 (98%)	193 (96%)	7 (4%)	2 (1%)	15	54
11	4	193/198 (98%)	183 (95%)	9 (5%)	1 (0%)	29	69
11	k	193/198 (98%)	183 (95%)	8 (4%)	2 (1%)	15	54
12	5	210/287 (73%)	199 (95%)	10 (5%)	1 (0%)	29	69
12	l	210/287 (73%)	198 (94%)	11 (5%)	1 (0%)	29	69
13	6	220/241 (91%)	206 (94%)	12 (6%)	2 (1%)	17	56

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
13	m	220/241 (91%)	206 (94%)	12 (6%)	2 (1%)	17	56
14	7	227/266 (85%)	206 (91%)	18 (8%)	3 (1%)	12	48
14	n	227/266 (85%)	210 (92%)	17 (8%)	0	100	100
15	W	195/268 (73%)	177 (91%)	17 (9%)	1 (0%)	29	69
16	V	287/306 (94%)	261 (91%)	22 (8%)	4 (1%)	11	46
17	T	264/274 (96%)	239 (90%)	24 (9%)	1 (0%)	34	72
18	X	125/156 (80%)	107 (86%)	17 (14%)	1 (1%)	19	60
19	Y	87/89 (98%)	77 (88%)	7 (8%)	3 (3%)	3	26
20	Z	902/993 (91%)	822 (91%)	63 (7%)	17 (2%)	8	38
21	N	828/945 (88%)	796 (96%)	28 (3%)	4 (0%)	29	69
22	S	473/523 (90%)	437 (92%)	27 (6%)	9 (2%)	8	38
23	P	438/445 (98%)	418 (95%)	17 (4%)	3 (1%)	22	62
24	Q	432/434 (100%)	397 (92%)	30 (7%)	5 (1%)	13	50
25	R	403/429 (94%)	377 (94%)	23 (6%)	3 (1%)	22	62
26	U	288/338 (85%)	276 (96%)	11 (4%)	1 (0%)	41	76
27	O	386/393 (98%)	372 (96%)	14 (4%)	0	100	100
28	H	387/467 (83%)	355 (92%)	25 (6%)	7 (2%)	8	40
29	I	382/437 (87%)	331 (87%)	42 (11%)	9 (2%)	6	33
30	K	392/428 (92%)	360 (92%)	30 (8%)	2 (0%)	29	69
31	L	386/437 (88%)	349 (90%)	33 (8%)	4 (1%)	15	54
32	M	419/434 (96%)	374 (89%)	35 (8%)	10 (2%)	6	33
33	J	403/405 (100%)	356 (88%)	42 (10%)	5 (1%)	13	50
34	8	368/499 (74%)	329 (89%)	30 (8%)	9 (2%)	6	33
35	9	74/128 (58%)	70 (95%)	4 (5%)	0	100	100
All	All	14205/15766 (90%)	13230 (93%)	832 (6%)	143 (1%)	20	54

All (143) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	b	3	ASP
4	d	204	GLN
5	e	128	SER
9	i	200	SER
9	i	222	PRO

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	k	50	ALA
13	m	138	SER
2	B	3	ASP
4	D	101	GLU
4	D	204	GLN
5	E	128	SER
9	2	200	SER
10	3	126	LEU
10	3	183	TRP
11	4	50	ALA
13	6	138	SER
14	7	110	ASP
16	V	59	ASP
16	V	271	VAL
17	T	138	ASP
19	Y	4	ASP
19	Y	32	ASP
20	Z	5	SER
20	Z	142	ASP
20	Z	173	ALA
20	Z	174	GLU
20	Z	309	GLN
20	Z	366	LYS
20	Z	443	ASP
20	Z	498	ALA
20	Z	728	LYS
20	Z	802	ASP
20	Z	926	ASN
21	N	87	ASP
21	N	361	ASN
21	N	529	GLN
22	S	69	LEU
22	S	449	LEU
24	Q	387	TYR
25	R	71	LEU
25	R	72	VAL
25	R	280	ILE
28	H	95	HIS
28	H	152	ILE
28	H	314	VAL
28	H	372	ASP
28	H	465	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	H	466	TYR
29	I	102	ASN
29	I	125	MET
29	I	213	ILE
29	I	345	ASP
30	K	344	ARG
30	K	416	LYS
31	L	275	PRO
31	L	291	PHE
32	M	96	ASN
32	M	106	VAL
32	M	179	THR
32	M	316	SER
32	M	427	SER
32	M	429	SER
33	J	71	TYR
33	J	400	VAL
34	8	209	ASP
34	8	245	ALA
34	8	497	PHE
5	e	18	GLU
9	i	251	ASP
13	m	40	ASP
4	D	5	ASP
9	2	222	PRO
13	6	40	ASP
20	Z	85	VAL
20	Z	939	ALA
22	S	153	GLU
22	S	450	ASN
23	P	90	LYS
24	Q	51	ARG
32	M	97	SER
32	M	424	ALA
33	J	11	VAL
34	8	466	ASP
2	b	17	LYS
3	c	40	ALA
4	d	205	THR
6	f	205	SER
7	g	71	ASP
2	B	17	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
3	C	40	ALA
6	F	205	SER
7	G	71	ASP
16	V	112	PRO
16	V	186	GLN
18	X	116	ALA
19	Y	68	GLU
20	Z	377	ALA
26	U	179	ARG
28	H	459	SER
29	I	103	PRO
29	I	105	SER
31	L	245	PHE
34	8	331	ARG
4	d	102	ASP
5	e	53	ARG
20	Z	963	ALA
22	S	84	ASP
23	P	403	GLU
31	L	114	GLU
32	M	87	ASP
34	8	106	GLN
34	8	487	ASP
4	d	101	GLU
4	D	102	ASP
4	D	205	THR
21	N	861	TYR
22	S	112	ASN
22	S	327	ILE
23	P	89	LEU
24	Q	47	ASP
24	Q	110	SER
24	Q	286	TYR
32	M	317	SER
33	J	141	LYS
34	8	151	ALA
4	d	103	PRO
10	j	156	PRO
10	j	183	TRP
14	7	111	ASN
14	7	249	ASN
29	I	95	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
29	I	137	ASP
33	J	353	CYS
34	8	294	ASN
20	Z	233	LEU
15	W	22	PRO
20	Z	940	GLY
12	l	113	ASN
22	S	83	PRO
29	I	84	PRO
11	k	4	ILE
12	5	113	ASN
22	S	115	PRO

5.3.2 Protein sidechains ⓘ

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/210 (98%)	198 (96%)	8 (4%)	32	56
1	a	206/210 (98%)	197 (96%)	9 (4%)	28	53
2	B	208/209 (100%)	192 (92%)	16 (8%)	13	37
2	b	208/209 (100%)	192 (92%)	16 (8%)	13	37
3	C	203/216 (94%)	197 (97%)	6 (3%)	41	63
3	c	203/216 (94%)	197 (97%)	6 (3%)	41	63
4	D	209/226 (92%)	199 (95%)	10 (5%)	25	51
4	d	209/226 (92%)	200 (96%)	9 (4%)	29	54
5	E	200/215 (93%)	189 (94%)	11 (6%)	21	47
5	e	200/215 (93%)	187 (94%)	13 (6%)	17	42
6	F	190/193 (98%)	178 (94%)	12 (6%)	18	43
6	f	190/193 (98%)	178 (94%)	12 (6%)	18	43
7	G	200/239 (84%)	189 (94%)	11 (6%)	21	47
7	g	200/239 (84%)	188 (94%)	12 (6%)	19	44

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
8	1	162/178 (91%)	134 (83%)	28 (17%)	2	11
8	h	162/178 (91%)	136 (84%)	26 (16%)	2	13
9	2	185/214 (86%)	144 (78%)	41 (22%)	1	6
9	i	185/214 (86%)	155 (84%)	30 (16%)	2	13
10	3	172/173 (99%)	137 (80%)	35 (20%)	1	7
10	j	172/173 (99%)	145 (84%)	27 (16%)	2	14
11	4	173/175 (99%)	131 (76%)	42 (24%)	0	4
11	k	173/175 (99%)	133 (77%)	40 (23%)	1	5
12	5	169/235 (72%)	130 (77%)	39 (23%)	1	5
12	l	169/235 (72%)	130 (77%)	39 (23%)	1	5
13	6	185/201 (92%)	160 (86%)	25 (14%)	4	17
13	m	185/201 (92%)	154 (83%)	31 (17%)	2	12
14	7	195/224 (87%)	190 (97%)	5 (3%)	46	67
14	n	195/224 (87%)	192 (98%)	3 (2%)	65	80
15	W	171/230 (74%)	166 (97%)	5 (3%)	42	64
16	V	253/268 (94%)	247 (98%)	6 (2%)	49	69
17	T	249/256 (97%)	245 (98%)	4 (2%)	62	79
18	X	116/144 (81%)	112 (97%)	4 (3%)	37	60
19	Y	81/81 (100%)	81 (100%)	0	100	100
20	Z	773/850 (91%)	749 (97%)	24 (3%)	40	62
21	N	698/797 (88%)	684 (98%)	14 (2%)	55	74
22	S	447/489 (91%)	429 (96%)	18 (4%)	31	55
23	P	412/415 (99%)	407 (99%)	5 (1%)	71	84
24	Q	391/391 (100%)	379 (97%)	12 (3%)	40	62
25	R	356/379 (94%)	354 (99%)	2 (1%)	86	92
26	U	263/308 (85%)	261 (99%)	2 (1%)	81	89
27	O	363/368 (99%)	359 (99%)	4 (1%)	73	84
28	H	330/399 (83%)	313 (95%)	17 (5%)	23	48
29	I	341/385 (89%)	333 (98%)	8 (2%)	50	71
30	K	346/374 (92%)	333 (96%)	13 (4%)	33	57
31	L	332/377 (88%)	320 (96%)	12 (4%)	35	59

Continued on next page...

Continued from previous page...

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
32	M	364/375 (97%)	349 (96%)	15 (4%)	30	55
33	J	352/352 (100%)	345 (98%)	7 (2%)	55	74
34	8	337/449 (75%)	327 (97%)	10 (3%)	41	63
35	9	68/116 (59%)	66 (97%)	2 (3%)	42	64
All	All	12357/13619 (91%)	11611 (94%)	746 (6%)	23	44

All (746) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	13	ASP
1	a	67	THR
1	a	78	THR
1	a	95	LEU
1	a	96	ARG
1	a	112	MET
1	a	171	THR
1	a	187	LYS
1	a	193	HIS
2	b	11	THR
2	b	15	SER
2	b	35	LEU
2	b	53	SER
2	b	109	LEU
2	b	123	GLN
2	b	128	ARG
2	b	146	SER
2	b	166	LYS
2	b	177	LYS
2	b	178	ARG
2	b	201	GLU
2	b	229	THR
2	b	231	LYS
2	b	234	ARG
2	b	240	SER
3	c	81	THR
3	c	125	HIS
3	c	165	VAL
3	c	170	SER
3	c	174	THR
3	c	203	SER
4	d	11	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
4	d	66	LYS
4	d	149	GLN
4	d	153	SER
4	d	157	SER
4	d	167	ASN
4	d	170	THR
4	d	218	ASP
4	d	237	GLU
5	e	10	ARG
5	e	14	THR
5	e	36	THR
5	e	72	ARG
5	e	81	LEU
5	e	104	ASP
5	e	112	LEU
5	e	121	LEU
5	e	122	ARG
5	e	177	GLU
5	e	223	THR
5	e	225	GLN
5	e	250	GLU
6	f	5	ASN
6	f	38	LEU
6	f	69	HIS
6	f	72	LEU
6	f	115	LYS
6	f	117	GLN
6	f	119	ASN
6	f	139	LYS
6	f	143	HIS
6	f	154	THR
6	f	207	THR
6	f	226	ASP
7	g	15	PHE
7	g	17	PRO
7	g	46	VAL
7	g	57	LYS
7	g	93	ARG
7	g	137	ILE
7	g	179	LEU
7	g	185	GLU
7	g	202	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	g	209	GLU
7	g	218	TRP
7	g	245	LYS
8	h	10	THR
8	h	18	LYS
8	h	29	THR
8	h	31	THR
8	h	40	THR
8	h	44	THR
8	h	52	CYS
8	h	61	THR
8	h	71	HIS
8	h	77	SER
8	h	89	SER
8	h	103	THR
8	h	112	ASP
8	h	113	ASP
8	h	114	LYS
8	h	128	VAL
8	h	133	TYR
8	h	138	SER
8	h	144	TYR
8	h	147	CYS
8	h	155	MET
8	h	156	SER
8	h	166	HIS
8	h	169	SER
8	h	173	LYS
8	h	178	SER
9	i	30	THR
9	i	31	THR
9	i	38	ASN
9	i	49	SER
9	i	51	GLN
9	i	57	ASP
9	i	63	LEU
9	i	65	ARG
9	i	66	ILE
9	i	84	VAL
9	i	88	ILE
9	i	92	ILE
9	i	97	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	i	98	TYR
9	i	101	ARG
9	i	106	VAL
9	i	118	LYS
9	i	128	ILE
9	i	153	TYR
9	i	156	LEU
9	i	170	HIS
9	i	177	LYS
9	i	181	ILE
9	i	186	ASP
9	i	188	ILE
9	i	198	SER
9	i	200	SER
9	i	209	ILE
9	i	211	LYS
9	i	255	GLU
10	j	3	ASP
10	j	7	ILE
10	j	8	ASN
10	j	18	LYS
10	j	33	SER
10	j	40	PHE
10	j	41	GLU
10	j	53	ILE
10	j	59	ASP
10	j	63	LEU
10	j	65	GLU
10	j	74	TYR
10	j	77	LYS
10	j	87	PHE
10	j	93	SER
10	j	94	SER
10	j	114	SER
10	j	115	LYS
10	j	116	SER
10	j	188	TYR
10	j	193	ASP
10	j	194	GLU
10	j	196	VAL
10	j	202	MET
10	j	203	ARG

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
10	j	204	GLN
10	j	205	ASP
11	k	12	SER
11	k	17	SER
11	k	18	SER
11	k	26	SER
11	k	29	LYS
11	k	45	SER
11	k	52	ASP
11	k	65	GLN
11	k	67	TYR
11	k	68	SER
11	k	69	ILE
11	k	70	ARG
11	k	76	SER
11	k	78	GLN
11	k	81	SER
11	k	91	SER
11	k	92	ILE
11	k	93	ARG
11	k	98	TYR
11	k	99	GLN
11	k	101	ASN
11	k	120	ASP
11	k	121	TYR
11	k	125	LYS
11	k	135	TYR
11	k	136	SER
11	k	139	TYR
11	k	143	LEU
11	k	145	ASP
11	k	162	LYS
11	k	163	LEU
11	k	166	GLN
11	k	169	GLU
11	k	175	ASP
11	k	176	PHE
11	k	177	LYS
11	k	180	ILE
11	k	182	LYS
11	k	186	LYS
11	k	192	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	l	77	THR
12	l	81	PHE
12	l	84	GLN
12	l	100	TRP
12	l	104	GLN
12	l	107	LYS
12	l	110	ILE
12	l	115	PHE
12	l	120	MET
12	l	127	CYS
12	l	138	CYS
12	l	139	ARG
12	l	140	LEU
12	l	147	GLU
12	l	148	ARG
12	l	159	SER
12	l	160	ASN
12	l	162	VAL
12	l	179	TYR
12	l	182	LYS
12	l	183	GLU
12	l	186	THR
12	l	192	SER
12	l	195	THR
12	l	196	ARG
12	l	198	LYS
12	l	203	CYS
12	l	214	VAL
12	l	215	LEU
12	l	217	SER
12	l	245	TYR
12	l	246	SER
12	l	253	TYR
12	l	256	THR
12	l	257	GLU
12	l	267	ASP
12	l	274	LYS
12	l	283	ASN
12	l	286	ILE
13	m	15	ASP
13	m	30	VAL
13	m	39	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	m	41	TYR
13	m	46	ARG
13	m	47	TYR
13	m	50	LYS
13	m	56	ASP
13	m	58	ILE
13	m	72	LEU
13	m	78	ASN
13	m	83	TYR
13	m	93	SER
13	m	94	ILE
13	m	109	ARG
13	m	116	HIS
13	m	118	ILE
13	m	124	GLU
13	m	131	TYR
13	m	134	ASP
13	m	138	SER
13	m	140	GLU
13	m	141	ARG
13	m	143	GLN
13	m	181	LYS
13	m	186	GLU
13	m	194	ASP
13	m	201	GLU
13	m	208	ASP
13	m	217	LYS
13	m	228	LYS
14	n	63	TYR
14	n	102	ASP
14	n	137	ARG
1	A	13	ASP
1	A	67	THR
1	A	95	LEU
1	A	96	ARG
1	A	112	MET
1	A	171	THR
1	A	187	LYS
1	A	193	HIS
2	B	11	THR
2	B	15	SER
2	B	35	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
2	B	53	SER
2	B	109	LEU
2	B	123	GLN
2	B	128	ARG
2	B	146	SER
2	B	166	LYS
2	B	177	LYS
2	B	178	ARG
2	B	201	GLU
2	B	229	THR
2	B	231	LYS
2	B	234	ARG
2	B	240	SER
3	C	81	THR
3	C	125	HIS
3	C	165	VAL
3	C	170	SER
3	C	174	THR
3	C	203	SER
4	D	6	ARG
4	D	11	PHE
4	D	90	ARG
4	D	119	ARG
4	D	122	GLN
4	D	142	ASP
4	D	144	GLU
4	D	208	LYS
4	D	219	SER
4	D	227	GLU
5	E	36	THR
5	E	72	ARG
5	E	81	LEU
5	E	104	ASP
5	E	112	LEU
5	E	121	LEU
5	E	122	ARG
5	E	177	GLU
5	E	223	THR
5	E	225	GLN
5	E	250	GLU
6	F	5	ASN
6	F	38	LEU

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
6	F	69	HIS
6	F	72	LEU
6	F	115	LYS
6	F	117	GLN
6	F	119	ASN
6	F	139	LYS
6	F	143	HIS
6	F	154	THR
6	F	207	THR
6	F	226	ASP
7	G	15	PHE
7	G	17	PRO
7	G	46	VAL
7	G	57	LYS
7	G	93	ARG
7	G	137	ILE
7	G	185	GLU
7	G	190	ARG
7	G	218	TRP
7	G	232	LYS
7	G	236	LEU
8	1	10	THR
8	1	18	LYS
8	1	29	THR
8	1	31	THR
8	1	40	THR
8	1	44	THR
8	1	52	CYS
8	1	61	THR
8	1	71	HIS
8	1	77	SER
8	1	89	SER
8	1	103	THR
8	1	112	ASP
8	1	113	ASP
8	1	114	LYS
8	1	128	VAL
8	1	133	TYR
8	1	138	SER
8	1	144	TYR
8	1	147	CYS
8	1	155	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
8	1	156	SER
8	1	166	HIS
8	1	169	SER
8	1	173	LYS
8	1	178	SER
8	1	203	GLU
8	1	204	GLN
9	2	30	THR
9	2	31	THR
9	2	38	ASN
9	2	49	SER
9	2	51	GLN
9	2	57	ASP
9	2	63	LEU
9	2	65	ARG
9	2	66	ILE
9	2	84	VAL
9	2	88	ILE
9	2	92	ILE
9	2	97	LEU
9	2	98	TYR
9	2	101	ARG
9	2	106	VAL
9	2	118	LYS
9	2	126	TYR
9	2	128	ILE
9	2	153	TYR
9	2	156	LEU
9	2	170	HIS
9	2	177	LYS
9	2	181	ILE
9	2	186	ASP
9	2	188	ILE
9	2	198	SER
9	2	200	SER
9	2	209	ILE
9	2	211	LYS
9	2	212	ASP
9	2	217	ARG
9	2	219	TYR
9	2	220	LEU
9	2	224	VAL

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
9	2	228	LYS
9	2	230	LYS
9	2	231	SER
9	2	244	GLU
9	2	245	SER
9	2	254	GLU
10	3	3	ASP
10	3	7	ILE
10	3	8	ASN
10	3	18	LYS
10	3	33	SER
10	3	40	PHE
10	3	41	GLU
10	3	53	ILE
10	3	59	ASP
10	3	63	LEU
10	3	65	GLU
10	3	74	TYR
10	3	77	LYS
10	3	87	PHE
10	3	93	SER
10	3	94	SER
10	3	114	SER
10	3	115	LYS
10	3	116	SER
10	3	125	ASP
10	3	141	THR
10	3	149	MET
10	3	152	SER
10	3	154	TYR
10	3	166	THR
10	3	172	LEU
10	3	183	TRP
10	3	188	TYR
10	3	193	ASP
10	3	194	GLU
10	3	196	VAL
10	3	202	MET
10	3	203	ARG
10	3	204	GLN
10	3	205	ASP
11	4	1	MET

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
11	4	3	ILE
11	4	12	SER
11	4	17	SER
11	4	18	SER
11	4	26	SER
11	4	29	LYS
11	4	45	SER
11	4	52	ASP
11	4	65	GLN
11	4	67	TYR
11	4	68	SER
11	4	69	ILE
11	4	70	ARG
11	4	76	SER
11	4	78	GLN
11	4	81	SER
11	4	91	SER
11	4	92	ILE
11	4	93	ARG
11	4	98	TYR
11	4	99	GLN
11	4	101	ASN
11	4	120	ASP
11	4	121	TYR
11	4	125	LYS
11	4	135	TYR
11	4	136	SER
11	4	139	TYR
11	4	143	LEU
11	4	145	ASP
11	4	162	LYS
11	4	163	LEU
11	4	166	GLN
11	4	169	GLU
11	4	175	ASP
11	4	176	PHE
11	4	177	LYS
11	4	180	ILE
11	4	182	LYS
11	4	186	LYS
11	4	192	VAL
12	5	77	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
12	5	81	PHE
12	5	84	GLN
12	5	100	TRP
12	5	104	GLN
12	5	107	LYS
12	5	110	ILE
12	5	115	PHE
12	5	120	MET
12	5	127	CYS
12	5	138	CYS
12	5	139	ARG
12	5	140	LEU
12	5	147	GLU
12	5	148	ARG
12	5	159	SER
12	5	160	ASN
12	5	162	VAL
12	5	179	TYR
12	5	182	LYS
12	5	183	GLU
12	5	186	THR
12	5	192	SER
12	5	195	THR
12	5	196	ARG
12	5	198	LYS
12	5	203	CYS
12	5	214	VAL
12	5	215	LEU
12	5	217	SER
12	5	245	TYR
12	5	246	SER
12	5	253	TYR
12	5	256	THR
12	5	257	GLU
12	5	267	ASP
12	5	274	LYS
12	5	283	ASN
12	5	286	ILE
13	6	15	ASP
13	6	30	VAL
13	6	39	THR
13	6	41	TYR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
13	6	46	ARG
13	6	47	TYR
13	6	50	LYS
13	6	56	ASP
13	6	58	ILE
13	6	72	LEU
13	6	78	ASN
13	6	124	GLU
13	6	131	TYR
13	6	134	ASP
13	6	138	SER
13	6	140	GLU
13	6	141	ARG
13	6	143	GLN
13	6	181	LYS
13	6	186	GLU
13	6	194	ASP
13	6	201	GLU
13	6	208	ASP
13	6	217	LYS
13	6	228	LYS
14	7	43	SER
14	7	127	GLU
14	7	194	ARG
14	7	242	LYS
14	7	254	PHE
15	W	1	MET
15	W	22	PRO
15	W	84	LYS
15	W	87	MET
15	W	175	THR
16	V	31	SER
16	V	47	MET
16	V	179	LEU
16	V	182	LYS
16	V	211	LYS
16	V	223	SER
17	T	28	PRO
17	T	88	TYR
17	T	125	GLU
17	T	135	ASN
18	X	25	THR

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
18	X	96	ARG
18	X	112	ASN
18	X	119	LYS
20	Z	40	GLU
20	Z	82	MET
20	Z	113	SER
20	Z	213	LYS
20	Z	217	GLU
20	Z	258	PRO
20	Z	277	GLU
20	Z	309	GLN
20	Z	317	GLN
20	Z	352	LYS
20	Z	424	SER
20	Z	471	LEU
20	Z	479	THR
20	Z	503	ASP
20	Z	528	LEU
20	Z	557	GLU
20	Z	630	LYS
20	Z	798	ARG
20	Z	815	MET
20	Z	824	ASN
20	Z	873	LEU
20	Z	892	SER
20	Z	909	ARG
20	Z	943	LYS
21	N	42	GLU
21	N	210	SER
21	N	269	LEU
21	N	311	ILE
21	N	330	THR
21	N	340	HIS
21	N	417	ARG
21	N	479	GLU
21	N	490	LEU
21	N	632	LYS
21	N	671	LEU
21	N	716	GLN
21	N	747	HIS
21	N	911	LYS
22	S	36	LYS

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
22	S	43	LYS
22	S	101	LYS
22	S	138	MET
22	S	192	GLU
22	S	202	ASN
22	S	249	SER
22	S	265	SER
22	S	287	SER
22	S	304	SER
22	S	331	SER
22	S	400	LYS
22	S	405	ARG
22	S	425	ARG
22	S	435	LYS
22	S	454	SER
22	S	464	ARG
22	S	478	SER
23	P	1	MET
23	P	2	SER
23	P	120	GLU
23	P	206	LYS
23	P	408	SER
24	Q	8	LEU
24	Q	12	ARG
24	Q	18	LYS
24	Q	47	ASP
24	Q	71	LYS
24	Q	98	LYS
24	Q	167	LYS
24	Q	195	LYS
24	Q	198	LEU
24	Q	207	SER
24	Q	252	HIS
24	Q	387	TYR
25	R	78	ASP
25	R	336	LYS
26	U	160	THR
26	U	180	ASP
27	O	80	LYS
27	O	112	LYS
27	O	157	LEU
27	O	285	SER

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
28	H	71	GLU
28	H	72	SER
28	H	87	ASP
28	H	88	ARG
28	H	162	ARG
28	H	180	LYS
28	H	194	SER
28	H	202	GLU
28	H	216	ASP
28	H	282	LYS
28	H	307	PHE
28	H	321	ASP
28	H	373	ARG
28	H	374	LYS
28	H	458	SER
28	H	461	SER
28	H	464	MET
29	I	72	GLU
29	I	97	GLU
29	I	102	ASN
29	I	139	GLU
29	I	255	LYS
29	I	277	SER
29	I	300	ARG
29	I	373	GLU
30	K	117	SER
30	K	121	ARG
30	K	124	SER
30	K	199	GLU
30	K	204	ASP
30	K	249	GLU
30	K	306	PHE
30	K	344	ARG
30	K	345	ASP
30	K	361	SER
30	K	387	MET
30	K	399	ARG
30	K	414	GLN
31	L	123	SER
31	L	141	LYS
31	L	177	GLU
31	L	243	PHE

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	L	272	GLU
31	L	281	ASP
31	L	330	PRO
31	L	345	ARG
31	L	413	ASP
31	L	421	LYS
31	L	426	LYS
31	L	435	GLN
32	M	96	ASN
32	M	100	THR
32	M	109	ASP
32	M	110	ASN
32	M	124	ARG
32	M	131	MET
32	M	174	GLU
32	M	213	ARG
32	M	261	LYS
32	M	289	LYS
32	M	292	ASP
32	M	305	MET
32	M	411	LYS
32	M	428	LYS
32	M	429	SER
33	J	1	MET
33	J	57	PHE
33	J	131	ASP
33	J	278	GLN
33	J	295	ASN
33	J	309	ARG
33	J	390	MET
34	8	153	ASP
34	8	175	SER
34	8	177	LYS
34	8	182	ILE
34	8	204	PHE
34	8	221	MET
34	8	404	GLU
34	8	422	LYS
34	8	454	ASP
34	8	493	MET
35	9	31	GLN
35	9	63	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (93) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	92	ASN
1	a	184	ASN
1	a	209	HIS
1	a	251	GLN
3	c	94	HIS
3	c	177	GLN
4	d	79	ASN
6	f	100	ASN
6	f	110	HIS
7	g	64	ASN
7	g	204	HIS
7	g	207	ASN
8	h	78	GLN
8	h	129	HIS
9	i	51	GLN
9	i	91	ASN
9	i	115	HIS
9	i	223	ASN
10	j	8	ASN
10	j	48	HIS
10	j	204	GLN
11	k	147	HIS
11	k	166	GLN
12	l	160	ASN
12	l	251	ASN
12	l	265	ASN
13	m	16	ASN
13	m	88	ASN
13	m	143	GLN
13	m	203	HIS
14	n	59	ASN
1	A	184	ASN
1	A	209	HIS
1	A	251	GLN
3	C	89	ASN
3	C	94	HIS
3	C	152	ASN
3	C	173	GLN
4	D	70	HIS
4	D	149	GLN
6	F	100	ASN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
7	G	43	ASN
7	G	68	GLN
8	1	69	GLN
8	1	78	GLN
8	1	129	HIS
9	2	51	GLN
9	2	91	ASN
9	2	115	HIS
9	2	173	GLN
9	2	223	ASN
10	3	8	ASN
10	3	48	HIS
10	3	89	GLN
11	4	147	HIS
11	4	166	GLN
12	5	160	ASN
12	5	251	ASN
12	5	265	ASN
13	6	87	HIS
13	6	116	HIS
13	6	143	GLN
13	6	203	HIS
14	7	107	ASN
16	V	190	HIS
17	T	17	ASN
18	X	30	GLN
18	X	131	ASN
20	Z	26	ASN
20	Z	361	HIS
21	N	280	GLN
21	N	360	GLN
21	N	565	ASN
21	N	616	HIS
23	P	417	HIS
24	Q	252	HIS
25	R	340	GLN
25	R	378	ASN
27	O	323	ASN
28	H	387	ASN
29	I	239	GLN
29	I	431	ASN
30	K	72	GLN

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type
31	L	273	HIS
32	M	24	ASN
32	M	74	GLN
33	J	204	HIS
33	J	295	ASN
33	J	376	HIS
33	J	393	ASN
34	8	172	GLN
34	8	313	GLN
34	8	438	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\# Z > 2$	Counts	RMSZ	$\# Z > 2$
35	GLZ	9	76	35	3,3,3	0.17	0	0,2,2	-	-

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	GLZ	9	76	35	-	0/0/1/1	-

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

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	ATP	H	501	37	26,33,33	1.25	2 (7%)	31,52,52	1.72	7 (22%)
36	ATP	I	501	37	26,33,33	1.30	2 (7%)	31,52,52	1.15	3 (9%)
36	ATP	L	501	37	26,33,33	1.48	5 (19%)	31,52,52	1.55	6 (19%)
36	ATP	M	501	-	26,33,33	2.09	4 (15%)	31,52,52	1.76	6 (19%)
36	ATP	K	501	37	26,33,33	1.41	3 (11%)	31,52,52	1.59	7 (22%)
38	ADP	J	501	-	24,29,29	1.82	6 (25%)	29,45,45	1.34	5 (17%)

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	ATP	H	501	37	-	5/18/38/38	0/3/3/3
36	ATP	I	501	37	-	8/18/38/38	0/3/3/3
36	ATP	L	501	37	-	3/18/38/38	0/3/3/3
36	ATP	M	501	-	-	3/18/38/38	0/3/3/3

Continued on next page...

Continued from previous page...

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	K	501	37	-	6/18/38/38	0/3/3/3
38	ADP	J	501	-	-	2/12/32/32	0/3/3/3

All (22) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	M	501	ATP	O4'-C1'	6.74	1.50	1.41
36	M	501	ATP	C4-N3	-4.97	1.28	1.35
36	M	501	ATP	C8-N7	-4.81	1.26	1.34
36	K	501	ATP	C8-N7	-4.60	1.26	1.34
38	J	501	ADP	C2-N3	4.18	1.38	1.32
38	J	501	ADP	O4'-C4'	-4.08	1.35	1.45
36	L	501	ATP	C2'-C1'	3.90	1.59	1.53
38	J	501	ADP	O2'-C2'	-3.81	1.34	1.43
36	H	501	ATP	C2'-C1'	3.50	1.59	1.53
38	J	501	ADP	C2-N1	2.83	1.39	1.33
36	K	501	ATP	C2-N3	2.83	1.36	1.32
36	I	501	ATP	C4-N3	2.83	1.39	1.35
36	L	501	ATP	C4-N3	-2.77	1.31	1.35
36	M	501	ATP	C2-N3	2.66	1.36	1.32
38	J	501	ADP	C4-N3	-2.45	1.32	1.35
36	L	501	ATP	PG-O1G	2.44	1.58	1.50
36	I	501	ATP	C5'-C4'	2.41	1.59	1.51
36	H	501	ATP	C5-N7	-2.34	1.31	1.39
38	J	501	ADP	C3'-C4'	2.25	1.58	1.53
36	L	501	ATP	C2-N1	2.24	1.38	1.33
36	L	501	ATP	C2-N3	2.08	1.35	1.32
36	K	501	ATP	C2'-C1'	2.01	1.56	1.53

All (34) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	H	501	ATP	PA-O3A-PB	5.13	150.41	132.83
36	M	501	ATP	C5-C6-N6	4.30	126.88	120.35
36	K	501	ATP	N6-C6-N1	3.99	126.86	118.57
36	M	501	ATP	PA-O3A-PB	3.88	146.16	132.83
38	J	501	ADP	C5-C6-N6	3.74	126.04	120.35
36	H	501	ATP	C5-C6-N6	3.53	125.71	120.35
36	M	501	ATP	C5-C6-N1	-3.36	112.73	120.35
36	L	501	ATP	O4'-C1'-C2'	-3.36	102.01	106.93
36	H	501	ATP	C5-C6-N1	-2.99	113.58	120.35
36	I	501	ATP	C4-C5-N7	-2.96	106.31	109.40

Continued on next page...

Continued from previous page...

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	L	501	ATP	PA-O3A-PB	2.94	142.90	132.83
36	L	501	ATP	C3'-C2'-C1'	2.92	105.38	100.98
36	K	501	ATP	PA-O3A-PB	2.87	142.66	132.83
36	K	501	ATP	O3G-PG-O2G	2.86	118.56	107.64
36	L	501	ATP	O3G-PG-O2G	2.84	118.51	107.64
36	M	501	ATP	O5'-C5'-C4'	2.59	117.91	108.99
36	H	501	ATP	O2B-PB-O1B	2.44	124.29	112.24
36	M	501	ATP	O4'-C1'-C2'	-2.40	103.42	106.93
36	K	501	ATP	N3-C2-N1	-2.37	124.98	128.68
38	J	501	ADP	O3'-C3'-C4'	2.35	117.84	111.05
36	M	501	ATP	O3B-PG-O1G	-2.30	98.44	111.19
36	K	501	ATP	C5-C6-N1	-2.28	115.19	120.35
36	L	501	ATP	C2'-C3'-C4'	-2.27	98.23	102.64
36	K	501	ATP	O3G-PG-O3B	-2.21	97.22	104.64
38	J	501	ADP	O5'-C5'-C4'	2.20	116.56	108.99
36	K	501	ATP	O4'-C4'-C5'	2.19	116.58	109.37
36	H	501	ATP	O3B-PG-O1G	-2.19	99.04	111.19
36	I	501	ATP	PA-O3A-PB	2.14	140.18	132.83
38	J	501	ADP	N3-C2-N1	-2.14	125.34	128.68
36	H	501	ATP	O2A-PA-O5'	-2.12	97.92	107.75
38	J	501	ADP	C5-C6-N1	-2.11	115.57	120.35
36	H	501	ATP	C4-C5-N7	-2.07	107.24	109.40
36	L	501	ATP	O3'-C3'-C4'	2.07	117.03	111.05
36	I	501	ATP	C5-C6-N6	2.06	123.48	120.35

There are no chirality outliers.

All (27) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
36	H	501	ATP	PB-O3B-PG-O2G
36	H	501	ATP	C5'-O5'-PA-O2A
36	H	501	ATP	C5'-O5'-PA-O3A
36	I	501	ATP	PB-O3B-PG-O2G
36	I	501	ATP	C5'-O5'-PA-O1A
36	I	501	ATP	C5'-O5'-PA-O2A
36	K	501	ATP	PB-O3B-PG-O2G
36	K	501	ATP	PB-O3B-PG-O3G
36	K	501	ATP	C5'-O5'-PA-O3A
36	L	501	ATP	C5'-O5'-PA-O3A
36	M	501	ATP	C5'-O5'-PA-O1A
38	J	501	ADP	C5'-O5'-PA-O3A
36	I	501	ATP	PB-O3A-PA-O5'

Continued on next page...

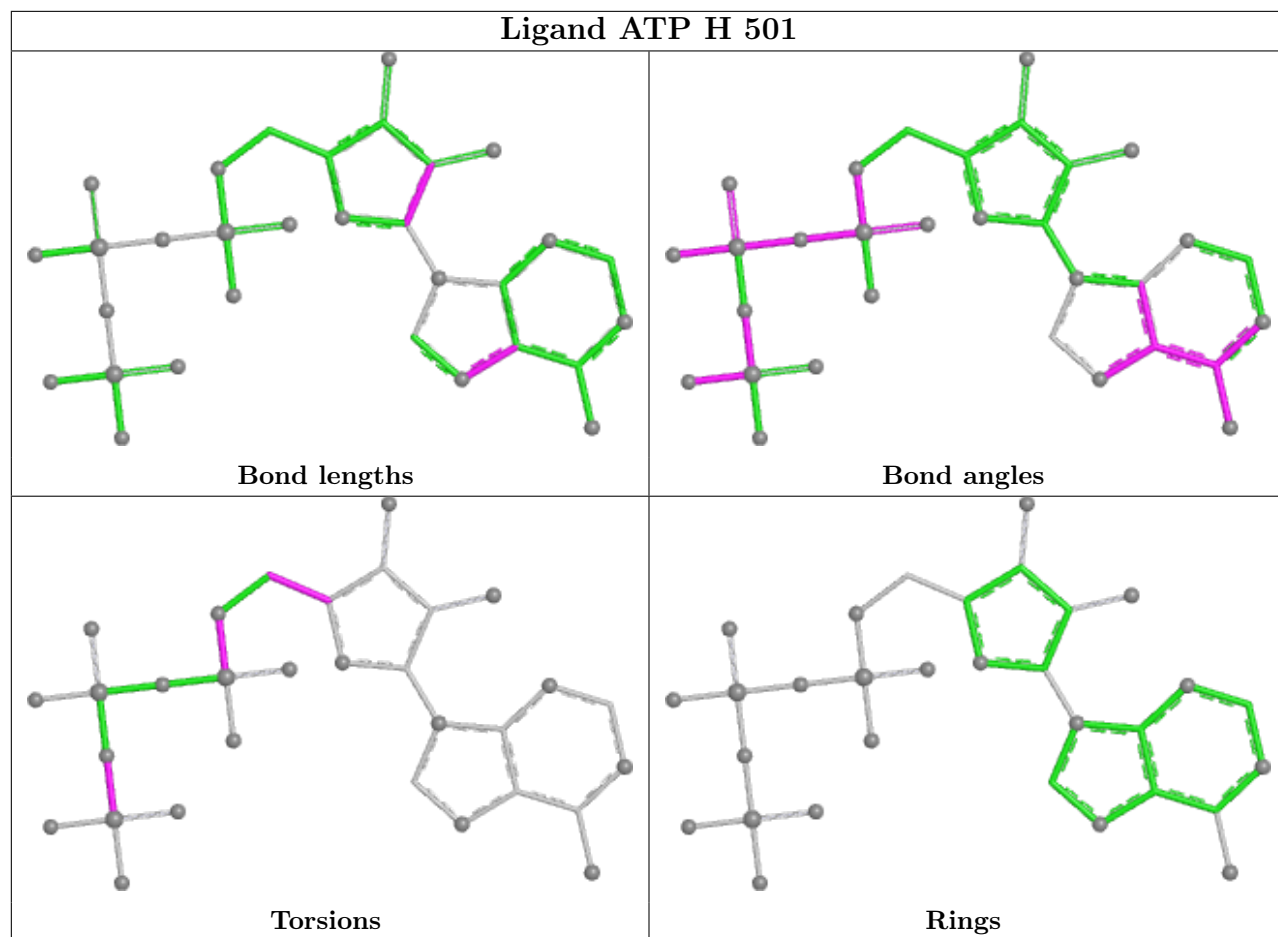
Continued from previous page...

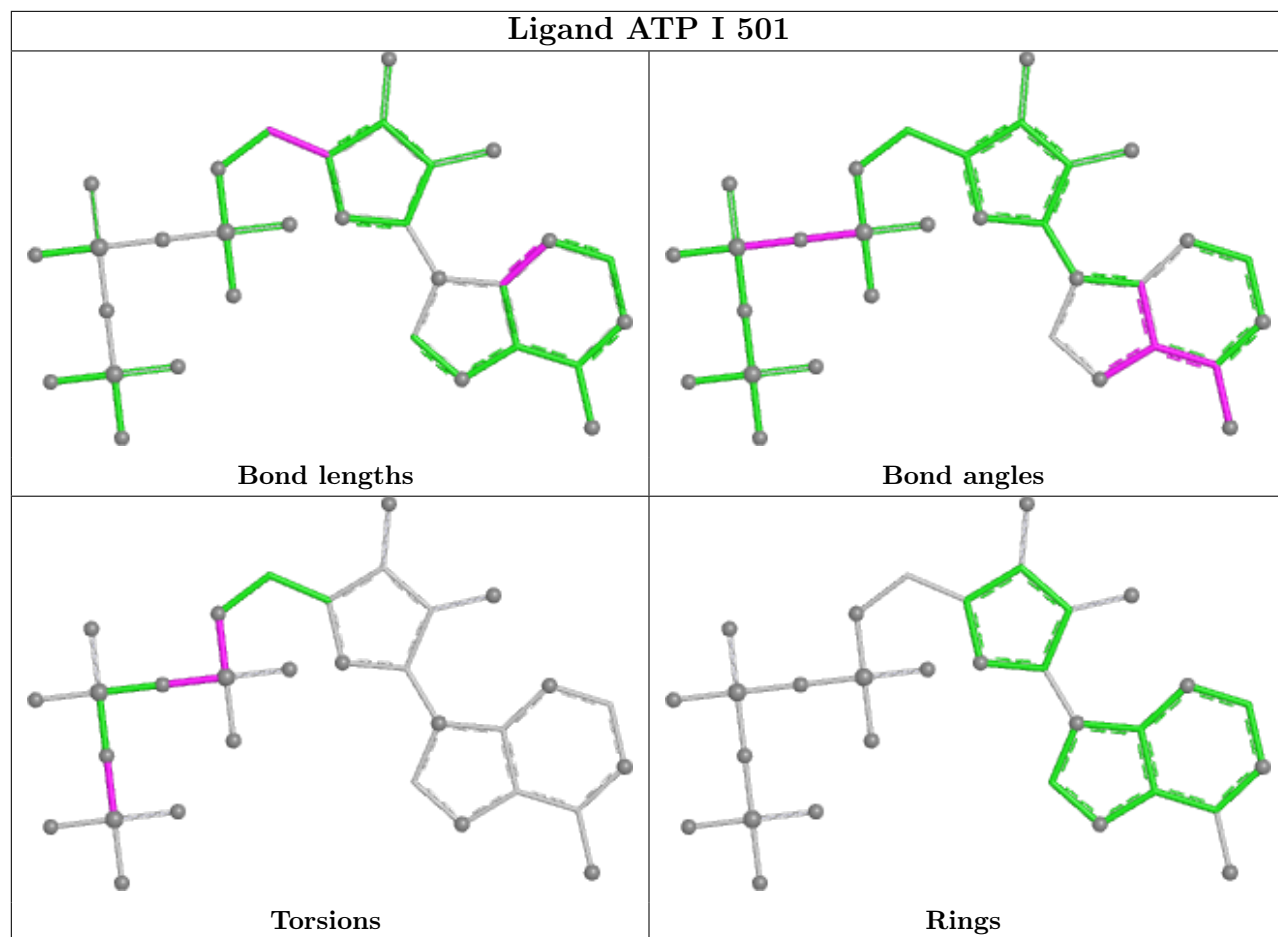
Mol	Chain	Res	Type	Atoms
36	I	501	ATP	C5'-O5'-PA-O3A
36	K	501	ATP	C5'-O5'-PA-O1A
36	L	501	ATP	C5'-O5'-PA-O2A
38	J	501	ADP	C5'-O5'-PA-O1A
36	L	501	ATP	PA-O3A-PB-O1B
36	M	501	ATP	C4'-C5'-O5'-PA
36	I	501	ATP	PB-O3A-PA-O1A
36	H	501	ATP	O4'-C4'-C5'-O5'
36	K	501	ATP	PB-O3B-PG-O1G
36	H	501	ATP	PB-O3B-PG-O3G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

There are no ring outliers.

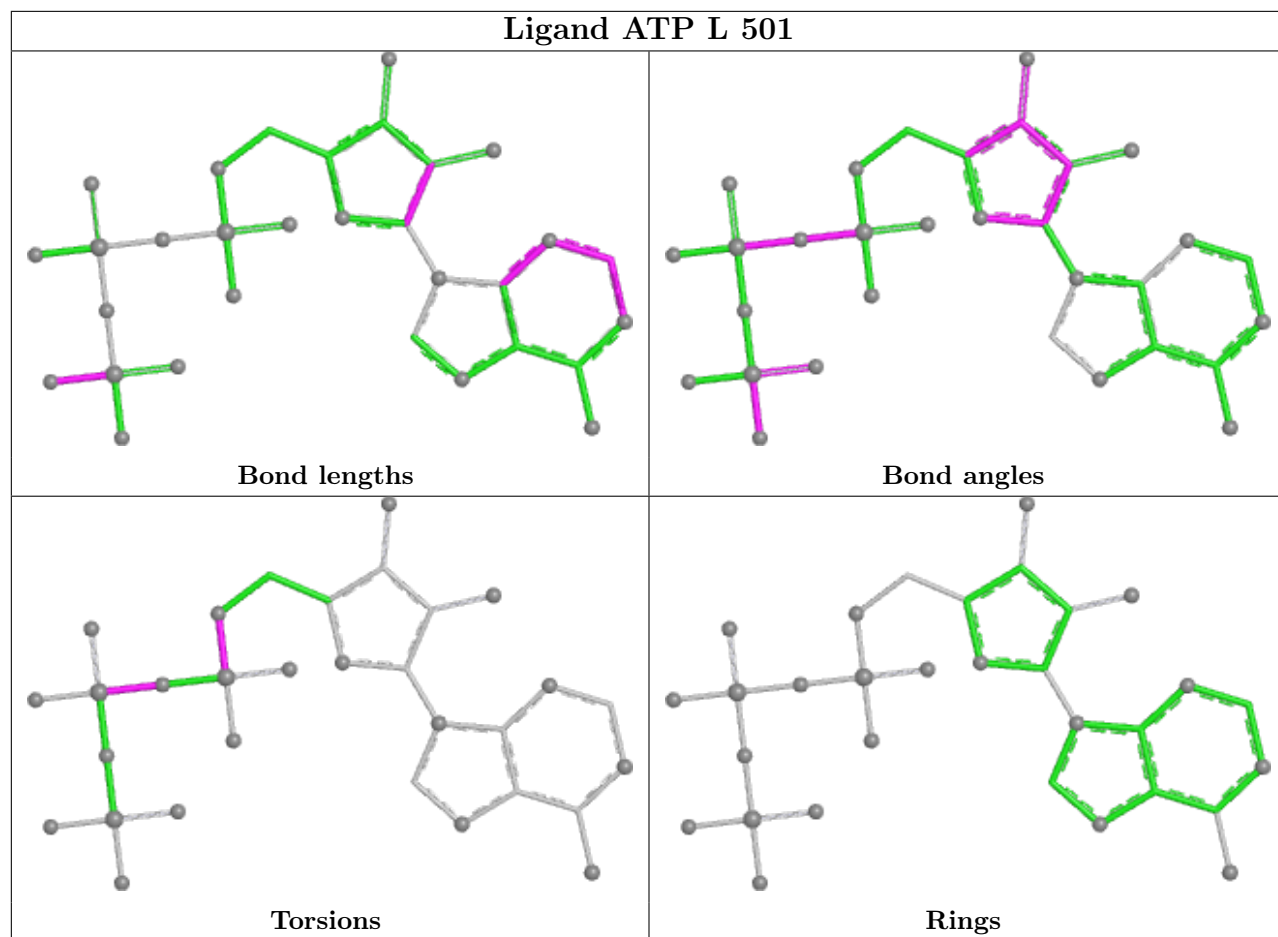
No monomer is involved in short contacts.

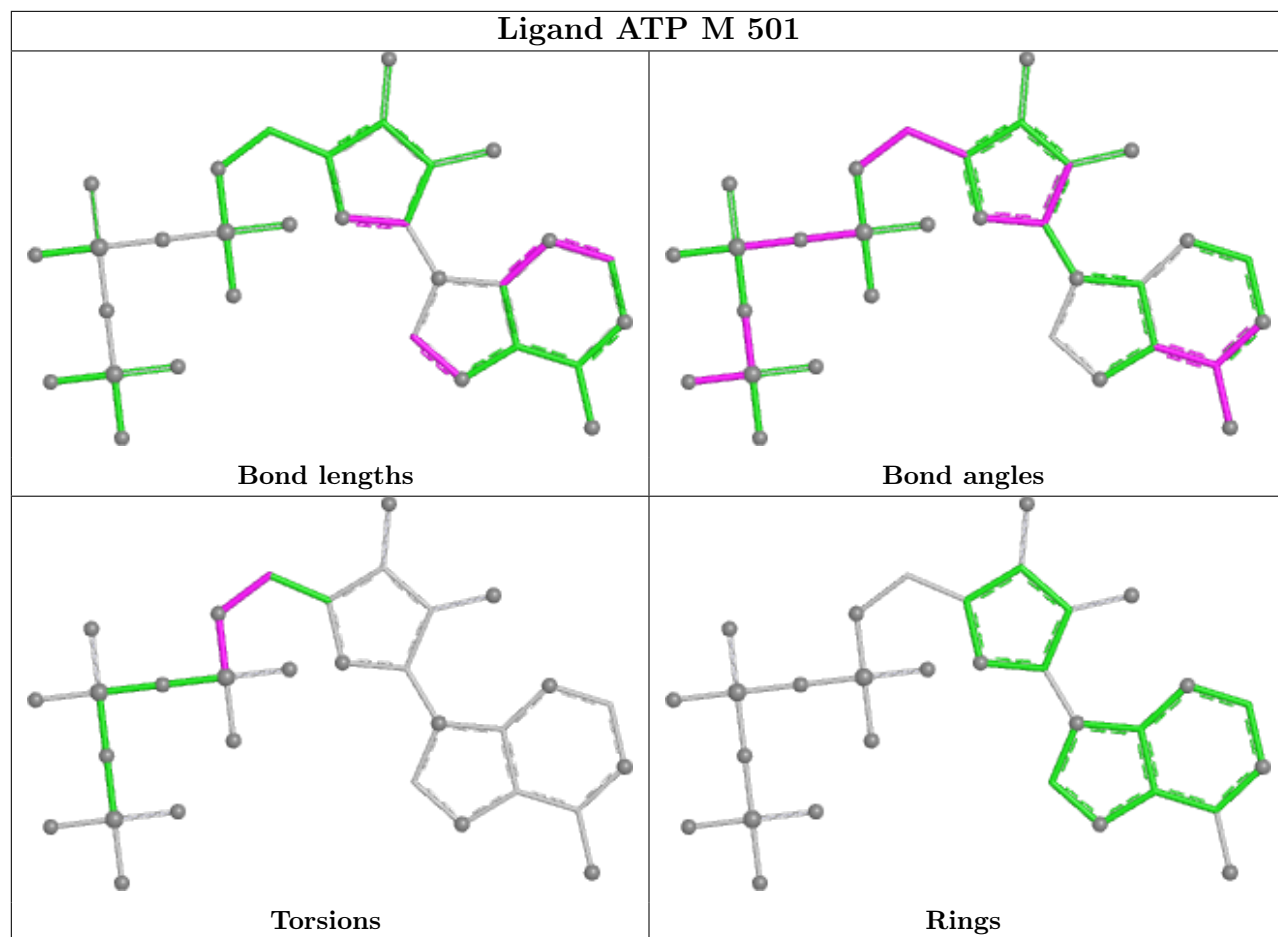
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



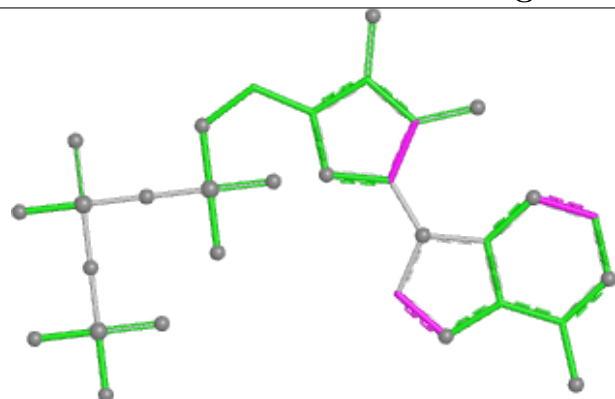


Ligand ATP L 501

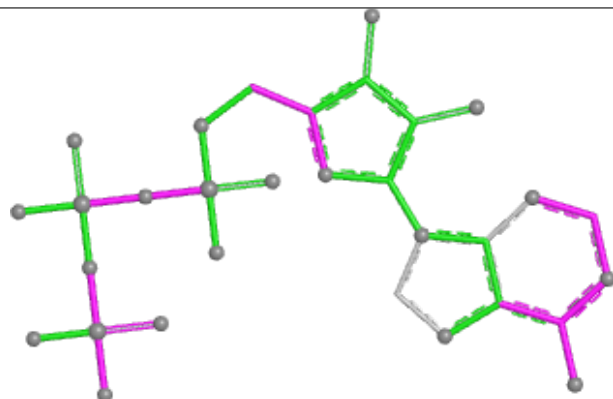




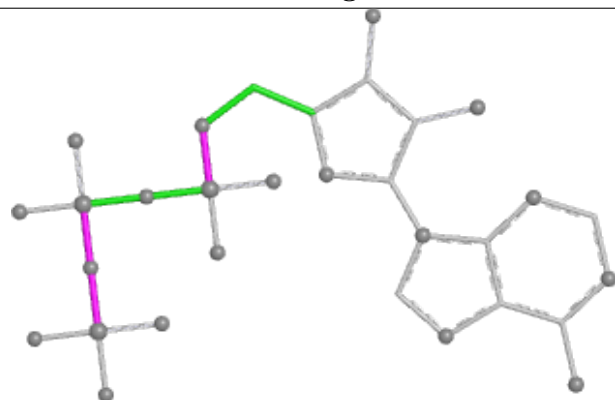
Ligand ATP K 501



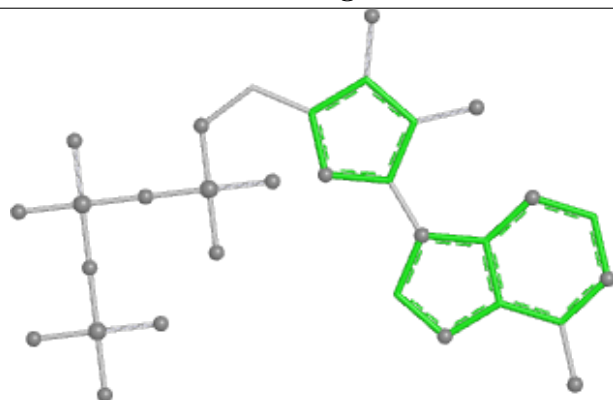
Bond lengths



Bond angles

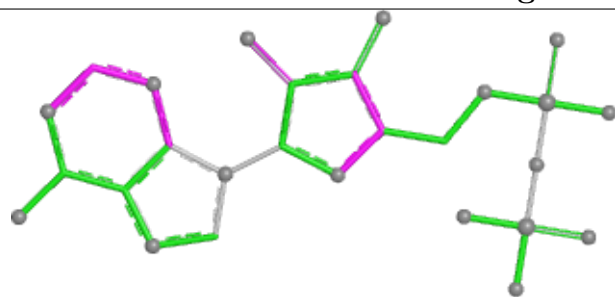


Torsions

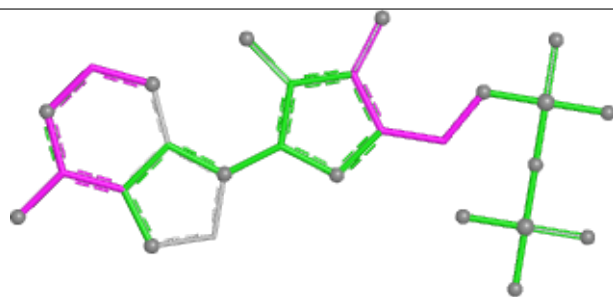


Rings

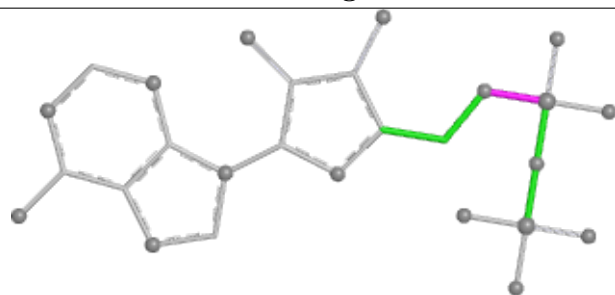
Ligand ADP J 501



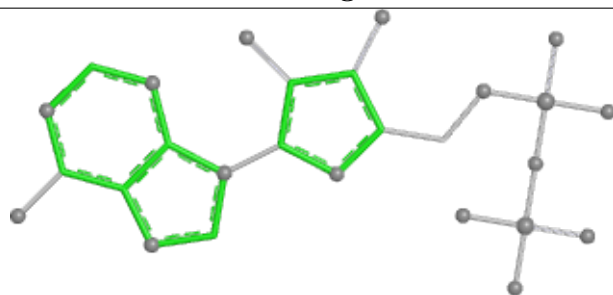
Bond lengths



Bond angles



Torsions



Rings

5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

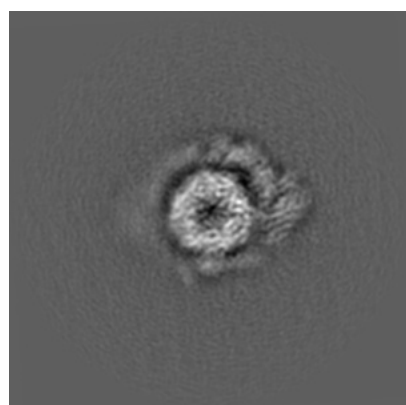
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-14084. These allow visual inspection of the internal detail of the map and identification of artifacts.

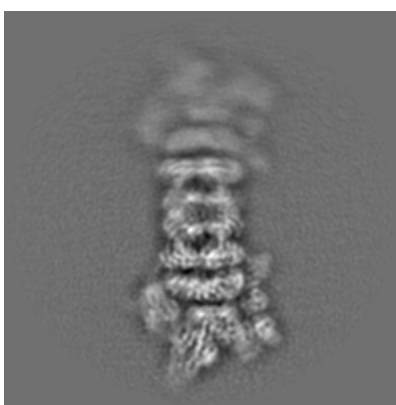
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

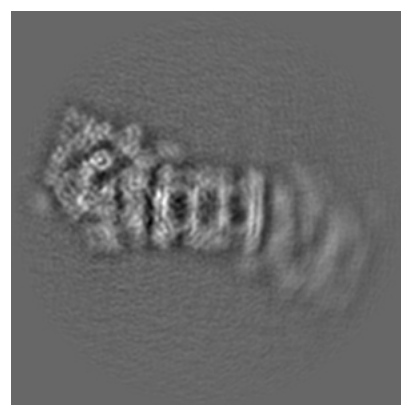
6.1.1 Primary map



X



Y

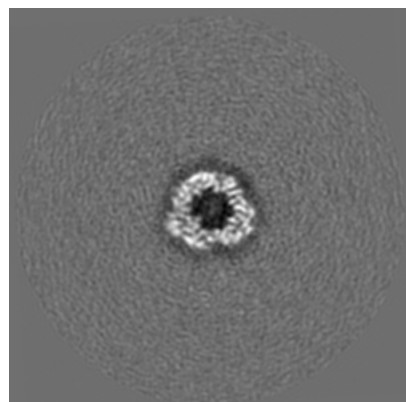


Z

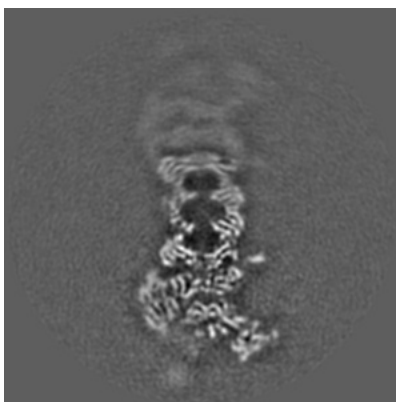
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

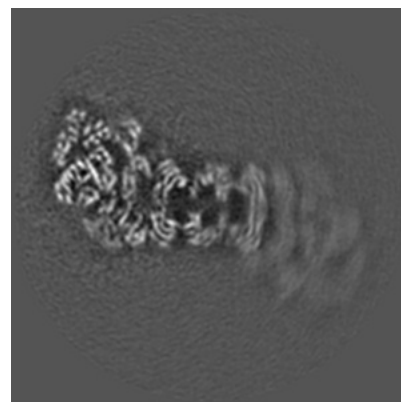
6.2.1 Primary map



X Index: 192



Y Index: 192

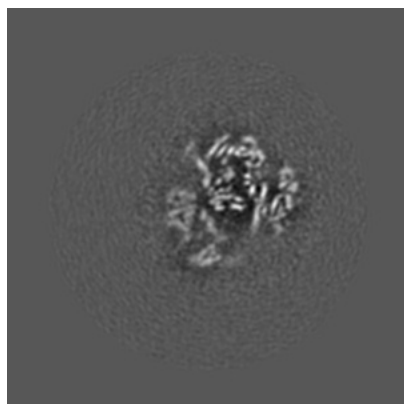


Z Index: 192

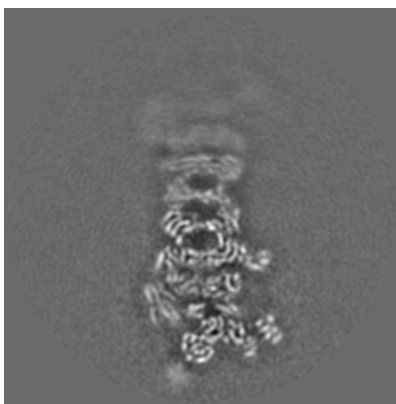
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

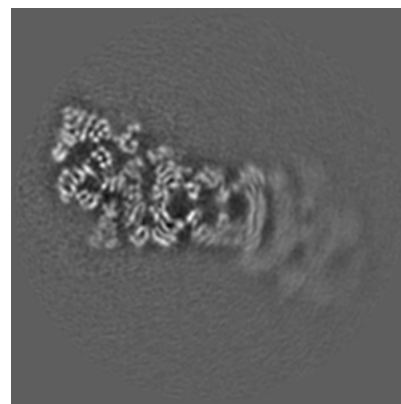
6.3.1 Primary map



X Index: 82



Y Index: 204

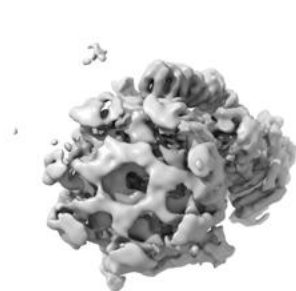


Z Index: 197

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

6.4 Orthogonal surface views [i](#)

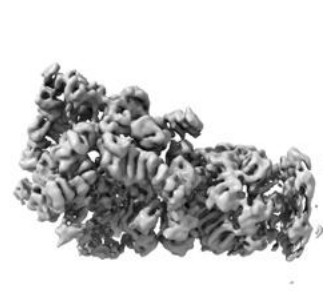
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.8. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

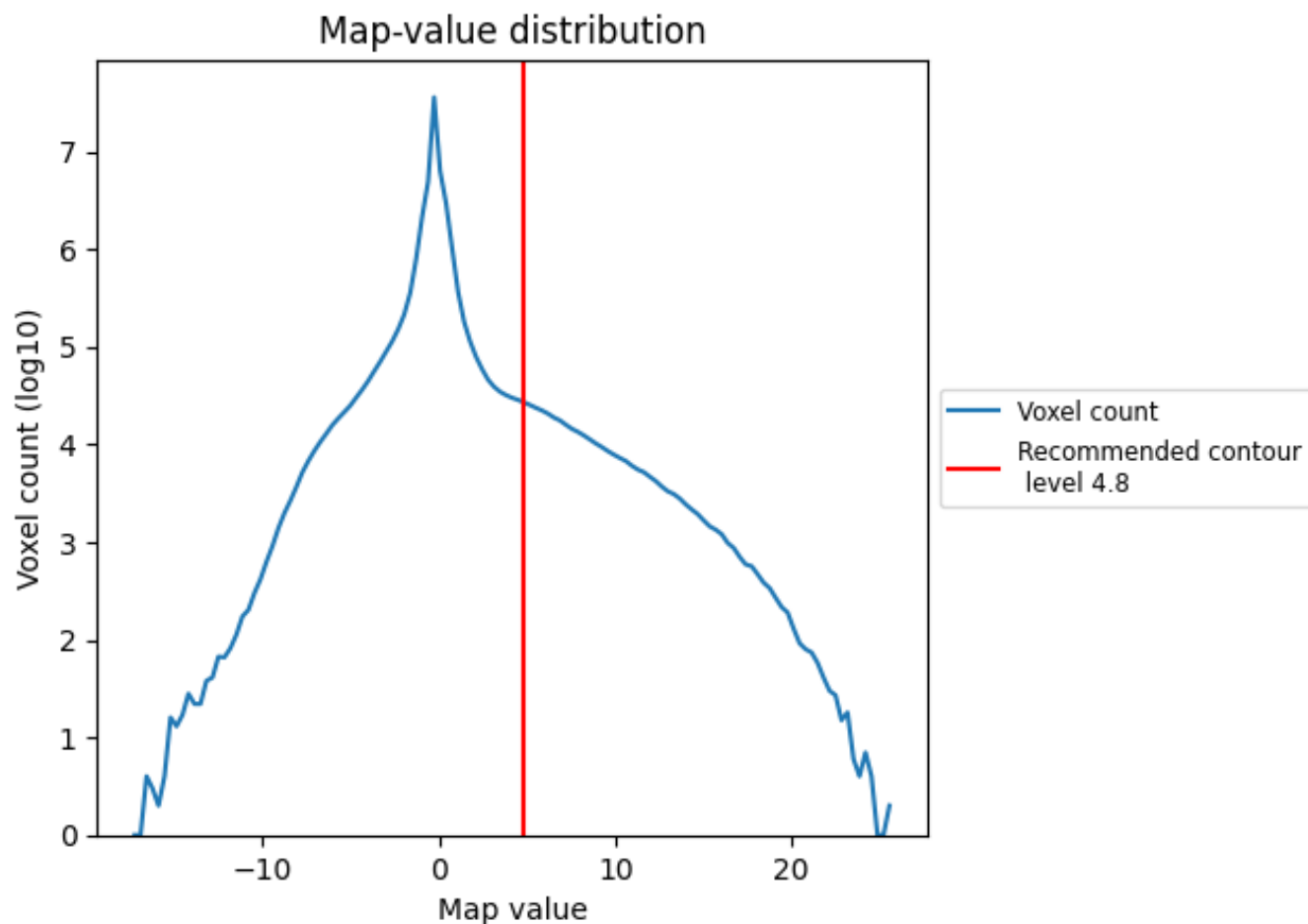
6.5 Mask visualisation

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

7 Map analysis [i](#)

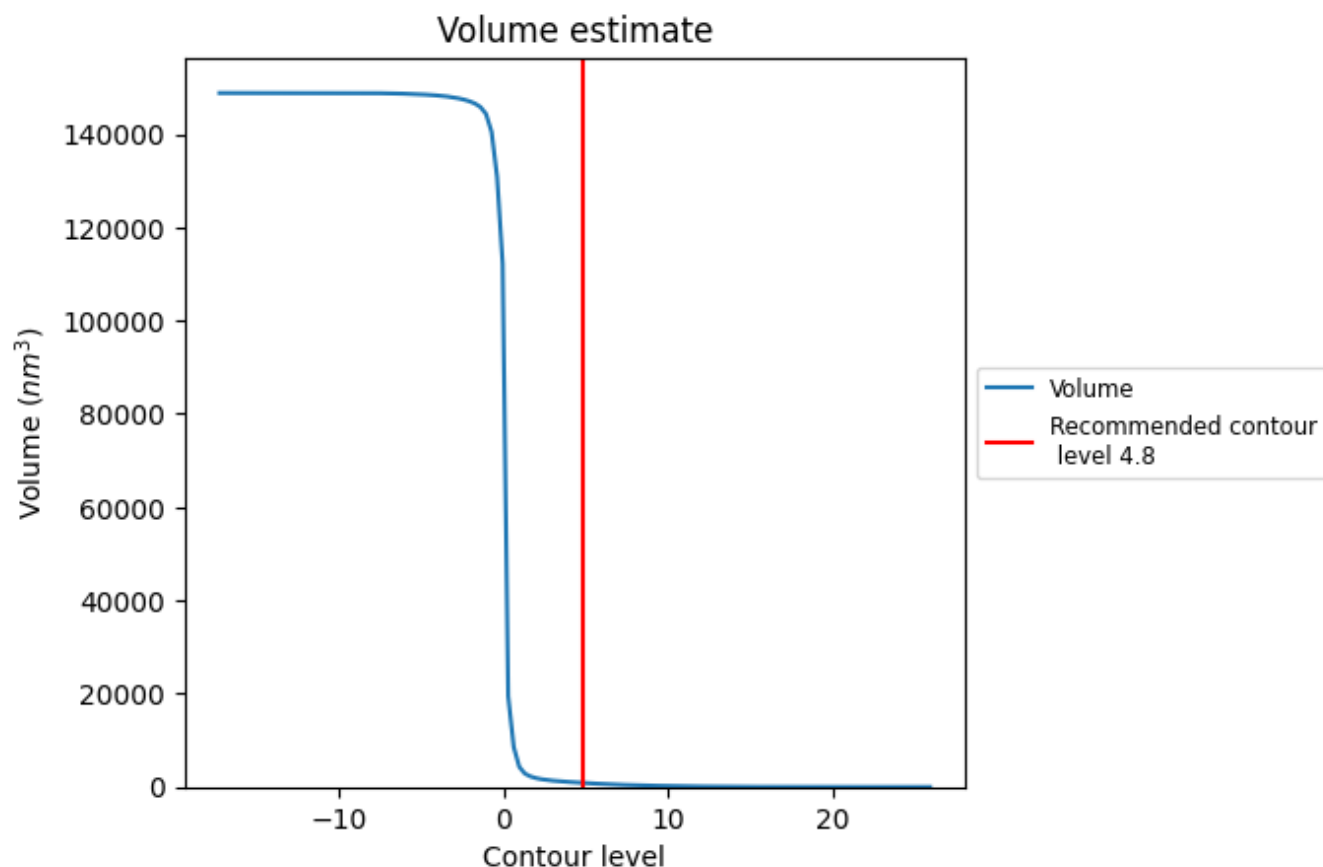
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution [i](#)



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.

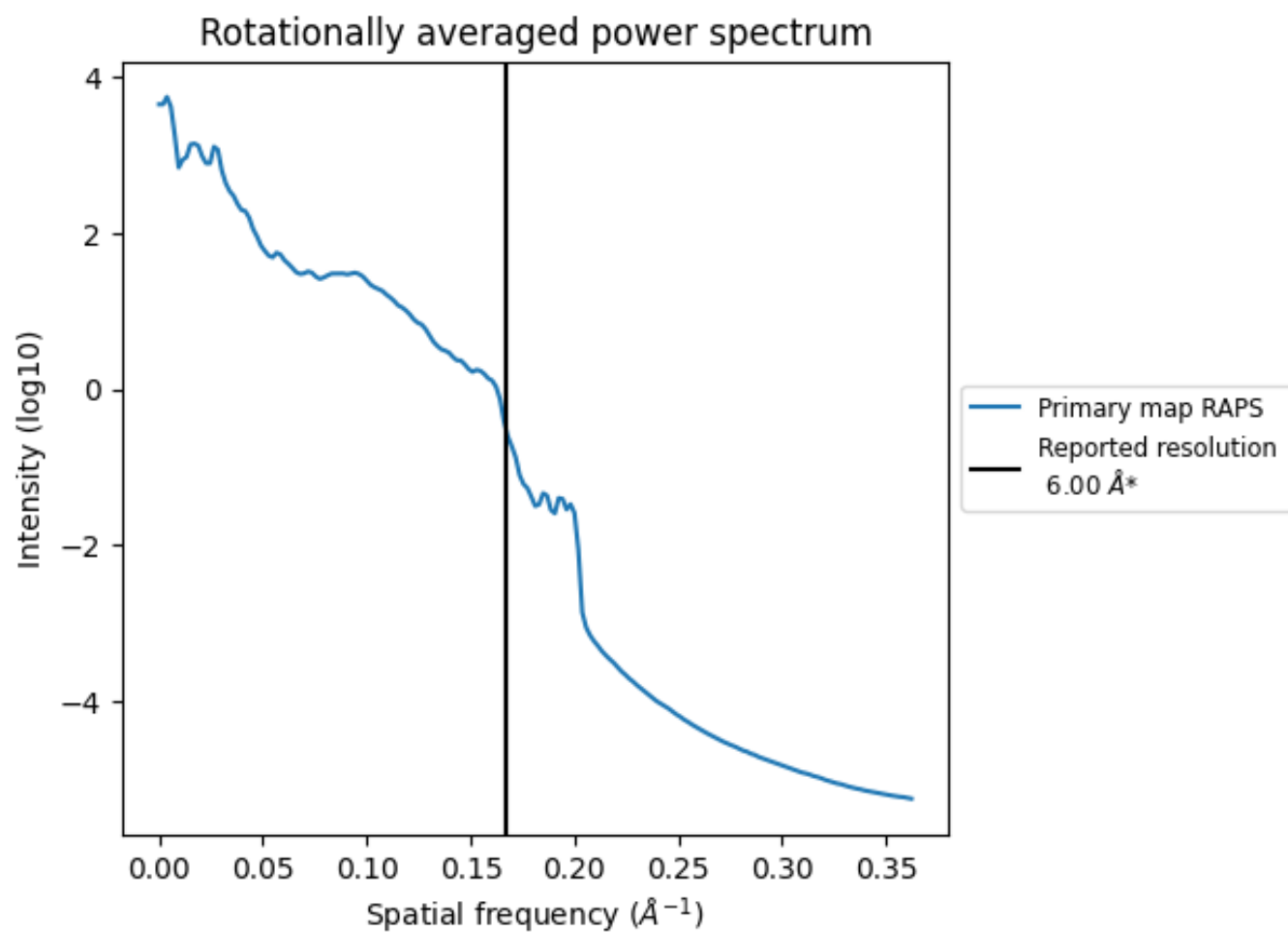
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 874 nm^3 ; this corresponds to an approximate mass of 789 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 ⓘ



*Reported resolution corresponds to spatial frequency of 0.167 Å⁻¹

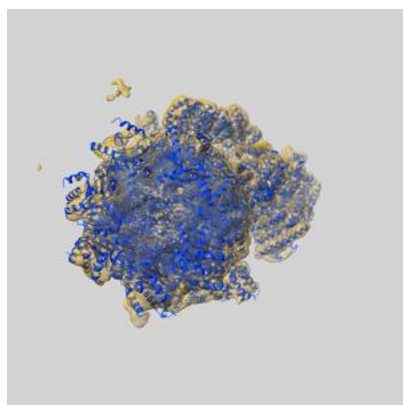
8 Fourier-Shell correlation

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

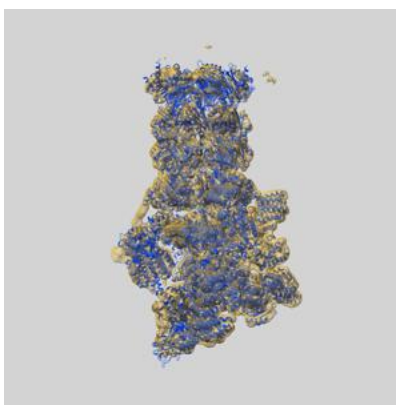
9 Map-model fit [i](#)

This section contains information regarding the fit between EMDB map EMD-14084 and PDB model 7QO5. Per-residue inclusion information can be found in section 3 on page 13.

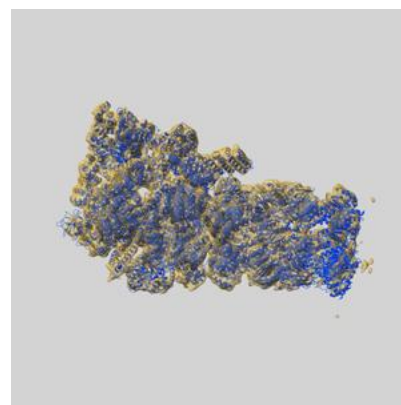
9.1 Map-model overlay [i](#)



X



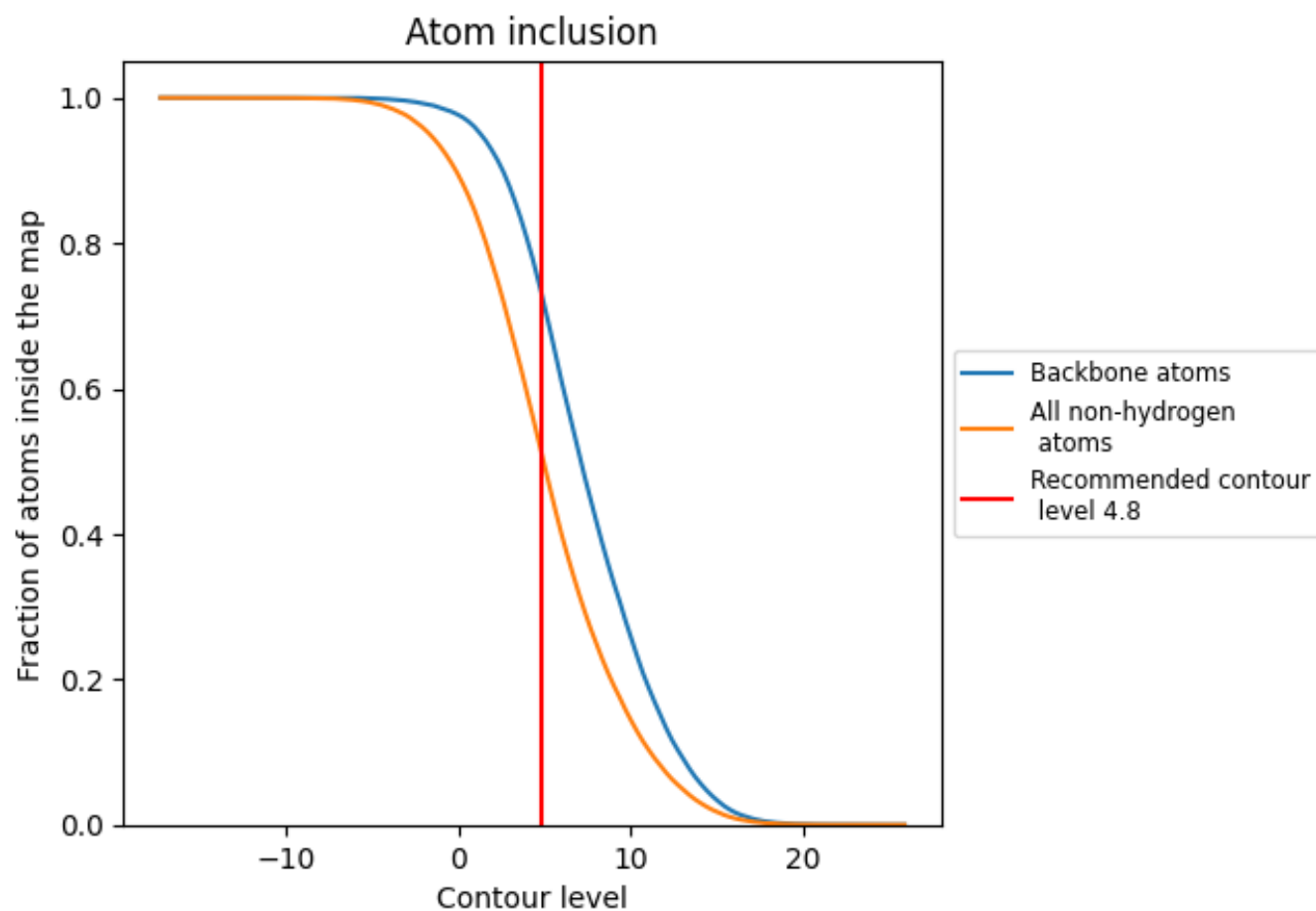
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 4.8 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 Atom inclusion [i](#)



At the recommended contour level, 74% of all backbone atoms, 52% of all non-hydrogen atoms, are inside the map.