Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 01:03 am GMT

PDB ID	:	6FVY
EMDB ID	:	EMD-4324
Title	:	26S proteasome, s6 state
Authors	:	Eisele, M.R.; Reed, R.G.; Rudack, T.; Schweitzer, A.; Beck, F.; Nagy, I.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Tomko, R.J.; Sakata, E.
Deposited on	:	2018-03-05
Resolution	:	6.10 Å(reported)

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

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

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

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

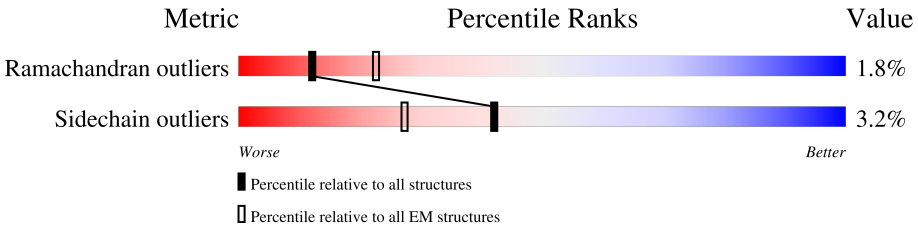
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.10 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	244	73% 24%
1	a	244	32% 75% 23%
2	B	248	76% 20%
2	b	248	38% 79% 18%
3	C	241	5% 76% 22%
3	c	241	37% 79% 17%
4	D	252	73% 19% 6%
4	d	252	41% 78% 20%
5	E	245	80% 19%

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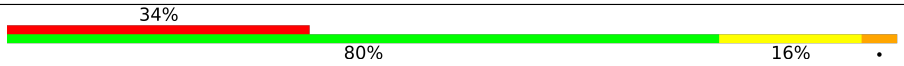
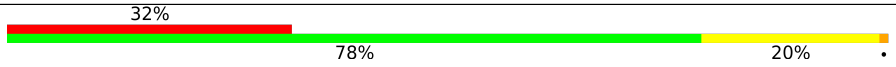
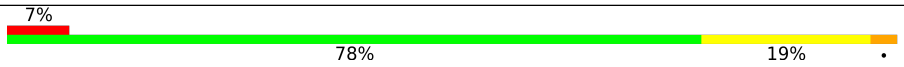
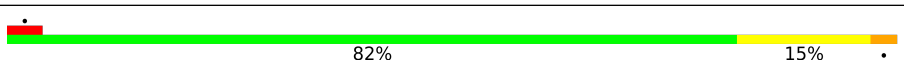
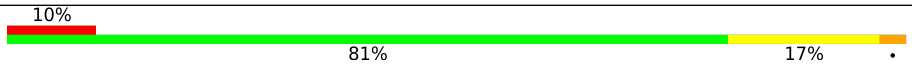
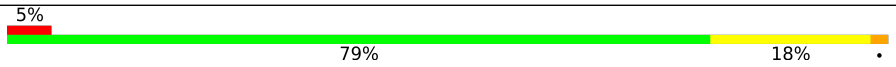
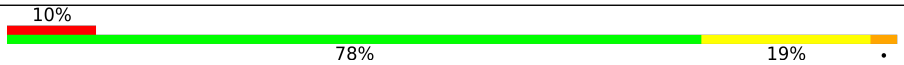
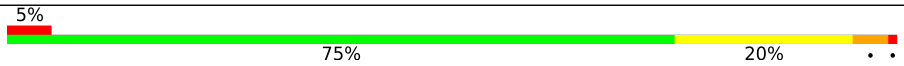
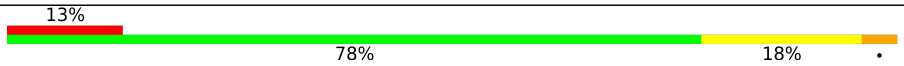
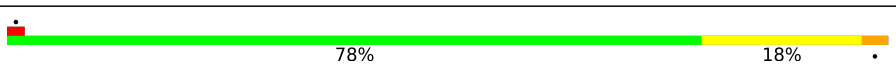
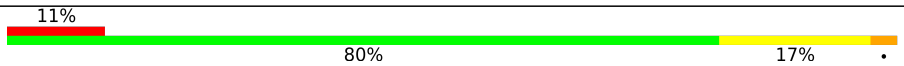
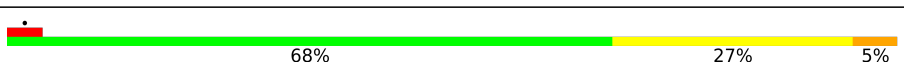
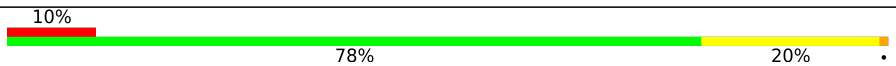
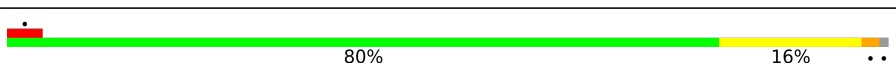
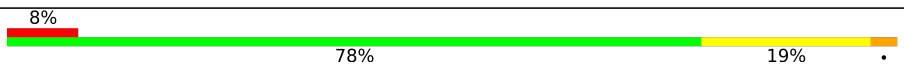
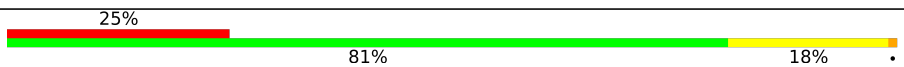
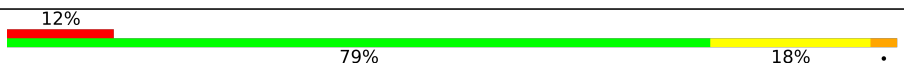
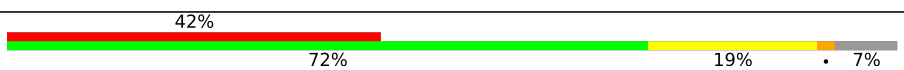
Mol	Chain	Length	Quality of chain
5	e	245	
6	F	232	
6	f	232	
7	G	245	
7	g	245	
8	1	196	
8	h	196	
9	2	226	
9	i	226	
10	3	204	
10	j	204	
11	4	195	
11	k	195	
12	5	212	
12	l	212	
13	6	222	
13	m	222	
14	7	232	
14	n	232	
15	W	197	
16	V	289	
17	T	266	
18	X	127	
19	Y	89	
20	Z	970	

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Mol	Chain	Length	Quality of chain
21	N	922	13% 81% 17%
22	S	475	16% 75% 22%
23	P	440	80% 19%
24	Q	434	6% 79% 16%
25	R	405	6% 77% 18%
26	U	304	13% 84% 14%
27	O	388	10% 79% 20%
28	H	426	30% 73% 22%
29	I	385	21% 79% 18%
30	K	394	14% 77% 19%
31	L	388	13% 74% 21%
32	M	421	26% 77% 19%
33	J	405	19% 78% 18%

2 Entry composition

There are 36 unique types of molecules in this entry. The entry contains 110555 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	244	Total	C	N	O	S	0	0
			1924	1223	323	370	8		
1	A	244	Total	C	N	O	S	0	0
			1924	1223	323	370	8		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	b	248	Total	C	N	O	S	0	0
			1900	1210	313	374	3		
2	B	248	Total	C	N	O	S	0	0
			1900	1210	313	374	3		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	252	Total	C	N	O	S	0	0
			1986	1237	351	394	4		
4	D	238	Total	C	N	O	S	0	0
			1863	1166	326	367	4		

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

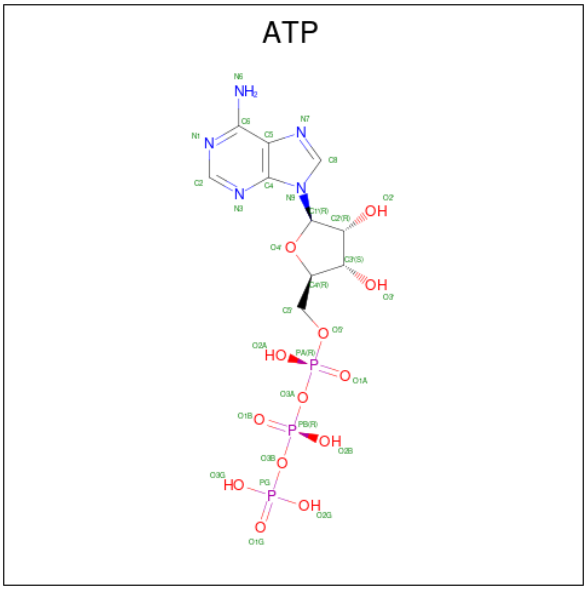
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

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

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

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

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



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

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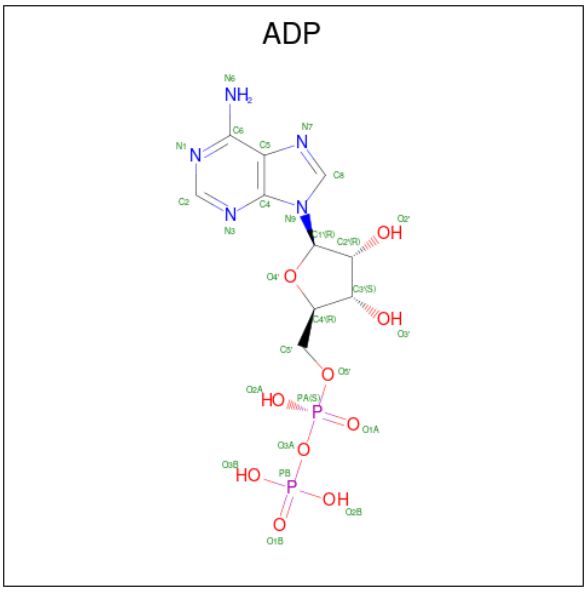
Mol	Chain	Residues	Atoms					AltConf
34	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	J	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

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

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



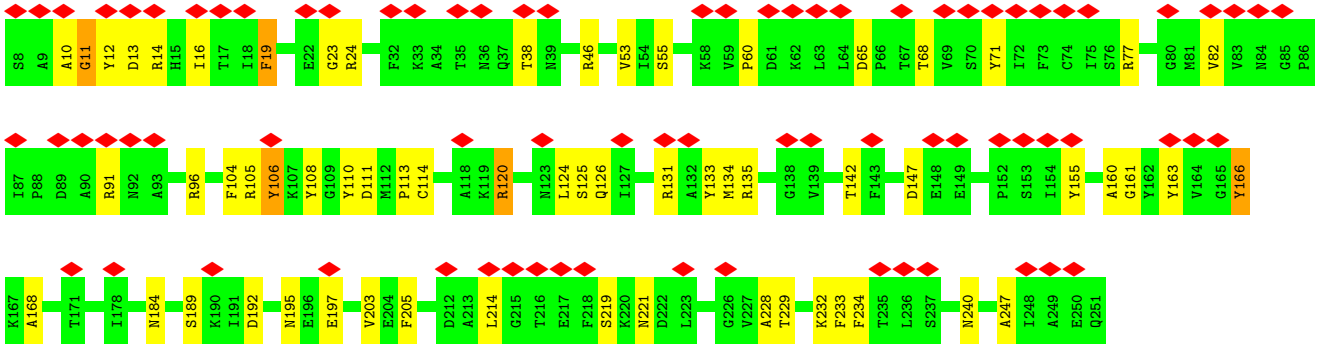
Mol	Chain	Residues	Atoms					AltConf
36	L	1	Total	C	N	O	P	0
			27	10	5	10	2	
36	M	1	Total	C	N	O	P	0
			27	10	5	10	2	

3 Residue-property plots (i)

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

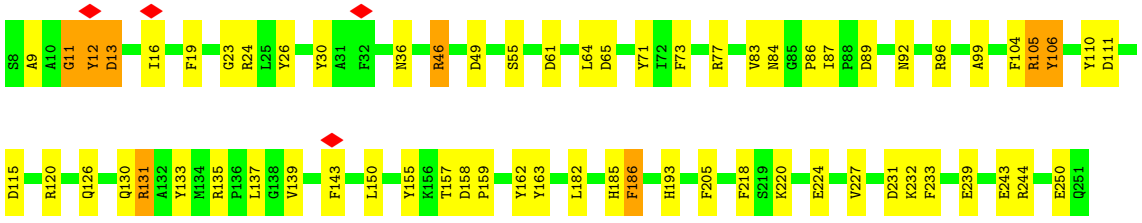
• Molecule 1: Proteasome subunit alpha type-1

Chain a:



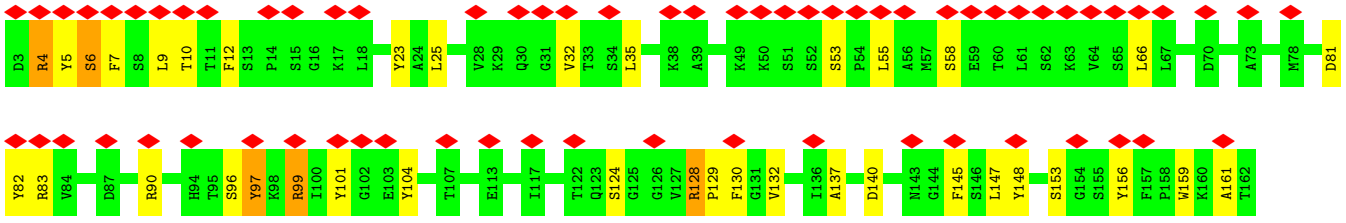
• Molecule 1: Proteasome subunit alpha type-1

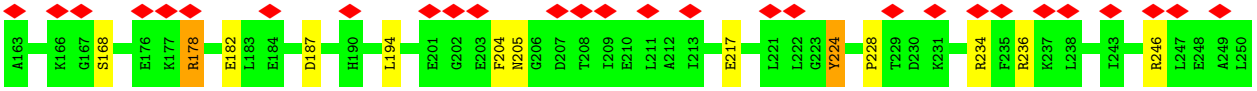
Chain A:



• Molecule 2: Proteasome subunit alpha type-2

Chain b:



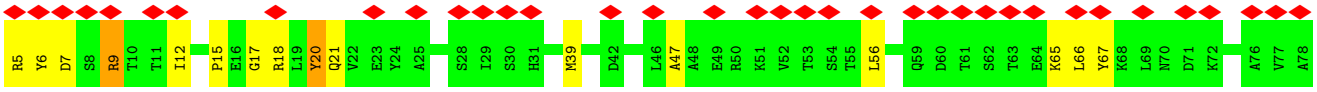


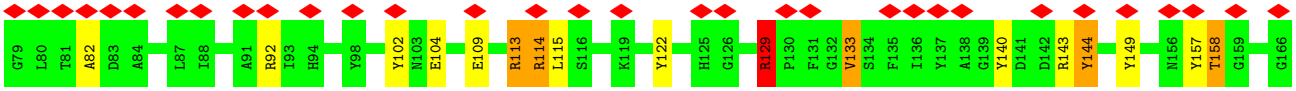
• Molecule 2: Proteasome subunit alpha type-2

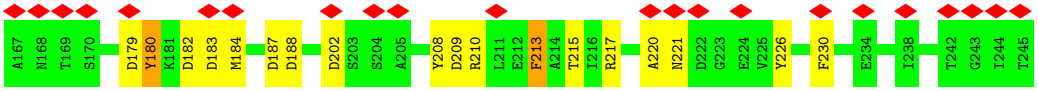
Chain B:

• Molecule 3: Proteasome subunit alpha type-3

Chain c:

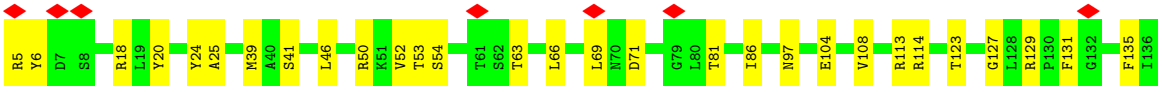


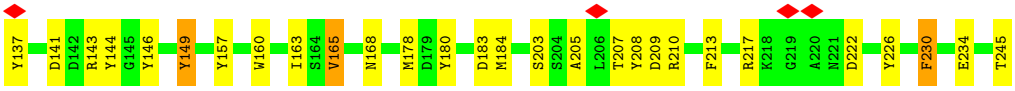




• Molecule 3: Proteasome subunit alpha type-3

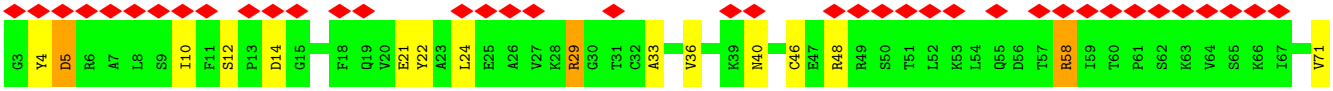
Chain C:

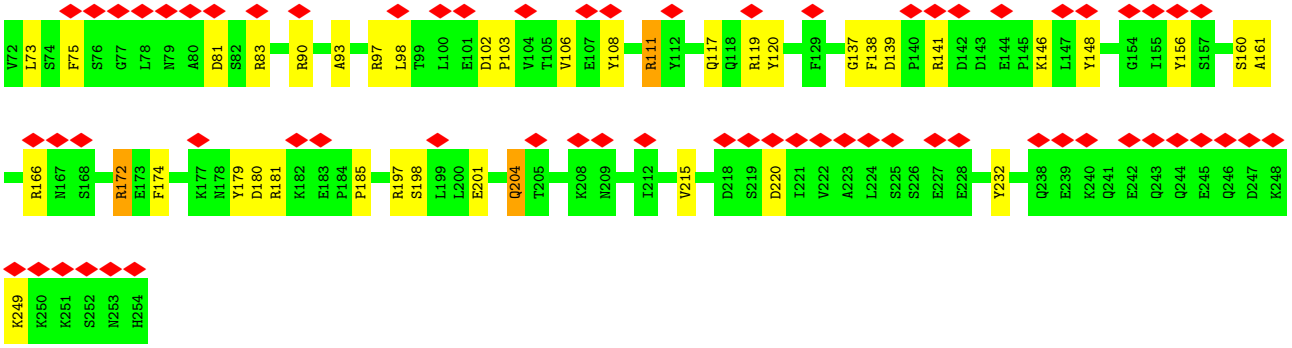




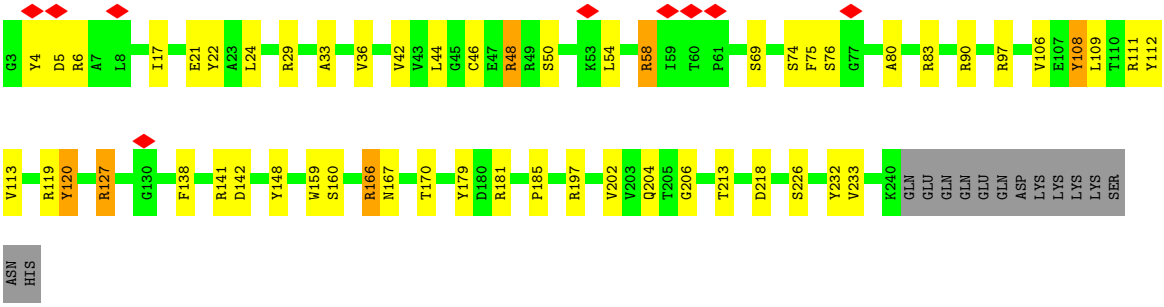
• Molecule 4: Proteasome subunit alpha type-4

Chain d:

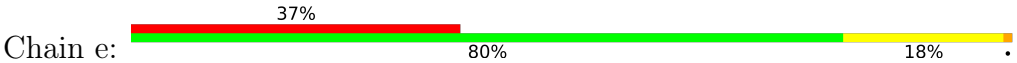


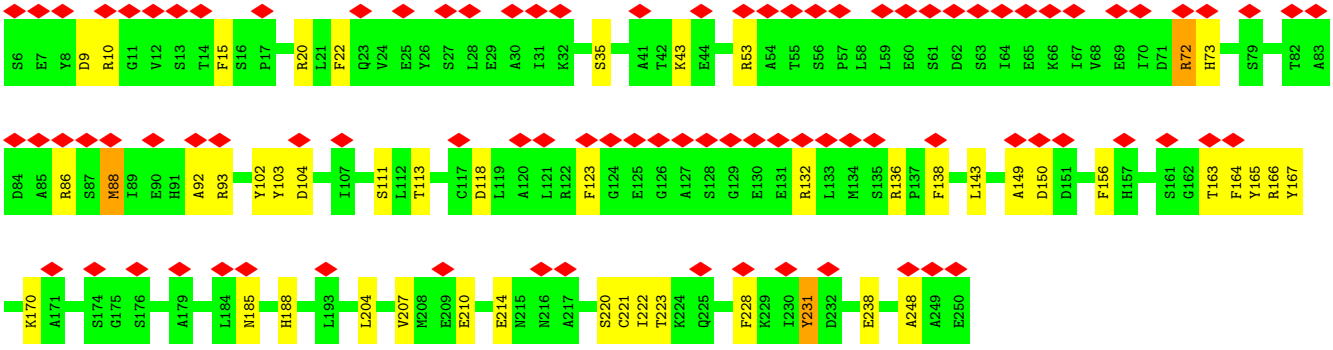


• Molecule 4: Proteasome subunit alpha type-4

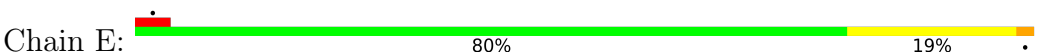


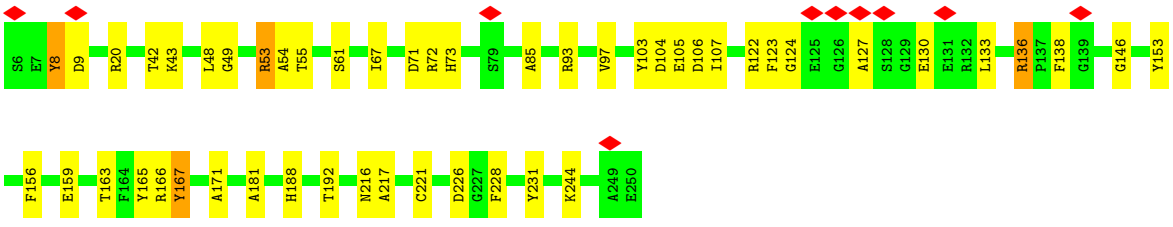
• Molecule 5: Proteasome subunit alpha type-5





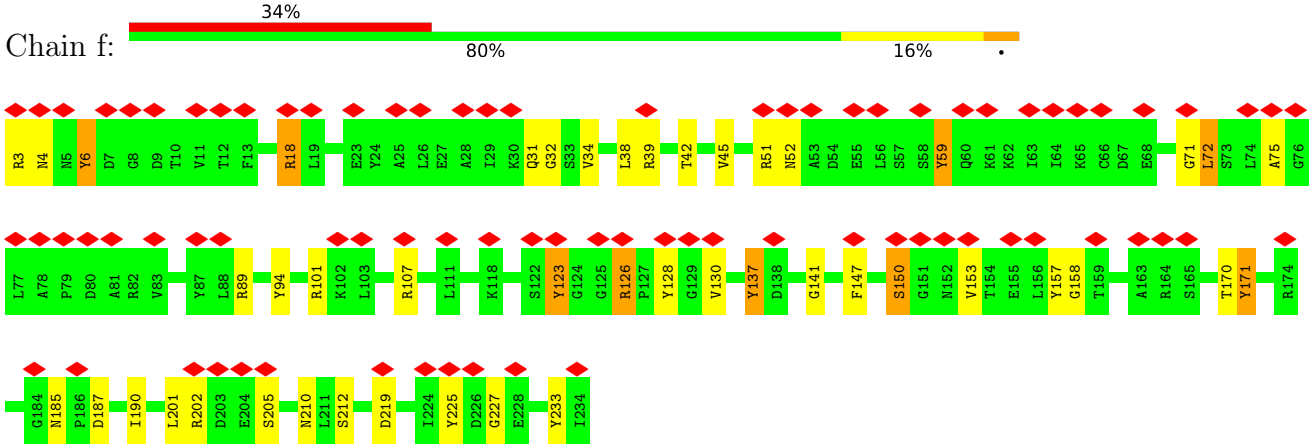
• Molecule 5: Proteasome subunit alpha type-5





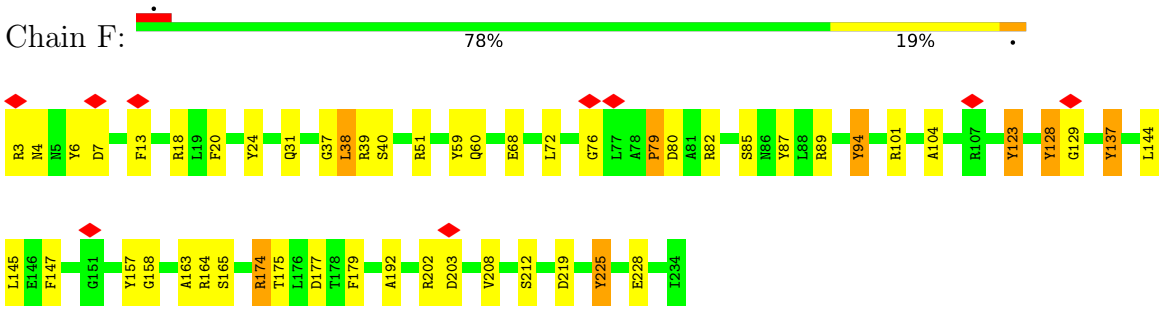
• Molecule 6: Proteasome subunit alpha type-6

Chain f:



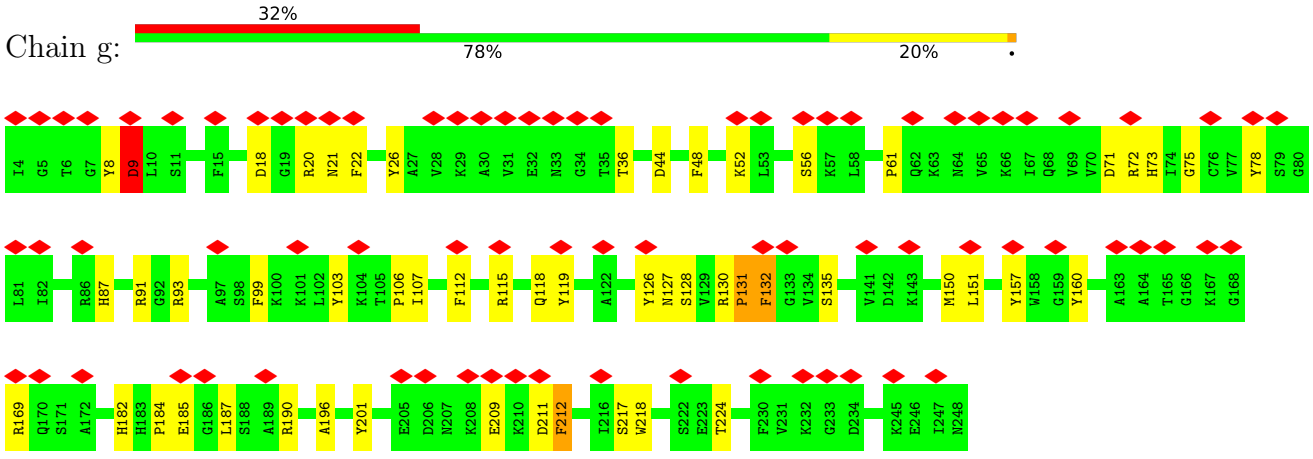
• Molecule 6: Proteasome subunit alpha type-6

Chain F:



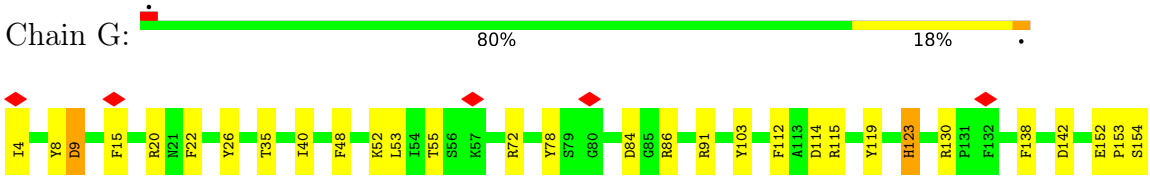
• Molecule 7: Probable proteasome subunit alpha type-7

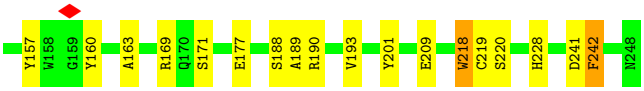
Chain g:



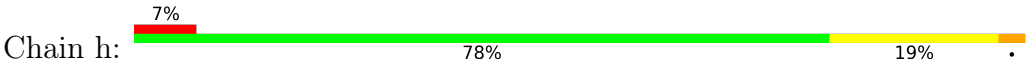
• Molecule 7: Probable proteasome subunit alpha type-7

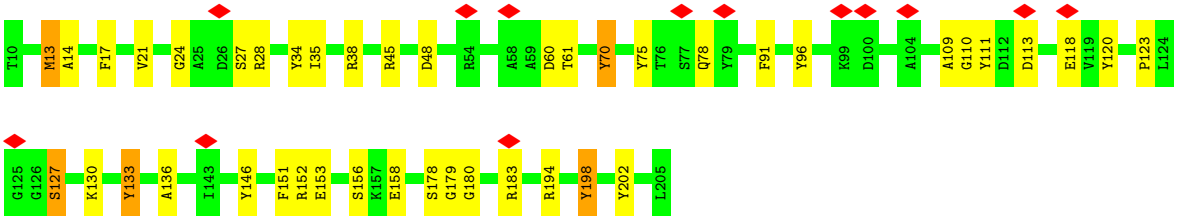
Chain G:



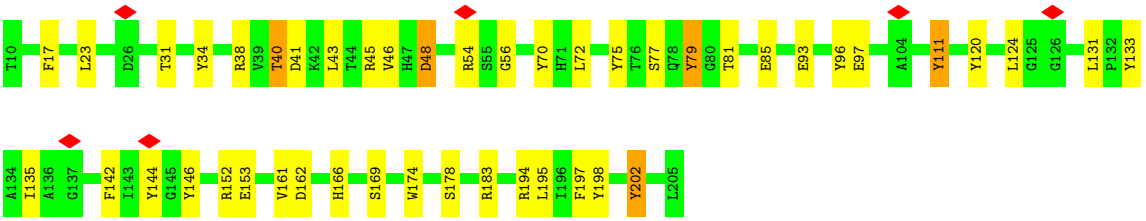


• Molecule 8: Proteasome subunit beta type-1

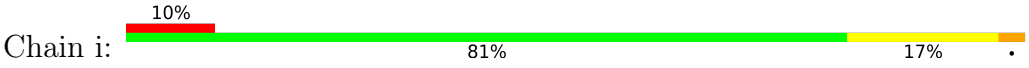


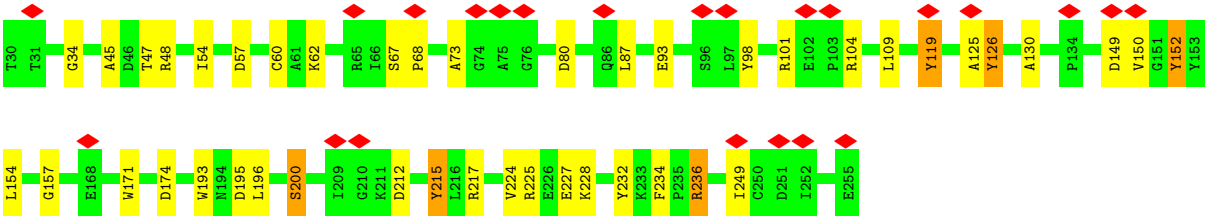


• Molecule 8: Proteasome subunit beta type-1

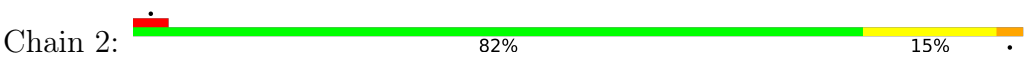


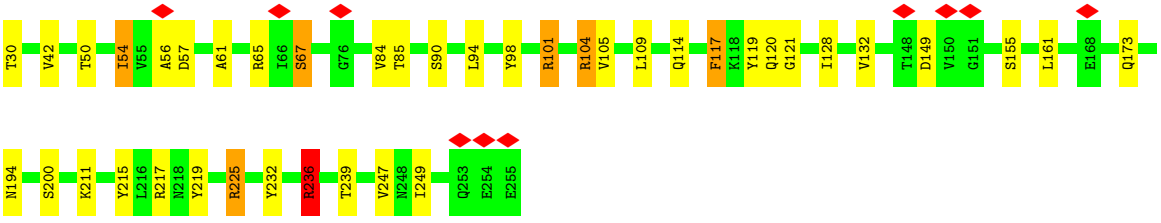
• Molecule 9: Proteasome subunit beta type-2





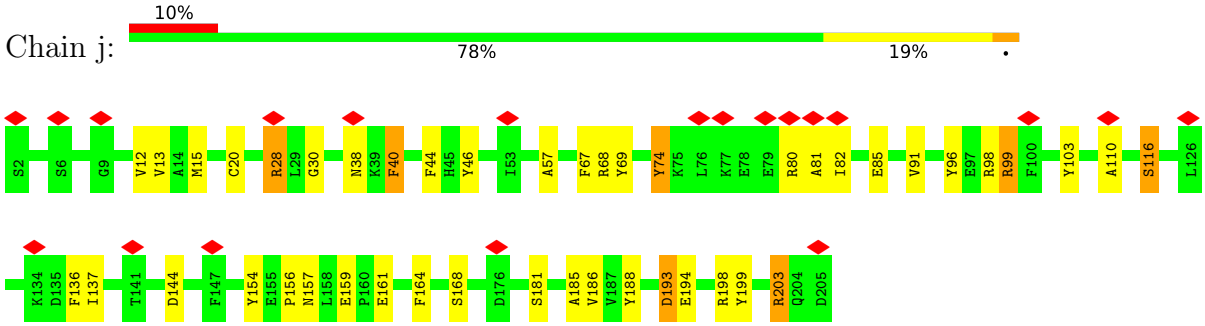
• Molecule 9: Proteasome subunit beta type-2





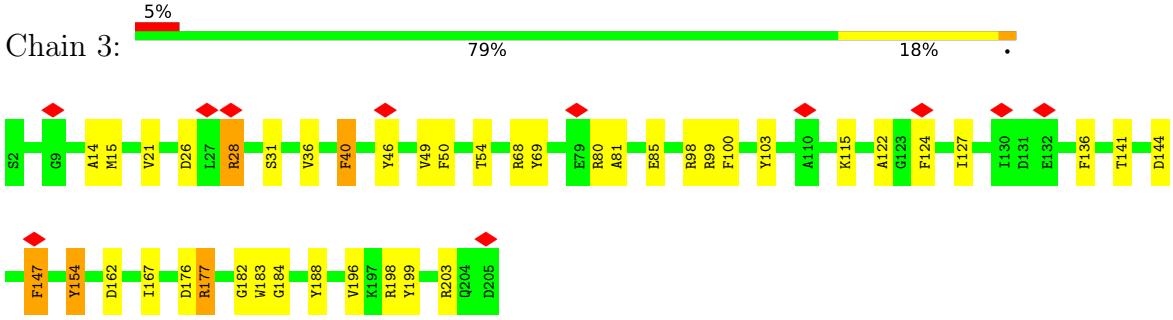
• Molecule 10: Proteasome subunit beta type-3

Chain j:



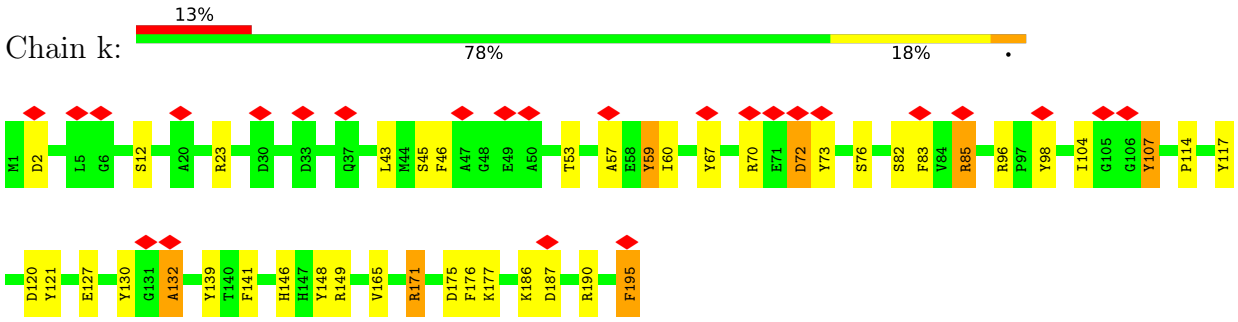
• Molecule 10: Proteasome subunit beta type-3

Chain 3:



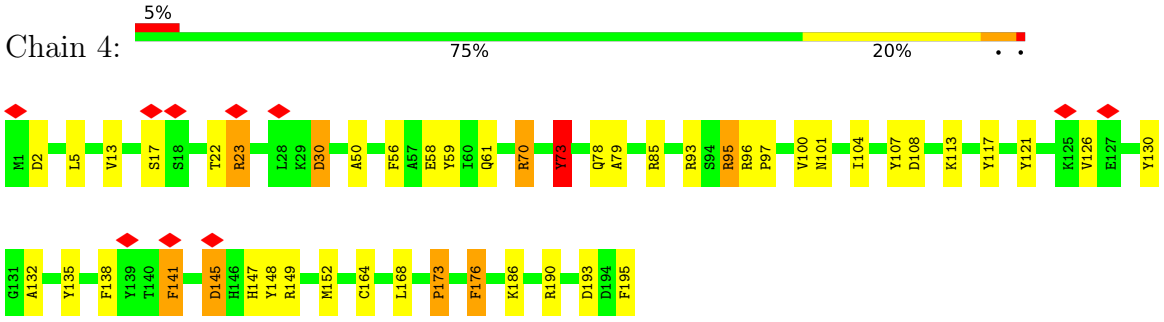
• Molecule 11: Proteasome subunit beta type-4

Chain k:



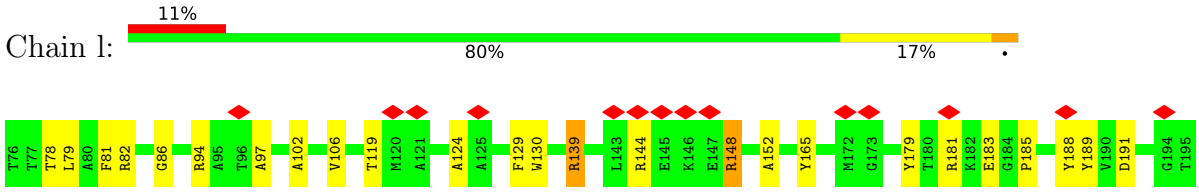
• Molecule 11: Proteasome subunit beta type-4

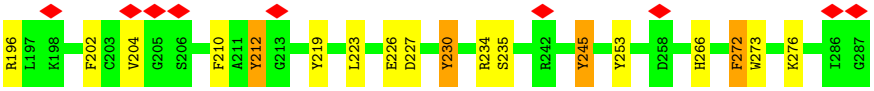
Chain 4:



• Molecule 12: Proteasome subunit beta type-5

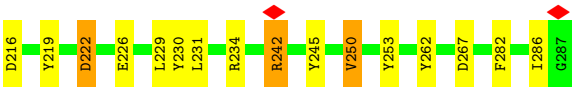
Chain l:





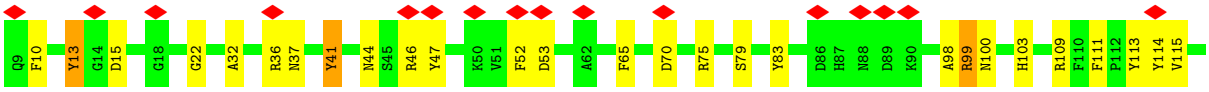
• Molecule 12: Proteasome subunit beta type-5

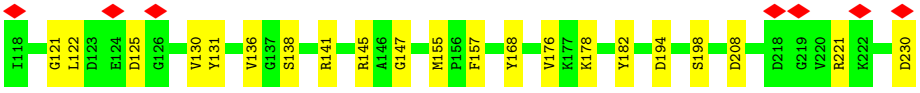
Chain 5:



• Molecule 13: Proteasome subunit beta type-6

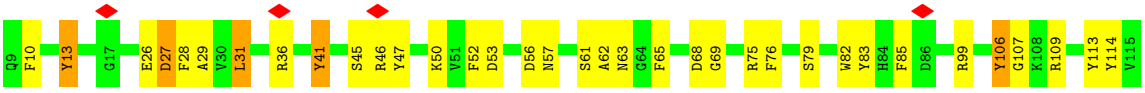
Chain m:

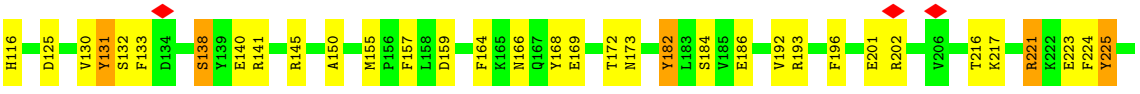




• Molecule 13: Proteasome subunit beta type-6

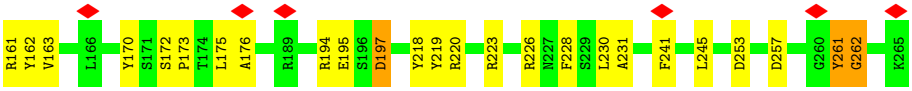
Chain 6:





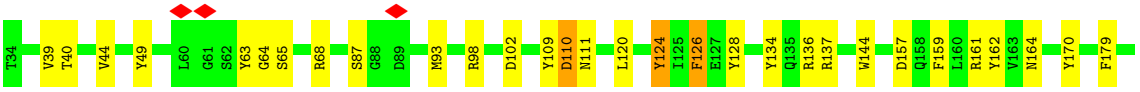
• Molecule 14: Proteasome subunit beta type-7

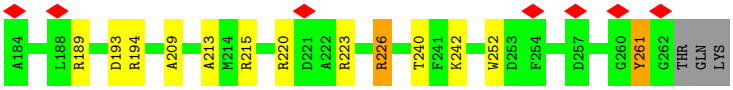
Chain n:



• Molecule 14: Proteasome subunit beta type-7

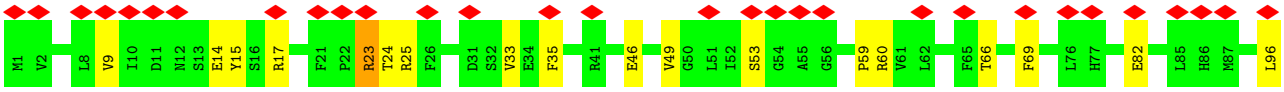
Chain 7:

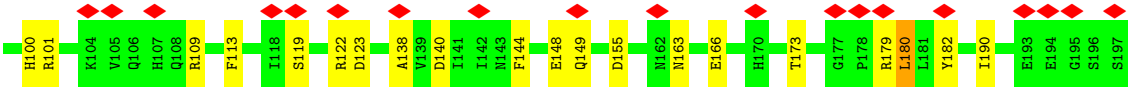




• Molecule 15: 26S proteasome regulatory subunit RPN10

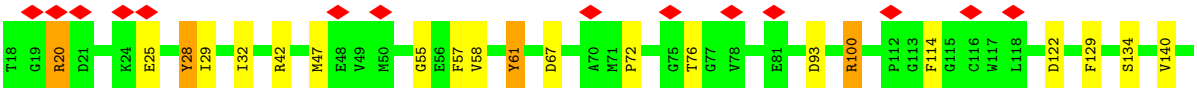
Chain W:

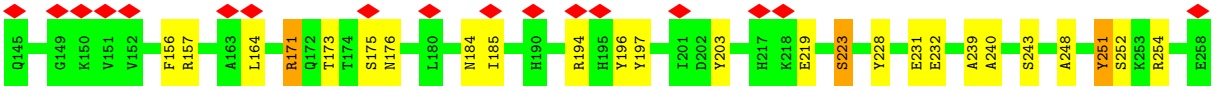


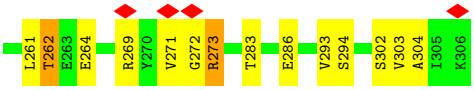


• Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:

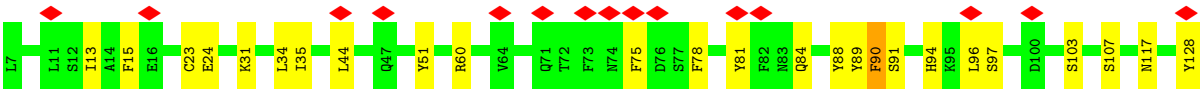


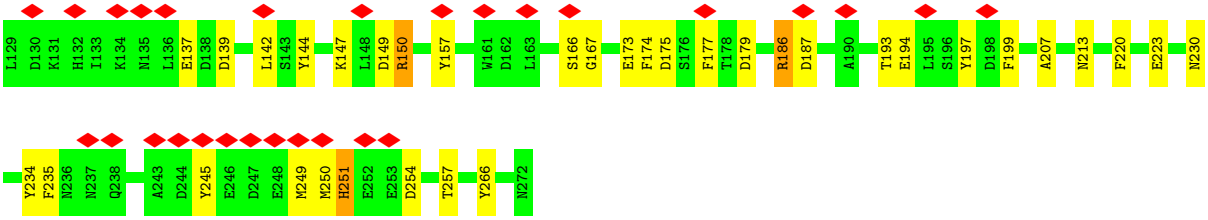




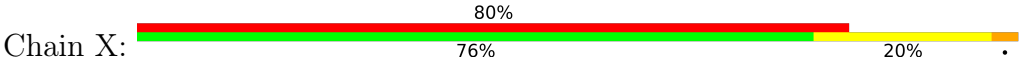
• Molecule 17: 26S proteasome regulatory subunit RPN12

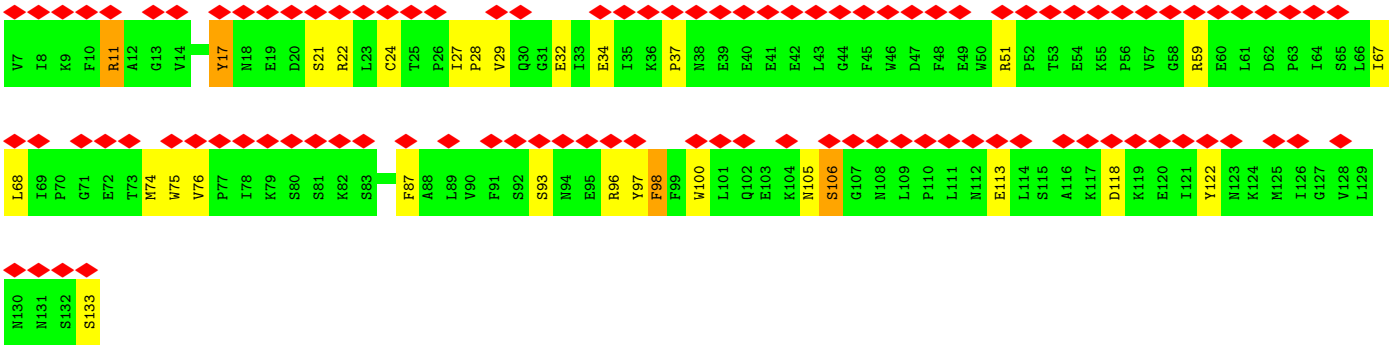
Chain T:



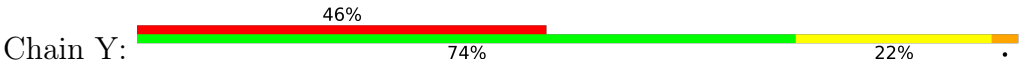


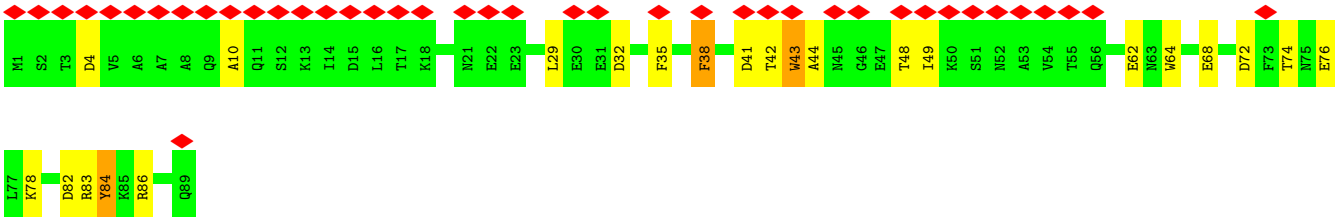
• Molecule 18: 26S proteasome regulatory subunit RPN13



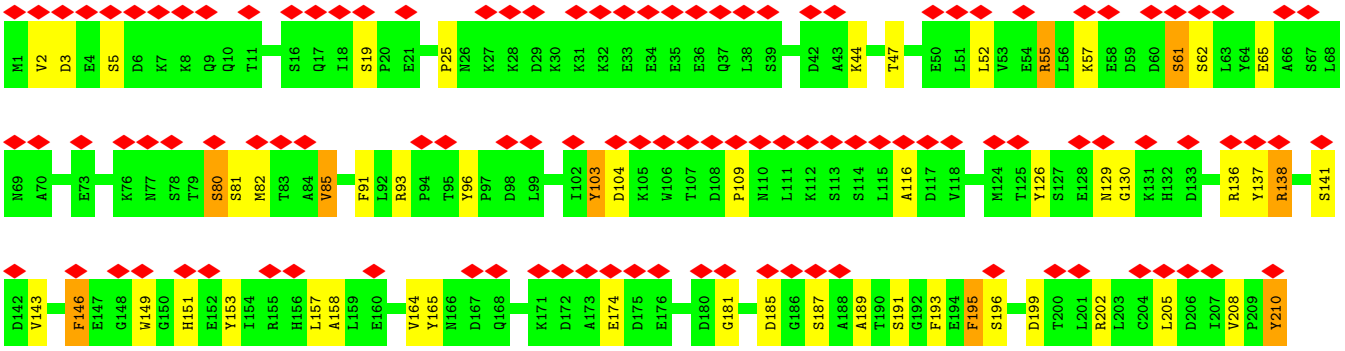


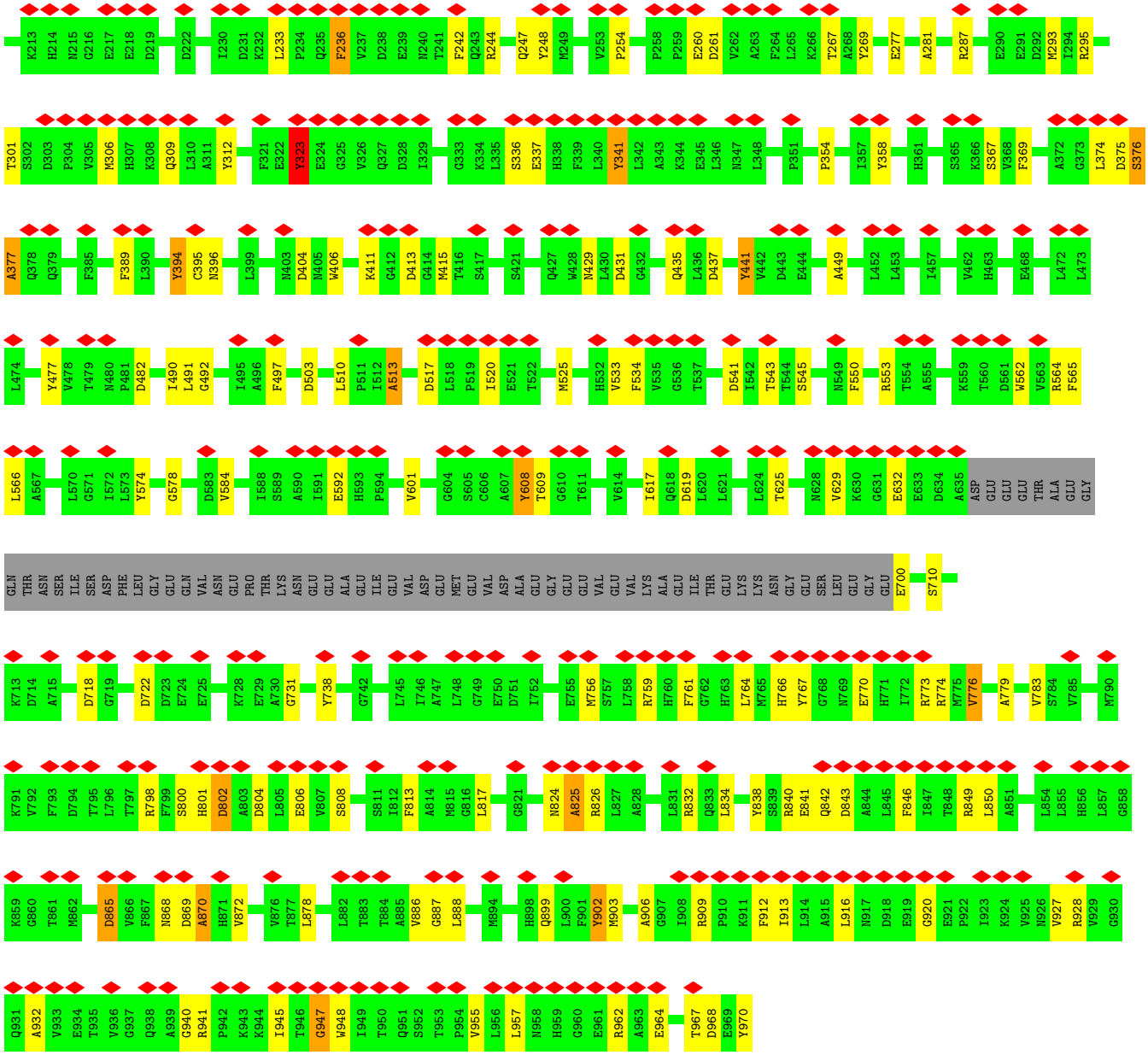
• Molecule 19: 26S proteasome complex subunit SEM1





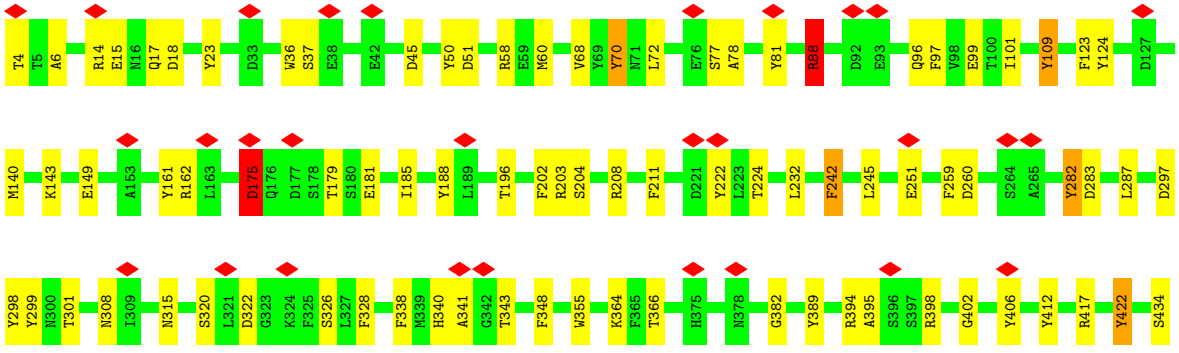
• Molecule 20: 26S proteasome regulatory subunit RPN1

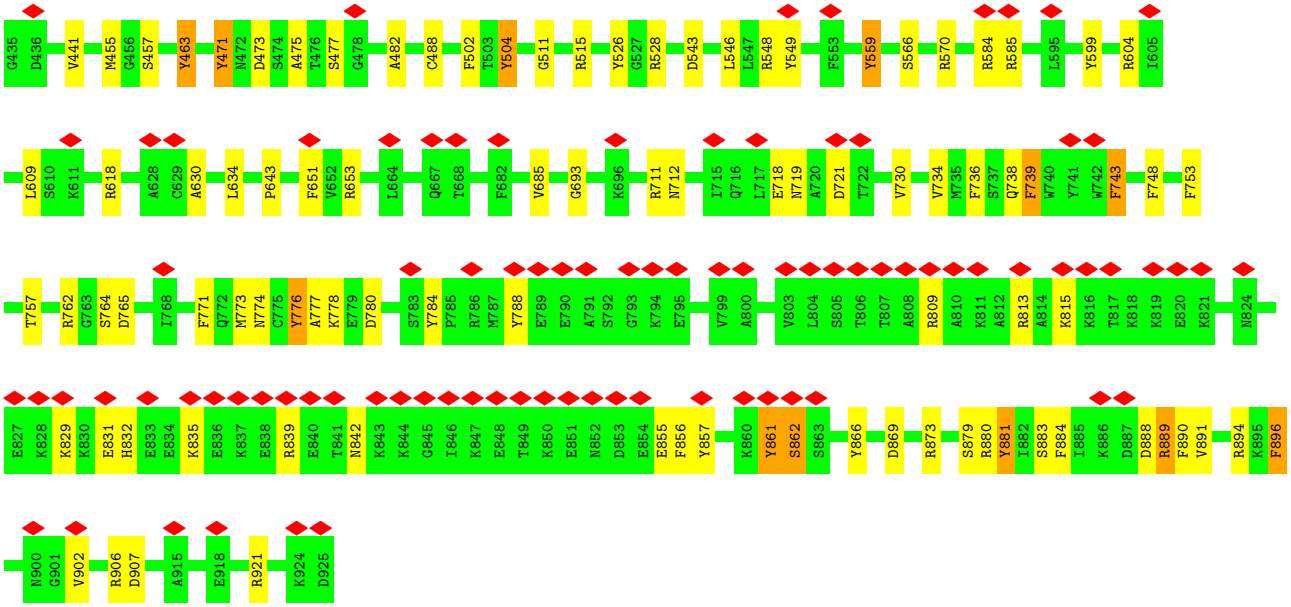




• Molecule 21: 26S proteasome regulatory subunit RPN2

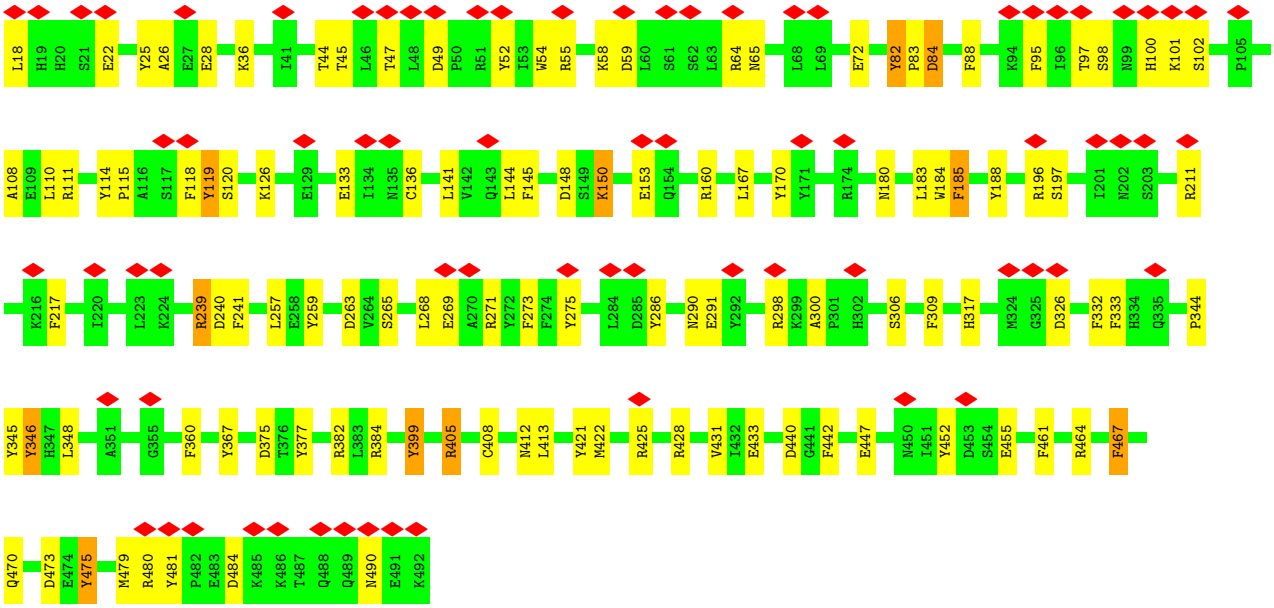
Chain N:





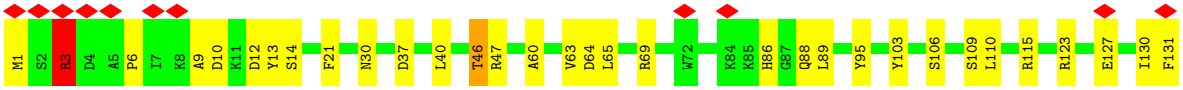
• Molecule 22: 26S proteasome regulatory subunit RPN3

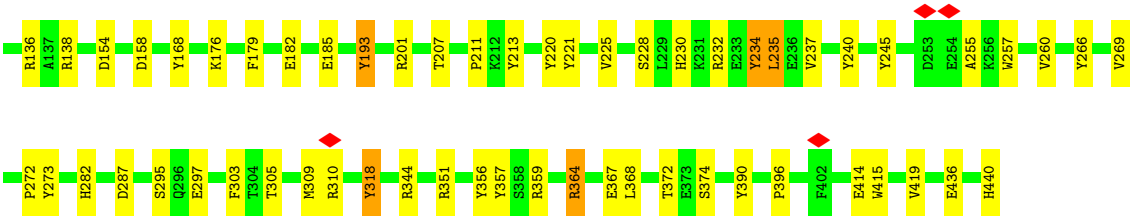
Chain S:



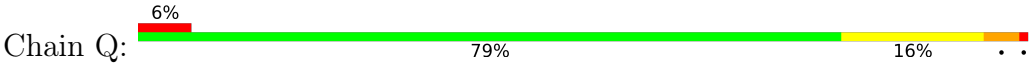
• Molecule 23: 26S proteasome regulatory subunit RPN5

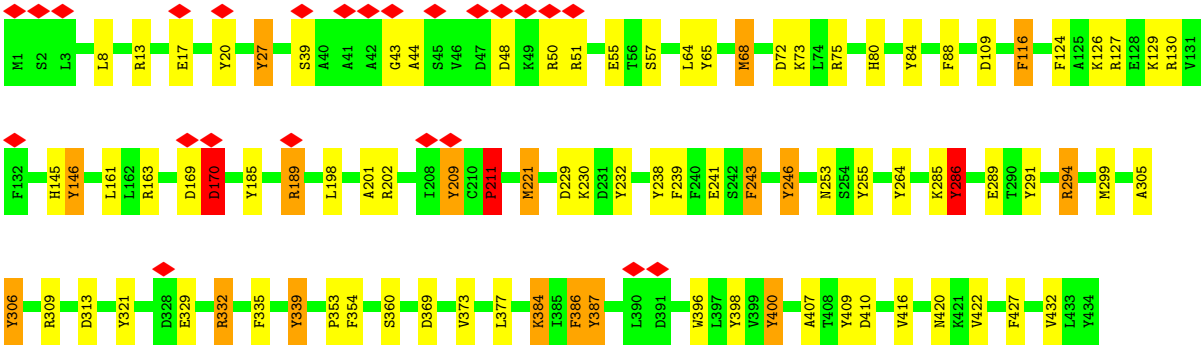
Chain P:



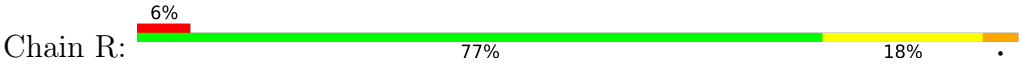


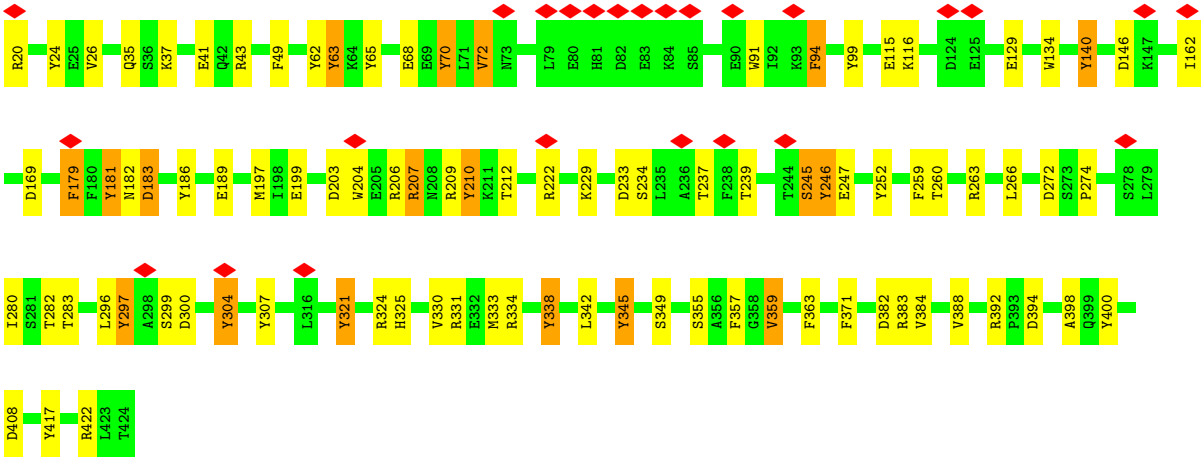
• Molecule 24: 26S proteasome regulatory subunit RPN6



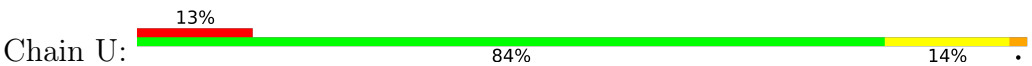


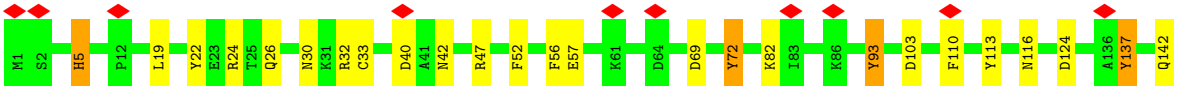
• Molecule 25: 26S proteasome regulatory subunit RPN7

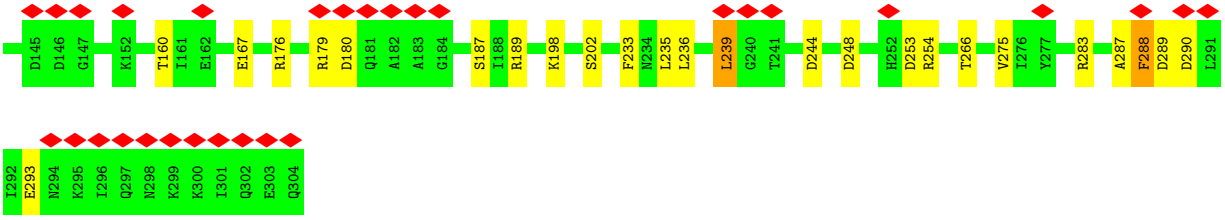




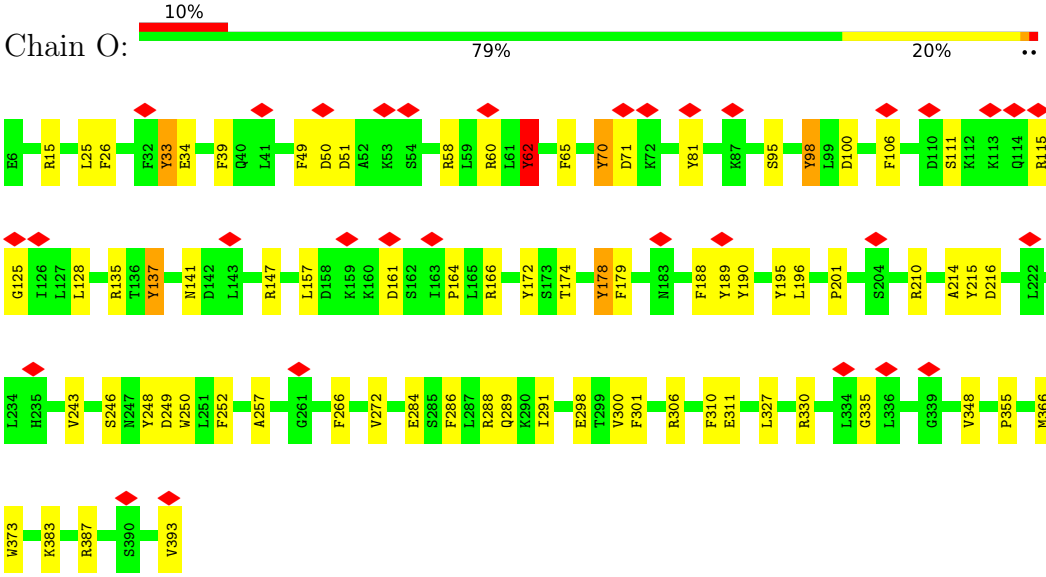
• Molecule 26: 26S proteasome regulatory subunit RPN8



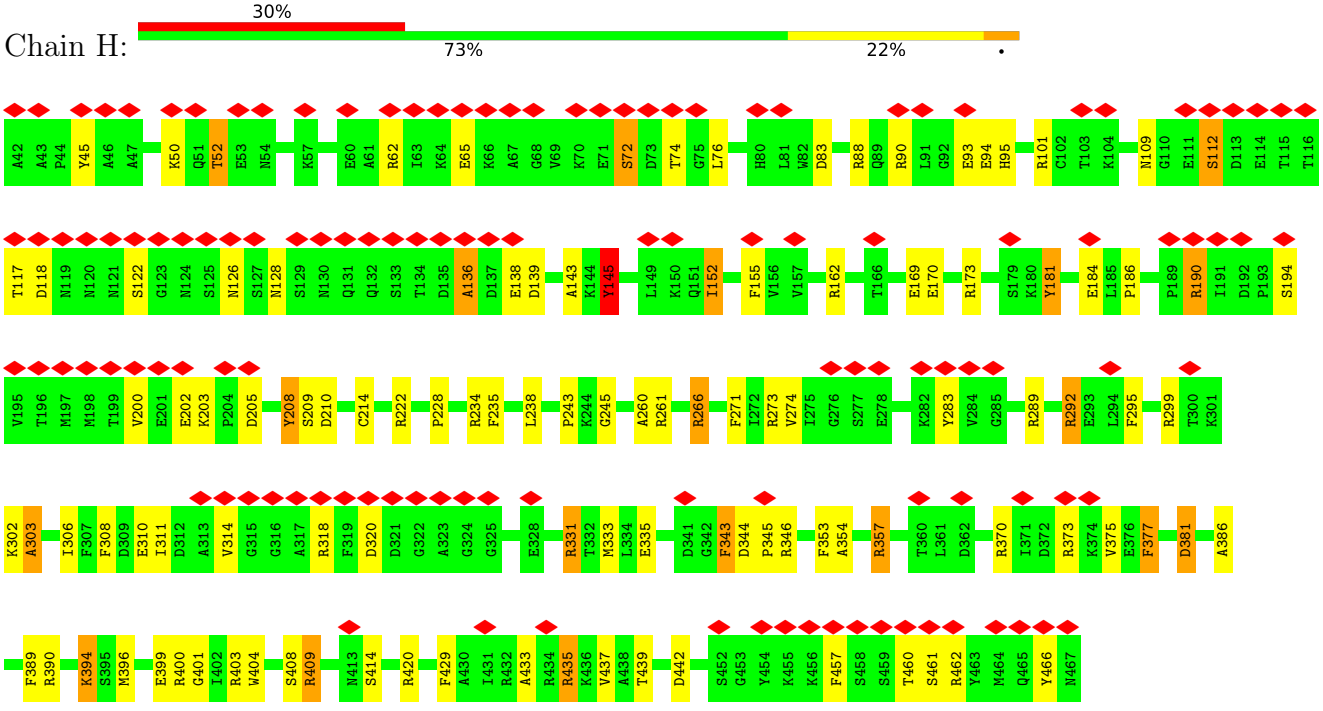




• Molecule 27: 26S proteasome regulatory subunit RPN9

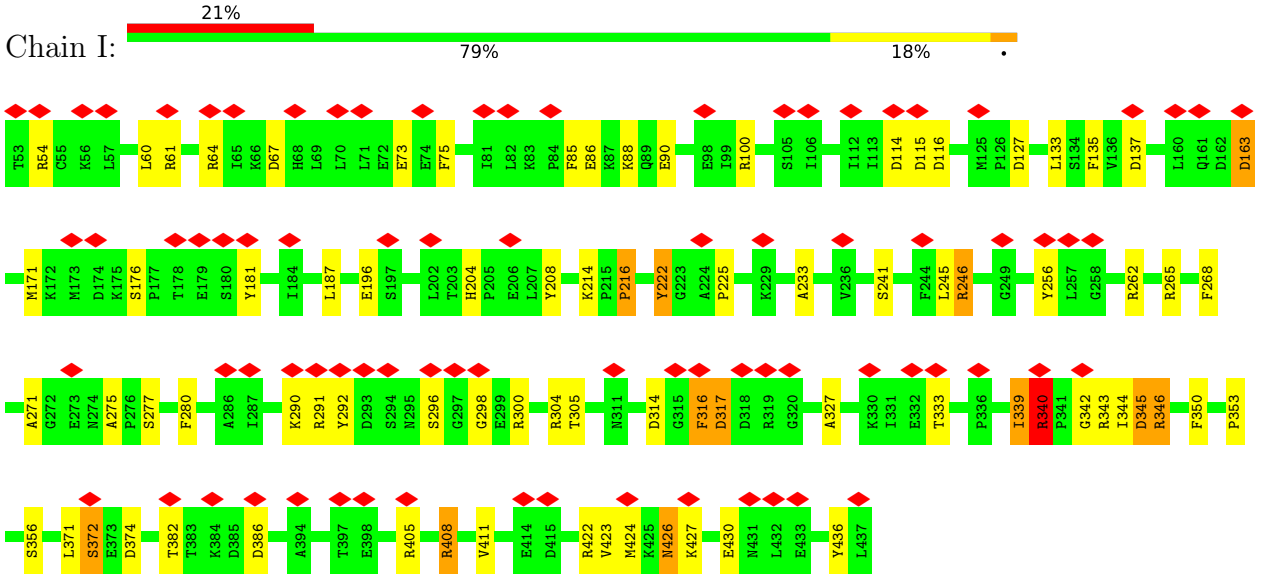


• Molecule 28: 26S proteasome regulatory subunit 7 homolog



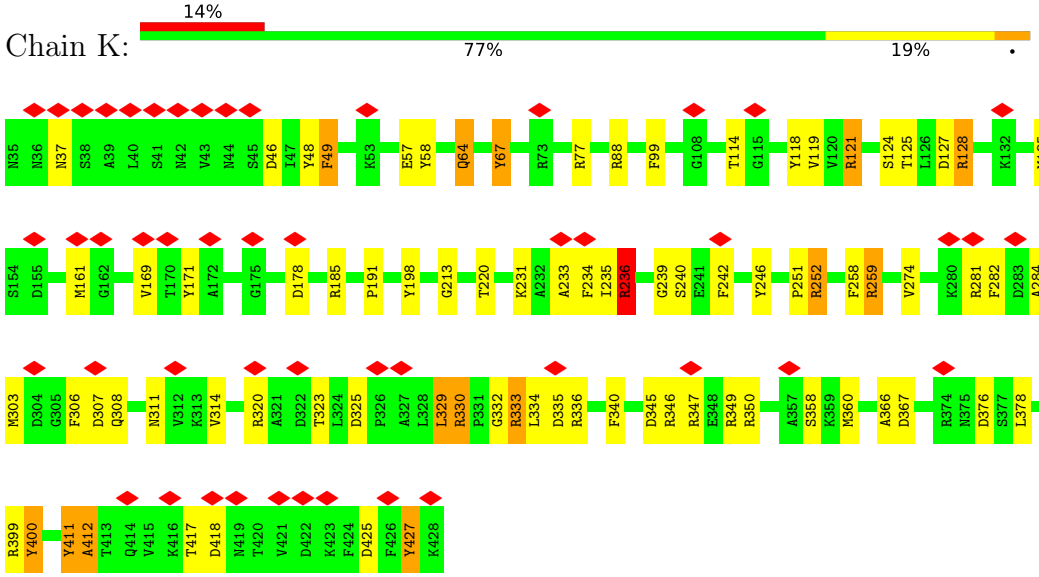
• Molecule 29: 26S proteasome regulatory subunit 4 homolog

Chain I:



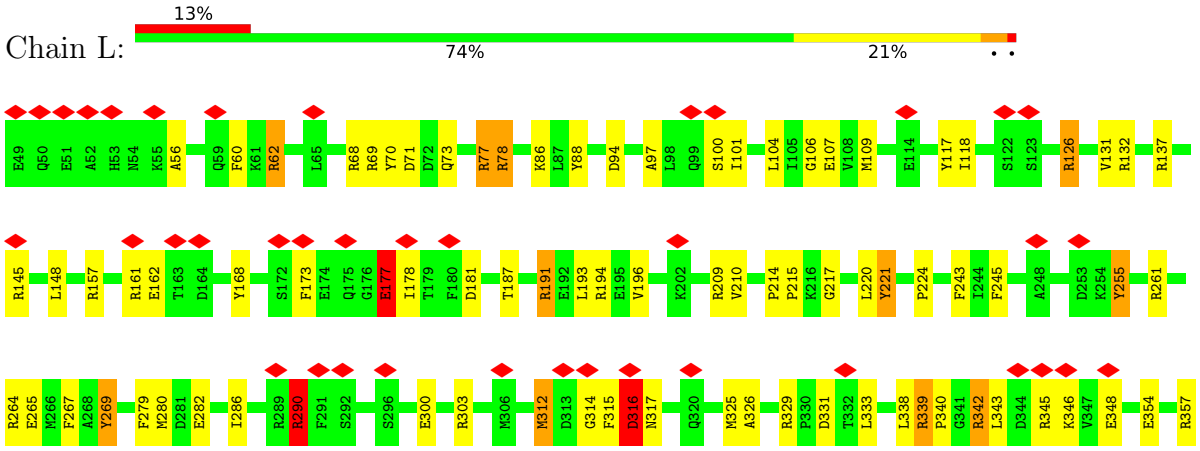
• Molecule 30: 26S proteasome regulatory subunit 6B homolog

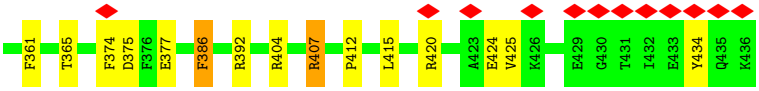
Chain K:



• Molecule 31: 26S proteasome subunit RPT4

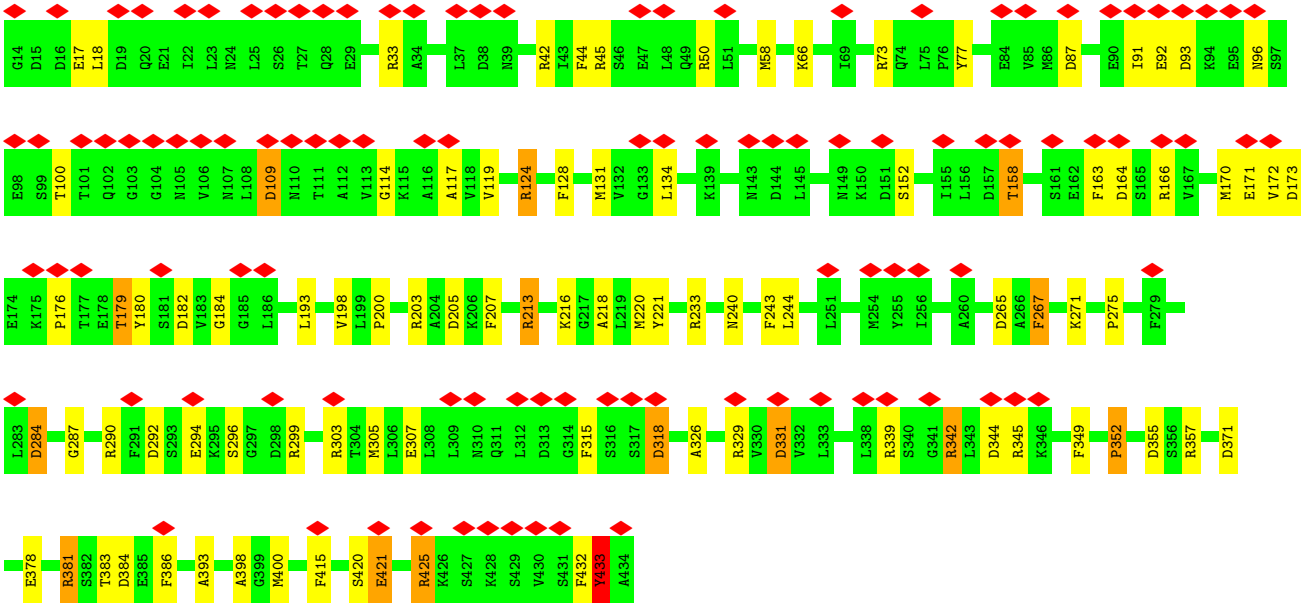
Chain L:





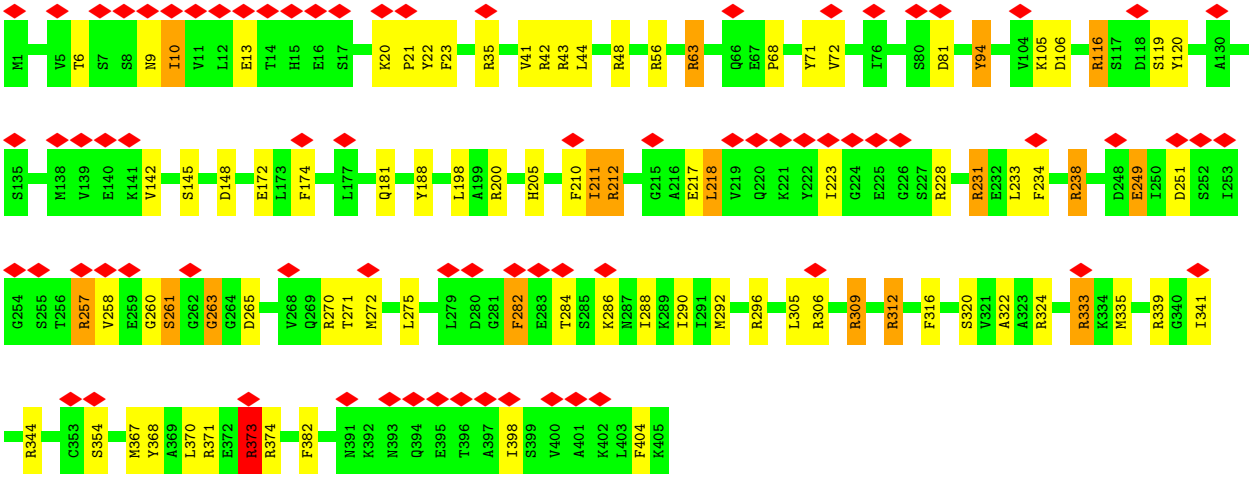
• Molecule 32: 26S proteasome regulatory subunit 6A

Chain M:



• Molecule 33: 26S proteasome regulatory subunit 8 homolog

Chain J:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	184988	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.121	Depositor
Minimum map value	-0.078	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.004	Depositor
Recommended contour level	0.012	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, ATP, MG

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.76	19/1962 (1.0%)	2.03	53/2656 (2.0%)
1	a	1.72	11/1962 (0.6%)	2.03	57/2656 (2.1%)
2	B	1.71	18/1937 (0.9%)	2.01	54/2622 (2.1%)
2	b	1.74	21/1937 (1.1%)	1.88	39/2622 (1.5%)
3	C	1.76	21/1914 (1.1%)	1.91	51/2591 (2.0%)
3	c	1.69	17/1914 (0.9%)	1.95	50/2591 (1.9%)
4	D	1.84	25/1892 (1.3%)	2.05	50/2562 (2.0%)
4	d	1.76	22/2016 (1.1%)	1.88	31/2723 (1.1%)
5	E	1.69	13/1915 (0.7%)	1.96	49/2579 (1.9%)
5	e	1.70	13/1915 (0.7%)	1.94	45/2579 (1.7%)
6	F	1.79	22/1811 (1.2%)	1.88	43/2447 (1.8%)
6	f	1.73	19/1811 (1.0%)	1.95	46/2447 (1.9%)
7	G	1.81	25/1945 (1.3%)	1.91	43/2625 (1.6%)
7	g	1.69	16/1945 (0.8%)	1.91	47/2625 (1.8%)
8	1	1.78	16/1541 (1.0%)	2.02	48/2087 (2.3%)
8	h	1.70	12/1541 (0.8%)	1.86	33/2087 (1.6%)
9	2	1.67	7/1751 (0.4%)	1.86	36/2373 (1.5%)
9	i	1.70	14/1751 (0.8%)	1.92	38/2373 (1.6%)
10	3	1.69	11/1611 (0.7%)	1.93	38/2174 (1.7%)
10	j	1.79	18/1611 (1.1%)	2.01	36/2174 (1.7%)
11	4	1.82	16/1590 (1.0%)	1.96	38/2142 (1.8%)
11	k	1.79	18/1590 (1.1%)	2.01	41/2142 (1.9%)
12	5	1.78	15/1681 (0.9%)	1.95	42/2274 (1.8%)
12	l	1.76	11/1681 (0.7%)	2.03	52/2274 (2.3%)
13	6	1.83	33/1795 (1.8%)	1.98	58/2420 (2.4%)
13	m	1.82	20/1795 (1.1%)	1.93	38/2420 (1.6%)
14	7	1.75	17/1821 (0.9%)	1.99	45/2470 (1.8%)
14	n	1.70	17/1847 (0.9%)	1.98	57/2503 (2.3%)
15	W	1.69	10/1558 (0.6%)	1.80	24/2111 (1.1%)
16	V	1.70	20/2309 (0.9%)	1.92	44/3115 (1.4%)
17	T	1.69	15/2236 (0.7%)	1.87	44/3017 (1.5%)
18	X	1.74	7/1059 (0.7%)	1.92	23/1432 (1.6%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
19	Y	1.70	8/741 (1.1%)	1.89	17/1000 (1.7%)
20	Z	1.97	77/7123 (1.1%)	1.93	168/9645 (1.7%)
21	N	1.70	65/7273 (0.9%)	1.87	149/9822 (1.5%)
22	S	1.72	37/3967 (0.9%)	1.98	117/5355 (2.2%)
23	P	1.65	21/3664 (0.6%)	1.85	74/4940 (1.5%)
24	Q	1.72	39/3556 (1.1%)	1.87	79/4787 (1.7%)
25	R	1.71	32/3314 (1.0%)	1.96	82/4469 (1.8%)
26	U	1.64	10/2461 (0.4%)	1.86	45/3327 (1.4%)
27	O	1.69	26/3247 (0.8%)	1.88	73/4380 (1.7%)
28	H	1.74	30/3363 (0.9%)	2.05	96/4532 (2.1%)
29	I	1.71	25/3061 (0.8%)	1.87	61/4121 (1.5%)
30	K	1.71	20/3156 (0.6%)	1.94	72/4261 (1.7%)
31	L	1.72	33/3129 (1.1%)	1.94	77/4204 (1.8%)
32	M	1.70	36/3323 (1.1%)	1.91	78/4478 (1.7%)
33	J	2.33	32/3212 (1.0%)	1.88	63/4316 (1.5%)
All	All	1.76	1030/112234 (0.9%)	1.93	2644/151550 (1.7%)

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

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

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Mol	Chain	#Chirality outliers	#Planarity outliers
10	j	0	5
11	4	0	7
11	k	0	5
12	5	0	4
12	l	0	6
13	6	0	7
13	m	0	4
14	7	0	6
14	n	0	4
15	W	0	4
16	V	0	6
17	T	0	3
18	X	0	4
19	Y	0	1
20	Z	0	15
21	N	0	21
22	S	0	11
23	P	0	11
24	Q	0	14
25	R	0	13
26	U	0	5
27	O	0	5
28	H	0	13
29	I	0	11
30	K	0	18
31	L	0	21
32	M	0	7
33	J	0	17
All	All	0	353

All (1030) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	286	LYS	CD-CE	69.91	3.26	1.51
20	Z	738	TYR	CZ-OH	60.17	2.40	1.37
20	Z	948	TRP	CZ3-CH2	41.74	2.06	1.40
20	Z	948	TRP	CZ2-CH2	41.54	2.16	1.37
33	J	234	PHE	CG-CD2	28.46	1.81	1.38
33	J	234	PHE	CG-CD1	27.81	1.80	1.38
33	J	234	PHE	CE2-CZ	21.33	1.77	1.37
33	J	234	PHE	CD2-CE2	21.07	1.81	1.39
33	J	234	PHE	CE1-CZ	20.80	1.76	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	234	PHE	CD1-CE1	15.25	1.69	1.39
20	Z	738	TYR	CE1-CZ	10.68	1.52	1.38
17	T	186	ARG	CD-NE	9.49	1.62	1.46
13	m	141	ARG	CD-NE	9.33	1.62	1.46
29	I	296	SER	CA-CB	8.96	1.66	1.52
20	Z	948	TRP	CD2-CE2	8.93	1.52	1.41
12	l	144	ARG	NE-CZ	8.73	1.44	1.33
15	W	109	ARG	CZ-NH2	8.51	1.44	1.33
5	E	61	SER	CA-CB	8.47	1.65	1.52
20	Z	962	ARG	CD-NE	8.43	1.60	1.46
20	Z	948	TRP	CE2-CZ2	8.38	1.54	1.39
4	d	201	GLU	CD-OE2	8.37	1.34	1.25
32	M	345	ARG	NE-CZ	8.37	1.44	1.33
11	k	76	SER	CA-CB	8.24	1.65	1.52
12	5	245	TYR	CE2-CZ	8.24	1.49	1.38
21	N	643	PRO	N-CD	-8.23	1.36	1.47
29	I	86	GLU	CG-CD	8.16	1.64	1.51
2	B	178	ARG	CZ-NH1	8.15	1.43	1.33
28	H	409	ARG	NE-CZ	8.12	1.43	1.33
31	L	407	ARG	NE-CZ	8.07	1.43	1.33
19	Y	86	ARG	CZ-NH1	8.05	1.43	1.33
20	Z	738	TYR	CE2-CZ	7.96	1.48	1.38
28	H	93	GLU	CG-CD	7.95	1.63	1.51
25	R	324	ARG	NE-CZ	7.94	1.43	1.33
17	T	167	GLY	N-CA	-7.90	1.34	1.46
3	C	114	ARG	CZ-NH2	7.83	1.43	1.33
13	m	47	TYR	CG-CD1	7.78	1.49	1.39
29	I	61	ARG	NE-CZ	7.78	1.43	1.33
24	Q	255	TYR	CE2-CZ	7.78	1.48	1.38
7	G	130	ARG	CD-NE	7.76	1.59	1.46
24	Q	39	SER	CA-CB	7.75	1.64	1.52
22	S	22	GLU	CD-OE1	7.75	1.34	1.25
28	H	370	ARG	NE-CZ	7.71	1.43	1.33
29	I	316	PHE	CE1-CZ	7.61	1.51	1.37
4	d	90	ARG	CZ-NH2	7.57	1.42	1.33
30	K	306	PHE	CG-CD2	7.54	1.50	1.38
3	C	41	SER	CA-CB	7.53	1.64	1.52
30	K	128	ARG	CZ-NH1	7.52	1.42	1.33
20	Z	269	TYR	CZ-OH	7.51	1.50	1.37
21	N	412	TYR	CE2-CZ	7.43	1.48	1.38
22	S	211	ARG	CD-NE	7.43	1.59	1.46
16	V	264	GLU	CG-CD	7.42	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	18	ARG	CZ-NH2	7.41	1.42	1.33
33	J	339	ARG	NE-CZ	7.39	1.42	1.33
14	n	136	ARG	CD-NE	7.37	1.58	1.46
31	L	209	ARG	NE-CZ	7.37	1.42	1.33
7	G	152	GLU	CG-CD	7.36	1.62	1.51
6	F	165	SER	CB-OG	7.35	1.51	1.42
6	F	51	ARG	NE-CZ	7.33	1.42	1.33
20	Z	545	SER	CA-CB	7.33	1.64	1.52
8	1	75	TYR	CG-CD1	7.33	1.48	1.39
24	Q	17	GLU	CG-CD	7.31	1.62	1.51
20	Z	909	ARG	NE-CZ	7.28	1.42	1.33
33	J	309	ARG	CZ-NH2	7.27	1.42	1.33
24	Q	387	TYR	CG-CD2	7.27	1.48	1.39
29	I	356	SER	CA-CB	7.26	1.63	1.52
24	Q	289	GLU	CG-CD	7.24	1.62	1.51
18	X	113	GLU	CG-CD	7.23	1.62	1.51
4	D	141	ARG	NE-CZ	7.22	1.42	1.33
29	I	405	ARG	NE-CZ	7.22	1.42	1.33
7	g	126	TYR	CZ-OH	7.21	1.50	1.37
29	I	181	TYR	CE2-CZ	7.20	1.48	1.38
21	N	515	ARG	NE-CZ	7.19	1.42	1.33
11	k	96	ARG	CZ-NH1	7.17	1.42	1.33
27	O	15	ARG	NE-CZ	7.16	1.42	1.33
5	e	53	ARG	CD-NE	7.15	1.58	1.46
9	i	98	TYR	CZ-OH	7.14	1.50	1.37
24	Q	294	ARG	NE-CZ	7.12	1.42	1.33
20	Z	165	TYR	CE1-CZ	7.12	1.47	1.38
5	e	103	TYR	CB-CG	-7.11	1.41	1.51
8	1	194	ARG	CZ-NH1	7.11	1.42	1.33
12	5	188	TYR	CZ-OH	7.11	1.50	1.37
21	N	15	GLU	CB-CG	7.09	1.65	1.52
3	C	104	GLU	CD-OE2	7.08	1.33	1.25
16	V	223	SER	CA-CB	7.08	1.63	1.52
13	m	168	TYR	CZ-OH	7.08	1.49	1.37
32	M	294	GLU	CD-OE1	7.07	1.33	1.25
3	c	143	ARG	CZ-NH2	7.05	1.42	1.33
21	N	585	ARG	CZ-NH1	7.05	1.42	1.33
29	I	262	ARG	CZ-NH1	7.05	1.42	1.33
1	a	71	TYR	CE2-CZ	7.01	1.47	1.38
20	Z	710	SER	CA-CB	7.01	1.63	1.52
20	Z	798	ARG	CZ-NH1	7.00	1.42	1.33
25	R	63	TYR	CB-CG	7.00	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	218	ASP	CB-CG	7.00	1.66	1.51
33	J	354	SER	CB-OG	6.99	1.51	1.42
29	I	430	GLU	CG-CD	6.99	1.62	1.51
1	A	23	GLY	CA-C	-6.98	1.40	1.51
21	N	566	SER	CA-CB	6.98	1.63	1.52
30	K	88	ARG	CZ-NH1	6.97	1.42	1.33
5	E	53	ARG	CD-NE	6.97	1.58	1.46
14	n	172	SER	CA-CB	6.96	1.63	1.52
24	Q	232	TYR	CG-CD1	6.96	1.48	1.39
20	Z	389	PHE	CE2-CZ	6.96	1.50	1.37
20	Z	849	ARG	CZ-NH1	6.95	1.42	1.33
32	M	92	GLU	CG-CD	6.94	1.62	1.51
21	N	693	GLY	N-CA	-6.94	1.35	1.46
18	X	28	PRO	N-CD	-6.92	1.38	1.47
24	Q	127	ARG	NE-CZ	6.92	1.42	1.33
13	m	221	ARG	CZ-NH1	6.92	1.42	1.33
9	i	217	ARG	NE-CZ	6.91	1.42	1.33
1	A	120	ARG	NE-CZ	6.90	1.42	1.33
10	j	164	PHE	CG-CD2	6.88	1.49	1.38
27	O	250	TRP	CD2-CE3	-6.88	1.30	1.40
31	L	354	GLU	CG-CD	6.87	1.62	1.51
17	T	157	TYR	CZ-OH	6.87	1.49	1.37
3	C	50	ARG	NE-CZ	6.86	1.42	1.33
25	R	392	ARG	CD-NE	6.85	1.58	1.46
20	Z	948	TRP	CE3-CZ3	6.85	1.50	1.38
22	S	428	ARG	CZ-NH2	6.84	1.42	1.33
27	O	125	GLY	N-CA	-6.84	1.35	1.46
30	K	252	ARG	CZ-NH1	6.83	1.42	1.33
2	b	82	TYR	CB-CG	6.82	1.61	1.51
25	R	207	ARG	CZ-NH2	6.79	1.41	1.33
25	R	94	PHE	CG-CD1	6.79	1.49	1.38
11	4	59	TYR	CD2-CE2	6.79	1.49	1.39
22	S	382	ARG	CZ-NH2	6.79	1.41	1.33
28	H	245	GLY	CA-C	-6.78	1.41	1.51
33	J	22	TYR	CB-CG	6.78	1.61	1.51
13	6	145	ARG	CZ-NH2	6.75	1.41	1.33
20	Z	5	SER	CA-CB	6.75	1.63	1.52
16	V	114	PHE	CG-CD2	6.75	1.48	1.38
8	h	120	TYR	CE1-CZ	6.74	1.47	1.38
24	Q	329	GLU	CB-CG	6.74	1.65	1.52
8	1	169	SER	CA-CB	6.73	1.63	1.52
20	Z	565	PHE	CG-CD1	6.72	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	883	SER	CA-CB	6.71	1.63	1.52
6	f	3	ARG	CZ-NH2	6.71	1.41	1.33
22	S	425	ARG	CD-NE	6.71	1.57	1.46
22	S	275	TYR	CG-CD1	6.70	1.47	1.39
7	G	91	ARG	CZ-NH2	6.70	1.41	1.33
20	Z	759	ARG	CD-NE	6.69	1.57	1.46
21	N	585	ARG	CD-NE	6.68	1.57	1.46
2	b	23	TYR	CE1-CZ	6.67	1.47	1.38
28	H	208	TYR	CE2-CZ	6.67	1.47	1.38
1	a	23	GLY	CA-C	-6.66	1.41	1.51
20	Z	941	ARG	CZ-NH2	6.66	1.41	1.33
21	N	417	ARG	NE-CZ	6.66	1.41	1.33
7	G	169	ARG	CD-NE	6.66	1.57	1.46
32	M	42	ARG	CZ-NH2	6.65	1.41	1.33
15	W	17	ARG	NE-CZ	6.65	1.41	1.33
31	L	69	ARG	CD-NE	6.65	1.57	1.46
30	K	236	ARG	CD-NE	6.65	1.57	1.46
4	D	6	ARG	CZ-NH2	6.64	1.41	1.33
32	M	152	SER	CA-CB	6.64	1.62	1.52
30	K	346	ARG	CD-NE	6.63	1.57	1.46
13	6	106	TYR	CZ-OH	6.59	1.49	1.37
16	V	302	SER	CA-CB	6.59	1.62	1.52
20	Z	909	ARG	CD-NE	6.58	1.57	1.46
21	N	884	PHE	CG-CD2	6.58	1.48	1.38
1	a	166	TYR	CE1-CZ	6.58	1.47	1.38
4	D	58	ARG	CZ-NH2	6.57	1.41	1.33
11	4	70	ARG	CZ-NH1	6.57	1.41	1.33
4	d	198	SER	CA-CB	6.56	1.62	1.52
29	I	292	TYR	CG-CD1	6.56	1.47	1.39
7	G	201	TYR	CG-CD2	6.56	1.47	1.39
25	R	181	TYR	CB-CG	6.56	1.61	1.51
1	A	155	TYR	CE1-CZ	6.54	1.47	1.38
13	6	229	ARG	NE-CZ	6.54	1.41	1.33
15	W	15	TYR	CB-CG	-6.54	1.41	1.51
4	D	108	TYR	CG-CD2	6.53	1.47	1.39
18	X	106	SER	CA-CB	6.52	1.62	1.52
17	T	103	SER	CA-CB	6.51	1.62	1.52
20	Z	149	TRP	CB-CG	6.51	1.61	1.50
8	h	28	ARG	CZ-NH1	6.51	1.41	1.33
23	P	414	GLU	CG-CD	6.51	1.61	1.51
4	D	181	ARG	CD-NE	6.51	1.57	1.46
14	n	223	ARG	NE-CZ	6.51	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	608	TYR	CG-CD2	6.50	1.47	1.39
14	7	98	ARG	CZ-NH2	6.48	1.41	1.33
29	I	304	ARG	CZ-NH1	6.48	1.41	1.33
24	Q	354	PHE	CE2-CZ	6.48	1.49	1.37
32	M	329	ARG	NE-CZ	6.45	1.41	1.33
3	C	6	TYR	CG-CD1	6.45	1.47	1.39
11	4	85	ARG	CZ-NH1	6.44	1.41	1.33
6	F	145	LEU	CA-CB	6.43	1.68	1.53
20	Z	800	SER	CB-OG	6.43	1.50	1.42
27	O	115	ARG	CZ-NH1	6.43	1.41	1.33
25	R	189	GLU	CB-CG	6.43	1.64	1.52
31	L	217	GLY	N-CA	-6.43	1.36	1.46
10	j	68	ARG	CZ-NH2	6.42	1.41	1.33
9	2	42	VAL	CA-CB	6.41	1.68	1.54
25	R	115	GLU	CB-CG	6.41	1.64	1.52
25	R	252	TYR	CE2-CZ	6.41	1.46	1.38
12	5	245	TYR	CG-CD2	6.41	1.47	1.39
9	i	93	GLU	CD-OE2	6.41	1.32	1.25
9	i	101	ARG	CZ-NH1	6.41	1.41	1.33
32	M	171	GLU	CD-OE2	6.41	1.32	1.25
7	g	190	ARG	CZ-NH1	6.40	1.41	1.33
13	6	113	TYR	CZ-OH	6.40	1.48	1.37
4	D	4	TYR	CZ-OH	6.39	1.48	1.37
29	I	436	TYR	CE2-CZ	6.39	1.46	1.38
11	4	96	ARG	CZ-NH1	6.39	1.41	1.33
29	I	277	SER	CA-CB	6.39	1.62	1.52
22	S	298	ARG	NE-CZ	6.38	1.41	1.33
22	S	55	ARG	CZ-NH1	6.38	1.41	1.33
20	Z	369	PHE	CG-CD1	6.37	1.48	1.38
4	d	22	TYR	CG-CD1	6.36	1.47	1.39
1	a	82	VAL	CA-CB	-6.36	1.41	1.54
13	m	99	ARG	CZ-NH1	6.35	1.41	1.33
4	D	166	ARG	CD-NE	6.35	1.57	1.46
13	m	52	PHE	CG-CD2	6.35	1.48	1.38
27	O	195	TYR	CG-CD2	6.34	1.47	1.39
21	N	394	ARG	CD-NE	6.33	1.57	1.46
33	J	270	ARG	CZ-NH1	6.33	1.41	1.33
3	C	234	GLU	CG-CD	6.33	1.61	1.51
20	Z	947	GLY	CA-C	-6.33	1.41	1.51
14	7	126	PHE	CG-CD2	6.33	1.48	1.38
13	6	169	GLU	CA-CB	6.32	1.67	1.53
27	O	298	GLU	CG-CD	6.32	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	C	217	ARG	NE-CZ	6.31	1.41	1.33
3	C	113	ARG	CZ-NH2	6.31	1.41	1.33
7	g	72	ARG	CZ-NH2	6.30	1.41	1.33
21	N	88	ARG	CZ-NH2	6.29	1.41	1.33
24	Q	255	TYR	CZ-OH	6.29	1.48	1.37
15	W	46	GLU	CD-OE1	6.28	1.32	1.25
26	U	253	ASP	CA-CB	6.27	1.67	1.53
6	f	202	ARG	CZ-NH1	6.26	1.41	1.33
10	3	85	GLU	CG-CD	-6.26	1.42	1.51
32	M	296	SER	CA-CB	6.25	1.62	1.52
13	6	28	PHE	CA-CB	6.25	1.67	1.53
28	H	462	ARG	CZ-NH2	6.25	1.41	1.33
16	V	20	ARG	NE-CZ	6.25	1.41	1.33
23	P	9	ALA	CA-CB	6.24	1.65	1.52
29	I	208	TYR	CG-CD2	6.24	1.47	1.39
31	L	357	ARG	NE-CZ	6.24	1.41	1.33
22	S	160	ARG	CD-NE	6.23	1.57	1.46
33	J	145	SER	CA-CB	6.23	1.62	1.52
6	f	51	ARG	NE-CZ	6.23	1.41	1.33
9	2	219	TYR	CG-CD2	6.23	1.47	1.39
20	Z	295	ARG	CZ-NH1	6.23	1.41	1.33
25	R	186	TYR	CG-CD1	6.23	1.47	1.39
13	6	75	ARG	NE-CZ	6.22	1.41	1.33
4	D	206	GLY	N-CA	-6.22	1.36	1.46
10	j	20	CYS	CB-SG	6.22	1.92	1.82
7	G	228	HIS	CB-CG	6.21	1.61	1.50
26	U	110	PHE	CG-CD2	6.21	1.48	1.38
33	J	200	ARG	NE-CZ	6.21	1.41	1.33
24	Q	185	TYR	CE2-CZ	6.21	1.46	1.38
6	F	60	GLN	N-CA	-6.21	1.33	1.46
25	R	68	GLU	CD-OE2	-6.20	1.18	1.25
13	6	13	TYR	CZ-OH	6.20	1.48	1.37
22	S	286	TYR	CE1-CZ	6.20	1.46	1.38
31	L	264	ARG	NE-CZ	6.20	1.41	1.33
22	S	170	TYR	CG-CD1	6.19	1.47	1.39
22	S	298	ARG	CZ-NH2	6.19	1.41	1.33
21	N	739	PHE	CG-CD1	6.19	1.48	1.38
18	X	93	SER	CA-CB	6.18	1.62	1.52
21	N	58	ARG	CZ-NH1	6.18	1.41	1.33
21	N	338	PHE	CB-CG	6.18	1.61	1.51
21	N	889	ARG	CD-NE	6.18	1.56	1.46
10	j	154	TYR	CD2-CE2	6.18	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	96	ARG	NE-CZ	6.18	1.41	1.33
16	V	171	ARG	CD-NE	6.18	1.56	1.46
12	5	212	TYR	CZ-OH	6.17	1.48	1.37
4	d	166	ARG	CZ-NH1	6.17	1.41	1.33
25	R	355	SER	CA-CB	6.16	1.62	1.52
1	a	120	ARG	CZ-NH1	6.16	1.41	1.33
22	S	271	ARG	NE-CZ	6.16	1.41	1.33
3	C	137	TYR	CD1-CE1	6.15	1.48	1.39
13	6	99	ARG	NE-CZ	6.15	1.41	1.33
8	1	54	ARG	NE-CZ	6.14	1.41	1.33
33	J	217	GLU	CG-CD	6.13	1.61	1.51
21	N	282	TYR	CE1-CZ	6.13	1.46	1.38
11	k	114	PRO	N-CD	-6.13	1.39	1.47
7	G	190	ARG	CZ-NH1	6.13	1.41	1.33
25	R	209	ARG	CZ-NH2	6.13	1.41	1.33
17	T	245	TYR	CE1-CZ	6.13	1.46	1.38
21	N	251	GLU	CG-CD	6.13	1.61	1.51
12	l	212	TYR	C-N	6.12	1.44	1.33
22	S	332	PHE	CB-CG	6.12	1.61	1.51
24	Q	50	ARG	CD-NE	6.12	1.56	1.46
24	Q	398	TYR	CE1-CZ	6.12	1.46	1.38
13	6	107	GLY	N-CA	-6.12	1.36	1.46
22	S	120	SER	CA-CB	6.12	1.62	1.52
28	H	222	ARG	CZ-NH1	6.12	1.41	1.33
24	Q	360	SER	CA-CB	6.11	1.62	1.52
10	3	115	LYS	CA-CB	6.10	1.67	1.53
23	P	201	ARG	CZ-NH2	6.10	1.41	1.33
5	E	122	ARG	CZ-NH2	6.10	1.41	1.33
23	P	185	GLU	CB-CG	6.10	1.63	1.52
4	d	108	TYR	CE2-CZ	6.09	1.46	1.38
24	Q	50	ARG	CZ-NH1	6.09	1.41	1.33
8	h	27	SER	CA-CB	6.09	1.62	1.52
12	l	230	TYR	CG-CD1	6.08	1.47	1.39
19	Y	42	THR	C-N	6.08	1.48	1.34
17	T	91	SER	CA-CB	6.07	1.62	1.52
4	d	119	ARG	CD-NE	6.07	1.56	1.46
10	j	194	GLU	CB-CG	6.07	1.63	1.52
21	N	857	TYR	CE1-CZ	-6.07	1.30	1.38
25	R	252	TYR	CZ-OH	6.06	1.48	1.37
11	4	190	ARG	CD-NE	6.06	1.56	1.46
25	R	24	TYR	CE1-CZ	6.06	1.46	1.38
12	5	234	ARG	CZ-NH2	6.06	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	307	GLU	CG-CD	6.06	1.61	1.51
5	E	167	TYR	CG-CD2	6.05	1.47	1.39
6	F	68	GLU	CB-CG	6.05	1.63	1.52
30	K	349	ARG	CZ-NH2	6.05	1.41	1.33
13	m	22	GLY	CA-C	-6.04	1.42	1.51
27	O	201	PRO	N-CA	-6.04	1.36	1.47
13	m	109	ARG	CZ-NH1	6.04	1.40	1.33
12	l	234	ARG	CD-NE	6.04	1.56	1.46
32	M	50	ARG	CZ-NH1	6.04	1.40	1.33
30	K	121	ARG	NE-CZ	6.03	1.40	1.33
9	i	236	ARG	CD-NE	6.03	1.56	1.46
23	P	13	TYR	CG-CD1	6.02	1.47	1.39
12	5	120	MET	CA-C	-6.01	1.37	1.52
14	n	134	TYR	CE1-CZ	6.01	1.46	1.38
6	F	129	GLY	CA-C	-6.01	1.42	1.51
19	Y	78	LYS	CA-CB	6.01	1.67	1.53
23	P	273	TYR	CG-CD2	6.01	1.47	1.39
24	Q	409	TYR	CB-CG	-6.01	1.42	1.51
30	K	411	TYR	CG-CD1	6.01	1.47	1.39
3	c	5	ARG	NE-CZ	6.00	1.40	1.33
20	Z	826	ARG	NE-CZ	6.00	1.40	1.33
21	N	906	ARG	NE-CZ	6.00	1.40	1.33
11	k	82	SER	CA-CB	6.00	1.61	1.52
2	b	83	ARG	CZ-NH1	6.00	1.40	1.33
10	j	198	ARG	CZ-NH1	6.00	1.40	1.33
20	Z	195	PHE	CG-CD1	6.00	1.47	1.38
4	d	29	ARG	CZ-NH2	5.99	1.40	1.33
32	M	166	ARG	CZ-NH2	5.99	1.40	1.33
25	R	62	TYR	CZ-OH	5.99	1.48	1.37
6	F	228	GLU	CG-CD	5.98	1.60	1.51
13	m	198	SER	CA-CB	5.98	1.61	1.52
33	J	296	ARG	NE-CZ	5.98	1.40	1.33
7	G	153	PRO	N-CD	-5.97	1.39	1.47
33	J	371	ARG	CD-NE	5.97	1.56	1.46
1	A	135	ARG	NE-CZ	5.97	1.40	1.33
31	L	215	PRO	N-CD	-5.96	1.39	1.47
25	R	392	ARG	CZ-NH2	5.96	1.40	1.33
24	Q	50	ARG	NE-CZ	5.96	1.40	1.33
31	L	265	GLU	CA-CB	5.95	1.67	1.53
23	P	297	GLU	CD-OE1	5.95	1.32	1.25
27	O	60	ARG	NE-CZ	5.95	1.40	1.33
7	G	20	ARG	NE-CZ	5.94	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	185	GLU	CD-OE2	5.94	1.32	1.25
3	C	6	TYR	CD2-CE2	5.94	1.48	1.39
16	V	55	GLY	CA-C	-5.94	1.42	1.51
18	X	51	ARG	NE-CZ	5.94	1.40	1.33
11	k	98	TYR	CZ-OH	5.93	1.48	1.37
7	g	128	SER	CA-CB	5.92	1.61	1.52
31	L	420	ARG	NE-CZ	5.92	1.40	1.33
7	g	127	ASN	CB-CG	5.92	1.64	1.51
4	D	159	TRP	CD2-CE3	-5.92	1.31	1.40
19	Y	43	TRP	NE1-CE2	5.92	1.45	1.37
8	1	178	SER	C-N	5.92	1.43	1.33
5	E	165	TYR	CE1-CZ	5.92	1.46	1.38
21	N	434	SER	CA-CB	5.92	1.61	1.52
4	D	76	SER	CA-CB	5.91	1.61	1.52
17	T	194	GLU	CG-CD	5.91	1.60	1.51
8	1	23	LEU	C-N	5.91	1.43	1.33
14	n	262	GLY	N-CA	-5.91	1.37	1.46
12	5	282	PHE	CG-CD2	5.91	1.47	1.38
13	6	61	SER	CA-CB	5.91	1.61	1.52
21	N	839	ARG	NE-CZ	5.90	1.40	1.33
2	b	182	GLU	CD-OE2	5.90	1.32	1.25
2	B	83	ARG	CZ-NH2	5.90	1.40	1.33
5	E	153	TYR	CZ-OH	5.90	1.47	1.37
27	O	335	GLY	N-CA	-5.90	1.37	1.46
21	N	259	PHE	CG-CD2	5.89	1.47	1.38
32	M	398	ALA	C-N	5.89	1.43	1.33
9	i	217	ARG	CZ-NH2	5.89	1.40	1.33
3	c	217	ARG	CZ-NH1	5.89	1.40	1.33
21	N	208	ARG	NE-CZ	5.89	1.40	1.33
13	m	79	SER	CB-OG	5.89	1.50	1.42
16	V	28	TYR	CG-CD2	5.88	1.46	1.39
30	K	118	TYR	CG-CD2	5.88	1.46	1.39
32	M	357	ARG	CZ-NH2	5.88	1.40	1.33
20	Z	354	PRO	N-CD	-5.88	1.39	1.47
22	S	211	ARG	CZ-NH2	5.88	1.40	1.33
4	D	29	ARG	CZ-NH1	5.88	1.40	1.33
3	c	6	TYR	CG-CD2	5.88	1.46	1.39
2	b	130	PHE	CE2-CZ	5.87	1.48	1.37
8	1	45	ARG	NE-CZ	5.87	1.40	1.33
13	6	114	TYR	CG-CD2	5.87	1.46	1.39
30	K	399	ARG	NE-CZ	5.87	1.40	1.33
4	D	160	SER	CA-CB	5.86	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	114	TYR	CG-CD1	5.86	1.46	1.39
13	6	63	ASN	CB-CG	5.86	1.64	1.51
14	7	226	ARG	CD-NE	5.86	1.56	1.46
26	U	167	GLU	CG-CD	5.86	1.60	1.51
29	I	100	ARG	CZ-NH1	5.86	1.40	1.33
5	e	238	GLU	CG-CD	5.86	1.60	1.51
1	A	131	ARG	CZ-NH2	5.86	1.40	1.33
20	Z	395	CYS	CB-SG	-5.86	1.72	1.81
28	H	400	ARG	CZ-NH1	5.86	1.40	1.33
6	F	89	ARG	CZ-NH2	5.85	1.40	1.33
5	E	49	GLY	N-CA	-5.85	1.37	1.46
33	J	48	ARG	CZ-NH2	5.85	1.40	1.33
5	e	188	HIS	N-CA	-5.85	1.34	1.46
5	E	159	GLU	CD-OE2	5.85	1.32	1.25
4	d	137	GLY	CA-C	-5.84	1.42	1.51
30	K	48	TYR	CE2-CZ	5.84	1.46	1.38
20	Z	553	ARG	CZ-NH2	5.84	1.40	1.33
22	S	197	SER	CA-CB	5.83	1.61	1.52
8	h	133	TYR	CG-CD1	5.83	1.46	1.39
20	Z	832	ARG	CZ-NH2	5.83	1.40	1.33
6	f	32	GLY	CA-C	5.83	1.61	1.51
13	6	79	SER	N-CA	-5.83	1.34	1.46
25	R	43	ARG	NE-CZ	5.83	1.40	1.33
1	A	239	GLU	CB-CG	5.83	1.63	1.52
25	R	204	TRP	CZ2-CH2	5.83	1.48	1.37
25	R	207	ARG	CD-NE	5.83	1.56	1.46
4	D	127	ARG	CZ-NH2	5.82	1.40	1.33
20	Z	813	PHE	CE2-CZ	5.82	1.48	1.37
11	k	121	TYR	CB-CG	-5.82	1.43	1.51
20	Z	174	GLU	CD-OE1	5.82	1.32	1.25
21	N	711	ARG	NE-CZ	5.81	1.40	1.33
30	K	198	TYR	CZ-OH	5.81	1.47	1.37
11	4	97	PRO	N-CD	-5.81	1.39	1.47
30	K	336	ARG	CZ-NH2	5.81	1.40	1.33
4	D	120	TYR	CD2-CE2	5.81	1.48	1.39
4	D	58	ARG	CD-NE	5.80	1.56	1.46
29	I	291	ARG	CD-NE	5.80	1.56	1.46
20	Z	970	TYR	CG-CD1	5.80	1.46	1.39
25	R	129	GLU	CG-CD	-5.80	1.43	1.51
29	I	353	PRO	N-CD	-5.80	1.39	1.47
5	e	214	GLU	CG-CD	5.79	1.60	1.51
4	d	111	ARG	CZ-NH2	5.79	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	I	90	GLU	CG-CD	5.79	1.60	1.51
10	j	203	ARG	CZ-NH2	5.79	1.40	1.33
10	3	99	ARG	CD-NE	5.79	1.56	1.46
27	O	135	ARG	NE-CZ	5.79	1.40	1.33
32	M	213	ARG	NE-CZ	5.79	1.40	1.33
2	b	99	ARG	NE-CZ	5.79	1.40	1.33
4	D	74	SER	CA-CB	5.78	1.61	1.52
13	6	82	TRP	CE3-CZ3	5.78	1.48	1.38
14	7	136	ARG	CD-NE	5.78	1.56	1.46
21	N	203	ARG	CD-NE	5.78	1.56	1.46
28	H	435	ARG	CD-NE	5.78	1.56	1.46
16	V	194	ARG	CZ-NH2	5.78	1.40	1.33
24	Q	72	ASP	CA-CB	5.77	1.66	1.53
3	C	114	ARG	CD-NE	5.77	1.56	1.46
9	2	155	SER	CA-CB	5.77	1.61	1.52
10	3	80	ARG	CD-NE	5.77	1.56	1.46
21	N	298	TYR	CE2-CZ	5.77	1.46	1.38
12	l	139	ARG	CZ-NH2	5.77	1.40	1.33
7	g	190	ARG	NE-CZ	5.76	1.40	1.33
31	L	88	TYR	CE2-CZ	5.76	1.46	1.38
31	L	132	ARG	NE-CZ	5.76	1.40	1.33
32	M	45	ARG	CD-NE	5.76	1.56	1.46
6	F	6	TYR	CB-CG	-5.76	1.43	1.51
13	6	184	SER	CA-CB	5.76	1.61	1.52
24	Q	286	TYR	CE1-CZ	5.76	1.46	1.38
7	g	131	PRO	CA-CB	5.76	1.65	1.53
25	R	384	VAL	CB-CG2	5.76	1.65	1.52
4	D	21	GLU	CG-CD	5.75	1.60	1.51
27	O	210	ARG	CZ-NH2	5.75	1.40	1.33
28	H	65	GLU	CD-OE2	5.75	1.31	1.25
31	L	342	ARG	NE-CZ	5.75	1.40	1.33
21	N	894	ARG	CZ-NH2	5.74	1.40	1.33
4	d	21	GLU	CG-CD	5.74	1.60	1.51
10	j	30	GLY	N-CA	-5.74	1.37	1.46
22	S	452	TYR	CZ-OH	5.74	1.47	1.37
21	N	880	ARG	CZ-NH2	5.74	1.40	1.33
28	H	409	ARG	CD-NE	5.73	1.56	1.46
7	G	8	TYR	CE1-CZ	5.73	1.46	1.38
8	h	70	TYR	CZ-OH	5.72	1.47	1.37
7	G	190	ARG	CD-NE	5.72	1.56	1.46
20	Z	838	TYR	CG-CD1	5.72	1.46	1.39
24	Q	246	TYR	CG-CD2	5.71	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	355	TRP	CG-CD1	5.71	1.44	1.36
21	N	204	SER	CB-OG	5.71	1.49	1.42
30	K	57	GLU	CD-OE2	5.71	1.31	1.25
32	M	342	ARG	CZ-NH1	5.70	1.40	1.33
2	b	204	PHE	CG-CD2	5.70	1.47	1.38
13	6	28	PHE	CG-CD1	5.70	1.47	1.38
21	N	320	SER	CA-CB	5.69	1.61	1.52
25	R	41	GLU	CG-CD	5.69	1.60	1.51
7	G	91	ARG	CZ-NH1	5.69	1.40	1.33
29	I	346	ARG	CZ-NH2	5.69	1.40	1.33
31	L	69	ARG	NE-CZ	5.69	1.40	1.33
6	F	123	TYR	CG-CD1	5.69	1.46	1.39
28	H	90	ARG	CZ-NH2	5.69	1.40	1.33
3	c	143	ARG	NE-CZ	5.68	1.40	1.33
12	5	114	PRO	N-CD	-5.68	1.39	1.47
2	b	236	ARG	CZ-NH1	5.68	1.40	1.33
7	G	26	TYR	CB-CG	-5.68	1.43	1.51
8	1	31	THR	C-N	5.68	1.43	1.33
6	f	39	ARG	NE-CZ	5.68	1.40	1.33
10	j	28	ARG	CZ-NH1	5.68	1.40	1.33
20	Z	55	ARG	CZ-NH2	5.68	1.40	1.33
1	a	96	ARG	CZ-NH1	5.67	1.40	1.33
20	Z	55	ARG	NE-CZ	5.67	1.40	1.33
32	M	299	ARG	CZ-NH2	5.67	1.40	1.33
13	m	182	TYR	CG-CD1	5.67	1.46	1.39
10	3	188	TYR	CG-CD1	5.67	1.46	1.39
8	h	179	GLY	N-CA	-5.67	1.37	1.46
20	Z	513	ALA	CA-CB	5.66	1.64	1.52
5	e	221	CYS	CB-SG	5.66	1.91	1.82
24	Q	291	TYR	CZ-OH	5.66	1.47	1.37
14	n	175	LEU	CA-C	-5.65	1.38	1.52
9	2	101	ARG	CD-NE	5.65	1.56	1.46
21	N	398	ARG	CZ-NH2	5.65	1.40	1.33
28	H	390	ARG	NE-CZ	5.64	1.40	1.33
14	7	65	SER	CA-CB	5.64	1.61	1.52
24	Q	13	ARG	CZ-NH1	5.64	1.40	1.33
33	J	263	GLY	N-CA	5.64	1.54	1.46
6	f	3	ARG	NE-CZ	5.64	1.40	1.33
9	i	45	ALA	CA-C	-5.64	1.38	1.52
23	P	182	GLU	CD-OE2	5.64	1.31	1.25
10	3	98	ARG	CZ-NH2	5.63	1.40	1.33
4	d	12	SER	CA-CB	5.63	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	181	ARG	CZ-NH2	5.63	1.40	1.33
6	F	158	GLY	N-CA	-5.63	1.37	1.46
6	F	37	GLY	N-CA	5.63	1.54	1.46
13	6	131	TYR	CZ-OH	5.63	1.47	1.37
22	S	82	TYR	CG-CD2	5.63	1.46	1.39
27	O	178	TYR	CG-CD1	5.62	1.46	1.39
22	S	64	ARG	CZ-NH1	5.62	1.40	1.33
7	G	157	TYR	CE2-CZ	5.62	1.45	1.38
21	N	549	TYR	CG-CD1	5.62	1.46	1.39
14	7	252	TRP	N-CA	-5.61	1.35	1.46
2	b	23	TYR	CG-CD1	5.61	1.46	1.39
5	e	20	ARG	CZ-NH2	5.61	1.40	1.33
2	B	83	ARG	CZ-NH1	5.61	1.40	1.33
32	M	163	PHE	CA-CB	5.61	1.66	1.53
21	N	58	ARG	CD-NE	5.61	1.55	1.46
2	B	176	GLU	CG-CD	-5.60	1.43	1.51
29	I	291	ARG	CZ-NH2	5.60	1.40	1.33
4	d	75	PHE	CG-CD2	5.60	1.47	1.38
11	4	148	TYR	CB-CG	-5.60	1.43	1.51
33	J	205	HIS	CB-CG	5.60	1.60	1.50
2	b	217	GLU	CG-CD	5.60	1.60	1.51
13	6	225	TYR	CE1-CZ	5.59	1.45	1.38
3	c	129	ARG	NE-CZ	5.59	1.40	1.33
16	V	273	ARG	CZ-NH1	5.59	1.40	1.33
17	T	223	GLU	CB-CG	5.59	1.62	1.52
19	Y	64	TRP	CD2-CE2	5.59	1.48	1.41
12	5	81	PHE	CG-CD1	5.59	1.47	1.38
31	L	100	SER	CA-CB	5.59	1.61	1.52
22	S	447	GLU	CD-OE2	5.58	1.31	1.25
2	b	148	TYR	CG-CD1	5.58	1.46	1.39
28	H	209	SER	CA-CB	5.58	1.61	1.52
33	J	120	TYR	CZ-OH	5.58	1.47	1.37
5	e	210	GLU	CG-CD	5.58	1.60	1.51
23	P	123	ARG	NE-CZ	5.58	1.40	1.33
24	Q	400	TYR	CZ-OH	5.58	1.47	1.37
25	R	140	TYR	CG-CD1	5.58	1.46	1.39
19	Y	83	ARG	CZ-NH1	5.58	1.40	1.33
27	O	190	TYR	CE1-CZ	5.58	1.45	1.38
26	U	137	TYR	CG-CD2	5.57	1.46	1.39
8	h	96	TYR	CZ-OH	5.57	1.47	1.37
2	B	197	LYS	CB-CG	5.57	1.67	1.52
13	m	113	TYR	CE2-CZ	5.57	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	49	TYR	CD1-CE1	5.57	1.47	1.39
12	l	196	ARG	NE-CZ	5.57	1.40	1.33
13	6	36	ARG	CZ-NH1	5.57	1.40	1.33
12	5	226	GLU	CG-CD	5.57	1.60	1.51
8	1	38	ARG	NE-CZ	5.56	1.40	1.33
15	W	138	ALA	CA-C	-5.56	1.38	1.52
27	O	228	TYR	CE2-CZ	5.56	1.45	1.38
33	J	188	TYR	CE2-CZ	5.56	1.45	1.38
7	g	130	ARG	CZ-NH1	5.55	1.40	1.33
23	P	318	TYR	CE1-CZ	5.55	1.45	1.38
3	C	230	PHE	CG-CD1	5.55	1.47	1.38
1	A	162	TYR	CZ-OH	5.55	1.47	1.37
32	M	233	ARG	CZ-NH1	5.55	1.40	1.33
1	A	135	ARG	CZ-NH2	5.54	1.40	1.33
5	E	153	TYR	CE2-CZ	5.54	1.45	1.38
24	Q	209	TYR	CE2-CZ	5.54	1.45	1.38
6	f	123	TYR	CB-CG	5.54	1.59	1.51
32	M	33	ARG	CZ-NH1	5.54	1.40	1.33
3	c	149	TYR	CD2-CE2	-5.54	1.31	1.39
9	i	215	TYR	CE1-CZ	5.53	1.45	1.38
22	S	360	PHE	CB-CG	5.53	1.60	1.51
4	D	111	ARG	NE-CZ	5.53	1.40	1.33
20	Z	774	ARG	NE-CZ	5.53	1.40	1.33
11	k	171	ARG	CZ-NH1	5.53	1.40	1.33
7	G	154	SER	CA-CB	5.53	1.61	1.52
11	k	107	TYR	CG-CD2	5.52	1.46	1.39
13	m	141	ARG	CZ-NH2	5.52	1.40	1.33
14	n	63	TYR	CE2-CZ	5.52	1.45	1.38
20	Z	248	TYR	CG-CD2	5.52	1.46	1.39
21	N	718	GLU	CD-OE2	5.52	1.31	1.25
10	j	74	TYR	CE2-CZ	5.52	1.45	1.38
11	k	107	TYR	CE2-CZ	5.52	1.45	1.38
12	5	242	ARG	CD-NE	5.52	1.55	1.46
32	M	221	TYR	CZ-OH	5.52	1.47	1.37
12	5	262	TYR	CE2-CZ	5.51	1.45	1.38
30	K	282	PHE	CD1-CE1	5.51	1.50	1.39
1	a	110	TYR	CE1-CZ	5.51	1.45	1.38
1	A	244	ARG	CZ-NH1	5.51	1.40	1.33
4	D	167	ASN	CB-CG	5.51	1.63	1.51
5	E	165	TYR	CG-CD2	5.51	1.46	1.39
6	f	59	TYR	CG-CD2	5.50	1.46	1.39
13	m	121	GLY	N-CA	-5.50	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	68	ARG	CZ-NH1	5.50	1.40	1.33
33	J	212	ARG	CZ-NH1	5.50	1.40	1.33
4	d	249	LYS	C-N	5.50	1.46	1.34
5	E	53	ARG	NE-CZ	5.50	1.40	1.33
28	H	145	TYR	CE2-CZ	5.50	1.45	1.38
32	M	433	TYR	CE2-CZ	5.50	1.45	1.38
11	k	130	TYR	CE2-CZ	5.50	1.45	1.38
7	G	22	PHE	CG-CD1	5.49	1.47	1.38
22	S	346	TYR	CE2-CZ	5.49	1.45	1.38
12	l	130	TRP	CZ3-CH2	5.49	1.48	1.40
7	G	103	TYR	CE1-CZ	5.49	1.45	1.38
20	Z	525	MET	N-CA	-5.49	1.35	1.46
28	H	238	LEU	C-N	5.49	1.43	1.33
2	B	82	TYR	CG-CD2	5.49	1.46	1.39
20	Z	181	GLY	CA-C	-5.49	1.43	1.51
33	J	257	ARG	CZ-NH1	5.49	1.40	1.33
17	T	197	TYR	CE1-CZ	5.49	1.45	1.38
6	f	6	TYR	CD1-CE1	5.48	1.47	1.39
10	j	103	TYR	CG-CD2	5.48	1.46	1.39
11	k	45	SER	CA-CB	5.48	1.61	1.52
21	N	921	ARG	CD-NE	5.48	1.55	1.46
24	Q	57	SER	CA-CB	5.48	1.61	1.52
5	e	164	PHE	CG-CD2	5.48	1.47	1.38
13	6	140	GLU	CD-OE2	5.48	1.31	1.25
7	G	86	ARG	NE-CZ	5.47	1.40	1.33
12	5	203	CYS	CB-SG	5.47	1.91	1.82
22	S	480	ARG	CZ-NH1	5.47	1.40	1.33
13	6	99	ARG	CZ-NH1	5.47	1.40	1.33
32	M	378	GLU	CG-CD	5.47	1.60	1.51
1	A	55	SER	N-CA	-5.47	1.35	1.46
25	R	65	TYR	CE1-CZ	5.47	1.45	1.38
26	U	239	LEU	C-N	5.46	1.42	1.33
20	Z	928	ARG	CA-C	-5.46	1.38	1.52
2	b	104	TYR	CZ-OH	5.46	1.47	1.37
14	7	261	TYR	CD2-CE2	5.46	1.47	1.39
22	S	55	ARG	NE-CZ	5.46	1.40	1.33
6	f	205	SER	CA-CB	5.46	1.61	1.52
11	4	50	ALA	C-N	5.46	1.42	1.33
20	Z	81	SER	CA-CB	5.46	1.61	1.52
21	N	298	TYR	CG-CD2	5.46	1.46	1.39
20	Z	153	TYR	CD2-CE2	-5.45	1.31	1.39
24	Q	339	TYR	CZ-OH	5.45	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Y	83	ARG	NE-CZ	5.45	1.40	1.33
33	J	35	ARG	CD-NE	5.45	1.55	1.46
2	B	186	GLU	CD-OE1	5.45	1.31	1.25
7	G	123	HIS	CB-CG	-5.45	1.40	1.50
21	N	149	GLU	CD-OE1	5.45	1.31	1.25
8	1	38	ARG	CZ-NH2	5.44	1.40	1.33
17	T	15	PHE	CB-CG	5.44	1.60	1.51
24	Q	255	TYR	CG-CD1	5.44	1.46	1.39
29	I	246	ARG	CD-NE	5.44	1.55	1.46
20	Z	244	ARG	NE-CZ	5.44	1.40	1.33
6	F	225	TYR	CG-CD1	5.44	1.46	1.39
8	1	75	TYR	CE2-CZ	5.44	1.45	1.38
13	6	223	GLU	CG-CD	-5.44	1.43	1.51
10	3	80	ARG	CZ-NH1	5.43	1.40	1.33
17	T	81	TYR	CB-CG	5.43	1.59	1.51
10	j	85	GLU	CD-OE1	5.43	1.31	1.25
20	Z	948	TRP	CD2-CE3	5.43	1.48	1.40
14	n	98	ARG	CZ-NH1	5.43	1.40	1.33
11	k	176	PHE	CA-C	-5.43	1.38	1.52
15	W	53	SER	CB-OG	5.43	1.49	1.42
21	N	862	SER	CA-CB	5.43	1.61	1.52
23	P	115	ARG	CD-NE	5.43	1.55	1.46
9	i	48	ARG	CZ-NH2	5.42	1.40	1.33
19	Y	76	GLU	CG-CD	5.42	1.60	1.51
33	J	21	PRO	N-CD	-5.42	1.40	1.47
20	Z	964	GLU	CG-CD	5.42	1.60	1.51
21	N	88	ARG	NE-CZ	5.42	1.40	1.33
6	f	158	GLY	CA-C	-5.42	1.43	1.51
7	g	212	PHE	CG-CD2	5.42	1.46	1.38
21	N	50	TYR	CE1-CZ	5.42	1.45	1.38
26	U	187	SER	CA-CB	5.41	1.61	1.52
26	U	275	VAL	N-CA	5.41	1.57	1.46
20	Z	773	ARG	NE-CZ	5.41	1.40	1.33
14	n	161	ARG	CZ-NH2	5.41	1.40	1.33
31	L	194	ARG	CZ-NH2	5.41	1.40	1.33
4	d	33	ALA	CA-CB	5.40	1.63	1.52
11	k	85	ARG	CD-NE	5.40	1.55	1.46
1	A	224	GLU	CB-CG	5.40	1.62	1.52
27	O	311	GLU	CB-CG	5.40	1.62	1.52
31	L	342	ARG	CZ-NH2	5.40	1.40	1.33
21	N	528	ARG	CZ-NH2	5.40	1.40	1.33
20	Z	832	ARG	CZ-NH1	5.40	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	6	109	ARG	CZ-NH2	5.40	1.40	1.33
21	N	181	GLU	CG-CD	5.40	1.60	1.51
32	M	342	ARG	NE-CZ	5.40	1.40	1.33
2	b	153	SER	CA-CB	5.40	1.61	1.52
11	k	190	ARG	C-N	5.40	1.46	1.34
13	6	75	ARG	CZ-NH1	5.39	1.40	1.33
14	7	220	ARG	NE-CZ	5.39	1.40	1.33
24	Q	55	GLU	CA-CB	5.39	1.65	1.53
31	L	404	ARG	CZ-NH1	5.39	1.40	1.33
6	f	72	LEU	CA-CB	5.39	1.66	1.53
10	3	167	ILE	N-CA	-5.39	1.35	1.46
2	b	90	ARG	CZ-NH1	5.38	1.40	1.33
4	d	83	ARG	CD-NE	5.38	1.55	1.46
11	4	148	TYR	CE2-CZ	5.38	1.45	1.38
4	d	83	ARG	CZ-NH2	5.38	1.40	1.33
2	B	179	TRP	NE1-CE2	5.38	1.44	1.37
20	Z	62	SER	CB-OG	5.38	1.49	1.42
3	C	245	THR	N-CA	-5.37	1.35	1.46
5	e	136	ARG	CD-NE	5.37	1.55	1.46
12	l	188	TYR	CG-CD2	5.37	1.46	1.39
1	A	250	GLU	CD-OE2	5.37	1.31	1.25
16	V	228	TYR	CG-CD1	5.37	1.46	1.39
31	L	224	PRO	CA-CB	5.37	1.64	1.53
25	R	304	TYR	CZ-OH	5.37	1.47	1.37
23	P	127	GLU	CD-OE2	5.36	1.31	1.25
16	V	269	ARG	CZ-NH1	5.36	1.40	1.33
10	3	177	ARG	NE-CZ	5.36	1.40	1.33
6	F	51	ARG	CZ-NH2	5.36	1.40	1.33
20	Z	202	ARG	CZ-NH2	5.36	1.40	1.33
8	h	45	ARG	CD-NE	5.36	1.55	1.46
6	f	94	TYR	CE2-CZ	5.35	1.45	1.38
6	f	150	SER	CA-CB	5.35	1.60	1.52
12	5	82	ARG	CZ-NH1	5.35	1.40	1.33
32	M	124	ARG	NE-CZ	5.35	1.40	1.33
2	b	178	ARG	CZ-NH1	5.35	1.40	1.33
8	1	144	TYR	CZ-OH	5.35	1.47	1.37
3	C	137	TYR	CG-CD2	5.34	1.46	1.39
15	W	119	SER	CA-CB	5.34	1.60	1.52
14	7	215	ARG	CZ-NH2	5.34	1.40	1.33
32	M	290	ARG	CZ-NH1	5.34	1.40	1.33
14	n	170	TYR	CE2-CZ	5.34	1.45	1.38
22	S	36	LYS	CA-CB	5.34	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	128	ARG	NE-CZ	5.34	1.40	1.33
15	W	166	GLU	CA-CB	5.34	1.65	1.53
23	P	138	ARG	CZ-NH1	5.34	1.40	1.33
8	h	38	ARG	NE-CZ	5.33	1.40	1.33
7	G	72	ARG	CZ-NH1	5.33	1.40	1.33
9	2	236	ARG	CZ-NH1	5.33	1.40	1.33
13	6	116	HIS	CG-CD2	5.33	1.44	1.35
23	P	109	SER	CA-CB	5.33	1.60	1.52
28	H	373	ARG	CD-NE	5.33	1.55	1.46
1	a	166	TYR	CZ-OH	5.33	1.47	1.37
2	b	58	SER	CA-CB	5.33	1.60	1.52
10	j	159	GLU	CD-OE1	5.33	1.31	1.25
22	S	271	ARG	CZ-NH1	5.33	1.40	1.33
2	B	120	GLU	CG-CD	5.33	1.59	1.51
21	N	548	ARG	NE-CZ	5.33	1.40	1.33
3	C	217	ARG	CZ-NH1	5.33	1.40	1.33
21	N	477	SER	C-N	5.33	1.42	1.33
28	H	331	ARG	CZ-NH1	5.33	1.40	1.33
13	m	147	GLY	N-CA	-5.32	1.38	1.46
8	1	93	GLU	CB-CG	5.32	1.62	1.52
8	1	124	LEU	C-N	5.32	1.42	1.33
14	7	161	ARG	CD-NE	5.32	1.55	1.46
12	l	86	GLY	N-CA	-5.32	1.38	1.46
21	N	382	GLY	CA-C	-5.32	1.43	1.51
24	Q	306	TYR	CD2-CE2	5.32	1.47	1.39
31	L	412	PRO	N-CD	-5.32	1.40	1.47
6	f	141	GLY	N-CA	-5.32	1.38	1.46
7	g	87	HIS	CA-CB	5.32	1.65	1.53
3	C	144	TYR	CG-CD1	5.32	1.46	1.39
15	W	82	GLU	CG-CD	5.32	1.59	1.51
22	S	184	TRP	CE3-CZ3	5.32	1.47	1.38
14	7	226	ARG	CZ-NH1	5.31	1.40	1.33
24	Q	88	PHE	CE1-CZ	5.31	1.47	1.37
28	H	343	PHE	CE1-CZ	5.31	1.47	1.37
3	c	104	GLU	CD-OE1	5.31	1.31	1.25
13	6	186	GLU	CD-OE2	5.31	1.31	1.25
17	T	166	SER	CA-CB	5.31	1.60	1.52
10	j	136	PHE	CG-CD2	5.31	1.46	1.38
10	3	28	ARG	NE-CZ	5.31	1.40	1.33
25	R	247	GLU	CD-OE1	5.31	1.31	1.25
33	J	404	PHE	CG-CD2	5.31	1.46	1.38
21	N	906	ARG	CZ-NH2	5.30	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	196	ARG	CZ-NH1	5.30	1.40	1.33
22	S	217	PHE	CB-CG	5.30	1.60	1.51
3	c	230	PHE	CE1-CZ	5.30	1.47	1.37
3	C	113	ARG	CZ-NH1	5.30	1.40	1.33
6	F	31	GLN	C-N	5.30	1.42	1.33
20	Z	93	ARG	NE-CZ	5.30	1.40	1.33
23	P	436	GLU	CD-OE2	5.30	1.31	1.25
29	I	133	LEU	CA-CB	5.30	1.66	1.53
25	R	209	ARG	CD-NE	5.29	1.55	1.46
2	B	62	SER	CA-CB	5.29	1.60	1.52
20	Z	767	TYR	C-N	5.29	1.42	1.33
12	5	242	ARG	NE-CZ	5.29	1.40	1.33
27	O	106	PHE	CG-CD1	5.29	1.46	1.38
8	h	146	TYR	CD1-CE1	5.29	1.47	1.39
8	1	56	GLY	N-CA	-5.29	1.38	1.46
31	L	300	GLU	CD-OE1	5.28	1.31	1.25
8	h	110	GLY	CA-C	-5.28	1.43	1.51
31	L	126	ARG	NE-CZ	5.28	1.40	1.33
1	a	91	ARG	NE-CZ	5.28	1.40	1.33
11	4	113	LYS	N-CA	-5.28	1.35	1.46
21	N	921	ARG	NE-CZ	5.28	1.40	1.33
31	L	424	GLU	CG-CD	5.28	1.59	1.51
14	n	74	ARG	CZ-NH1	5.27	1.40	1.33
30	K	346	ARG	NE-CZ	5.27	1.40	1.33
16	V	254	ARG	NE-CZ	5.27	1.39	1.33
13	m	114	TYR	CB-CG	-5.26	1.43	1.51
20	Z	193	PHE	CG-CD2	5.26	1.46	1.38
15	W	25	ARG	NE-CZ	5.26	1.39	1.33
1	a	189	SER	CB-OG	-5.26	1.35	1.42
7	G	177	GLU	CD-OE2	5.26	1.31	1.25
24	Q	427	PHE	CG-CD2	5.26	1.46	1.38
6	f	227	GLY	CA-C	-5.26	1.43	1.51
2	B	156	TYR	CE2-CZ	5.26	1.45	1.38
4	d	4	TYR	CZ-OH	5.25	1.46	1.37
4	D	69	SER	CA-CB	5.25	1.60	1.52
6	F	79	PRO	N-CD	-5.25	1.40	1.47
21	N	653	ARG	NE-CZ	5.25	1.39	1.33
27	O	98	TYR	CG-CD1	5.25	1.46	1.39
10	j	110	ALA	CA-CB	5.25	1.63	1.52
31	L	97	ALA	CA-C	-5.25	1.39	1.52
7	G	138	PHE	CG-CD2	5.25	1.46	1.38
18	X	32	GLU	CD-OE2	5.25	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	324	ARG	CZ-NH2	5.25	1.39	1.33
11	4	95	ARG	CZ-NH1	5.24	1.39	1.33
3	c	210	ARG	CZ-NH1	5.24	1.39	1.33
9	i	154	LEU	CA-CB	5.24	1.65	1.53
2	B	31	GLY	N-CA	-5.24	1.38	1.46
10	j	38	ASN	CB-CG	5.24	1.63	1.51
23	P	103	TYR	CE1-CZ	5.24	1.45	1.38
1	A	105	ARG	NE-CZ	5.24	1.39	1.33
32	M	303	ARG	NE-CZ	5.24	1.39	1.33
7	g	106	PRO	CA-C	-5.24	1.42	1.52
1	A	155	TYR	CE2-CZ	5.24	1.45	1.38
2	B	104	TYR	CZ-OH	5.24	1.46	1.37
20	Z	196	SER	CA-CB	5.23	1.60	1.52
16	V	252	SER	CA-CB	5.23	1.60	1.52
20	Z	260	GLU	CD-OE2	5.23	1.31	1.25
2	B	234	ARG	CZ-NH1	5.23	1.39	1.33
20	Z	157	LEU	C-N	5.23	1.46	1.34
21	N	315	ASN	N-CA	-5.23	1.35	1.46
2	B	242	GLU	CB-CG	5.22	1.62	1.52
21	N	743	PHE	C-N	-5.22	1.24	1.34
13	m	131	TYR	CZ-OH	5.22	1.46	1.37
28	H	396	MET	CA-C	-5.22	1.39	1.52
2	B	232	GLY	C-N	5.22	1.44	1.34
25	R	222	ARG	CZ-NH1	5.22	1.39	1.33
7	g	169	ARG	CD-NE	5.21	1.55	1.46
6	F	94	TYR	CZ-OH	5.21	1.46	1.37
31	L	386	PHE	CG-CD2	5.21	1.46	1.38
10	3	80	ARG	NE-CZ	5.21	1.39	1.33
11	4	173	PRO	CA-CB	-5.21	1.43	1.53
11	k	60	ILE	CA-CB	-5.21	1.42	1.54
27	O	330	ARG	NE-CZ	5.20	1.39	1.33
31	L	78	ARG	NE-CZ	5.20	1.39	1.33
20	Z	138	ARG	CZ-NH2	5.20	1.39	1.33
26	U	176	ARG	CZ-NH2	5.20	1.39	1.33
32	M	420	SER	CA-CB	5.20	1.60	1.52
11	k	85	ARG	NE-CZ	5.20	1.39	1.33
13	m	83	TYR	CB-CG	-5.20	1.43	1.51
21	N	77	SER	CA-CB	5.20	1.60	1.52
32	M	203	ARG	NE-CZ	5.20	1.39	1.33
21	N	299	TYR	CE1-CZ	5.19	1.45	1.38
28	H	414	SER	CB-OG	5.19	1.49	1.42
27	O	372	GLU	CB-CG	5.19	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	O	166	ARG	CZ-NH1	5.19	1.39	1.33
33	J	223	ILE	C-N	5.19	1.42	1.33
29	I	73	GLU	CD-OE2	-5.19	1.20	1.25
13	6	138	SER	CA-CB	5.18	1.60	1.52
24	Q	396	TRP	CE3-CZ3	5.18	1.47	1.38
29	I	382	THR	CA-C	-5.18	1.39	1.52
9	2	121	GLY	N-CA	5.18	1.53	1.46
14	7	64	GLY	CA-C	-5.17	1.43	1.51
6	f	123	TYR	CE2-CZ	5.17	1.45	1.38
21	N	14	ARG	CD-NE	5.17	1.55	1.46
5	E	123	PHE	CG-CD1	5.17	1.46	1.38
7	G	119	TYR	CD1-CE1	5.17	1.47	1.39
27	O	387	ARG	CZ-NH1	5.17	1.39	1.33
24	Q	50	ARG	CZ-NH2	5.17	1.39	1.33
12	l	223	LEU	N-CA	-5.17	1.36	1.46
13	6	10	PHE	CG-CD2	5.17	1.46	1.38
6	f	202	ARG	NE-CZ	5.16	1.39	1.33
7	g	75	GLY	CA-C	-5.16	1.43	1.51
28	H	88	ARG	CZ-NH2	5.16	1.39	1.33
13	6	131	TYR	CG-CD1	5.16	1.45	1.39
16	V	286	GLU	CG-CD	5.16	1.59	1.51
21	N	101	ILE	C-N	5.16	1.46	1.34
5	e	231	TYR	CZ-OH	5.16	1.46	1.37
8	h	34	TYR	CZ-OH	5.16	1.46	1.37
11	k	190	ARG	NE-CZ	5.16	1.39	1.33
14	n	92	ASP	CB-CG	5.16	1.62	1.51
22	S	119	TYR	CZ-OH	5.16	1.46	1.37
3	C	18	ARG	NE-CZ	5.15	1.39	1.33
20	Z	718	ASP	N-CA	5.15	1.56	1.46
28	H	94	GLU	CG-CD	5.15	1.59	1.51
7	g	185	GLU	CD-OE1	5.15	1.31	1.25
27	O	164	PRO	N-CA	-5.15	1.38	1.47
6	f	157	TYR	CZ-OH	5.15	1.46	1.37
24	Q	84	TYR	CE2-CZ	5.15	1.45	1.38
30	K	350	ARG	CZ-NH2	5.15	1.39	1.33
20	Z	312	TYR	CE2-CZ	5.15	1.45	1.38
10	j	67	PHE	CE2-CZ	5.14	1.47	1.37
2	B	219	PRO	N-CD	-5.14	1.40	1.47
31	L	145	ARG	CZ-NH2	5.14	1.39	1.33
3	C	20	TYR	CE2-CZ	5.14	1.45	1.38
14	7	170	TYR	CE2-CZ	5.14	1.45	1.38
32	M	339	ARG	CZ-NH2	5.14	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	98	ARG	NE-CZ	5.13	1.39	1.33
14	7	189	ARG	CZ-NH2	5.13	1.39	1.33
31	L	168	TYR	CE1-CZ	5.13	1.45	1.38
31	L	434	TYR	CD2-CE2	5.13	1.47	1.39
32	M	344	ASP	CA-CB	5.13	1.65	1.53
2	B	247	LEU	CA-CB	5.13	1.65	1.53
7	g	18	ASP	CB-CG	5.13	1.62	1.51
13	m	65	PHE	CE1-CZ	5.13	1.47	1.37
2	b	178	ARG	NE-CZ	5.13	1.39	1.33
4	d	141	ARG	NE-CZ	5.13	1.39	1.33
4	D	90	ARG	CD-NE	5.13	1.55	1.46
7	G	4	ILE	C-N	5.13	1.42	1.33
9	2	149	ASP	CB-CG	5.13	1.62	1.51
20	Z	337	GLU	CB-CG	5.13	1.61	1.52
20	Z	927	VAL	CB-CG2	5.13	1.63	1.52
3	c	67	TYR	CD2-CE2	5.12	1.47	1.39
28	H	390	ARG	CZ-NH2	5.12	1.39	1.33
28	H	408	SER	CA-CB	5.12	1.60	1.52
4	d	48	ARG	CZ-NH2	5.12	1.39	1.33
3	C	127	GLY	CA-C	-5.12	1.43	1.51
3	c	180	TYR	CE2-CZ	5.12	1.45	1.38
3	C	226	TYR	CG-CD1	5.12	1.45	1.39
16	V	254	ARG	CZ-NH1	5.12	1.39	1.33
20	Z	912	PHE	CE1-CZ	5.12	1.47	1.37
3	c	114	ARG	CZ-NH2	5.12	1.39	1.33
32	M	342	ARG	CZ-NH2	5.12	1.39	1.33
9	i	232	TYR	CE1-CZ	5.12	1.45	1.38
4	D	120	TYR	CG-CD1	5.12	1.45	1.39
26	U	176	ARG	CZ-NH1	5.12	1.39	1.33
1	A	104	PHE	CG-CD1	5.11	1.46	1.38
17	T	88	TYR	CE1-CZ	5.11	1.45	1.38
27	O	249	ASP	CB-CG	5.11	1.62	1.51
32	M	180	TYR	CE2-CZ	5.11	1.45	1.38
2	b	148	TYR	CG-CD2	5.11	1.45	1.39
1	A	26	TYR	CG-CD1	5.11	1.45	1.39
16	V	25	GLU	CG-CD	-5.11	1.44	1.51
3	c	122	TYR	CZ-OH	5.11	1.46	1.37
6	F	128	TYR	CD2-CE2	5.11	1.47	1.39
24	Q	309	ARG	CZ-NH2	5.11	1.39	1.33
1	A	9	ALA	CA-C	-5.10	1.39	1.52
27	O	229	ASN	N-CA	-5.10	1.36	1.46
28	H	289	ARG	CZ-NH1	5.10	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	209	ARG	CD-NE	5.10	1.55	1.46
30	K	239	GLY	N-CA	-5.10	1.38	1.46
4	D	148	TYR	CZ-OH	5.09	1.46	1.37
14	7	120	LEU	CA-C	-5.09	1.39	1.52
31	L	329	ARG	CZ-NH2	5.09	1.39	1.33
10	j	203	ARG	NE-CZ	5.09	1.39	1.33
2	b	124	SER	CB-OG	5.09	1.48	1.42
20	Z	492	GLY	CA-C	-5.09	1.43	1.51
25	R	49	PHE	CG-CD2	5.09	1.46	1.38
11	4	190	ARG	NE-CZ	5.09	1.39	1.33
27	O	189	TYR	CG-CD1	5.09	1.45	1.39
13	6	45	SER	CA-C	-5.08	1.39	1.52
28	H	181	TYR	CZ-OH	5.08	1.46	1.37
13	m	36	ARG	NE-CZ	5.08	1.39	1.33
20	Z	849	ARG	CD-NE	5.08	1.55	1.46
32	M	198	VAL	CA-CB	-5.08	1.44	1.54
1	A	84	ASN	CB-CG	5.08	1.62	1.51
24	Q	332	ARG	CD-NE	5.08	1.55	1.46
33	J	238	ARG	CD-NE	5.08	1.55	1.46
20	Z	592	GLU	CD-OE1	-5.08	1.20	1.25
21	N	736	PHE	CG-CD2	5.08	1.46	1.38
7	G	171	SER	CB-OG	5.07	1.48	1.42
20	Z	261	ASP	CB-CG	5.07	1.62	1.51
25	R	334	ARG	CD-NE	5.07	1.55	1.46
7	g	184	PRO	N-CA	-5.07	1.38	1.47
32	M	184	GLY	CA-C	-5.06	1.43	1.51
6	F	3	ARG	CZ-NH1	5.06	1.39	1.33
14	7	93	MET	CA-CB	5.06	1.65	1.53
20	Z	435	GLN	CG-CD	5.06	1.62	1.51
9	i	62	LYS	CB-CG	5.06	1.66	1.52
21	N	857	TYR	CE2-CZ	5.06	1.45	1.38
4	D	138	PHE	CG-CD2	5.06	1.46	1.38
6	F	177	ASP	CB-CG	5.06	1.62	1.51
11	4	138	PHE	CE1-CZ	5.06	1.47	1.37
23	P	106	SER	CA-CB	5.06	1.60	1.52
20	Z	565	PHE	CB-CG	5.06	1.59	1.51
16	V	28	TYR	CE1-CZ	5.05	1.45	1.38
1	a	161	GLY	N-CA	5.05	1.53	1.46
14	n	220	ARG	CZ-NH1	5.05	1.39	1.33
20	Z	700	GLU	CG-CD	5.05	1.59	1.51
22	S	480	ARG	CZ-NH2	5.05	1.39	1.33
11	k	171	ARG	CD-NE	5.05	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	840	ARG	CZ-NH2	5.05	1.39	1.33
24	Q	146	TYR	CE2-CZ	5.05	1.45	1.38
32	M	425	ARG	CZ-NH2	5.04	1.39	1.33
20	Z	801	HIS	CB-CG	-5.04	1.41	1.50
22	S	286	TYR	CG-CD2	5.04	1.45	1.39
28	H	162	ARG	CA-CB	5.04	1.65	1.53
11	4	108	ASP	N-CA	-5.04	1.36	1.46
22	S	239	ARG	NE-CZ	5.04	1.39	1.33
31	L	106	GLY	N-CA	-5.04	1.38	1.46
14	n	128	TYR	CZ-OH	5.04	1.46	1.37
6	F	24	TYR	CD2-CE2	5.04	1.47	1.39
3	c	92	ARG	CD-NE	5.04	1.55	1.46
9	i	224	VAL	N-CA	-5.04	1.36	1.46
14	n	137	ARG	CZ-NH1	5.04	1.39	1.33
2	b	55	LEU	N-CA	-5.04	1.36	1.46
4	d	148	TYR	CZ-OH	5.04	1.46	1.37
5	E	167	TYR	CB-CG	-5.04	1.44	1.51
22	S	110	LEU	N-CA	-5.03	1.36	1.46
23	P	414	GLU	C-N	5.03	1.45	1.34
9	i	193	TRP	CG-CD2	5.03	1.52	1.43
21	N	570	ARG	CZ-NH2	5.03	1.39	1.33
20	Z	189	ALA	CA-CB	5.03	1.63	1.52
25	R	20	ARG	NE-CZ	5.03	1.39	1.33
27	O	157	LEU	N-CA	-5.03	1.36	1.46
29	I	340	ARG	CZ-NH1	5.03	1.39	1.33
5	e	111	SER	CA-CB	5.03	1.60	1.52
26	U	179	ARG	CZ-NH1	5.03	1.39	1.33
1	A	159	PRO	N-CD	-5.02	1.40	1.47
22	S	273	PHE	CG-CD2	5.02	1.46	1.38
12	l	102	ALA	CA-C	-5.02	1.39	1.52
31	L	210	VAL	C-N	5.02	1.42	1.33
28	H	433	ALA	CA-CB	5.02	1.62	1.52
3	c	15	PRO	N-CD	-5.02	1.40	1.47
8	1	133	TYR	CG-CD2	5.02	1.45	1.39
21	N	511	GLY	CA-C	5.02	1.59	1.51
23	P	310	ARG	CZ-NH1	5.02	1.39	1.33
33	J	404	PHE	CE2-CZ	5.02	1.46	1.37
21	N	402	GLY	C-N	5.02	1.42	1.33
28	H	335	GLU	CG-CD	5.02	1.59	1.51
13	6	69	GLY	N-CA	-5.01	1.38	1.46
16	V	203	TYR	CZ-OH	5.01	1.46	1.37
24	Q	65	TYR	CZ-OH	5.01	1.46	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	346	ARG	CZ-NH2	5.01	1.39	1.33
33	J	228	ARG	CD-NE	5.01	1.54	1.46
16	V	228	TYR	CZ-OH	5.01	1.46	1.37
17	T	177	PHE	CE2-CZ	5.01	1.46	1.37
21	N	902	VAL	CA-CB	-5.01	1.44	1.54
23	P	440	HIS	C-OXT	5.01	1.32	1.23
21	N	23	TYR	CE2-CZ	5.00	1.45	1.38
18	X	59	ARG	NE-CZ	5.00	1.39	1.33
21	N	881	TYR	CG-CD1	-5.00	1.32	1.39
5	e	86	ARG	CZ-NH2	5.00	1.39	1.33
6	F	144	LEU	CA-CB	5.00	1.65	1.53
17	T	144	TYR	CZ-OH	5.00	1.46	1.37
22	S	405	ARG	CZ-NH2	5.00	1.39	1.33

All (2644) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	197	ARG	NE-CZ-NH2	-20.22	110.19	120.30
28	H	62	ARG	NE-CZ-NH2	-19.43	110.58	120.30
20	Z	948	TRP	CZ3-CH2-CZ2	-19.17	98.59	121.60
1	a	110	TYR	CB-CG-CD1	-19.04	109.57	121.00
21	N	417	ARG	NE-CZ-NH1	-17.94	111.33	120.30
10	3	68	ARG	NE-CZ-NH2	-17.60	111.50	120.30
12	l	82	ARG	NE-CZ-NH1	17.32	128.96	120.30
1	a	46	ARG	NE-CZ-NH2	-17.22	111.69	120.30
25	R	94	PHE	CB-CG-CD1	-16.93	108.95	120.80
1	a	46	ARG	NE-CZ-NH1	16.66	128.63	120.30
22	S	399	TYR	CB-CG-CD2	-16.61	111.04	121.00
28	H	429	PHE	CB-CG-CD1	16.25	132.17	120.80
6	F	24	TYR	CB-CG-CD2	-15.89	111.47	121.00
20	Z	553	ARG	NE-CZ-NH2	-15.83	112.38	120.30
2	B	174	PHE	CB-CG-CD1	15.56	131.69	120.80
28	H	429	PHE	CB-CG-CD2	-15.23	110.14	120.80
25	R	210	TYR	CB-CG-CD2	-15.20	111.88	121.00
31	L	392	ARG	NE-CZ-NH2	-15.19	112.70	120.30
28	H	353	PHE	CB-CG-CD1	-15.06	110.25	120.80
10	j	199	TYR	CB-CG-CD1	-14.91	112.05	121.00
5	e	10	ARG	NE-CZ-NH2	-14.91	112.85	120.30
25	R	43	ARG	NE-CZ-NH1	14.84	127.72	120.30
5	e	102	TYR	CB-CG-CD2	14.75	129.85	121.00
27	O	166	ARG	NE-CZ-NH1	14.67	127.64	120.30
24	Q	309	ARG	NE-CZ-NH1	14.62	127.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	299	ARG	NE-CZ-NH2	-14.55	113.02	120.30
5	E	231	TYR	CB-CG-CD1	-14.46	112.32	121.00
22	S	111	ARG	NE-CZ-NH2	-14.37	113.12	120.30
22	S	196	ARG	NE-CZ-NH2	-14.34	113.13	120.30
5	E	165	TYR	CB-CG-CD1	-14.16	112.50	121.00
28	H	299	ARG	NE-CZ-NH1	14.14	127.37	120.30
1	A	96	ARG	NE-CZ-NH2	-14.04	113.28	120.30
10	j	99	ARG	NE-CZ-NH2	13.96	127.28	120.30
24	Q	309	ARG	NE-CZ-NH2	-13.96	113.32	120.30
8	1	144	TYR	CB-CG-CD2	13.92	129.35	121.00
16	V	196	TYR	CB-CG-CD2	13.89	129.33	121.00
30	K	347	ARG	NE-CZ-NH2	-13.79	113.41	120.30
4	D	127	ARG	NE-CZ-NH2	-13.75	113.42	120.30
20	Z	165	TYR	CB-CG-CD1	-13.66	112.80	121.00
14	7	128	TYR	CB-CG-CD2	-13.65	112.81	121.00
22	S	345	TYR	CB-CG-CD2	13.62	129.17	121.00
27	O	26	PHE	CB-CG-CD1	-13.55	111.32	120.80
22	S	346	TYR	CB-CG-CD2	-13.54	112.88	121.00
26	U	283	ARG	NE-CZ-NH1	13.51	127.05	120.30
10	3	198	ARG	NE-CZ-NH2	-13.48	113.56	120.30
20	Z	236	PHE	CB-CG-CD2	-13.40	111.42	120.80
22	S	399	TYR	CB-CG-CD1	13.32	128.99	121.00
30	K	411	TYR	CB-CG-CD1	-13.32	113.01	121.00
1	A	12	TYR	CB-CG-CD2	-13.31	113.02	121.00
24	Q	264	TYR	CB-CG-CD2	-13.22	113.07	121.00
28	H	62	ARG	NE-CZ-NH1	13.22	126.91	120.30
2	B	23	TYR	CB-CG-CD2	-13.20	113.08	121.00
1	a	163	TYR	CB-CG-CD2	-13.17	113.10	121.00
30	K	400	TYR	CB-CG-CD2	13.14	128.88	121.00
23	P	303	PHE	CB-CG-CD2	-13.13	111.61	120.80
27	O	369	ARG	NE-CZ-NH2	13.11	126.85	120.30
28	H	353	PHE	CB-CG-CD2	13.05	129.94	120.80
27	O	106	PHE	CB-CG-CD1	13.03	129.92	120.80
16	V	196	TYR	CB-CG-CD1	-12.94	113.24	121.00
2	B	75	TYR	CB-CG-CD1	12.92	128.75	121.00
16	V	251	TYR	CB-CG-CD1	12.84	128.70	121.00
10	j	199	TYR	CB-CG-CD2	12.81	128.69	121.00
21	N	203	ARG	NE-CZ-NH2	-12.81	113.90	120.30
14	7	179	PHE	CB-CG-CD1	-12.72	111.90	120.80
31	L	194	ARG	NE-CZ-NH2	-12.71	113.95	120.30
17	T	128	TYR	CB-CG-CD1	12.70	128.62	121.00
28	H	318	ARG	NE-CZ-NH2	-12.70	113.95	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	312	TYR	CB-CG-CD2	-12.65	113.41	121.00
12	l	181	ARG	NE-CZ-NH1	12.56	126.58	120.30
17	T	128	TYR	CB-CG-CD2	-12.54	113.47	121.00
11	k	195	PHE	CB-CG-CD2	-12.52	112.03	120.80
1	A	106	TYR	CB-CG-CD2	-12.45	113.53	121.00
2	B	75	TYR	CB-CG-CD2	-12.39	113.57	121.00
13	m	46	ARG	NE-CZ-NH1	12.32	126.46	120.30
20	Z	138	ARG	NE-CZ-NH1	12.30	126.45	120.30
33	J	43	ARG	NE-CZ-NH2	-12.29	114.15	120.30
5	E	165	TYR	CB-CG-CD2	12.27	128.36	121.00
32	M	45	ARG	NE-CZ-NH1	12.22	126.41	120.30
31	L	255	TYR	CB-CG-CD2	-12.22	113.67	121.00
28	H	346	ARG	NE-CZ-NH2	-12.18	114.21	120.30
1	A	73	PHE	CB-CG-CD1	-12.14	112.30	120.80
26	U	176	ARG	NE-CZ-NH1	12.10	126.35	120.30
31	L	70	TYR	CB-CG-CD2	12.10	128.26	121.00
25	R	321	TYR	CB-CG-CD1	-12.10	113.74	121.00
6	f	3	ARG	NE-CZ-NH2	-12.09	114.26	120.30
7	g	157	TYR	CB-CG-CD1	-12.09	113.75	121.00
4	D	22	TYR	CB-CG-CD2	-12.01	113.80	121.00
22	S	111	ARG	NE-CZ-NH1	11.96	126.28	120.30
25	R	43	ARG	NE-CZ-NH2	-11.94	114.33	120.30
13	m	46	ARG	NE-CZ-NH2	-11.90	114.35	120.30
12	5	245	TYR	CB-CG-CD2	-11.90	113.86	121.00
14	n	109	TYR	CB-CG-CD1	11.88	128.13	121.00
1	A	233	PHE	CB-CG-CD1	-11.85	112.51	120.80
10	j	164	PHE	CB-CG-CD2	-11.83	112.52	120.80
10	j	164	PHE	CB-CG-CD1	11.83	129.08	120.80
30	K	400	TYR	CB-CG-CD1	-11.82	113.91	121.00
18	X	87	PHE	CB-CG-CD2	-11.78	112.55	120.80
20	Z	210	TYR	CB-CG-CD1	11.77	128.06	121.00
14	7	98	ARG	NE-CZ-NH2	11.76	126.18	120.30
32	M	425	ARG	NE-CZ-NH2	-11.74	114.43	120.30
21	N	162	ARG	NE-CZ-NH2	-11.74	114.43	120.30
22	S	382	ARG	NE-CZ-NH2	-11.73	114.43	120.30
22	S	25	TYR	CB-CG-CD1	-11.71	113.97	121.00
27	O	137	TYR	CB-CG-CD1	-11.67	114.00	121.00
8	h	60	ASP	CB-CG-OD1	-11.63	107.83	118.30
22	S	405	ARG	NE-CZ-NH1	11.63	126.11	120.30
1	A	12	TYR	CB-CG-CD1	11.62	127.97	121.00
21	N	161	TYR	CB-CG-CD2	-11.62	114.03	121.00
6	f	59	TYR	CB-CG-CD1	11.61	127.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	226	ARG	NE-CZ-NH1	11.57	126.08	120.30
23	P	351	ARG	NE-CZ-NH2	-11.56	114.52	120.30
9	i	48	ARG	NE-CZ-NH2	-11.54	114.53	120.30
14	7	159	PHE	CB-CG-CD2	-11.52	112.74	120.80
31	L	209	ARG	NE-CZ-NH1	-11.46	114.57	120.30
14	7	137	ARG	NE-CZ-NH2	-11.46	114.57	120.30
26	U	52	PHE	CB-CG-CD1	-11.45	112.79	120.80
25	R	94	PHE	CB-CG-CD2	11.44	128.81	120.80
2	B	142	PHE	CB-CG-CD2	-11.43	112.80	120.80
14	n	218	TYR	CB-CG-CD1	11.41	127.84	121.00
12	l	179	TYR	CB-CG-CD1	11.38	127.83	121.00
31	L	345	ARG	NE-CZ-NH2	-11.37	114.62	120.30
1	A	120	ARG	NE-CZ-NH2	-11.35	114.62	120.30
33	J	228	ARG	NE-CZ-NH1	11.34	125.97	120.30
31	L	157	ARG	NE-CZ-NH2	11.34	125.97	120.30
23	P	3	ARG	NE-CZ-NH2	-11.33	114.63	120.30
32	M	357	ARG	NE-CZ-NH2	-11.31	114.64	120.30
21	N	861	TYR	CB-CG-CD1	-11.30	114.22	121.00
33	J	116	ARG	NE-CZ-NH2	11.29	125.95	120.30
8	1	45	ARG	NE-CZ-NH1	-11.20	114.70	120.30
28	H	400	ARG	NE-CZ-NH1	11.17	125.89	120.30
21	N	857	TYR	CB-CG-CD2	-11.15	114.31	121.00
15	W	23	ARG	NE-CZ-NH1	11.15	125.88	120.30
16	V	251	TYR	CB-CG-CD2	-11.14	114.31	121.00
12	l	188	TYR	CB-CG-CD1	-11.14	114.32	121.00
30	K	347	ARG	NE-CZ-NH1	11.13	125.86	120.30
28	H	90	ARG	NE-CZ-NH2	11.12	125.86	120.30
6	F	24	TYR	CB-CG-CD1	11.11	127.67	121.00
7	g	91	ARG	NE-CZ-NH2	11.10	125.85	120.30
22	S	239	ARG	NE-CZ-NH2	-11.04	114.78	120.30
2	B	174	PHE	CB-CG-CD2	-11.03	113.08	120.80
3	C	129	ARG	NE-CZ-NH1	11.02	125.81	120.30
5	E	20	ARG	NE-CZ-NH2	-11.01	114.79	120.30
20	Z	126	TYR	CB-CG-CD2	-11.00	114.40	121.00
22	S	196	ARG	NE-CZ-NH1	11.00	125.80	120.30
20	Z	941	ARG	NE-CZ-NH2	-10.99	114.81	120.30
3	C	24	TYR	CB-CG-CD2	-10.97	114.42	121.00
3	c	6	TYR	CB-CG-CD2	10.95	127.57	121.00
1	a	131	ARG	NE-CZ-NH1	10.94	125.77	120.30
2	b	4	ARG	NE-CZ-NH1	10.91	125.75	120.30
5	e	138	PHE	CB-CG-CD2	-10.90	113.17	120.80
2	B	156	TYR	CB-CG-CD2	10.85	127.51	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	j	40	PHE	CB-CG-CD2	-10.83	113.22	120.80
25	R	210	TYR	CB-CG-CD1	10.81	127.48	121.00
32	M	166	ARG	NE-CZ-NH1	10.79	125.69	120.30
33	J	309	ARG	NE-CZ-NH1	10.74	125.67	120.30
4	D	141	ARG	NE-CZ-NH2	-10.72	114.94	120.30
6	f	3	ARG	NE-CZ-NH1	10.70	125.65	120.30
4	d	138	PHE	CB-CG-CD1	-10.69	113.31	120.80
21	N	328	PHE	CB-CG-CD1	10.69	128.28	120.80
14	n	136	ARG	NE-CZ-NH2	-10.69	114.96	120.30
14	7	134	TYR	CB-CG-CD1	-10.67	114.60	121.00
3	c	230	PHE	CB-CG-CD1	10.67	128.27	120.80
22	S	452	TYR	CB-CG-CD2	10.67	127.40	121.00
20	Z	242	PHE	CB-CG-CD1	10.67	128.27	120.80
11	4	70	ARG	NE-CZ-NH2	-10.66	114.97	120.30
10	j	98	ARG	NE-CZ-NH2	-10.66	114.97	120.30
22	S	464	ARG	NE-CZ-NH2	-10.64	114.98	120.30
8	1	144	TYR	CB-CG-CD1	-10.61	114.63	121.00
20	Z	199	ASP	CB-CG-OD1	10.61	127.85	118.30
6	F	157	TYR	CB-CG-CD1	-10.61	114.64	121.00
27	O	288	ARG	NE-CZ-NH1	10.60	125.60	120.30
11	4	73	TYR	CB-CG-CD1	-10.57	114.66	121.00
3	c	114	ARG	NE-CZ-NH2	-10.57	115.02	120.30
33	J	43	ARG	NE-CZ-NH1	10.55	125.58	120.30
14	n	109	TYR	CB-CG-CD2	-10.55	114.67	121.00
6	f	107	ARG	NE-CZ-NH2	10.53	125.56	120.30
8	1	48	ASP	CB-CG-OD2	-10.52	108.83	118.30
26	U	24	ARG	NE-CZ-NH1	10.47	125.53	120.30
23	P	273	TYR	CB-CG-CD1	10.45	127.27	121.00
11	4	96	ARG	NE-CZ-NH1	-10.44	115.08	120.30
11	k	23	ARG	NE-CZ-NH1	10.43	125.52	120.30
9	i	98	TYR	CB-CG-CD2	-10.42	114.75	121.00
27	O	306	ARG	NE-CZ-NH1	-10.40	115.10	120.30
4	D	179	TYR	CB-CG-CD1	-10.38	114.77	121.00
29	I	246	ARG	NE-CZ-NH1	10.38	125.49	120.30
23	P	3	ARG	NE-CZ-NH1	10.37	125.49	120.30
14	7	134	TYR	CB-CG-CD2	10.37	127.22	121.00
6	f	101	ARG	NE-CZ-NH2	-10.37	115.11	120.30
26	U	288	PHE	CB-CG-CD2	-10.33	113.57	120.80
33	J	23	PHE	CB-CG-CD1	10.31	128.02	120.80
22	S	375	ASP	CB-CG-OD1	-10.31	109.02	118.30
23	P	13	TYR	CB-CG-CD2	-10.31	114.81	121.00
8	h	60	ASP	CB-CG-OD2	10.30	127.57	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	162	ARG	NE-CZ-NH1	10.29	125.45	120.30
28	H	261	ARG	NE-CZ-NH2	-10.29	115.15	120.30
11	4	93	ARG	NE-CZ-NH2	-10.28	115.16	120.30
22	S	428	ARG	NE-CZ-NH2	-10.28	115.16	120.30
6	f	94	TYR	CB-CG-CD2	10.26	127.16	121.00
24	Q	246	TYR	CB-CG-CD1	-10.24	114.86	121.00
11	k	195	PHE	CB-CG-CD1	10.21	127.95	120.80
32	M	124	ARG	NE-CZ-NH1	10.20	125.40	120.30
2	b	23	TYR	CB-CG-CD2	-10.19	114.89	121.00
32	M	203	ARG	NE-CZ-NH2	-10.17	115.22	120.30
10	j	144	ASP	CB-CG-OD2	-10.17	109.15	118.30
12	5	150	SER	N-CA-CB	10.17	125.75	110.50
16	V	194	ARG	NE-CZ-NH1	10.16	125.38	120.30
20	Z	323	TYR	CB-CG-CD2	10.16	127.10	121.00
20	Z	738	TYR	CD1-CE1-CZ	10.16	128.95	119.80
3	c	230	PHE	CB-CG-CD2	-10.16	113.69	120.80
7	G	15	PHE	CB-CG-CD2	-10.15	113.69	120.80
25	R	246	TYR	CG-CD1-CE1	-10.14	113.19	121.30
12	l	94	ARG	NE-CZ-NH1	10.12	125.36	120.30
28	H	289	ARG	NE-CZ-NH1	10.12	125.36	120.30
4	D	179	TYR	CB-CG-CD2	10.10	127.06	121.00
29	I	54	ARG	NE-CZ-NH1	10.09	125.35	120.30
2	B	234	ARG	NE-CZ-NH1	10.09	125.34	120.30
27	O	266	PHE	CB-CG-CD1	-10.09	113.74	120.80
29	I	327	ALA	N-CA-CB	10.07	124.20	110.10
20	Z	138	ARG	NE-CZ-NH2	-10.07	115.27	120.30
20	Z	738	TYR	CE1-CZ-CE2	-10.06	103.70	119.80
10	j	188	TYR	CB-CG-CD2	10.06	127.04	121.00
13	6	221	ARG	NE-CZ-NH2	-10.04	115.28	120.30
3	C	24	TYR	CB-CG-CD1	10.03	127.02	121.00
17	T	60	ARG	NE-CZ-NH1	10.03	125.32	120.30
22	S	82	TYR	CB-CG-CD2	10.03	127.02	121.00
5	E	122	ARG	NE-CZ-NH1	10.03	125.31	120.30
31	L	420	ARG	NE-CZ-NH2	-10.03	115.29	120.30
8	h	194	ARG	NE-CZ-NH1	10.02	125.31	120.30
28	H	409	ARG	NE-CZ-NH2	-10.02	115.29	120.30
30	K	185	ARG	NE-CZ-NH2	-10.01	115.29	120.30
4	D	58	ARG	NE-CZ-NH2	-10.00	115.30	120.30
33	J	23	PHE	CB-CG-CD2	-10.00	113.80	120.80
5	E	231	TYR	CB-CG-CD2	10.00	127.00	121.00
1	a	163	TYR	CB-CG-CD1	9.99	127.00	121.00
8	1	54	ARG	NE-CZ-NH1	9.99	125.30	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	231	ARG	NE-CZ-NH1	9.98	125.29	120.30
18	X	87	PHE	CB-CG-CD1	9.97	127.78	120.80
29	I	343	ARG	NE-CZ-NH1	9.95	125.27	120.30
21	N	559	TYR	CB-CG-CD2	-9.93	115.04	121.00
7	g	169	ARG	NE-CZ-NH1	9.92	125.26	120.30
13	m	36	ARG	NE-CZ-NH1	-9.92	115.34	120.30
11	4	176	PHE	CB-CG-CD1	-9.91	113.86	120.80
8	1	120	TYR	CB-CG-CD1	-9.91	115.05	121.00
7	g	99	PHE	CB-CG-CD2	9.91	127.74	120.80
21	N	463	TYR	CB-CG-CD1	-9.90	115.06	121.00
4	d	156	TYR	CB-CG-CD2	-9.90	115.06	121.00
22	S	480	ARG	NE-CZ-NH2	9.89	125.25	120.30
5	e	102	TYR	CB-CG-CD1	-9.88	115.07	121.00
28	H	45	TYR	CB-CG-CD2	-9.88	115.07	121.00
14	7	179	PHE	CB-CG-CD2	9.87	127.71	120.80
5	e	165	TYR	CB-CG-CD2	-9.84	115.10	121.00
32	M	42	ARG	NE-CZ-NH1	9.83	125.22	120.30
25	R	263	ARG	NE-CZ-NH1	9.82	125.21	120.30
31	L	77	ARG	NE-CZ-NH1	9.82	125.21	120.30
22	S	185	PHE	CB-CG-CD2	-9.82	113.92	120.80
23	P	37	ASP	CB-CG-OD2	9.82	127.14	118.30
30	K	236	ARG	NE-CZ-NH2	-9.81	115.39	120.30
17	T	78	PHE	CB-CG-CD1	9.80	127.66	120.80
28	H	308	PHE	CB-CG-CD2	9.80	127.66	120.80
8	1	152	ARG	NE-CZ-NH1	9.79	125.20	120.30
5	E	54	ALA	N-CA-CB	9.79	123.80	110.10
30	K	320	ARG	NE-CZ-NH2	9.74	125.17	120.30
12	l	189	TYR	CB-CG-CD1	-9.74	115.16	121.00
21	N	771	PHE	CB-CG-CD1	-9.73	113.99	120.80
14	n	218	TYR	CB-CG-CD2	-9.72	115.17	121.00
28	H	222	ARG	NE-CZ-NH1	9.71	125.16	120.30
3	c	122	TYR	CB-CG-CD2	9.70	126.82	121.00
29	I	61	ARG	NE-CZ-NH2	-9.70	115.45	120.30
2	b	12	PHE	CB-CG-CD2	-9.68	114.02	120.80
4	d	119	ARG	NE-CZ-NH1	9.67	125.14	120.30
16	V	157	ARG	NE-CZ-NH1	9.67	125.14	120.30
28	H	222	ARG	NE-CZ-NH2	-9.66	115.47	120.30
14	7	124	TYR	CG-CD1-CE1	-9.65	113.58	121.30
14	n	162	TYR	CB-CG-CD2	-9.64	115.22	121.00
26	U	113	TYR	CB-CG-CD2	9.64	126.78	121.00
3	C	5	ARG	NE-CZ-NH1	9.63	125.11	120.30
9	2	117	PHE	CB-CG-CD1	-9.61	114.08	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	100	PHE	CB-CG-CD1	-9.59	114.09	120.80
31	L	267	PHE	CB-CG-CD2	-9.58	114.09	120.80
16	V	156	PHE	CB-CG-CD1	-9.58	114.10	120.80
2	B	128	ARG	NE-CZ-NH1	9.57	125.08	120.30
9	2	98	TYR	CB-CG-CD1	-9.55	115.27	121.00
7	G	130	ARG	NE-CZ-NH1	-9.55	115.53	120.30
21	N	299	TYR	CB-CG-CD2	9.55	126.73	121.00
21	N	299	TYR	CB-CG-CD1	-9.53	115.28	121.00
1	a	104	PHE	CB-CG-CD2	-9.53	114.13	120.80
7	g	103	TYR	CB-CG-CD1	-9.52	115.29	121.00
7	g	99	PHE	CB-CG-CD1	-9.50	114.15	120.80
18	X	98	PHE	CB-CG-CD2	-9.50	114.15	120.80
27	O	115	ARG	NE-CZ-NH2	-9.49	115.55	120.30
11	k	148	TYR	CB-CG-CD1	-9.49	115.31	121.00
23	P	95	TYR	CB-CG-CD2	-9.49	115.31	121.00
28	H	235	PHE	CB-CG-CD1	9.48	127.44	120.80
25	R	297	TYR	CB-CG-CD1	-9.43	115.34	121.00
13	6	196	PHE	CB-CG-CD2	-9.42	114.20	120.80
27	O	51	ASP	CB-CG-OD1	9.42	126.78	118.30
21	N	584	ARG	NE-CZ-NH1	-9.41	115.59	120.30
28	H	377	PHE	CB-CG-CD2	-9.41	114.22	120.80
7	G	112	PHE	CB-CG-CD2	9.40	127.38	120.80
4	D	127	ARG	NE-CZ-NH1	9.38	124.99	120.30
32	M	425	ARG	NE-CZ-NH1	9.38	124.99	120.30
13	6	41	TYR	CB-CG-CD1	-9.38	115.37	121.00
14	7	220	ARG	NE-CZ-NH2	-9.38	115.61	120.30
33	J	324	ARG	NE-CZ-NH2	-9.37	115.61	120.30
11	4	117	TYR	CB-CG-CD1	9.34	126.60	121.00
30	K	411	TYR	CB-CG-CD2	9.34	126.61	121.00
16	V	42	ARG	NE-CZ-NH1	9.32	124.96	120.30
11	4	141	PHE	CB-CG-CD2	9.32	127.32	120.80
17	T	157	TYR	CB-CG-CD1	-9.29	115.42	121.00
25	R	252	TYR	CB-CG-CD2	-9.29	115.43	121.00
13	6	164	PHE	CB-CG-CD1	9.28	127.29	120.80
3	c	113	ARG	NE-CZ-NH1	-9.27	115.66	120.30
5	e	166	ARG	NE-CZ-NH1	9.27	124.94	120.30
3	c	6	TYR	CB-CG-CD1	-9.27	115.44	121.00
30	K	399	ARG	NE-CZ-NH2	-9.27	115.67	120.30
21	N	526	TYR	CB-CG-CD1	9.26	126.56	121.00
11	4	85	ARG	NE-CZ-NH1	9.25	124.92	120.30
8	1	133	TYR	CB-CG-CD1	9.23	126.54	121.00
17	T	78	PHE	CB-CG-CD2	-9.23	114.34	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	422	MET	CG-SD-CE	-9.23	85.43	100.20
6	f	107	ARG	NE-CZ-NH1	-9.23	115.69	120.30
23	P	368	LEU	CB-CG-CD2	9.21	126.65	111.00
12	l	212	TYR	CB-CG-CD2	-9.21	115.48	121.00
4	D	111	ARG	NE-CZ-NH1	9.20	124.90	120.30
21	N	762	ARG	NE-CZ-NH1	9.20	124.90	120.30
23	P	37	ASP	CB-CG-OD1	-9.18	110.04	118.30
22	S	88	PHE	CB-CG-CD2	-9.18	114.38	120.80
3	c	67	TYR	CB-CG-CD1	-9.17	115.50	121.00
19	Y	35	PHE	CB-CG-CD1	9.16	127.21	120.80
29	I	75	PHE	CB-CG-CD2	-9.16	114.39	120.80
33	J	71	TYR	CB-CG-CD1	9.13	126.48	121.00
6	f	123	TYR	CB-CG-CD2	-9.13	115.52	121.00
12	5	80	ALA	N-CA-CB	9.12	122.87	110.10
10	3	68	ARG	NH1-CZ-NH2	9.10	129.41	119.40
11	k	132	ALA	N-CA-CB	9.09	122.83	110.10
15	W	101	ARG	NE-CZ-NH1	9.09	124.84	120.30
28	H	145	TYR	CB-CG-CD1	9.09	126.45	121.00
31	L	117	TYR	CB-CG-CD1	9.08	126.45	121.00
24	Q	332	ARG	NE-CZ-NH2	-9.08	115.76	120.30
15	W	122	ARG	NE-CZ-NH1	-9.08	115.76	120.30
5	e	20	ARG	NE-CZ-NH2	9.07	124.84	120.30
11	k	70	ARG	NE-CZ-NH1	9.07	124.84	120.30
4	d	148	TYR	CB-CG-CD2	9.07	126.44	121.00
30	K	99	PHE	CB-CG-CD1	-9.07	114.45	120.80
13	m	145	ARG	NE-CZ-NH2	9.06	124.83	120.30
11	k	23	ARG	NE-CZ-NH2	9.06	124.83	120.30
12	5	115	PHE	CB-CG-CD2	-9.04	114.47	120.80
24	Q	163	ARG	NE-CZ-NH2	9.04	124.82	120.30
31	L	68	ARG	NE-CZ-NH1	-9.03	115.79	120.30
23	P	351	ARG	NE-CZ-NH1	9.02	124.81	120.30
1	a	105	ARG	NE-CZ-NH1	9.02	124.81	120.30
19	Y	38	PHE	CB-CG-CD2	-9.01	114.49	120.80
24	Q	51	ARG	NE-CZ-NH1	9.00	124.80	120.30
6	F	101	ARG	NE-CZ-NH2	-8.99	115.80	120.30
33	J	306	ARG	NE-CZ-NH2	8.99	124.80	120.30
4	D	112	TYR	CG-CD1-CE1	-8.99	114.11	121.30
3	c	114	ARG	NE-CZ-NH1	8.97	124.79	120.30
1	A	24	ARG	NE-CZ-NH1	8.97	124.79	120.30
28	H	462	ARG	NE-CZ-NH2	-8.97	115.81	120.30
28	H	308	PHE	CB-CG-CD1	-8.97	114.52	120.80
22	S	55	ARG	NE-CZ-NH1	-8.96	115.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	162	TYR	CB-CG-CD1	8.96	126.38	121.00
18	X	97	TYR	CB-CG-CD2	-8.94	115.64	121.00
5	E	103	TYR	CB-CG-CD1	-8.92	115.65	121.00
1	a	110	TYR	CB-CG-CD2	8.91	126.35	121.00
23	P	240	TYR	CB-CG-CD2	-8.89	115.66	121.00
31	L	191	ARG	NE-CZ-NH2	8.89	124.75	120.30
22	S	25	TYR	CB-CG-CD2	8.89	126.33	121.00
32	M	207	PHE	CB-CG-CD2	-8.89	114.58	120.80
21	N	208	ARG	NE-CZ-NH2	-8.88	115.86	120.30
7	G	160	TYR	CB-CG-CD2	-8.87	115.68	121.00
21	N	559	TYR	CB-CG-CD1	8.87	126.32	121.00
11	k	23	ARG	NH1-CZ-NH2	-8.86	109.65	119.40
29	I	304	ARG	NE-CZ-NH1	8.86	124.73	120.30
3	C	129	ARG	NE-CZ-NH2	-8.86	115.87	120.30
20	Z	126	TYR	CB-CG-CD1	8.86	126.32	121.00
2	B	90	ARG	NE-CZ-NH1	8.85	124.73	120.30
11	k	117	TYR	CB-CG-CD1	-8.85	115.69	121.00
21	N	328	PHE	CB-CG-CD2	-8.84	114.61	120.80
31	L	69	ARG	NE-CZ-NH1	-8.84	115.88	120.30
21	N	161	TYR	CB-CG-CD1	8.83	126.30	121.00
27	O	161	ASP	CB-CG-OD1	-8.82	110.36	118.30
7	G	201	TYR	CG-CD2-CE2	-8.82	114.24	121.30
1	a	108	TYR	CB-CG-CD2	8.81	126.28	121.00
24	Q	264	TYR	CB-CG-CD1	8.80	126.28	121.00
29	I	75	PHE	CB-CG-CD1	8.80	126.96	120.80
10	3	98	ARG	NE-CZ-NH2	-8.78	115.91	120.30
9	2	236	ARG	NE-CZ-NH1	8.77	124.69	120.30
11	k	141	PHE	CB-CG-CD2	-8.77	114.66	120.80
7	g	130	ARG	NE-CZ-NH2	-8.77	115.92	120.30
8	1	146	TYR	CB-CG-CD1	8.76	126.25	121.00
7	g	93	ARG	NE-CZ-NH2	-8.74	115.93	120.30
12	l	230	TYR	CB-CG-CD2	8.73	126.24	121.00
1	A	231	ASP	CB-CG-OD2	-8.73	110.45	118.30
1	a	160	ALA	CB-CA-C	-8.72	97.02	110.10
30	K	252	ARG	NE-CZ-NH2	-8.72	115.94	120.30
30	K	141	ARG	NE-CZ-NH1	8.71	124.66	120.30
20	Z	287	ARG	NE-CZ-NH1	8.70	124.65	120.30
31	L	132	ARG	NE-CZ-NH1	-8.69	115.95	120.30
12	l	94	ARG	NE-CZ-NH2	-8.69	115.95	120.30
3	C	217	ARG	NE-CZ-NH1	-8.69	115.96	120.30
31	L	77	ARG	NE-CZ-NH2	-8.66	115.97	120.30
30	K	121	ARG	NE-CZ-NH1	8.65	124.63	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	301	PHE	CB-CG-CD2	-8.64	114.75	120.80
7	g	160	TYR	CB-CG-CD1	8.64	126.18	121.00
2	b	148	TYR	CB-CG-CD1	8.64	126.18	121.00
21	N	202	PHE	CB-CG-CD2	-8.64	114.75	120.80
21	N	771	PHE	CB-CG-CD2	8.63	126.84	120.80
22	S	114	TYR	CB-CG-CD1	-8.63	115.82	121.00
25	R	203	ASP	CB-CG-OD2	8.62	126.06	118.30
33	J	404	PHE	CB-CG-CD1	8.62	126.83	120.80
6	f	94	TYR	CB-CG-CD1	-8.61	115.83	121.00
12	5	245	TYR	CB-CG-CD1	8.60	126.16	121.00
25	R	383	ARG	NE-CZ-NH2	-8.60	116.00	120.30
20	Z	358	TYR	CB-CG-CD1	8.58	126.15	121.00
7	G	115	ARG	NE-CZ-NH1	-8.57	116.01	120.30
23	P	245	TYR	CB-CG-CD1	-8.57	115.86	121.00
33	J	35	ARG	NE-CZ-NH1	8.57	124.58	120.30
9	i	234	PHE	CB-CG-CD1	8.55	126.79	120.80
28	H	145	TYR	CB-CG-CD2	-8.55	115.87	121.00
1	A	46	ARG	NE-CZ-NH1	8.55	124.57	120.30
20	Z	738	TYR	CZ-CE2-CD2	8.55	127.49	119.80
3	c	182	ASP	CB-CG-OD2	-8.54	110.61	118.30
14	7	124	TYR	CB-CG-CD1	-8.54	115.88	121.00
9	i	126	TYR	CB-CG-CD2	-8.53	115.88	121.00
22	S	309	PHE	CB-CG-CD2	8.53	126.77	120.80
3	C	143	ARG	NE-CZ-NH1	8.53	124.56	120.30
26	U	124	ASP	CB-CG-OD2	-8.53	110.63	118.30
22	S	481	TYR	CB-CG-CD2	-8.52	115.89	121.00
11	4	73	TYR	CB-CG-CD2	8.51	126.11	121.00
17	T	266	TYR	CB-CG-CD2	8.51	126.11	121.00
22	S	95	PHE	CB-CG-CD1	-8.50	114.85	120.80
20	Z	912	PHE	CB-CG-CD1	-8.48	114.86	120.80
31	L	303	ARG	NE-CZ-NH2	-8.48	116.06	120.30
13	6	168	TYR	CB-CG-CD2	-8.47	115.92	121.00
14	n	161	ARG	NE-CZ-NH1	8.46	124.53	120.30
9	i	152	TYR	CB-CG-CD2	-8.46	115.93	121.00
31	L	261	ARG	NE-CZ-NH2	-8.46	116.07	120.30
25	R	206	ARG	NE-CZ-NH2	-8.46	116.07	120.30
33	J	316	PHE	CB-CG-CD2	-8.45	114.88	120.80
32	M	33	ARG	NE-CZ-NH2	-8.45	116.08	120.30
5	e	72	ARG	NE-CZ-NH2	8.44	124.52	120.30
2	B	4	ARG	NE-CZ-NH2	-8.43	116.08	120.30
21	N	394	ARG	NE-CZ-NH1	-8.42	116.09	120.30
7	G	8	TYR	CB-CG-CD2	-8.41	115.95	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	345	ARG	NE-CZ-NH1	8.40	124.50	120.30
12	5	96	THR	CA-CB-CG2	-8.39	100.65	112.40
16	V	122	ASP	CB-CG-OD2	-8.39	110.75	118.30
12	l	272	PHE	CB-CG-CD2	-8.39	114.93	120.80
33	J	148	ASP	CB-CG-OD2	8.38	125.84	118.30
21	N	398	ARG	NE-CZ-NH2	-8.38	116.11	120.30
5	e	93	ARG	NE-CZ-NH1	8.37	124.49	120.30
14	7	128	TYR	CB-CG-CD1	8.34	126.00	121.00
4	D	181	ARG	NE-CZ-NH2	-8.32	116.14	120.30
11	4	176	PHE	CB-CG-CD2	8.32	126.62	120.80
28	H	400	ARG	NE-CZ-NH2	-8.31	116.14	120.30
14	n	261	TYR	CB-CG-CD2	8.30	125.98	121.00
15	W	182	TYR	CB-CG-CD1	-8.30	116.02	121.00
20	Z	738	TYR	OH-CZ-CE2	8.30	142.50	120.10
33	J	286	LYS	CD-CE-NZ	8.30	130.78	111.70
27	O	249	ASP	CB-CG-OD1	8.29	125.77	118.30
12	l	202	PHE	CB-CG-CD1	-8.29	115.00	120.80
28	H	266	ARG	NE-CZ-NH2	-8.29	116.16	120.30
20	Z	840	ARG	NE-CZ-NH1	8.28	124.44	120.30
29	I	135	PHE	CB-CG-CD1	8.27	126.59	120.80
28	H	389	PHE	CB-CG-CD1	-8.25	115.02	120.80
5	e	103	TYR	CB-CG-CD2	8.24	125.95	121.00
22	S	332	PHE	CB-CG-CD1	8.24	126.57	120.80
10	3	198	ARG	NE-CZ-NH1	8.24	124.42	120.30
5	e	35	SER	N-CA-CB	8.24	122.85	110.50
5	E	228	PHE	CB-CG-CD2	8.24	126.56	120.80
20	Z	367	SER	N-CA-CB	8.23	122.85	110.50
21	N	406	TYR	CB-CG-CD2	-8.23	116.06	121.00
30	K	427	TYR	CB-CG-CD1	8.22	125.93	121.00
20	Z	199	ASP	CB-CG-OD2	-8.21	110.91	118.30
5	E	231	TYR	CG-CD2-CE2	-8.20	114.74	121.30
24	Q	64	LEU	CB-CG-CD2	8.20	124.94	111.00
20	Z	375	ASP	CB-CG-OD1	-8.20	110.92	118.30
17	T	220	PHE	CB-CG-CD1	-8.20	115.06	120.80
20	Z	193	PHE	CB-CG-CD1	8.19	126.54	120.80
4	d	29	ARG	NE-CZ-NH1	8.19	124.40	120.30
24	Q	75	ARG	NE-CZ-NH1	8.19	124.39	120.30
1	a	131	ARG	NE-CZ-NH2	-8.19	116.21	120.30
3	c	102	TYR	CB-CG-CD1	8.18	125.91	121.00
20	Z	369	PHE	CB-CG-CD1	8.18	126.52	120.80
17	T	175	ASP	CB-CG-OD1	8.17	125.65	118.30
3	c	213	PHE	CB-CG-CD1	8.17	126.52	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	369	ARG	NE-CZ-NH1	-8.15	116.23	120.30
1	A	135	ARG	NE-CZ-NH1	8.14	124.37	120.30
17	T	220	PHE	CB-CG-CD2	8.14	126.50	120.80
26	U	32	ARG	NE-CZ-NH1	-8.14	116.23	120.30
33	J	71	TYR	CB-CG-CD2	-8.13	116.12	121.00
15	W	60	ARG	NE-CZ-NH2	-8.13	116.23	120.30
6	F	7	ASP	CB-CG-OD2	8.12	125.61	118.30
2	B	23	TYR	CG-CD2-CE2	-8.12	114.81	121.30
32	M	243	PHE	CB-CG-CD2	-8.11	115.12	120.80
31	L	279	PHE	CB-CG-CD2	-8.11	115.12	120.80
3	C	143	ARG	NE-CZ-NH2	-8.10	116.25	120.30
20	Z	948	TRP	CE2-CD2-CE3	8.10	128.42	118.70
1	A	110	TYR	CB-CG-CD2	8.10	125.86	121.00
14	7	87	SER	N-CA-CB	8.10	122.64	110.50
7	g	115	ARG	NE-CZ-NH1	8.09	124.35	120.30
13	m	130	VAL	CA-CB-CG2	-8.09	98.77	110.90
4	D	120	TYR	CG-CD2-CE2	-8.08	114.83	121.30
17	T	150	ARG	NE-CZ-NH1	8.07	124.33	120.30
25	R	203	ASP	CB-CG-OD1	-8.07	111.04	118.30
23	P	359	ARG	NE-CZ-NH1	8.07	124.33	120.30
14	n	34	THR	CA-CB-CG2	-8.06	101.11	112.40
23	P	344	ARG	NE-CZ-NH2	8.06	124.33	120.30
5	E	138	PHE	CB-CG-CD1	-8.06	115.16	120.80
20	Z	843	ASP	CB-CG-OD2	8.06	125.55	118.30
32	M	318	ASP	CB-CG-OD2	-8.05	111.05	118.30
7	g	71	ASP	CB-CG-OD2	8.05	125.54	118.30
6	f	75	ALA	N-CA-CB	8.05	121.36	110.10
11	k	187	ASP	CB-CG-OD1	8.04	125.54	118.30
14	n	63	TYR	CB-CG-CD1	-8.04	116.18	121.00
24	Q	124	PHE	CB-CG-CD2	-8.03	115.18	120.80
28	H	457	PHE	CB-CG-CD2	-8.03	115.18	120.80
12	l	181	ARG	NE-CZ-NH2	-8.02	116.29	120.30
5	e	167	TYR	CB-CG-CD2	-8.02	116.19	121.00
12	5	133	TRP	CB-CG-CD2	-8.02	116.17	126.60
21	N	14	ARG	NE-CZ-NH2	-8.02	116.29	120.30
11	k	72	ASP	CB-CG-OD2	8.02	125.51	118.30
12	5	82	ARG	NE-CZ-NH1	8.01	124.30	120.30
11	4	85	ARG	NE-CZ-NH2	-8.00	116.30	120.30
27	O	62	TYR	CB-CG-CD1	8.00	125.80	121.00
23	P	303	PHE	CB-CG-CD1	8.00	126.40	120.80
25	R	65	TYR	CB-CG-CD2	8.00	125.80	121.00
31	L	280	MET	CG-SD-CE	-8.00	87.41	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	120	TYR	CZ-CE2-CD2	7.99	126.99	119.80
7	G	169	ARG	NE-CZ-NH2	-7.99	116.31	120.30
2	B	70	ASP	CB-CG-OD2	7.98	125.48	118.30
28	H	354	ALA	N-CA-CB	7.98	121.27	110.10
29	I	181	TYR	CB-CG-CD1	7.97	125.78	121.00
32	M	33	ARG	NE-CZ-NH1	7.96	124.28	120.30
27	O	190	TYR	CB-CG-CD2	-7.96	116.22	121.00
33	J	238	ARG	NE-CZ-NH2	-7.96	116.32	120.30
26	U	189	ARG	NE-CZ-NH2	7.96	124.28	120.30
17	T	186	ARG	NE-CZ-NH1	-7.94	116.33	120.30
20	Z	202	ARG	NE-CZ-NH2	-7.93	116.33	120.30
6	f	59	TYR	CB-CG-CD2	-7.93	116.24	121.00
3	C	149	TYR	CB-CG-CD2	-7.92	116.25	121.00
20	Z	738	TYR	CB-CG-CD2	7.92	125.75	121.00
30	K	185	ARG	NE-CZ-NH1	7.92	124.26	120.30
7	g	132	PHE	CB-CG-CD2	-7.92	115.26	120.80
22	S	184	TRP	CB-CG-CD1	7.91	137.29	127.00
16	V	100	ARG	NE-CZ-NH1	7.91	124.26	120.30
1	a	155	TYR	CB-CG-CD1	-7.91	116.25	121.00
4	d	141	ARG	NE-CZ-NH1	7.90	124.25	120.30
30	K	252	ARG	NE-CZ-NH1	7.89	124.25	120.30
20	Z	47	THR	CA-CB-CG2	-7.89	101.35	112.40
2	B	12	PHE	CB-CG-CD2	7.88	126.32	120.80
14	7	170	TYR	CB-CG-CD2	7.88	125.73	121.00
21	N	338	PHE	CB-CG-CD1	7.87	126.31	120.80
1	a	233	PHE	CB-CG-CD1	-7.86	115.30	120.80
11	4	130	TYR	CB-CG-CD1	-7.86	116.28	121.00
27	O	135	ARG	NE-CZ-NH2	-7.86	116.37	120.30
6	f	39	ARG	NE-CZ-NH2	-7.86	116.37	120.30
13	6	159	ASP	CB-CG-OD1	-7.85	111.23	118.30
28	H	420	ARG	NE-CZ-NH2	7.85	124.23	120.30
31	L	70	TYR	CB-CG-CD1	-7.85	116.29	121.00
22	S	367	TYR	CB-CG-CD2	7.84	125.70	121.00
24	Q	299	MET	CA-CB-CG	7.83	126.62	113.30
10	j	40	PHE	CB-CG-CD1	7.83	126.28	120.80
33	J	228	ARG	NE-CZ-NH2	-7.83	116.38	120.30
5	e	138	PHE	CB-CG-CD1	7.83	126.28	120.80
20	Z	210	TYR	CB-CG-CD2	-7.82	116.31	121.00
4	D	29	ARG	NE-CZ-NH2	7.82	124.21	120.30
26	U	56	PHE	CB-CG-CD1	-7.82	115.33	120.80
24	Q	146	TYR	CB-CG-CD2	-7.82	116.31	121.00
26	U	24	ARG	NE-CZ-NH2	-7.82	116.39	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	179	TYR	CB-CG-CD2	-7.82	116.31	121.00
32	M	164	ASP	CB-CG-OD1	-7.81	111.27	118.30
24	Q	246	TYR	CB-CG-CD2	7.81	125.69	121.00
29	I	292	TYR	CB-CG-CD2	-7.81	116.31	121.00
20	Z	236	PHE	CB-CG-CD1	7.81	126.27	120.80
28	H	466	TYR	CB-CG-CD2	-7.81	116.31	121.00
6	f	101	ARG	NE-CZ-NH1	7.80	124.20	120.30
23	P	123	ARG	NE-CZ-NH1	-7.80	116.40	120.30
25	R	388	VAL	CG1-CB-CG2	-7.79	98.43	110.90
27	O	26	PHE	CB-CG-CD2	7.79	126.25	120.80
27	O	210	ARG	NE-CZ-NH2	-7.79	116.40	120.30
6	f	187	ASP	CB-CG-OD2	-7.79	111.29	118.30
21	N	417	ARG	NH1-CZ-NH2	7.79	127.97	119.40
7	g	157	TYR	CB-CG-CD2	7.79	125.67	121.00
2	b	130	PHE	CB-CG-CD1	-7.78	115.35	120.80
2	b	23	TYR	CB-CG-CD1	7.77	125.66	121.00
21	N	762	ARG	NE-CZ-NH2	-7.77	116.41	120.30
8	h	28	ARG	NE-CZ-NH1	7.77	124.19	120.30
29	I	316	PHE	CB-CG-CD1	-7.77	115.36	120.80
20	Z	137	TYR	CB-CG-CD1	7.77	125.66	121.00
3	c	144	TYR	CB-CG-CD1	7.76	125.66	121.00
23	P	69	ARG	NE-CZ-NH2	-7.76	116.42	120.30
20	Z	91	PHE	CB-CG-CD1	7.75	126.23	120.80
15	W	35	PHE	CB-CG-CD1	7.75	126.23	120.80
16	V	156	PHE	CB-CG-CD2	7.74	126.22	120.80
20	Z	948	TRP	CG-CD2-CE3	-7.74	126.94	133.90
4	D	48	ARG	NE-CZ-NH1	7.73	124.17	120.30
21	N	788	TYR	CB-CG-CD1	7.73	125.64	121.00
2	B	216	ASP	CB-CG-OD1	7.72	125.24	118.30
28	H	101	ARG	NE-CZ-NH2	-7.71	116.44	120.30
6	f	39	ARG	NE-CZ-NH1	7.71	124.16	120.30
8	h	91	PHE	CB-CG-CD1	7.71	126.19	120.80
23	P	136	ARG	NE-CZ-NH1	7.71	124.15	120.30
28	H	439	THR	CA-CB-CG2	-7.70	101.62	112.40
5	E	136	ARG	NE-CZ-NH2	7.70	124.15	120.30
24	Q	189	ARG	NE-CZ-NH2	-7.70	116.45	120.30
26	U	288	PHE	CB-CG-CD1	7.69	126.19	120.80
20	Z	323	TYR	CB-CG-CD1	-7.69	116.39	121.00
12	l	253	TYR	CB-CG-CD2	7.67	125.60	121.00
13	m	99	ARG	NE-CZ-NH2	-7.67	116.47	120.30
21	N	259	PHE	CB-CG-CD1	7.67	126.17	120.80
8	h	136	ALA	N-CA-CB	7.66	120.83	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	223	ARG	NE-CZ-NH2	-7.66	116.47	120.30
31	L	255	TYR	CG-CD2-CE2	-7.66	115.17	121.30
30	K	259	ARG	NE-CZ-NH2	-7.65	116.47	120.30
4	d	73	LEU	CB-CG-CD2	7.64	123.99	111.00
13	m	178	LYS	N-CA-CB	7.63	124.34	110.60
19	Y	82	ASP	CB-CG-OD1	7.63	125.17	118.30
22	S	271	ARG	NE-CZ-NH2	-7.63	116.48	120.30
32	M	109	ASP	CB-CG-OD1	7.63	125.17	118.30
31	L	312	MET	CG-SD-CE	-7.63	87.99	100.20
26	U	52	PHE	CB-CG-CD2	7.63	126.14	120.80
25	R	300	ASP	CB-CG-OD1	-7.62	111.44	118.30
32	M	213	ARG	NE-CZ-NH1	7.62	124.11	120.30
28	H	404	TRP	CG-CD2-CE3	-7.62	127.04	133.90
20	Z	137	TYR	CB-CG-CD2	-7.62	116.43	121.00
32	M	158	THR	CA-CB-CG2	-7.61	101.74	112.40
33	J	322	ALA	N-CA-CB	7.61	120.76	110.10
14	7	170	TYR	CB-CG-CD1	-7.61	116.43	121.00
1	a	77	ARG	NE-CZ-NH1	7.61	124.11	120.30
14	n	170	TYR	CB-CG-CD2	-7.61	116.44	121.00
21	N	651	PHE	CB-CG-CD2	-7.60	115.48	120.80
1	a	104	PHE	CB-CG-CD1	7.58	126.11	120.80
32	M	386	PHE	CB-CG-CD1	7.58	126.10	120.80
31	L	279	PHE	CB-CG-CD1	7.57	126.10	120.80
21	N	884	PHE	CB-CG-CD1	7.57	126.10	120.80
25	R	342	LEU	CB-CG-CD1	-7.57	98.13	111.00
12	5	230	TYR	CB-CG-CD2	7.57	125.54	121.00
14	n	253	ASP	CB-CG-OD1	-7.57	111.49	118.30
28	H	373	ARG	NE-CZ-NH1	7.55	124.07	120.30
21	N	224	THR	CA-CB-CG2	-7.55	101.83	112.40
9	i	80	ASP	CB-CG-OD1	7.54	125.09	118.30
24	Q	427	PHE	CB-CG-CD1	-7.54	115.52	120.80
3	C	135	PHE	CB-CG-CD2	-7.53	115.53	120.80
8	1	183	ARG	NE-CZ-NH2	-7.53	116.54	120.30
21	N	398	ARG	NE-CZ-NH1	7.53	124.06	120.30
23	P	131	PHE	CB-CG-CD2	-7.53	115.53	120.80
13	6	113	TYR	CB-CG-CD2	-7.52	116.49	121.00
32	M	415	PHE	CB-CG-CD1	-7.52	115.54	120.80
25	R	304	TYR	CZ-CE2-CD2	7.51	126.56	119.80
10	j	161	GLU	OE1-CD-OE2	-7.50	114.30	123.30
32	M	290	ARG	NE-CZ-NH2	7.49	124.05	120.30
4	D	148	TYR	CB-CG-CD1	7.49	125.49	121.00
16	V	129	PHE	CB-CG-CD2	-7.48	115.56	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	46	LEU	N-CA-CB	7.48	125.36	110.40
11	k	70	ARG	NE-CZ-NH2	-7.48	116.56	120.30
14	7	161	ARG	NE-CZ-NH2	-7.47	116.56	120.30
8	h	133	TYR	CB-CG-CD2	7.47	125.48	121.00
20	Z	3	ASP	CB-CG-OD1	-7.47	111.58	118.30
24	Q	202	ARG	NE-CZ-NH1	7.47	124.03	120.30
7	g	196	ALA	N-CA-CB	7.46	120.55	110.10
10	3	154	TYR	CZ-CE2-CD2	7.46	126.52	119.80
21	N	866	TYR	CG-CD1-CE1	-7.46	115.33	121.30
8	1	70	TYR	CB-CG-CD2	-7.46	116.53	121.00
22	S	480	ARG	NH1-CZ-NH2	-7.46	111.20	119.40
6	F	40	SER	N-CA-CB	7.45	121.68	110.50
27	O	172	TYR	CB-CG-CD2	-7.45	116.53	121.00
22	S	263	ASP	CB-CG-OD2	-7.45	111.59	118.30
4	D	197	ARG	NH1-CZ-NH2	7.45	127.59	119.40
4	d	111	ARG	NE-CZ-NH1	7.44	124.02	120.30
7	g	212	PHE	CB-CG-CD1	7.44	126.01	120.80
2	B	157	PHE	CG-CD1-CE1	-7.44	112.61	120.80
21	N	773	MET	CG-SD-CE	7.44	112.11	100.20
6	f	126	ARG	NE-CZ-NH2	-7.43	116.58	120.30
8	h	45	ARG	NE-CZ-NH1	7.43	124.02	120.30
4	D	33	ALA	N-CA-CB	7.42	120.49	110.10
3	C	226	TYR	CB-CG-CD2	-7.42	116.55	121.00
11	4	149	ARG	NE-CZ-NH2	-7.41	116.59	120.30
21	N	869	ASP	CB-CG-OD1	-7.41	111.63	118.30
29	I	265	ARG	NE-CZ-NH2	-7.41	116.59	120.30
32	M	432	PHE	CB-CG-CD2	-7.41	115.61	120.80
2	B	103	GLU	N-CA-CB	7.41	123.94	110.60
5	E	103	TYR	CB-CG-CD2	7.41	125.45	121.00
6	F	179	PHE	CB-CG-CD2	-7.41	115.61	120.80
25	R	183	ASP	CB-CG-OD2	-7.41	111.63	118.30
6	F	175	THR	CA-CB-CG2	-7.41	102.03	112.40
10	j	69	TYR	CB-CG-CD2	-7.41	116.56	121.00
12	l	81	PHE	CB-CG-CD1	-7.41	115.62	120.80
25	R	70	TYR	CB-CG-CD1	7.40	125.44	121.00
3	C	178	MET	CG-SD-CE	-7.39	88.37	100.20
20	Z	165	TYR	CB-CG-CD2	7.39	125.43	121.00
30	K	323	THR	CA-CB-CG2	-7.39	102.06	112.40
32	M	299	ARG	NE-CZ-NH1	7.38	123.99	120.30
1	a	133	TYR	CG-CD1-CE1	7.38	127.20	121.30
8	1	70	TYR	CB-CG-CD1	7.38	125.43	121.00
27	O	248	TYR	CB-CG-CD1	-7.38	116.57	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	711	ARG	NE-CZ-NH1	7.38	123.99	120.30
10	3	103	TYR	CB-CG-CD2	-7.38	116.58	121.00
11	k	141	PHE	CG-CD2-CE2	-7.37	112.69	120.80
6	F	164	ARG	NE-CZ-NH1	-7.37	116.61	120.30
12	5	219	TYR	CB-CG-CD2	-7.37	116.58	121.00
17	T	250	MET	CG-SD-CE	-7.37	88.42	100.20
22	S	114	TYR	CB-CG-CD2	7.37	125.42	121.00
2	b	161	ALA	N-CA-CB	7.36	120.41	110.10
30	K	128	ARG	NE-CZ-NH1	-7.36	116.62	120.30
5	e	228	PHE	CB-CG-CD1	-7.36	115.65	120.80
32	M	87	ASP	CB-CG-OD2	-7.36	111.68	118.30
26	U	290	ASP	CB-CG-OD1	7.36	124.92	118.30
12	l	188	TYR	CG-CD1-CE1	-7.35	115.42	121.30
12	l	82	ARG	NH1-CZ-NH2	-7.35	111.32	119.40
23	P	115	ARG	NE-CZ-NH2	7.35	123.97	120.30
5	E	93	ARG	NE-CZ-NH1	7.33	123.97	120.30
14	7	124	TYR	CD1-CE1-CZ	7.33	126.40	119.80
12	5	230	TYR	CB-CG-CD1	-7.33	116.60	121.00
16	V	28	TYR	CB-CG-CD1	7.33	125.40	121.00
21	N	604	ARG	NE-CZ-NH1	-7.33	116.64	120.30
6	f	202	ARG	NE-CZ-NH1	-7.33	116.64	120.30
14	7	124	TYR	CG-CD2-CE2	-7.33	115.44	121.30
20	Z	808	SER	O-C-N	-7.32	110.99	122.70
21	N	890	PHE	CB-CG-CD1	7.32	125.92	120.80
4	d	102	ASP	CB-CG-OD2	7.32	124.88	118.30
1	A	73	PHE	CB-CG-CD2	7.32	125.92	120.80
11	4	138	PHE	CB-CG-CD2	-7.32	115.68	120.80
14	7	137	ARG	NE-CZ-NH1	7.32	123.96	120.30
27	O	137	TYR	CB-CG-CD2	7.31	125.39	121.00
11	4	23	ARG	NE-CZ-NH1	7.31	123.96	120.30
2	B	156	TYR	CZ-CE2-CD2	-7.31	113.22	119.80
3	C	180	TYR	CB-CG-CD1	-7.31	116.61	121.00
18	X	17	TYR	CB-CG-CD1	-7.31	116.61	121.00
20	Z	210	TYR	CA-CB-CG	-7.31	99.51	113.40
31	L	88	TYR	CB-CG-CD1	-7.31	116.62	121.00
14	n	220	ARG	NE-CZ-NH1	7.30	123.95	120.30
23	P	273	TYR	CB-CG-CD2	-7.30	116.62	121.00
10	j	80	ARG	NE-CZ-NH1	7.30	123.95	120.30
2	B	234	ARG	NE-CZ-NH2	-7.30	116.65	120.30
1	a	142	THR	N-CA-CB	7.29	124.16	110.30
32	M	44	PHE	CB-CG-CD1	-7.29	115.70	120.80
7	g	151	LEU	CB-CG-CD1	7.29	123.39	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	245	PHE	CB-CG-CD1	-7.29	115.70	120.80
7	g	169	ARG	NE-CZ-NH2	-7.29	116.66	120.30
2	b	12	PHE	CB-CG-CD1	7.28	125.90	120.80
3	C	81	THR	CA-CB-CG2	-7.28	102.21	112.40
7	G	84	ASP	CB-CG-OD2	-7.28	111.75	118.30
5	e	163	THR	CA-CB-CG2	-7.28	102.21	112.40
9	i	104	ARG	NE-CZ-NH2	-7.28	116.66	120.30
7	g	26	TYR	CB-CG-CD1	7.28	125.36	121.00
6	F	18	ARG	NE-CZ-NH2	-7.28	116.66	120.30
17	T	81	TYR	CB-CG-CD2	-7.28	116.64	121.00
21	N	394	ARG	NE-CZ-NH2	7.27	123.93	120.30
6	f	157	TYR	CB-CG-CD2	7.26	125.36	121.00
25	R	246	TYR	CB-CG-CD2	-7.26	116.64	121.00
31	L	62	ARG	NE-CZ-NH2	7.26	123.93	120.30
11	k	46	PHE	CB-CG-CD1	-7.26	115.72	120.80
12	l	210	PHE	CB-CG-CD2	7.25	125.88	120.80
20	Z	141	SER	N-CA-CB	-7.25	99.62	110.50
1	A	96	ARG	NE-CZ-NH1	7.25	123.92	120.30
20	Z	802	ASP	CB-CG-OD2	7.25	124.83	118.30
25	R	183	ASP	CB-CG-OD1	7.25	124.83	118.30
2	B	157	PHE	CB-CG-CD2	-7.25	115.73	120.80
28	H	390	ARG	NE-CZ-NH1	7.24	123.92	120.30
2	B	156	TYR	CG-CD2-CE2	7.24	127.09	121.30
2	B	23	TYR	CB-CG-CD1	7.24	125.34	121.00
33	J	312	ARG	NE-CZ-NH2	7.24	123.92	120.30
7	G	26	TYR	CG-CD2-CE2	7.23	127.09	121.30
20	Z	912	PHE	CB-CG-CD2	7.23	125.86	120.80
31	L	173	PHE	CB-CG-CD2	7.23	125.86	120.80
21	N	422	TYR	CB-CG-CD1	-7.23	116.67	121.00
24	Q	387	TYR	CG-CD2-CE2	-7.23	115.52	121.30
29	I	300	ARG	NE-CZ-NH2	-7.22	116.69	120.30
4	D	113	VAL	CA-CB-CG1	7.22	121.73	110.90
20	Z	208	VAL	CA-CB-CG2	-7.22	100.07	110.90
3	c	188	ASP	CB-CG-OD1	7.22	124.80	118.30
5	E	127	ALA	N-CA-CB	7.21	120.20	110.10
9	2	65	ARG	NE-CZ-NH1	-7.21	116.69	120.30
6	f	233	TYR	CB-CG-CD2	-7.20	116.68	121.00
20	Z	96	TYR	CB-CG-CD1	7.20	125.32	121.00
32	M	87	ASP	CB-CG-OD1	7.20	124.78	118.30
8	1	79	TYR	CG-CD2-CE2	-7.19	115.55	121.30
31	L	425	VAL	CG1-CB-CG2	7.19	122.41	110.90
25	R	417	TYR	CB-CG-CD2	-7.18	116.69	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	262	ARG	NE-CZ-NH2	7.18	123.89	120.30
32	M	386	PHE	CB-CG-CD2	-7.18	115.78	120.80
10	3	127	ILE	O-C-N	-7.17	111.00	123.20
10	3	103	TYR	CB-CG-CD1	7.17	125.30	121.00
32	M	432	PHE	CB-CG-CD1	7.17	125.82	120.80
22	S	367	TYR	CB-CG-CD1	-7.17	116.70	121.00
2	B	67	LEU	CB-CG-CD2	7.16	123.18	111.00
8	h	109	ALA	N-CA-CB	7.16	120.12	110.10
13	6	53	ASP	CB-CG-OD2	-7.16	111.86	118.30
7	g	8	TYR	CB-CG-CD2	-7.16	116.70	121.00
11	4	117	TYR	CB-CG-CD2	-7.16	116.70	121.00
13	m	75	ARG	NE-CZ-NH1	7.15	123.88	120.30
7	G	169	ARG	NE-CZ-NH1	7.15	123.88	120.30
11	4	100	VAL	CA-CB-CG2	-7.14	100.18	110.90
28	H	466	TYR	CB-CG-CD1	7.13	125.28	121.00
12	5	253	TYR	CB-CG-CD1	-7.12	116.73	121.00
22	S	333	PHE	CB-CG-CD1	7.12	125.78	120.80
18	X	75	TRP	CH2-CZ2-CE2	7.11	124.51	117.40
8	1	142	PHE	CB-CG-CD1	7.11	125.78	120.80
6	f	225	TYR	CG-CD1-CE1	-7.11	115.61	121.30
29	I	340	ARG	N-CA-CB	7.11	123.40	110.60
20	Z	431	ASP	CB-CG-OD2	-7.10	111.91	118.30
23	P	154	ASP	CB-CG-OD2	7.10	124.69	118.30
3	c	39	MET	CG-SD-CE	-7.10	88.84	100.20
21	N	788	TYR	CG-CD2-CE2	7.10	126.98	121.30
6	f	18	ARG	NE-CZ-NH1	7.10	123.85	120.30
10	j	98	ARG	NE-CZ-NH1	7.09	123.85	120.30
9	i	48	ARG	NE-CZ-NH1	7.09	123.84	120.30
4	D	75	PHE	CB-CG-CD1	7.08	125.76	120.80
4	D	119	ARG	NE-CZ-NH2	7.08	123.84	120.30
9	i	125	ALA	N-CA-CB	7.08	120.01	110.10
1	a	228	ALA	N-CA-CB	7.08	120.00	110.10
8	1	77	SER	N-CA-CB	7.08	121.11	110.50
10	3	154	TYR	CB-CG-CD1	-7.07	116.76	121.00
27	O	373	TRP	CB-CG-CD2	-7.07	117.42	126.60
29	I	408	ARG	NE-CZ-NH1	7.06	123.83	120.30
8	1	142	PHE	CB-CG-CD2	-7.06	115.86	120.80
1	A	143	PHE	CB-CG-CD2	-7.05	115.86	120.80
20	Z	865	ASP	CB-CG-OD1	7.05	124.64	118.30
22	S	54	TRP	CE2-CD2-CE3	7.04	127.15	118.70
23	P	47	ARG	NE-CZ-NH2	7.03	123.82	120.30
3	c	209	ASP	CB-CG-OD2	-7.03	111.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	72	ARG	NE-CZ-NH2	-7.03	116.78	120.30
29	I	54	ARG	NE-CZ-NH2	-7.03	116.79	120.30
28	H	357	ARG	NE-CZ-NH1	-7.03	116.79	120.30
9	2	85	THR	CA-CB-CG2	-7.02	102.57	112.40
7	G	35	THR	CA-CB-CG2	-7.02	102.58	112.40
6	f	225	TYR	CB-CG-CD1	-7.01	116.79	121.00
9	i	98	TYR	CB-CG-CD1	7.01	125.21	121.00
21	N	412	TYR	CG-CD2-CE2	-7.01	115.69	121.30
26	U	57	GLU	N-CA-CB	7.01	123.22	110.60
9	2	101	ARG	NE-CZ-NH1	7.01	123.80	120.30
12	l	196	ARG	NE-CZ-NH1	-7.00	116.80	120.30
7	g	9	ASP	N-CA-CB	7.00	123.20	110.60
8	h	194	ARG	NE-CZ-NH2	-7.00	116.80	120.30
8	1	194	ARG	NE-CZ-NH1	7.00	123.80	120.30
12	5	189	TYR	CB-CG-CD1	-7.00	116.80	121.00
2	b	246	ARG	NE-CZ-NH1	7.00	123.80	120.30
14	n	170	TYR	CB-CG-CD1	7.00	125.20	121.00
28	H	386	ALA	N-CA-CB	6.99	119.89	110.10
29	I	316	PHE	CB-CG-CD2	6.99	125.69	120.80
25	R	371	PHE	CB-CG-CD1	-6.98	115.92	120.80
9	2	225	ARG	NE-CZ-NH2	-6.98	116.81	120.30
7	g	160	TYR	CB-CG-CD2	-6.97	116.82	121.00
1	a	113	PRO	N-CD-CG	6.97	113.65	103.20
21	N	788	TYR	CB-CG-CD2	-6.97	116.82	121.00
10	j	116	SER	N-CA-CB	6.97	120.95	110.50
23	P	154	ASP	CB-CG-OD1	-6.97	112.03	118.30
31	L	392	ARG	NE-CZ-NH1	6.97	123.78	120.30
27	O	115	ARG	NE-CZ-NH1	6.96	123.78	120.30
18	X	74	MET	CG-SD-CE	-6.96	89.07	100.20
21	N	68	VAL	CA-CB-CG2	-6.96	100.46	110.90
1	a	147	ASP	CB-CG-OD1	6.95	124.56	118.30
9	i	212	ASP	CB-CG-OD1	6.95	124.56	118.30
32	M	58	MET	CG-SD-CE	-6.95	89.08	100.20
8	1	40	THR	N-CA-CB	6.95	123.50	110.30
19	Y	68	GLU	OE1-CD-OE2	6.94	131.63	123.30
2	B	187	ASP	CB-CG-OD1	-6.94	112.06	118.30
21	N	283	ASP	CB-CG-OD2	6.93	124.54	118.30
31	L	316	ASP	N-CA-CB	6.93	123.07	110.60
1	A	133	TYR	CG-CD1-CE1	-6.93	115.76	121.30
4	d	172	ARG	NE-CZ-NH1	6.92	123.76	120.30
23	P	64	ASP	CB-CG-OD1	6.92	124.53	118.30
2	B	205	ASN	N-CA-CB	6.92	123.05	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	177	PHE	CB-CG-CD2	6.92	125.64	120.80
25	R	363	PHE	CB-CG-CD2	-6.92	115.96	120.80
4	d	5	ASP	CB-CG-OD1	-6.91	112.08	118.30
21	N	283	ASP	CB-CG-OD1	-6.91	112.08	118.30
24	Q	239	PHE	CB-CG-CD1	6.91	125.64	120.80
2	B	82	TYR	CB-CG-CD1	-6.91	116.85	121.00
23	P	95	TYR	CB-CG-CD1	6.91	125.15	121.00
13	6	202	ARG	NE-CZ-NH1	6.91	123.75	120.30
21	N	861	TYR	CB-CG-CD2	6.90	125.14	121.00
33	J	265	ASP	CB-CG-OD2	-6.90	112.09	118.30
8	h	178	SER	N-CA-C	-6.89	92.39	111.00
9	i	150	VAL	CA-CB-CG2	-6.89	100.56	110.90
30	K	88	ARG	NE-CZ-NH1	-6.89	116.86	120.30
1	a	125	SER	N-CA-CB	6.88	120.83	110.50
12	l	188	TYR	CB-CG-CD2	6.88	125.13	121.00
19	Y	41	ASP	CB-CG-OD1	6.88	124.49	118.30
23	P	287	ASP	CB-CG-OD1	-6.88	112.11	118.30
3	C	50	ARG	NE-CZ-NH2	-6.88	116.86	120.30
20	Z	550	PHE	CB-CG-CD2	-6.87	115.99	120.80
10	3	144	ASP	CB-CG-OD2	-6.87	112.11	118.30
32	M	203	ARG	NE-CZ-NH1	6.87	123.74	120.30
2	b	81	ASP	CB-CG-OD1	6.87	124.48	118.30
22	S	55	ARG	NE-CZ-NH2	6.87	123.73	120.30
24	Q	88	PHE	CG-CD2-CE2	6.87	128.35	120.80
16	V	129	PHE	CB-CG-CD1	6.86	125.60	120.80
32	M	355	ASP	CB-CG-OD1	6.86	124.47	118.30
12	5	267	ASP	CB-CG-OD2	-6.86	112.13	118.30
23	P	13	TYR	CB-CG-CD1	6.85	125.11	121.00
2	B	229	THR	CA-CB-CG2	-6.85	102.81	112.40
3	c	102	TYR	CB-CG-CD2	-6.85	116.89	121.00
30	K	258	PHE	CB-CG-CD1	6.85	125.59	120.80
14	7	252	TRP	CB-CG-CD1	6.85	135.90	127.00
5	e	231	TYR	CB-CG-CD2	6.84	125.10	121.00
12	l	191	ASP	CB-CG-OD2	6.84	124.45	118.30
6	f	123	TYR	CB-CG-CD1	6.84	125.10	121.00
9	2	84	VAL	CA-CB-CG1	6.83	121.15	110.90
13	6	221	ARG	NE-CZ-NH1	6.83	123.72	120.30
1	a	133	TYR	CD1-CG-CD2	-6.83	110.39	117.90
8	1	54	ARG	NE-CZ-NH2	-6.83	116.89	120.30
13	m	32	ALA	N-CA-CB	6.83	119.66	110.10
5	E	167	TYR	CB-CG-CD1	6.83	125.10	121.00
12	5	165	TYR	CB-CG-CD2	6.83	125.10	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	392	ARG	NE-CZ-NH2	-6.82	116.89	120.30
17	T	254	ASP	CB-CG-OD2	-6.81	112.17	118.30
12	l	253	TYR	CG-CD2-CE2	6.81	126.75	121.30
33	J	309	ARG	NE-CZ-NH2	-6.81	116.89	120.30
14	n	261	TYR	CB-CG-CD1	-6.81	116.91	121.00
2	B	157	PHE	CD1-CE1-CZ	6.81	128.27	120.10
8	1	202	TYR	CB-CG-CD2	-6.81	116.92	121.00
2	b	90	ARG	NE-CZ-NH2	6.80	123.70	120.30
33	J	106	ASP	CB-CG-OD2	-6.80	112.18	118.30
24	Q	72	ASP	CB-CG-OD1	-6.80	112.18	118.30
32	M	109	ASP	CB-CG-OD2	-6.79	112.19	118.30
15	W	69	PHE	CB-CG-CD1	6.78	125.55	120.80
9	i	149	ASP	CB-CG-OD2	-6.78	112.20	118.30
7	G	242	PHE	CB-CG-CD2	-6.78	116.06	120.80
2	b	137	ALA	N-CA-CB	6.78	119.59	110.10
20	Z	843	ASP	CB-CG-OD1	-6.77	112.20	118.30
28	H	331	ARG	NE-CZ-NH1	6.77	123.69	120.30
5	e	132	ARG	NE-CZ-NH1	6.77	123.69	120.30
21	N	618	ARG	NE-CZ-NH2	-6.77	116.91	120.30
14	7	193	ASP	CB-CG-OD2	-6.77	112.21	118.30
13	m	10	PHE	CB-CG-CD2	-6.77	116.06	120.80
20	Z	941	ARG	NE-CZ-NH1	6.77	123.68	120.30
22	S	309	PHE	CB-CG-CD1	-6.77	116.06	120.80
14	n	228	PHE	CB-CG-CD2	-6.76	116.06	120.80
25	R	35	GLN	N-CA-CB	6.76	122.77	110.60
3	c	143	ARG	NE-CZ-NH2	-6.76	116.92	120.30
5	e	10	ARG	NH1-CZ-NH2	6.75	126.83	119.40
9	2	119	TYR	CG-CD1-CE1	-6.75	115.90	121.30
30	K	246	TYR	CB-CG-CD1	-6.75	116.95	121.00
3	c	144	TYR	CG-CD1-CE1	6.75	126.70	121.30
9	2	119	TYR	CB-CA-C	-6.75	96.90	110.40
1	A	110	TYR	O-C-N	6.74	133.49	122.70
33	J	116	ARG	NE-CZ-NH1	-6.74	116.93	120.30
12	5	144	ARG	NE-CZ-NH2	-6.74	116.93	120.30
30	K	48	TYR	CB-CG-CD2	-6.74	116.96	121.00
14	7	242	LYS	N-CA-CB	6.73	122.72	110.60
19	Y	83	ARG	NE-CZ-NH1	6.73	123.67	120.30
9	i	73	ALA	N-CA-CB	6.73	119.52	110.10
28	H	143	ALA	N-CA-CB	6.72	119.51	110.10
3	c	129	ARG	NE-CZ-NH2	-6.72	116.94	120.30
26	U	113	TYR	CB-CG-CD1	-6.72	116.97	121.00
11	k	139	TYR	CB-CG-CD1	-6.71	116.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	268	PHE	CB-CG-CD2	-6.71	116.10	120.80
14	n	134	TYR	CB-CG-CD2	-6.71	116.97	121.00
14	n	124	TYR	CG-CD2-CE2	-6.71	115.93	121.30
20	Z	287	ARG	NE-CZ-NH2	-6.71	116.95	120.30
13	6	50	LYS	CB-CA-C	-6.71	96.99	110.40
4	D	4	TYR	CZ-CE2-CD2	6.71	125.83	119.80
27	O	366	MET	CG-SD-CE	-6.70	89.47	100.20
7	g	190	ARG	NE-CZ-NH2	6.70	123.65	120.30
24	Q	146	TYR	CB-CG-CD1	6.70	125.02	121.00
27	O	373	TRP	CB-CG-CD1	6.70	135.71	127.00
3	c	179	ASP	CB-CG-OD1	-6.70	112.27	118.30
12	5	159	SER	N-CA-CB	6.70	120.54	110.50
21	N	857	TYR	CG-CD2-CE2	-6.69	115.95	121.30
21	N	861	TYR	CG-CD1-CE1	-6.69	115.95	121.30
5	E	122	ARG	NE-CZ-NH2	-6.69	116.95	120.30
17	T	157	TYR	CB-CG-CD2	6.69	125.01	121.00
14	7	63	TYR	CG-CD2-CE2	-6.69	115.95	121.30
3	C	157	TYR	CB-CG-CD2	-6.68	116.99	121.00
15	W	49	VAL	CA-CB-CG2	-6.68	100.87	110.90
33	J	286	LYS	CG-CD-CE	6.68	131.95	111.90
13	m	125	ASP	CB-CG-OD2	6.68	124.31	118.30
24	Q	255	TYR	CG-CD2-CE2	6.68	126.64	121.30
20	Z	96	TYR	CB-CG-CD2	-6.67	117.00	121.00
32	M	267	PHE	CB-CG-CD2	6.67	125.47	120.80
17	T	90	PHE	CB-CG-CD2	-6.67	116.13	120.80
10	3	15	MET	CG-SD-CE	-6.67	89.53	100.20
21	N	869	ASP	CB-CG-OD2	6.66	124.29	118.30
29	I	291	ARG	NE-CZ-NH1	6.66	123.63	120.30
23	P	269	VAL	CA-CB-CG1	6.66	120.89	110.90
7	G	190	ARG	NE-CZ-NH1	6.66	123.63	120.30
2	B	127	VAL	CA-CB-CG2	-6.66	100.92	110.90
4	D	166	ARG	NE-CZ-NH2	-6.66	116.97	120.30
32	M	117	ALA	CB-CA-C	-6.66	100.12	110.10
8	h	34	TYR	CB-CG-CD2	-6.65	117.01	121.00
28	H	273	ARG	NE-CZ-NH2	6.65	123.62	120.30
32	M	193	LEU	N-CA-CB	6.65	123.70	110.40
6	F	202	ARG	NE-CZ-NH1	6.65	123.62	120.30
7	G	20	ARG	NE-CZ-NH2	-6.65	116.98	120.30
25	R	363	PHE	CB-CG-CD1	6.65	125.45	120.80
20	Z	574	TYR	CB-CG-CD1	6.65	124.99	121.00
1	a	133	TYR	CB-CG-CD2	6.64	124.99	121.00
17	T	81	TYR	CG-CD2-CE2	-6.64	115.98	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	18	ARG	NE-CZ-NH2	-6.63	116.98	120.30
27	O	33	TYR	CB-CG-CD2	-6.63	117.02	121.00
31	L	420	ARG	NH1-CZ-NH2	6.63	126.69	119.40
24	Q	68	MET	CG-SD-CE	-6.62	89.60	100.20
27	O	50	ASP	CB-CG-OD2	6.62	124.26	118.30
5	e	15	PHE	CB-CG-CD2	-6.62	116.17	120.80
20	Z	406	TRP	CD1-CG-CD2	6.62	111.59	106.30
11	k	148	TYR	CB-CG-CD2	6.62	124.97	121.00
14	7	109	TYR	CB-CG-CD1	6.62	124.97	121.00
6	f	51	ARG	NE-CZ-NH2	-6.61	116.99	120.30
29	I	256	TYR	CB-CG-CD2	-6.61	117.03	121.00
22	S	384	ARG	NE-CZ-NH2	-6.61	117.00	120.30
33	J	367	MET	CG-SD-CE	-6.61	89.62	100.20
20	Z	767	TYR	CB-CG-CD2	-6.60	117.04	121.00
20	Z	804	ASP	CB-CG-OD2	6.60	124.24	118.30
24	Q	229	ASP	N-CA-CB	6.60	122.48	110.60
6	f	147	PHE	CB-CG-CD1	-6.60	116.18	120.80
6	F	174	ARG	NE-CZ-NH1	6.60	123.60	120.30
13	6	125	ASP	CB-CG-OD2	-6.59	112.37	118.30
33	J	282	PHE	CB-CG-CD2	-6.59	116.19	120.80
2	B	208	THR	CA-CB-CG2	-6.58	103.18	112.40
13	6	132	SER	N-CA-CB	6.58	120.38	110.50
2	B	156	TYR	CB-CG-CD1	-6.58	117.05	121.00
20	Z	916	LEU	CB-CG-CD2	6.58	122.19	111.00
22	S	150	LYS	N-CA-CB	6.58	122.45	110.60
5	E	8	TYR	CB-CG-CD2	-6.58	117.05	121.00
18	X	37	PRO	N-CA-CB	6.58	111.19	103.30
25	R	371	PHE	CB-CG-CD2	6.58	125.41	120.80
24	Q	398	TYR	CB-CA-C	-6.57	97.26	110.40
3	c	183	ASP	CB-CG-OD1	-6.57	112.39	118.30
14	7	209	ALA	C-N-CA	6.57	138.12	121.70
33	J	9	ASN	N-CA-CB	6.57	122.42	110.60
21	N	890	PHE	CB-CG-CD2	-6.56	116.21	120.80
22	S	344	PRO	N-CA-CB	6.56	111.17	103.30
3	C	144	TYR	CB-CG-CD2	-6.55	117.07	121.00
9	2	50	THR	CA-CB-CG2	-6.55	103.23	112.40
11	k	83	PHE	CB-CG-CD1	-6.55	116.22	120.80
15	W	109	ARG	NE-CZ-NH1	6.54	123.57	120.30
22	S	239	ARG	NE-CZ-NH1	6.54	123.57	120.30
9	2	104	ARG	CD-NE-CZ	-6.54	114.44	123.60
13	6	52	PHE	CB-CG-CD2	6.53	125.37	120.80
3	c	67	TYR	CB-CG-CD2	6.53	124.92	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	71	ASP	CB-CG-OD2	-6.53	112.42	118.30
28	H	295	PHE	CB-CG-CD1	-6.53	116.23	120.80
6	f	89	ARG	NE-CZ-NH1	6.53	123.56	120.30
33	J	94	TYR	CB-CG-CD2	6.53	124.92	121.00
12	l	202	PHE	CB-CG-CD2	6.53	125.37	120.80
25	R	357	PHE	CB-CG-CD1	-6.53	116.23	120.80
12	5	210	PHE	CB-CG-CD2	-6.53	116.23	120.80
31	L	137	ARG	NE-CZ-NH2	-6.52	117.04	120.30
1	A	162	TYR	CD1-CE1-CZ	6.52	125.67	119.80
15	W	123	ASP	CB-CG-OD2	6.52	124.17	118.30
2	B	145	PHE	CB-CG-CD2	6.52	125.36	120.80
12	5	219	TYR	CB-CG-CD1	6.52	124.91	121.00
20	Z	497	PHE	CB-CG-CD1	-6.52	116.24	120.80
22	S	467	PHE	CB-CG-CD2	-6.51	116.24	120.80
33	J	41	VAL	CA-CB-CG2	-6.51	101.13	110.90
30	K	198	TYR	CB-CG-CD2	-6.51	117.10	121.00
20	Z	341	TYR	CB-CG-CD2	6.50	124.90	121.00
21	N	23	TYR	CB-CG-CD1	6.50	124.90	121.00
20	Z	902	TYR	CG-CD2-CE2	6.50	126.50	121.30
20	Z	202	ARG	NE-CZ-NH1	6.49	123.55	120.30
24	Q	373	VAL	CA-CB-CG2	-6.49	101.16	110.90
25	R	297	TYR	CB-CG-CD2	6.49	124.89	121.00
10	j	186	VAL	CG1-CB-CG2	6.49	121.28	110.90
23	P	88	GLN	O-C-N	6.49	133.09	122.70
5	E	54	ALA	CB-CA-C	-6.49	100.37	110.10
11	4	149	ARG	NE-CZ-NH1	6.49	123.54	120.30
22	S	120	SER	N-CA-CB	6.48	120.23	110.50
25	R	179	PHE	CG-CD1-CE1	6.48	127.93	120.80
25	R	246	TYR	CD1-CE1-CZ	6.48	125.64	119.80
5	e	118	ASP	N-CA-CB	6.48	122.27	110.60
17	T	139	ASP	CB-CG-OD1	-6.48	112.47	118.30
21	N	211	PHE	CB-CG-CD2	-6.48	116.26	120.80
29	I	436	TYR	CB-CG-CD1	6.48	124.89	121.00
13	6	29	ALA	N-CA-CB	6.48	119.17	110.10
21	N	907	ASP	CB-CG-OD1	6.48	124.13	118.30
20	Z	482	ASP	CB-CG-OD1	-6.48	112.47	118.30
21	N	730	VAL	CG1-CB-CG2	-6.47	100.54	110.90
6	f	157	TYR	CB-CG-CD1	-6.47	117.12	121.00
1	A	231	ASP	CB-CG-OD1	6.47	124.12	118.30
24	Q	416	VAL	CA-CB-CG2	-6.47	101.20	110.90
5	E	244	LYS	N-CA-CB	6.47	122.24	110.60
12	5	250	VAL	CB-CA-C	-6.46	99.12	111.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	366	ALA	CB-CA-C	-6.46	100.41	110.10
32	M	44	PHE	CB-CG-CD2	6.46	125.32	120.80
19	Y	83	ARG	NE-CZ-NH2	-6.46	117.07	120.30
32	M	265	ASP	N-CA-CB	6.46	122.23	110.60
22	S	240	ASP	CB-CG-OD1	-6.46	112.49	118.30
33	J	174	PHE	CB-CG-CD2	6.46	125.32	120.80
20	Z	543	THR	O-C-N	-6.46	112.37	122.70
13	m	53	ASP	CB-CG-OD1	-6.45	112.49	118.30
1	A	157	THR	CA-CB-CG2	6.45	121.43	112.40
18	X	11	ARG	NE-CZ-NH2	6.45	123.53	120.30
1	a	197	GLU	CB-CA-C	-6.45	97.51	110.40
3	C	146	TYR	CB-CG-CD1	6.45	124.87	121.00
25	R	99	TYR	CB-CG-CD1	-6.45	117.13	121.00
4	d	93	ALA	O-C-N	-6.44	112.39	122.70
3	C	135	PHE	CB-CG-CD1	6.44	125.31	120.80
21	N	343	THR	CA-CB-CG2	-6.44	103.38	112.40
3	C	137	TYR	CB-CG-CD2	-6.43	117.14	121.00
4	D	4	TYR	CB-CG-CD2	-6.43	117.14	121.00
20	Z	962	ARG	NE-CZ-NH2	-6.43	117.08	120.30
32	M	207	PHE	CB-CG-CD1	6.43	125.30	120.80
33	J	374	ARG	NE-CZ-NH1	6.43	123.51	120.30
1	a	91	ARG	NE-CZ-NH2	6.43	123.51	120.30
4	D	80	ALA	CB-CA-C	-6.43	100.46	110.10
16	V	194	ARG	NE-CZ-NH2	-6.43	117.09	120.30
16	V	203	TYR	CB-CG-CD1	6.43	124.86	121.00
8	1	38	ARG	NE-CZ-NH1	6.42	123.51	120.30
20	Z	553	ARG	NH1-CZ-NH2	6.42	126.46	119.40
12	5	253	TYR	CB-CG-CD2	6.42	124.85	121.00
11	4	13	VAL	CA-CB-CG2	6.42	120.52	110.90
22	S	265	SER	N-CA-CB	6.41	120.12	110.50
1	a	229	THR	N-CA-CB	6.41	122.48	110.30
8	1	48	ASP	CB-CG-OD1	6.41	124.07	118.30
2	b	66	LEU	CB-CA-C	6.41	122.38	110.20
12	l	210	PHE	CB-CG-CD1	-6.41	116.31	120.80
32	M	342	ARG	NE-CZ-NH2	6.41	123.51	120.30
27	O	306	ARG	NE-CZ-NH2	6.41	123.50	120.30
13	m	13	TYR	CG-CD1-CE1	-6.40	116.18	121.30
21	N	721	ASP	CB-CA-C	-6.40	97.60	110.40
21	N	862	SER	N-CA-CB	6.40	120.10	110.50
28	H	136	ALA	N-CA-CB	6.40	119.06	110.10
16	V	164	LEU	CB-CG-CD2	6.39	121.87	111.00
9	i	157	GLY	CA-C-O	6.39	132.10	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	65	TYR	CB-CG-CD1	-6.39	117.17	121.00
22	S	98	SER	N-CA-CB	6.39	120.08	110.50
24	Q	243	PHE	CB-CG-CD1	6.38	125.27	120.80
3	c	65	LYS	N-CA-CB	6.38	122.09	110.60
14	7	110	ASP	CB-CG-OD2	-6.38	112.56	118.30
20	Z	80	SER	N-CA-CB	6.38	120.07	110.50
14	n	139	LYS	CA-CB-CG	6.37	127.42	113.40
1	A	158	ASP	CB-CG-OD2	6.37	124.04	118.30
14	7	240	THR	CA-CB-CG2	-6.37	103.48	112.40
19	Y	43	TRP	CG-CD2-CE3	-6.37	128.16	133.90
31	L	88	TYR	CG-CD1-CE1	-6.37	116.20	121.30
10	3	136	PHE	CB-CG-CD1	-6.37	116.34	120.80
4	D	111	ARG	NE-CZ-NH2	-6.36	117.12	120.30
10	3	80	ARG	NE-CZ-NH2	-6.36	117.12	120.30
2	B	142	PHE	CB-CG-CD1	6.36	125.25	120.80
9	i	200	SER	N-CA-CB	6.36	120.04	110.50
4	D	97	ARG	NE-CZ-NH1	-6.36	117.12	120.30
6	F	202	ARG	NE-CZ-NH2	-6.35	117.12	120.30
27	O	371	VAL	CA-CB-CG1	6.35	120.43	110.90
5	E	181	ALA	N-CA-CB	6.34	118.98	110.10
10	3	99	ARG	CB-CA-C	-6.34	97.71	110.40
11	4	95	ARG	NE-CZ-NH1	6.34	123.47	120.30
32	M	179	THR	N-CA-CB	6.34	122.36	110.30
33	J	382	PHE	CB-CG-CD1	-6.34	116.36	120.80
6	F	85	SER	N-CA-CB	6.34	120.01	110.50
6	f	3	ARG	C-N-CA	6.34	137.55	121.70
31	L	357	ARG	NE-CZ-NH1	6.34	123.47	120.30
32	M	73	ARG	NE-CZ-NH1	-6.34	117.13	120.30
6	f	171	TYR	CB-CG-CD1	-6.34	117.20	121.00
3	C	137	TYR	CG-CD1-CE1	-6.34	116.23	121.30
7	G	201	TYR	CD1-CE1-CZ	-6.34	114.10	119.80
21	N	734	VAL	CA-CB-CG1	6.34	120.40	110.90
25	R	417	TYR	CG-CD1-CE1	-6.33	116.23	121.30
30	K	213	GLY	N-CA-C	-6.33	97.27	113.10
13	6	41	TYR	CB-CG-CD2	6.33	124.80	121.00
4	D	148	TYR	CB-CG-CD2	-6.33	117.20	121.00
1	A	227	VAL	CG1-CB-CG2	-6.33	100.78	110.90
12	l	185	PRO	N-CA-CB	6.32	110.89	103.30
18	X	122	TYR	CB-CG-CD2	6.32	124.79	121.00
28	H	289	ARG	NE-CZ-NH2	-6.32	117.14	120.30
4	d	58	ARG	NE-CZ-NH2	-6.32	117.14	120.30
7	g	211	ASP	N-CA-C	-6.32	93.94	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	320	ASP	CB-CG-OD2	-6.32	112.61	118.30
22	S	399	TYR	N-CA-CB	6.31	121.96	110.60
23	P	115	ARG	NE-CZ-NH1	-6.31	117.14	120.30
33	J	370	LEU	CB-CG-CD2	6.31	121.73	111.00
6	F	7	ASP	CB-CG-OD1	-6.31	112.62	118.30
13	6	76	PHE	CD1-CE1-CZ	-6.31	112.53	120.10
16	V	240	ALA	CB-CA-C	-6.31	100.64	110.10
2	b	101	TYR	CB-CG-CD1	-6.30	117.22	121.00
27	O	100	ASP	CB-CG-OD2	6.30	123.97	118.30
3	C	5	ARG	NE-CZ-NH2	-6.30	117.15	120.30
6	f	201	LEU	CB-CG-CD1	-6.30	100.29	111.00
7	g	201	TYR	CG-CD1-CE1	6.30	126.34	121.30
33	J	142	VAL	CA-CB-CG1	-6.30	101.45	110.90
5	E	156	PHE	CB-CG-CD2	-6.30	116.39	120.80
13	6	52	PHE	CB-CG-CD1	-6.30	116.39	120.80
22	S	326	ASP	CA-CB-CG	-6.30	99.55	113.40
5	e	228	PHE	CB-CG-CD2	6.29	125.20	120.80
29	I	372	SER	N-CA-CB	6.29	119.94	110.50
16	V	231	GLU	OE1-CD-OE2	6.29	130.85	123.30
7	g	182	HIS	N-CA-CB	6.29	121.92	110.60
20	Z	394	TYR	CG-CD1-CE1	-6.29	116.27	121.30
22	S	479	MET	CA-CB-CG	6.29	123.99	113.30
12	l	191	ASP	CB-CG-OD1	-6.29	112.64	118.30
24	Q	410	ASP	CB-CG-OD2	-6.28	112.64	118.30
12	l	189	TYR	CG-CD2-CE2	-6.28	116.28	121.30
21	N	14	ARG	NE-CZ-NH1	6.28	123.44	120.30
2	B	214	ILE	N-CA-C	-6.27	94.07	111.00
5	e	10	ARG	CD-NE-CZ	-6.27	114.83	123.60
7	G	112	PHE	CG-CD1-CE1	6.27	127.69	120.80
11	k	67	TYR	CB-CG-CD2	-6.26	117.24	121.00
23	P	64	ASP	CB-CG-OD2	-6.26	112.66	118.30
4	D	120	TYR	CB-CG-CD2	-6.26	117.25	121.00
1	A	24	ARG	NE-CZ-NH2	-6.25	117.17	120.30
25	R	24	TYR	CD1-CE1-CZ	-6.25	114.17	119.80
31	L	326	ALA	CB-CA-C	-6.25	100.72	110.10
22	S	399	TYR	CB-CA-C	-6.25	97.90	110.40
20	Z	562	TRP	CD2-CE2-CZ2	-6.25	114.80	122.30
32	M	329	ARG	NE-CZ-NH1	-6.25	117.18	120.30
26	U	69	ASP	CB-CG-OD1	-6.24	112.68	118.30
10	3	147	PHE	CB-CG-CD2	-6.24	116.43	120.80
20	Z	841	GLU	OE1-CD-OE2	6.24	130.78	123.30
27	O	179	PHE	CB-CG-CD2	-6.24	116.43	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2	225	ARG	NE-CZ-NH1	6.24	123.42	120.30
26	U	275	VAL	CA-CB-CG2	-6.23	101.55	110.90
20	Z	377	ALA	N-CA-CB	6.23	118.83	110.10
6	F	20	PHE	CB-CG-CD1	-6.23	116.44	120.80
16	V	93	ASP	CB-CG-OD2	6.23	123.91	118.30
21	N	881	TYR	CB-CG-CD1	-6.23	117.26	121.00
11	4	79	ALA	CB-CA-C	-6.23	100.76	110.10
24	Q	321	TYR	CB-CG-CD1	-6.23	117.26	121.00
27	O	161	ASP	CB-CG-OD2	6.23	123.90	118.30
14	n	218	TYR	CA-CB-CG	-6.22	101.57	113.40
21	N	4	THR	CA-CB-CG2	-6.22	103.69	112.40
29	I	305	THR	N-CA-CB	6.22	122.12	110.30
8	1	96	TYR	CB-CG-CD1	6.22	124.73	121.00
8	h	61	THR	CA-CB-CG2	-6.21	103.70	112.40
2	B	82	TYR	CB-CG-CD2	6.21	124.73	121.00
16	V	293	VAL	CA-CB-CG2	-6.21	101.58	110.90
6	F	59	TYR	CB-CG-CD1	-6.21	117.27	121.00
12	5	139	ARG	NE-CZ-NH2	-6.21	117.19	120.30
21	N	260	ASP	CB-CG-OD2	6.21	123.89	118.30
23	P	168	TYR	CB-CG-CD1	-6.21	117.27	121.00
25	R	345	TYR	CB-CG-CD1	6.21	124.72	121.00
2	b	145	PHE	CG-CD2-CE2	6.21	127.62	120.80
10	j	15	MET	CB-CA-C	-6.21	97.99	110.40
7	g	103	TYR	CD1-CE1-CZ	6.20	125.38	119.80
14	n	49	TYR	CG-CD1-CE1	-6.20	116.34	121.30
32	M	326	ALA	N-CA-CB	6.20	118.78	110.10
21	N	51	ASP	CB-CA-C	-6.20	98.01	110.40
1	A	193	HIS	CB-CA-C	-6.19	98.01	110.40
16	V	269	ARG	NE-CZ-NH1	-6.19	117.20	120.30
22	S	28	GLU	N-CA-CB	6.19	121.75	110.60
24	Q	27	TYR	CG-CD1-CE1	-6.19	116.35	121.30
27	O	65	PHE	CB-CG-CD2	-6.19	116.47	120.80
31	L	375	ASP	CB-CG-OD2	-6.19	112.73	118.30
14	n	219	TYR	CB-CG-CD1	6.18	124.71	121.00
24	Q	332	ARG	NE-CZ-NH1	6.18	123.39	120.30
21	N	748	PHE	CB-CG-CD2	-6.18	116.47	120.80
24	Q	386	PHE	CB-CG-CD2	-6.18	116.48	120.80
7	G	193	VAL	CA-CB-CG1	6.17	120.16	110.90
22	S	148	ASP	CB-CG-OD2	6.17	123.86	118.30
3	C	209	ASP	CB-CG-OD1	-6.17	112.75	118.30
3	c	143	ARG	NE-CZ-NH1	6.17	123.38	120.30
7	g	130	ARG	NE-CZ-NH1	6.17	123.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	56	ALA	N-CA-CB	6.17	118.73	110.10
20	Z	564	ARG	CD-NE-CZ	6.16	132.23	123.60
2	b	187	ASP	CB-CG-OD2	-6.16	112.75	118.30
20	Z	369	PHE	CB-CG-CD2	-6.16	116.49	120.80
26	U	72	TYR	CB-CG-CD1	-6.16	117.31	121.00
33	J	198	LEU	CB-CG-CD1	6.16	121.47	111.00
22	S	257	LEU	CB-CG-CD1	6.15	121.46	111.00
30	K	396	ARG	NE-CZ-NH1	6.15	123.38	120.30
31	L	361	PHE	CB-CG-CD2	-6.15	116.49	120.80
12	l	148	ARG	NE-CZ-NH2	6.15	123.38	120.30
33	J	63	ARG	NE-CZ-NH1	6.15	123.38	120.30
3	c	20	TYR	N-CA-CB	6.15	121.67	110.60
30	K	48	TYR	CB-CG-CD1	6.15	124.69	121.00
33	J	322	ALA	CB-CA-C	-6.14	100.88	110.10
13	m	98	ALA	N-CA-CB	6.14	118.70	110.10
28	H	173	ARG	NE-CZ-NH1	-6.14	117.23	120.30
31	L	56	ALA	CB-CA-C	-6.14	100.89	110.10
24	Q	305	ALA	N-CA-CB	6.14	118.70	110.10
28	H	214	CYS	N-CA-C	-6.14	94.42	111.00
16	V	243	SER	N-CA-CB	6.14	119.71	110.50
1	a	24	ARG	NE-CZ-NH2	-6.14	117.23	120.30
13	m	114	TYR	CB-CG-CD2	-6.14	117.32	121.00
5	E	107	ILE	CG1-CB-CG2	6.13	124.89	111.40
10	j	12	VAL	N-CA-C	-6.13	94.45	111.00
20	Z	826	ARG	NE-CZ-NH2	-6.13	117.23	120.30
21	N	618	ARG	NE-CZ-NH1	-6.13	117.23	120.30
2	b	9	LEU	CB-CG-CD1	6.13	121.42	111.00
3	C	210	ARG	NE-CZ-NH2	-6.13	117.23	120.30
23	P	269	VAL	CA-CB-CG2	-6.13	101.71	110.90
22	S	332	PHE	CB-CG-CD2	-6.13	116.51	120.80
27	O	246	SER	N-CA-CB	6.13	119.69	110.50
8	h	118	GLU	OE1-CD-OE2	6.12	130.65	123.30
3	C	53	THR	N-CA-CB	6.12	121.94	110.30
20	Z	376	SER	N-CA-CB	6.12	119.68	110.50
27	O	225	ASP	CB-CG-OD1	-6.12	112.79	118.30
10	j	137	ILE	N-CA-C	-6.12	94.47	111.00
21	N	835	LYS	N-CA-CB	6.12	121.61	110.60
25	R	359	VAL	CA-CB-CG1	-6.12	101.72	110.90
22	S	184	TRP	CE3-CZ3-CH2	-6.12	114.47	121.20
7	g	78	TYR	CB-CG-CD2	-6.11	117.33	121.00
2	B	145	PHE	CB-CG-CD1	-6.11	116.53	120.80
32	M	400	MET	CG-SD-CE	-6.11	90.43	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	112	TYR	CB-CG-CD1	-6.10	117.34	121.00
25	R	321	TYR	CG-CD1-CE1	-6.10	116.42	121.30
29	I	317	ASP	N-CA-C	-6.10	94.52	111.00
31	L	88	TYR	CD1-CG-CD2	6.10	124.61	117.90
9	2	219	TYR	CD1-CE1-CZ	-6.10	114.31	119.80
21	N	780	ASP	CB-CG-OD2	6.10	123.79	118.30
20	Z	267	THR	N-CA-CB	6.09	121.88	110.30
3	c	82	ALA	CB-CA-C	-6.09	100.96	110.10
7	G	26	TYR	CB-CG-CD1	6.09	124.66	121.00
6	f	137	TYR	CB-CG-CD1	6.09	124.65	121.00
15	W	123	ASP	CB-CG-OD1	-6.09	112.82	118.30
23	P	364	ARG	NE-CZ-NH2	-6.09	117.25	120.30
14	n	110	ASP	CB-CG-OD2	-6.09	112.82	118.30
17	T	51	TYR	CB-CG-CD2	-6.09	117.35	121.00
11	k	149	ARG	N-CA-C	-6.08	94.57	111.00
4	D	138	PHE	CB-CG-CD1	-6.08	116.54	120.80
25	R	296	LEU	CB-CA-C	-6.08	98.64	110.20
30	K	360	MET	CG-SD-CE	-6.08	90.47	100.20
15	W	66	THR	CA-CB-CG2	-6.08	103.89	112.40
21	N	719	ASN	CA-CB-CG	-6.08	100.03	113.40
2	B	83	ARG	NE-CZ-NH2	6.08	123.34	120.30
6	F	87	TYR	CB-CG-CD1	-6.08	117.35	121.00
12	5	90	ALA	CB-CA-C	-6.07	100.99	110.10
22	S	452	TYR	CB-CG-CD1	-6.07	117.36	121.00
28	H	109	ASN	N-CA-CB	6.07	121.53	110.60
24	Q	285	LYS	CB-CA-C	-6.07	98.26	110.40
6	F	3	ARG	NE-CZ-NH2	-6.07	117.27	120.30
29	I	181	TYR	CG-CD1-CE1	6.07	126.16	121.30
4	D	17	ILE	N-CA-C	-6.07	94.62	111.00
24	Q	161	LEU	CB-CG-CD1	6.06	121.31	111.00
31	L	290	ARG	N-CA-C	-6.06	94.63	111.00
7	g	44	ASP	CB-CG-OD2	-6.06	112.84	118.30
4	d	36	VAL	CA-CB-CG2	-6.06	101.81	110.90
22	S	59	ASP	CA-CB-CG	-6.06	100.07	113.40
25	R	181	TYR	CB-CG-CD1	6.06	124.64	121.00
14	7	136	ARG	NE-CZ-NH2	-6.05	117.27	120.30
5	e	111	SER	O-C-N	-6.05	113.02	122.70
8	1	197	PHE	CB-CG-CD2	-6.05	116.56	120.80
22	S	484	ASP	CB-CG-OD1	-6.05	112.86	118.30
8	1	96	TYR	CZ-CE2-CD2	-6.04	114.36	119.80
14	7	223	ARG	NE-CZ-NH1	6.04	123.32	120.30
23	P	138	ARG	NE-CZ-NH2	-6.04	117.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	20	ARG	NE-CZ-NH1	6.04	123.32	120.30
7	g	135	SER	N-CA-CB	6.04	119.56	110.50
1	A	36	ASN	CB-CG-OD1	-6.03	109.53	121.60
16	V	248	ALA	N-CA-CB	6.03	118.55	110.10
5	e	92	ALA	CB-CA-C	-6.03	101.06	110.10
20	Z	153	TYR	CB-CG-CD2	-6.03	117.38	121.00
24	Q	109	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	A	12	TYR	C-N-CA	6.03	136.77	121.70
8	1	45	ARG	NH1-CZ-NH2	6.03	126.03	119.40
25	R	169	ASP	CB-CG-OD2	-6.03	112.87	118.30
10	j	68	ARG	NE-CZ-NH2	-6.03	117.29	120.30
21	N	604	ARG	NE-CZ-NH2	6.03	123.31	120.30
9	2	194	ASN	N-CA-CB	-6.02	99.76	110.60
7	g	56	SER	N-CA-CB	6.02	119.53	110.50
1	A	106	TYR	CZ-CE2-CD2	-6.02	114.38	119.80
3	c	122	TYR	CB-CG-CD1	-6.02	117.39	121.00
13	m	230	ASP	CB-CA-C	-6.02	98.36	110.40
13	6	65	PHE	CB-CG-CD1	6.02	125.01	120.80
21	N	37	SER	N-CA-CB	6.02	119.53	110.50
21	N	202	PHE	CB-CG-CD1	6.02	125.01	120.80
13	6	193	ARG	NE-CZ-NH2	-6.02	117.29	120.30
14	n	68	ARG	NE-CZ-NH1	-6.01	117.29	120.30
21	N	78	ALA	N-CA-CB	6.01	118.52	110.10
22	S	268	LEU	CB-CG-CD2	6.01	121.22	111.00
21	N	504	TYR	CD1-CE1-CZ	6.01	125.21	119.80
30	K	345	ASP	N-CA-C	-6.01	94.78	111.00
32	M	421	GLU	N-CA-CB	6.01	121.41	110.60
11	k	46	PHE	CD1-CG-CD2	6.01	126.11	118.30
23	P	21	PHE	CB-CG-CD1	-6.01	116.60	120.80
29	I	343	ARG	NH1-CZ-NH2	-6.01	112.79	119.40
17	T	254	ASP	CB-CG-OD1	6.00	123.70	118.30
14	7	157	ASP	CB-CG-OD2	-6.00	112.90	118.30
27	O	286	PHE	CB-CG-CD2	6.00	125.00	120.80
32	M	220	MET	CG-SD-CE	-6.00	90.60	100.20
15	W	33	VAL	CA-CB-CG2	-6.00	101.90	110.90
8	h	14	ALA	N-CA-C	-6.00	94.81	111.00
26	U	289	ASP	CB-CG-OD1	5.99	123.69	118.30
12	l	273	TRP	CE2-CD2-CG	-5.99	102.51	107.30
20	Z	281	ALA	N-CA-CB	5.99	118.49	110.10
2	b	32	VAL	CB-CA-C	-5.99	100.02	111.40
21	N	549	TYR	CG-CD1-CE1	-5.99	116.51	121.30
13	6	168	TYR	CG-CD2-CE2	-5.99	116.51	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	346	TYR	CB-CG-CD1	5.99	124.59	121.00
25	R	179	PHE	CB-CG-CD1	5.99	124.99	120.80
14	n	163	VAL	CA-CB-CG2	5.99	119.88	110.90
3	C	69	LEU	CB-CG-CD2	5.99	121.18	111.00
3	C	131	PHE	CG-CD2-CE2	-5.99	114.22	120.80
24	Q	65	TYR	CD1-CE1-CZ	5.98	125.19	119.80
33	J	261	SER	N-CA-CB	5.98	119.47	110.50
11	k	59	TYR	CB-CG-CD1	5.98	124.59	121.00
17	T	34	LEU	CB-CG-CD1	5.98	121.16	111.00
22	S	108	ALA	O-C-N	5.98	132.26	122.70
7	g	103	TYR	CG-CD1-CE1	-5.97	116.52	121.30
18	X	122	TYR	CB-CG-CD1	-5.97	117.42	121.00
23	P	158	ASP	CB-CG-OD2	-5.97	112.93	118.30
29	I	233	ALA	CB-CA-C	-5.97	101.14	110.10
3	c	208	TYR	CB-CG-CD1	-5.97	117.42	121.00
21	N	406	TYR	CB-CG-CD1	5.97	124.58	121.00
10	j	67	PHE	CB-CA-C	-5.97	98.47	110.40
9	2	61	ALA	N-CA-CB	5.97	118.45	110.10
33	J	211	ILE	N-CA-CB	5.97	124.52	110.80
21	N	599	TYR	CB-CG-CD2	-5.96	117.42	121.00
28	H	52	THR	N-CA-CB	5.96	121.63	110.30
4	d	220	ASP	CB-CG-OD2	-5.96	112.94	118.30
22	S	431	VAL	CA-CB-CG2	-5.96	101.96	110.90
28	H	234	ARG	NH1-CZ-NH2	-5.96	112.84	119.40
23	P	240	TYR	CB-CG-CD1	5.96	124.58	121.00
23	P	46	THR	CA-CB-CG2	-5.96	104.06	112.40
3	c	184	MET	CG-SD-CE	-5.96	90.67	100.20
9	i	68	PRO	N-CA-CB	-5.96	96.05	102.60
14	7	252	TRP	CB-CG-CD2	-5.96	118.86	126.60
28	H	461	SER	N-CA-CB	5.96	119.44	110.50
11	4	56	PHE	CB-CG-CD2	-5.95	116.63	120.80
13	m	194	ASP	CB-CG-OD1	-5.95	112.94	118.30
28	H	45	TYR	CZ-CE2-CD2	-5.95	114.45	119.80
13	6	85	PHE	CB-CG-CD1	5.95	124.96	120.80
31	L	60	PHE	CB-CG-CD1	5.94	124.96	120.80
3	c	220	ALA	N-CA-CB	5.94	118.42	110.10
19	Y	72	ASP	CB-CG-OD2	-5.94	112.95	118.30
20	Z	146	PHE	CB-CG-CD1	5.94	124.96	120.80
24	Q	48	ASP	CB-CG-OD1	5.94	123.64	118.30
12	l	230	TYR	CG-CD2-CE2	5.94	126.05	121.30
21	N	526	TYR	CB-CG-CD2	-5.93	117.44	121.00
11	k	96	ARG	NE-CZ-NH1	5.93	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	55	SER	N-CA-CB	5.93	119.39	110.50
12	5	229	LEU	N-CA-CB	5.93	122.26	110.40
13	6	27	ASP	CB-CG-OD1	-5.93	112.96	118.30
25	R	197	MET	CG-SD-CE	-5.93	90.71	100.20
1	A	155	TYR	CZ-CE2-CD2	-5.93	114.47	119.80
20	Z	375	ASP	CB-CG-OD2	5.93	123.64	118.30
30	K	161	MET	CG-SD-CE	-5.93	90.72	100.20
16	V	156	PHE	CD1-CE1-CZ	-5.93	112.99	120.10
20	Z	601	VAL	CG1-CB-CG2	5.93	120.38	110.90
4	d	179	TYR	CB-CG-CD1	-5.92	117.44	121.00
4	d	179	TYR	CG-CD1-CE1	-5.92	116.56	121.30
2	b	5	TYR	CB-CG-CD2	5.92	124.55	121.00
8	h	91	PHE	CB-CG-CD2	-5.92	116.66	120.80
30	K	412	ALA	CB-CA-C	-5.92	101.23	110.10
19	Y	84	TYR	CB-CG-CD1	-5.92	117.45	121.00
13	m	130	VAL	N-CA-C	-5.91	95.03	111.00
31	L	346	LYS	N-CA-CB	5.91	121.24	110.60
28	H	76	LEU	N-CA-C	-5.91	95.05	111.00
20	Z	906	ALA	N-CA-CB	5.91	118.37	110.10
12	l	165	TYR	CG-CD2-CE2	-5.91	116.58	121.30
12	5	245	TYR	CZ-CE2-CD2	-5.91	114.48	119.80
13	6	76	PHE	CB-CG-CD2	-5.91	116.67	120.80
31	L	331	ASP	CB-CG-OD2	-5.90	112.99	118.30
30	K	49	PHE	CB-CG-CD1	-5.90	116.67	120.80
7	G	15	PHE	CG-CD1-CE1	-5.90	114.31	120.80
8	1	120	TYR	CD1-CG-CD2	5.90	124.39	117.90
10	3	183	TRP	C-N-CA	5.90	134.69	122.30
30	K	349	ARG	NE-CZ-NH1	-5.90	117.35	120.30
30	K	387	MET	CA-CB-CG	5.90	123.33	113.30
3	c	133	VAL	CG1-CB-CG2	5.89	120.33	110.90
28	H	83	ASP	CB-CG-OD1	5.89	123.61	118.30
29	I	61	ARG	NE-CZ-NH1	5.89	123.25	120.30
5	E	53	ARG	NE-CZ-NH2	5.89	123.25	120.30
20	Z	887	GLY	N-CA-C	-5.89	98.37	113.10
32	M	166	ARG	NE-CZ-NH2	-5.89	117.35	120.30
1	a	168	ALA	N-CA-CB	5.89	118.35	110.10
13	6	182	TYR	CB-CG-CD2	-5.89	117.47	121.00
22	S	45	THR	CA-CB-CG2	-5.89	104.15	112.40
21	N	18	ASP	CB-CG-OD2	-5.89	113.00	118.30
1	a	91	ARG	NE-CZ-NH1	-5.89	117.36	120.30
20	Z	247	GLN	N-CA-CB	5.88	121.19	110.60
29	I	88	LYS	N-CA-CB	5.88	121.19	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	22	PHE	CB-CG-CD1	5.88	124.92	120.80
8	h	198	TYR	CB-CG-CD2	-5.88	117.47	121.00
2	B	246	ARG	NE-CZ-NH1	-5.88	117.36	120.30
27	O	81	TYR	N-CA-CB	5.88	121.18	110.60
31	L	221	TYR	CG-CD1-CE1	-5.88	116.60	121.30
9	i	225	ARG	NE-CZ-NH1	5.88	123.24	120.30
13	m	47	TYR	CB-CG-CD1	5.87	124.52	121.00
23	P	6	PRO	N-CA-CB	5.87	110.35	103.30
20	Z	870	ALA	N-CA-CB	-5.87	101.88	110.10
30	K	418	ASP	N-CA-CB	5.87	121.17	110.60
4	d	4	TYR	CB-CG-CD2	-5.87	117.48	121.00
9	2	128	ILE	N-CA-C	-5.87	95.15	111.00
13	6	166	ASN	N-CA-CB	5.87	121.17	110.60
20	Z	374	LEU	N-CA-CB	5.87	122.14	110.40
31	L	118	ILE	N-CA-C	-5.87	95.15	111.00
12	l	227	ASP	CB-CG-OD2	5.87	123.58	118.30
15	W	17	ARG	NE-CZ-NH1	5.87	123.23	120.30
8	1	97	GLU	OE1-CD-OE2	5.86	130.34	123.30
25	R	357	PHE	CG-CD1-CE1	-5.86	114.35	120.80
28	H	190	ARG	NE-CZ-NH2	-5.86	117.37	120.30
29	I	280	PHE	CZ-CE2-CD2	-5.86	113.07	120.10
12	5	242	ARG	NE-CZ-NH1	-5.86	117.37	120.30
15	W	9	VAL	N-CA-C	-5.86	95.19	111.00
8	h	127	SER	N-CA-CB	5.86	119.28	110.50
20	Z	513	ALA	N-CA-CB	5.86	118.30	110.10
29	I	171	MET	CG-SD-CE	-5.86	90.83	100.20
3	c	213	PHE	CB-CG-CD2	-5.85	116.70	120.80
20	Z	906	ALA	CB-CA-C	-5.85	101.32	110.10
11	4	130	TYR	CG-CD2-CE2	-5.85	116.62	121.30
11	4	132	ALA	N-CA-CB	5.85	118.29	110.10
26	U	19	LEU	CB-CG-CD2	-5.84	101.07	111.00
29	I	196	GLU	N-CA-CB	5.84	121.12	110.60
3	C	165	VAL	N-CA-C	-5.84	95.23	111.00
5	E	55	THR	CA-CB-CG2	-5.84	104.22	112.40
8	1	162	ASP	CB-CG-OD1	5.84	123.56	118.30
21	N	630	ALA	CB-CA-C	-5.84	101.34	110.10
32	M	381	ARG	NE-CZ-NH2	-5.84	117.38	120.30
24	Q	398	TYR	CG-CD1-CE1	-5.84	116.63	121.30
32	M	128	PHE	CB-CG-CD1	-5.84	116.71	120.80
7	G	142	ASP	CB-CG-OD1	5.84	123.55	118.30
33	J	404	PHE	CB-CG-CD2	-5.84	116.72	120.80
8	h	48	ASP	CB-CG-OD2	5.83	123.55	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	82	TYR	CB-CG-CD1	-5.83	117.50	121.00
18	X	100	TRP	N-CA-CB	5.83	121.10	110.60
20	Z	437	ASP	CB-CG-OD1	-5.83	113.05	118.30
29	I	222	TYR	CG-CD1-CE1	-5.83	116.63	121.30
13	6	155	MET	CA-C-N	5.83	133.43	117.10
15	W	155	ASP	CB-CG-OD1	5.83	123.55	118.30
22	S	95	PHE	CB-CG-CD2	5.83	124.88	120.80
6	F	219	ASP	CB-CG-OD2	-5.83	113.05	118.30
10	3	49	VAL	CG1-CB-CG2	5.83	120.22	110.90
8	h	156	SER	N-CA-CB	5.83	119.24	110.50
14	n	67	LEU	CB-CG-CD2	5.82	120.90	111.00
2	B	5	TYR	CB-CG-CD2	-5.82	117.51	121.00
26	U	110	PHE	CB-CG-CD2	-5.82	116.72	120.80
11	4	164	CYS	CB-CA-C	-5.82	98.75	110.40
23	P	419	VAL	CA-CB-CG2	-5.82	102.17	110.90
5	e	223	THR	N-CA-C	-5.82	95.29	111.00
30	K	378	LEU	CB-CG-CD2	5.82	120.89	111.00
23	P	225	VAL	CG1-CB-CG2	5.82	120.20	110.90
30	K	335	ASP	CB-CG-OD1	-5.82	113.07	118.30
24	Q	427	PHE	CB-CG-CD2	5.81	124.87	120.80
21	N	771	PHE	N-CA-CB	5.81	121.06	110.60
21	N	778	LYS	N-CA-C	-5.81	95.30	111.00
22	S	18	LEU	CB-CG-CD1	5.81	120.88	111.00
6	F	208	VAL	CA-CB-CG1	-5.81	102.19	110.90
28	H	228	PRO	N-CA-CB	5.81	110.27	103.30
30	K	119	VAL	N-CA-C	-5.81	95.31	111.00
4	d	138	PHE	CB-CG-CD2	5.81	124.87	120.80
31	L	221	TYR	CB-CG-CD2	-5.81	117.52	121.00
25	R	422	ARG	NE-CZ-NH1	-5.81	117.40	120.30
14	n	128	TYR	CG-CD2-CE2	5.80	125.94	121.30
4	d	97	ARG	NE-CZ-NH1	5.80	123.20	120.30
20	Z	776	VAL	CA-C-O	-5.80	107.91	120.10
12	l	81	PHE	CG-CD1-CE1	-5.80	114.42	120.80
6	F	164	ARG	NE-CZ-NH2	-5.80	117.40	120.30
33	J	292	MET	N-CA-CB	5.80	121.04	110.60
7	g	91	ARG	NH1-CZ-NH2	-5.80	113.02	119.40
13	m	157	PHE	CB-CG-CD2	-5.80	116.74	120.80
11	4	5	LEU	CB-CA-C	-5.80	99.18	110.20
22	S	442	PHE	CB-CG-CD1	-5.80	116.74	120.80
30	K	114	THR	O-C-N	-5.80	113.34	123.20
2	b	148	TYR	CB-CA-C	-5.80	98.80	110.40
25	R	162	ILE	N-CA-C	-5.80	95.35	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	97	TYR	CB-CG-CD2	5.79	124.48	121.00
11	k	177	LYS	N-CA-CB	5.79	121.03	110.60
8	1	43	LEU	N-CA-C	-5.79	95.36	111.00
26	U	287	ALA	CB-CA-C	-5.79	101.42	110.10
4	d	197	ARG	NE-CZ-NH2	-5.79	117.41	120.30
32	M	221	TYR	CB-CG-CD1	-5.79	117.53	121.00
20	Z	632	GLU	C-N-CA	5.78	136.16	121.70
21	N	764	SER	N-CA-CB	5.78	119.18	110.50
19	Y	4	ASP	CB-CG-OD1	-5.78	113.10	118.30
20	Z	872	VAL	CA-CB-CG1	-5.78	102.23	110.90
30	K	325	ASP	CB-CG-OD1	5.78	123.50	118.30
12	l	165	TYR	CB-CG-CD1	-5.78	117.53	121.00
2	b	25	LEU	CB-CG-CD2	5.78	120.82	111.00
12	5	202	PHE	CB-CG-CD2	-5.78	116.76	120.80
16	V	134	SER	O-C-N	-5.78	113.46	122.70
20	Z	806	GLU	OE1-CD-OE2	5.78	130.23	123.30
24	Q	129	LYS	CB-CA-C	-5.78	98.85	110.40
21	N	81	TYR	CB-CG-CD1	5.78	124.47	121.00
21	N	97	PHE	CB-CG-CD2	-5.78	116.76	120.80
7	G	112	PHE	CB-CG-CD1	-5.77	116.76	120.80
17	T	31	LYS	O-C-N	5.77	131.94	122.70
22	S	26	ALA	N-CA-CB	5.77	118.18	110.10
14	n	50	ASP	CB-CG-OD1	-5.77	113.11	118.30
10	3	54	THR	CA-CB-CG2	-5.77	104.32	112.40
21	N	776	TYR	N-CA-CB	5.77	120.99	110.60
29	I	374	ASP	CB-CG-OD2	5.77	123.49	118.30
9	i	171	TRP	CB-CG-CD1	5.77	134.50	127.00
17	T	142	LEU	CB-CA-C	-5.77	99.24	110.20
19	Y	35	PHE	CB-CG-CD2	-5.77	116.76	120.80
28	H	437	VAL	CA-CB-CG2	5.77	119.56	110.90
3	c	56	LEU	CB-CA-C	-5.77	99.24	110.20
20	Z	306	MET	CG-SD-CE	-5.77	90.97	100.20
23	P	374	SER	N-CA-CB	5.77	119.15	110.50
12	l	235	SER	N-CA-CB	5.76	119.14	110.50
13	m	47	TYR	CZ-CE2-CD2	5.76	124.99	119.80
24	Q	189	ARG	N-CA-CB	5.76	120.98	110.60
8	h	17	PHE	CB-CG-CD2	5.76	124.83	120.80
10	j	96	TYR	CB-CG-CD1	5.76	124.46	121.00
24	Q	201	ALA	CB-CA-C	-5.76	101.46	110.10
30	K	235	ILE	CA-C-N	5.76	129.88	117.20
24	Q	238	TYR	CD1-CE1-CZ	-5.76	114.62	119.80
33	J	272	MET	CA-CB-CG	5.76	123.09	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	967	THR	CA-CB-CG2	-5.76	104.34	112.40
2	B	159	TRP	CB-CA-C	-5.76	98.89	110.40
3	C	160	TRP	CZ3-CH2-CZ2	-5.76	114.69	121.60
4	D	22	TYR	CB-CG-CD1	5.76	124.45	121.00
28	H	112	SER	CB-CA-C	5.75	121.03	110.10
1	a	205	PHE	CB-CG-CD2	-5.75	116.78	120.80
20	Z	878	LEU	CB-CG-CD1	5.75	120.77	111.00
9	2	236	ARG	NE-CZ-NH2	-5.75	117.43	120.30
27	O	51	ASP	CB-CG-OD2	-5.75	113.13	118.30
27	O	120	LYS	N-CA-CB	5.75	120.94	110.60
31	L	290	ARG	NE-CZ-NH2	-5.75	117.43	120.30
33	J	181	GLN	N-CA-CB	5.75	120.94	110.60
13	m	13	TYR	CG-CD2-CE2	-5.75	116.70	121.30
13	6	168	TYR	CD1-CG-CD2	5.75	124.22	117.90
13	m	176	VAL	CA-CB-CG2	-5.74	102.29	110.90
2	b	178	ARG	NE-CZ-NH2	-5.74	117.43	120.30
13	6	224	PHE	CB-CG-CD1	5.74	124.82	120.80
21	N	140	MET	CG-SD-CE	5.74	109.38	100.20
23	P	12	ASP	CB-CG-OD2	5.74	123.46	118.30
4	d	98	LEU	O-C-N	-5.74	113.52	122.70
4	d	117	GLN	O-C-N	-5.74	113.52	122.70
16	V	261	LEU	C-N-CA	5.74	136.04	121.70
9	i	234	PHE	CB-CG-CD2	-5.73	116.79	120.80
13	m	182	TYR	CG-CD1-CE1	-5.73	116.71	121.30
9	2	57	ASP	CB-CG-OD1	5.73	123.46	118.30
9	2	117	PHE	CG-CD1-CE1	-5.73	114.49	120.80
22	S	286	TYR	CB-CG-CD1	-5.73	117.56	121.00
24	Q	43	GLY	C-N-CA	5.73	136.03	121.70
20	Z	406	TRP	CG-CD1-NE1	-5.73	104.37	110.10
27	O	216	ASP	CB-CG-OD1	-5.73	113.14	118.30
32	M	303	ARG	NE-CZ-NH2	-5.73	117.44	120.30
3	C	203	SER	N-CA-CB	5.73	119.09	110.50
23	P	266	TYR	CZ-CE2-CD2	5.73	124.95	119.80
20	Z	413	ASP	CB-CG-OD1	-5.72	113.15	118.30
30	K	220	THR	CA-CB-CG2	5.72	120.42	112.40
10	3	81	ALA	N-CA-CB	5.72	118.11	110.10
27	O	266	PHE	CB-CG-CD2	5.72	124.81	120.80
12	l	204	VAL	CB-CA-C	-5.72	100.53	111.40
1	A	19	PHE	CB-CG-CD1	-5.72	116.80	120.80
12	5	133	TRP	CE2-CD2-CG	-5.72	102.72	107.30
9	i	232	TYR	CB-CG-CD1	-5.72	117.57	121.00
14	n	50	ASP	CB-CG-OD2	5.72	123.45	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	60	ARG	NE-CZ-NH1	-5.72	117.44	120.30
16	V	176	ASN	N-CA-CB	5.71	120.89	110.60
21	N	776	TYR	CB-CG-CD1	5.71	124.43	121.00
10	j	116	SER	CB-CA-C	-5.71	99.25	110.10
2	B	204	PHE	CB-CG-CD1	5.71	124.80	120.80
2	B	70	ASP	CB-CG-OD1	-5.71	113.16	118.30
14	n	228	PHE	N-CA-CB	5.71	120.87	110.60
20	Z	441	TYR	CD1-CE1-CZ	5.71	124.94	119.80
14	n	35	GLN	CG-CD-OE1	-5.70	110.19	121.60
7	G	219	CYS	N-CA-C	-5.70	95.60	111.00
8	1	46	VAL	CA-CB-CG1	-5.70	102.35	110.90
20	Z	85	VAL	CA-C-N	5.70	133.07	117.10
2	b	97	TYR	CB-CG-CD1	-5.70	117.58	121.00
22	S	306	SER	N-CA-CB	5.70	119.05	110.50
9	2	249	ILE	CA-CB-CG2	-5.70	99.50	110.90
20	Z	825	ALA	N-CA-CB	5.70	118.08	110.10
24	Q	369	ASP	CB-CG-OD2	5.70	123.43	118.30
13	6	145	ARG	NE-CZ-NH1	5.70	123.15	120.30
29	I	271	ALA	CB-CA-C	-5.70	101.56	110.10
6	f	170	THR	CA-CB-CG2	5.69	120.37	112.40
25	R	272	ASP	N-CA-CB	5.69	120.85	110.60
2	b	7	PHE	CB-CG-CD1	5.69	124.78	120.80
10	j	193	ASP	CB-CG-OD2	-5.69	113.18	118.30
4	D	6	ARG	NE-CZ-NH2	-5.69	117.45	120.30
21	N	196	THR	CA-CB-CG2	5.69	120.37	112.40
5	E	48	LEU	CB-CA-C	-5.69	99.39	110.20
20	Z	413	ASP	CB-CG-OD2	5.69	123.42	118.30
5	E	217	ALA	N-CA-CB	5.68	118.06	110.10
33	J	120	TYR	CB-CG-CD1	5.68	124.41	121.00
24	Q	68	MET	N-CA-CB	5.68	120.83	110.60
29	I	127	ASP	CB-CG-OD1	5.68	123.41	118.30
30	K	340	PHE	CB-CG-CD2	-5.68	116.82	120.80
10	j	168	SER	N-CA-CB	5.68	119.02	110.50
5	E	97	VAL	CA-CB-CG2	-5.68	102.38	110.90
21	N	543	ASP	N-CA-CB	5.68	120.82	110.60
25	R	297	TYR	CZ-CE2-CD2	-5.68	114.69	119.80
5	e	88	MET	CG-SD-CE	-5.67	91.12	100.20
20	Z	510	LEU	CB-CG-CD2	5.67	120.65	111.00
4	d	5	ASP	CB-CG-OD2	5.67	123.41	118.30
4	D	166	ARG	NE-CZ-NH1	5.67	123.14	120.30
8	1	79	TYR	CD1-CE1-CZ	-5.67	114.69	119.80
1	a	124	LEU	CB-CG-CD1	5.67	120.64	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	190	ARG	NE-CZ-NH1	-5.67	117.47	120.30
26	U	110	PHE	CB-CG-CD1	5.67	124.77	120.80
2	b	132	VAL	CG1-CB-CG2	-5.67	101.83	110.90
16	V	254	ARG	NE-CZ-NH2	-5.67	117.47	120.30
21	N	880	ARG	NE-CZ-NH2	-5.67	117.47	120.30
3	c	144	TYR	CD1-CE1-CZ	-5.67	114.70	119.80
28	H	194	SER	N-CA-CB	5.67	119.00	110.50
1	a	133	TYR	CB-CG-CD1	5.66	124.40	121.00
7	g	217	SER	N-CA-CB	5.66	118.99	110.50
22	S	475	TYR	CB-CG-CD2	-5.66	117.60	121.00
25	R	345	TYR	CB-CA-C	-5.66	99.07	110.40
30	K	127	ASP	CB-CG-OD2	-5.66	113.20	118.30
32	M	77	TYR	N-CA-CB	5.66	120.79	110.60
19	Y	10	ALA	N-CA-CB	5.66	118.03	110.10
1	a	68	THR	CA-CB-CG2	-5.66	104.47	112.40
16	V	304	ALA	N-CA-CB	5.66	118.03	110.10
9	i	119	TYR	CB-CA-C	-5.66	99.08	110.40
13	6	201	GLU	N-CA-CB	5.66	120.79	110.60
32	M	271	LYS	CB-CA-C	-5.66	99.08	110.40
17	T	24	GLU	N-CA-CB	5.66	120.78	110.60
3	c	226	TYR	CB-CG-CD1	-5.65	117.61	121.00
13	m	44	ASN	CA-CB-CG	-5.65	100.97	113.40
3	c	187	ASP	CB-CG-OD1	5.64	123.38	118.30
23	P	390	TYR	CG-CD1-CE1	5.64	125.81	121.30
14	n	43	SER	N-CA-CB	5.64	118.96	110.50
9	2	119	TYR	CD1-CE1-CZ	5.64	124.88	119.80
13	6	76	PHE	CB-CG-CD1	5.64	124.75	120.80
16	V	294	SER	N-CA-CB	5.64	118.96	110.50
7	g	115	ARG	NE-CZ-NH2	-5.64	117.48	120.30
7	g	119	TYR	CB-CG-CD1	-5.64	117.62	121.00
9	2	54	ILE	CA-CB-CG1	5.64	121.71	111.00
23	P	207	THR	N-CA-CB	5.64	121.01	110.30
1	a	53	VAL	CG1-CB-CG2	5.63	119.92	110.90
23	P	65	LEU	CB-CG-CD2	5.63	120.58	111.00
30	K	367	ASP	CB-CG-OD2	-5.63	113.23	118.30
6	f	171	TYR	CG-CD1-CE1	-5.63	116.80	121.30
1	A	110	TYR	CG-CD1-CE1	5.63	125.81	121.30
12	5	144	ARG	O-C-N	-5.63	113.69	122.70
20	Z	441	TYR	CG-CD1-CE1	-5.63	116.79	121.30
30	K	46	ASP	CB-CG-OD2	5.63	123.37	118.30
1	a	147	ASP	CB-CG-OD2	-5.63	113.23	118.30
10	3	203	ARG	NE-CZ-NH1	5.63	123.11	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	236	ARG	NH1-CZ-NH2	5.63	125.59	119.40
30	K	178	ASP	CB-CG-OD2	5.63	123.36	118.30
5	E	124	GLY	N-CA-C	-5.62	99.04	113.10
7	G	78	TYR	CB-CG-CD2	-5.62	117.63	121.00
24	Q	8	LEU	CB-CG-CD2	5.62	120.56	111.00
12	l	204	VAL	CA-CB-CG2	-5.62	102.47	110.90
13	m	155	MET	N-CA-CB	5.62	120.72	110.60
22	S	95	PHE	CG-CD1-CE1	-5.62	114.62	120.80
3	c	157	TYR	CB-CG-CD2	-5.62	117.63	121.00
21	N	873	ARG	NE-CZ-NH2	-5.62	117.49	120.30
1	a	203	VAL	CA-CB-CG1	5.61	119.32	110.90
15	W	96	LEU	CB-CG-CD2	5.61	120.54	111.00
13	m	145	ARG	NE-CZ-NH1	-5.61	117.49	120.30
20	Z	93	ARG	NE-CZ-NH2	-5.61	117.50	120.30
8	1	152	ARG	NH1-CZ-NH2	-5.61	113.23	119.40
9	2	217	ARG	NE-CZ-NH2	-5.61	117.50	120.30
23	P	12	ASP	CB-CG-OD1	-5.61	113.25	118.30
22	S	188	TYR	CB-CG-CD2	-5.61	117.64	121.00
31	L	104	LEU	N-CA-C	-5.61	95.86	111.00
19	Y	41	ASP	CB-CG-OD2	-5.60	113.26	118.30
22	S	136	CYS	CA-CB-SG	5.60	124.08	114.00
23	P	193	TYR	CB-CG-CD1	-5.60	117.64	121.00
20	Z	970	TYR	CB-CG-CD2	5.60	124.36	121.00
2	B	101	TYR	CB-CG-CD2	5.60	124.36	121.00
23	P	415	TRP	CB-CA-C	-5.60	99.20	110.40
7	g	48	PHE	CB-CG-CD2	-5.60	116.88	120.80
10	j	91	VAL	CA-CB-CG2	-5.60	102.50	110.90
17	T	23	CYS	CB-CA-C	-5.60	99.21	110.40
21	N	109	TYR	CB-CG-CD1	5.60	124.36	121.00
29	I	60	LEU	N-CA-CB	5.60	121.59	110.40
20	Z	109	PRO	N-CD-CG	5.59	111.59	103.20
20	Z	242	PHE	CB-CG-CD2	-5.59	116.88	120.80
24	Q	432	VAL	CG1-CB-CG2	-5.59	101.95	110.90
26	U	103	ASP	N-CA-CB	5.59	120.67	110.60
28	H	122	SER	N-CA-CB	5.59	118.89	110.50
21	N	389	TYR	CB-CG-CD1	5.59	124.36	121.00
25	R	331	ARG	NE-CZ-NH2	-5.59	117.50	120.30
21	N	60	MET	CA-CB-CG	-5.59	103.80	113.30
11	k	175	ASP	CB-CG-OD1	-5.59	113.27	118.30
14	n	173	PRO	O-C-N	5.59	131.64	122.70
1	A	150	LEU	CB-CG-CD2	5.59	120.50	111.00
10	3	40	PHE	CB-CG-CD1	-5.59	116.89	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	27	ASP	CB-CG-OD2	5.59	123.33	118.30
24	Q	65	TYR	CB-CG-CD1	5.59	124.35	121.00
25	R	234	SER	N-CA-CB	5.59	118.89	110.50
3	c	140	TYR	CB-CG-CD2	5.59	124.35	121.00
32	M	50	ARG	CD-NE-CZ	5.59	131.42	123.60
4	D	42	VAL	O-C-N	-5.59	113.76	122.70
20	Z	129	ASN	CB-CA-C	-5.59	99.23	110.40
20	Z	970	TYR	CB-CG-CD1	-5.59	117.65	121.00
32	M	179	THR	CA-CB-CG2	-5.59	104.58	112.40
9	2	94	LEU	CB-CA-C	-5.58	99.59	110.20
14	7	261	TYR	CG-CD1-CE1	-5.58	116.83	121.30
3	C	108	VAL	CA-CB-CG1	-5.58	102.52	110.90
26	U	40	ASP	CB-CG-OD2	5.58	123.33	118.30
26	U	198	LYS	N-CA-CB	5.58	120.65	110.60
6	f	126	ARG	NE-CZ-NH1	5.58	123.09	120.30
9	i	130	ALA	N-CA-C	-5.58	95.93	111.00
20	Z	116	ALA	N-CA-CB	5.58	117.92	110.10
30	K	307	ASP	C-N-CA	5.58	135.65	121.70
21	N	422	TYR	CD1-CE1-CZ	5.58	124.82	119.80
27	O	252	PHE	CB-CG-CD1	-5.58	116.89	120.80
22	S	461	PHE	CB-CG-CD1	5.58	124.70	120.80
7	g	201	TYR	CB-CG-CD2	5.58	124.34	121.00
13	m	36	ARG	NE-CZ-NH2	5.58	123.09	120.30
16	V	67	ASP	CB-CG-OD2	5.58	123.32	118.30
20	Z	103	TYR	CG-CD1-CE1	-5.58	116.84	121.30
7	G	220	SER	N-CA-CB	5.57	118.86	110.50
20	Z	244	ARG	NE-CZ-NH2	5.57	123.09	120.30
23	P	235	LEU	CB-CG-CD2	5.57	120.47	111.00
15	W	113	PHE	CB-CG-CD2	-5.57	116.90	120.80
24	Q	306	TYR	CB-CG-CD1	-5.57	117.66	121.00
33	J	188	TYR	CB-CG-CD1	5.57	124.34	121.00
11	k	72	ASP	CB-CG-OD1	-5.57	113.29	118.30
3	C	54	SER	N-CA-CB	5.57	118.85	110.50
12	l	266	HIS	CA-CB-CG	-5.57	104.13	113.60
14	7	40	THR	CA-CB-CG2	-5.57	104.61	112.40
20	Z	358	TYR	CB-CG-CD2	-5.57	117.66	121.00
32	M	331	ASP	CB-CG-OD1	-5.57	113.29	118.30
27	O	215	TYR	CB-CG-CD2	5.56	124.34	121.00
20	Z	541	ASP	N-CA-CB	5.56	120.61	110.60
23	P	10	ASP	CB-CG-OD2	5.56	123.31	118.30
27	O	49	PHE	N-CA-CB	5.56	120.61	110.60
27	O	300	VAL	CG1-CB-CG2	5.56	119.80	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	196	VAL	CA-CB-CG1	5.56	119.24	110.90
20	Z	520	ILE	C-N-CA	5.56	135.60	121.70
20	Z	902	TYR	CB-CG-CD2	5.56	124.34	121.00
5	e	207	VAL	CA-CB-CG1	-5.56	102.56	110.90
6	F	163	ALA	CB-CA-C	-5.55	101.77	110.10
6	f	185	ASN	N-CA-CB	5.55	120.59	110.60
11	k	127	GLU	N-CA-CB	5.55	120.59	110.60
13	m	113	TYR	CB-CG-CD1	-5.55	117.67	121.00
6	f	210	ASN	O-C-N	-5.55	113.82	122.70
21	N	36	TRP	CG-CD2-CE3	-5.55	128.90	133.90
27	O	135	ARG	NH1-CZ-NH2	5.55	125.51	119.40
1	A	99	ALA	CB-CA-C	-5.55	101.78	110.10
16	V	171	ARG	NE-CZ-NH1	-5.55	117.53	120.30
1	a	106	TYR	CB-CG-CD2	-5.55	117.67	121.00
6	f	94	TYR	CZ-CE2-CD2	-5.55	114.81	119.80
30	K	418	ASP	CB-CG-OD2	-5.55	113.31	118.30
33	J	120	TYR	CB-CG-CD2	-5.55	117.67	121.00
14	7	44	VAL	N-CA-C	-5.54	96.03	111.00
27	O	106	PHE	CB-CA-C	-5.54	99.31	110.40
25	R	91	TRP	CA-CB-CG	5.54	124.23	113.70
31	L	194	ARG	NE-CZ-NH1	5.54	123.07	120.30
31	L	377	GLU	OE1-CD-OE2	5.54	129.95	123.30
3	c	215	THR	N-CA-C	-5.54	96.05	111.00
11	k	12	SER	N-CA-CB	5.54	118.81	110.50
2	B	216	ASP	CA-CB-CG	-5.54	101.22	113.40
33	J	6	THR	CA-CB-CG2	5.54	120.16	112.40
1	A	71	TYR	CG-CD2-CE2	-5.54	116.87	121.30
25	R	207	ARG	NE-CZ-NH1	5.54	123.07	120.30
24	Q	80	HIS	N-CA-CB	5.54	120.56	110.60
6	F	145	LEU	N-CA-CB	5.53	121.47	110.40
22	S	440	ASP	CB-CG-OD2	5.53	123.28	118.30
30	K	125	THR	CA-CB-CG2	-5.53	104.65	112.40
21	N	175	ASP	N-CA-CB	5.53	120.56	110.60
11	4	141	PHE	N-CA-CB	5.53	120.56	110.60
29	I	275	ALA	N-CA-CB	5.53	117.84	110.10
12	l	212	TYR	CG-CD2-CE2	-5.53	116.88	121.30
17	T	89	TYR	CB-CG-CD1	5.53	124.32	121.00
24	Q	422	VAL	CA-CB-CG1	5.53	119.19	110.90
10	j	44	PHE	CB-CG-CD1	5.53	124.67	120.80
21	N	548	ARG	N-CA-CB	5.52	120.54	110.60
5	E	156	PHE	CG-CD1-CE1	-5.52	114.73	120.80
20	Z	779	ALA	N-CA-CB	5.52	117.83	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	176	ALA	N-CA-CB	5.52	117.83	110.10
8	1	79	TYR	CG-CD1-CE1	5.52	125.72	121.30
6	f	42	THR	CA-CB-CG2	-5.52	104.67	112.40
22	S	102	SER	N-CA-CB	5.52	118.78	110.50
23	P	179	PHE	N-CA-CB	5.52	120.53	110.60
26	U	253	ASP	CB-CG-OD2	5.52	123.27	118.30
5	E	216	ASN	N-CA-CB	5.52	120.53	110.60
28	H	303	ALA	N-CA-CB	5.51	117.82	110.10
7	G	53	LEU	CB-CG-CD2	5.51	120.37	111.00
22	S	464	ARG	NH1-CZ-NH2	5.51	125.46	119.40
17	T	235	PHE	CB-CG-CD2	5.51	124.66	120.80
25	R	388	VAL	N-CA-C	-5.51	96.12	111.00
12	5	175	MET	CG-SD-CE	-5.51	91.39	100.20
28	H	302	LYS	N-CA-CB	5.51	120.51	110.60
11	k	146	HIS	O-C-N	-5.50	113.89	122.70
5	E	221	CYS	N-CA-CB	5.50	120.51	110.60
5	E	171	ALA	N-CA-CB	5.50	117.80	110.10
22	S	348	LEU	N-CA-CB	5.50	121.40	110.40
17	T	75	PHE	CB-CG-CD1	-5.50	116.95	120.80
2	B	11	THR	CA-CB-CG2	-5.50	104.70	112.40
24	Q	321	TYR	CG-CD2-CE2	-5.50	116.90	121.30
2	b	234	ARG	NE-CZ-NH2	-5.49	117.55	120.30
14	7	162	TYR	CB-CG-CD2	5.49	124.30	121.00
30	K	191	PRO	N-CD-CG	5.49	111.44	103.20
10	3	154	TYR	CD1-CE1-CZ	5.49	124.74	119.80
20	Z	865	ASP	CB-CG-OD2	-5.49	113.36	118.30
24	Q	432	VAL	CB-CA-C	-5.49	100.97	111.40
25	R	72	VAL	CB-CA-C	5.49	121.83	111.40
5	e	220	SER	N-CA-CB	5.49	118.73	110.50
1	a	192	ASP	CB-CG-OD2	5.49	123.24	118.30
20	Z	738	TYR	CB-CG-CD1	-5.49	117.71	121.00
14	n	231	ALA	CB-CA-C	-5.48	101.88	110.10
13	6	192	VAL	CA-CB-CG2	-5.48	102.67	110.90
1	a	234	PHE	CG-CD2-CE2	-5.48	114.77	120.80
22	S	241	PHE	CB-CG-CD1	5.48	124.64	120.80
21	N	348	PHE	CB-CG-CD2	5.48	124.64	120.80
1	a	65	ASP	CB-CG-OD1	5.48	123.23	118.30
1	a	134	MET	CG-SD-CE	5.48	108.96	100.20
9	i	101	ARG	NE-CZ-NH2	-5.47	117.56	120.30
22	S	412	ASN	N-CA-CB	5.47	120.45	110.60
12	l	144	ARG	NE-CZ-NH2	-5.47	117.56	120.30
14	n	39	VAL	N-CA-CB	5.47	123.54	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	98	ARG	NE-CZ-NH1	-5.47	117.56	120.30
3	C	144	TYR	CB-CG-CD1	5.47	124.28	121.00
31	L	374	PHE	CB-CG-CD2	5.47	124.63	120.80
26	U	235	LEU	CB-CG-CD1	5.47	120.30	111.00
4	D	44	LEU	N-CA-C	-5.47	96.23	111.00
23	P	110	LEU	CB-CG-CD2	5.47	120.30	111.00
6	f	71	GLY	N-CA-C	-5.47	99.43	113.10
21	N	471	TYR	CB-CG-CD2	-5.47	117.72	121.00
20	Z	44	LYS	O-C-N	-5.46	113.96	122.70
21	N	906	ARG	NE-CZ-NH1	5.46	123.03	120.30
29	I	176	SER	N-CA-CB	5.46	118.70	110.50
2	B	236	ARG	CD-NE-CZ	-5.46	115.95	123.60
3	C	160	TRP	CH2-CZ2-CE2	5.46	122.86	117.40
28	H	170	GLU	OE1-CD-OE2	5.46	129.85	123.30
32	M	355	ASP	CB-CG-OD2	-5.46	113.39	118.30
10	3	141	THR	CA-CB-CG2	-5.46	104.76	112.40
17	T	197	TYR	CB-CG-CD1	-5.46	117.72	121.00
27	O	372	GLU	OE1-CD-OE2	5.46	129.85	123.30
29	I	222	TYR	CB-CG-CD2	-5.46	117.72	121.00
3	C	20	TYR	CB-CG-CD1	-5.46	117.73	121.00
23	P	419	VAL	CA-CB-CG1	5.46	119.08	110.90
32	M	100	THR	C-N-CA	5.46	135.34	121.70
9	2	247	VAL	N-CA-C	-5.46	96.27	111.00
11	k	107	TYR	CZ-CE2-CD2	-5.45	114.89	119.80
6	F	203	ASP	N-CA-CB	5.45	120.42	110.60
25	R	186	TYR	CG-CD1-CE1	-5.45	116.94	121.30
30	K	252	ARG	CD-NE-CZ	-5.45	115.97	123.60
5	e	150	ASP	CB-CG-OD2	-5.45	113.39	118.30
28	H	271	PHE	CG-CD2-CE2	5.45	126.80	120.80
30	K	118	TYR	CD1-CE1-CZ	5.45	124.71	119.80
6	f	190	ILE	O-C-N	-5.45	113.98	122.70
13	6	172	THR	CA-CB-OG1	5.45	120.44	109.00
18	X	97	TYR	N-CA-CB	5.45	120.41	110.60
20	Z	61	SER	N-CA-CB	5.45	118.67	110.50
21	N	515	ARG	NE-CZ-NH1	-5.45	117.57	120.30
25	R	304	TYR	CG-CD2-CE2	-5.45	116.94	121.30
21	N	570	ARG	NE-CZ-NH1	-5.45	117.58	120.30
22	S	413	LEU	CB-CG-CD2	5.45	120.26	111.00
26	U	283	ARG	NH1-CZ-NH2	-5.45	113.41	119.40
31	L	162	GLU	N-CA-CB	5.45	120.41	110.60
24	Q	75	ARG	NH1-CZ-NH2	-5.45	113.41	119.40
1	a	96	ARG	NE-CZ-NH1	-5.44	117.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	164	PHE	N-CA-CB	5.44	120.40	110.60
25	R	206	ARG	CD-NE-CZ	-5.44	115.98	123.60
5	e	15	PHE	CB-CG-CD1	5.44	124.61	120.80
9	i	47	THR	CA-CB-CG2	-5.44	104.78	112.40
14	7	136	ARG	NE-CZ-NH1	5.44	123.02	120.30
21	N	341	ALA	CB-CA-C	-5.44	101.94	110.10
1	A	77	ARG	NE-CZ-NH1	5.44	123.02	120.30
4	D	36	VAL	CB-CA-C	-5.44	101.06	111.40
21	N	753	PHE	CB-CG-CD1	-5.44	116.99	120.80
31	L	290	ARG	CG-CD-NE	-5.44	100.37	111.80
33	J	13	GLU	N-CA-CB	5.44	120.39	110.60
5	e	136	ARG	NE-CZ-NH1	5.44	123.02	120.30
3	C	86	ILE	CA-CB-CG1	5.44	121.33	111.00
8	1	195	LEU	CB-CG-CD1	-5.44	101.76	111.00
24	Q	384	LYS	N-CA-CB	5.44	120.39	110.60
30	K	393	ARG	NE-CZ-NH2	5.44	123.02	120.30
4	D	54	LEU	CB-CG-CD1	5.44	120.24	111.00
26	U	93	TYR	CG-CD2-CE2	-5.44	116.95	121.30
33	J	258	VAL	CA-CB-CG2	-5.44	102.75	110.90
3	c	47	ALA	N-CA-CB	5.43	117.71	110.10
29	I	411	VAL	CA-CB-CG2	-5.43	102.75	110.90
29	I	85	PHE	CB-CG-CD1	-5.43	117.00	120.80
4	D	50	SER	N-CA-CB	5.43	118.64	110.50
21	N	502	PHE	CB-CG-CD2	5.43	124.60	120.80
5	e	149	ALA	CB-CA-C	-5.42	101.96	110.10
5	e	231	TYR	CB-CG-CD1	-5.42	117.75	121.00
14	n	241	PHE	CB-CG-CD1	5.42	124.60	120.80
5	E	20	ARG	NE-CZ-NH1	5.42	123.01	120.30
20	Z	185	ASP	CB-CG-OD2	-5.42	113.42	118.30
3	C	207	THR	N-CA-CB	5.42	120.60	110.30
7	G	189	ALA	CB-CA-C	-5.42	101.97	110.10
20	Z	164	VAL	CA-CB-CG2	5.42	119.03	110.90
24	Q	170	ASP	CB-CG-OD2	-5.42	113.42	118.30
8	h	111	TYR	CB-CG-CD2	5.42	124.25	121.00
9	i	215	TYR	CB-CG-CD1	-5.42	117.75	121.00
3	C	205	ALA	N-CA-CB	5.42	117.69	110.10
22	S	133	GLU	OE1-CD-OE2	5.42	129.80	123.30
1	a	120	ARG	CB-CG-CD	5.42	125.69	111.60
7	G	218	TRP	CB-CG-CD1	5.42	134.04	127.00
23	P	234	TYR	CA-CB-CG	-5.42	103.10	113.40
25	R	345	TYR	N-CA-CB	5.42	120.36	110.60
29	I	292	TYR	CB-CG-CD1	5.42	124.25	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	49	TYR	CG-CD2-CE2	5.42	125.63	121.30
1	a	113	PRO	N-CA-CB	5.41	109.80	103.30
5	E	146	GLY	O-C-N	5.41	131.36	122.70
20	Z	813	PHE	CB-CG-CD2	-5.41	117.01	120.80
25	R	349	SER	N-CA-CB	5.41	118.62	110.50
33	J	35	ARG	NH1-CZ-NH2	-5.41	113.44	119.40
9	2	30	THR	O-C-N	-5.41	114.04	122.70
21	N	6	ALA	N-CA-CB	5.41	117.68	110.10
29	I	187	LEU	CB-CG-CD2	5.41	120.20	111.00
2	b	10	THR	CA-CB-CG2	5.41	119.98	112.40
2	b	140	ASP	CB-CG-OD1	5.41	123.17	118.30
10	j	99	ARG	NH1-CZ-NH2	-5.41	113.45	119.40
21	N	457	SER	N-CA-CB	5.41	118.61	110.50
25	R	266	LEU	CB-CG-CD2	-5.41	101.81	111.00
4	d	108	TYR	O-C-N	5.41	131.35	122.70
5	e	123	PHE	CB-CG-CD2	5.41	124.58	120.80
20	Z	396	ASN	CB-CA-C	-5.41	99.59	110.40
7	G	163	ALA	N-CA-CB	5.40	117.67	110.10
13	m	10	PHE	CZ-CE2-CD2	-5.40	113.62	120.10
6	F	128	TYR	CG-CD2-CE2	-5.40	116.98	121.30
12	5	231	LEU	CB-CG-CD1	5.40	120.18	111.00
17	T	187	ASP	CB-CG-OD2	5.40	123.16	118.30
28	H	118	ASP	CB-CG-OD2	-5.40	113.44	118.30
1	a	19	PHE	CB-CG-CD1	5.40	124.58	120.80
1	A	64	LEU	CB-CG-CD2	5.40	120.18	111.00
1	a	111	ASP	C-N-CA	5.40	135.20	121.70
1	A	83	VAL	CA-CB-CG2	-5.40	102.80	110.90
23	P	60	ALA	N-CA-CB	5.40	117.66	110.10
28	H	200	VAL	CG1-CB-CG2	5.40	119.54	110.90
30	K	135	MET	CG-SD-CE	5.40	108.83	100.20
11	k	72	ASP	N-CA-CB	5.40	120.31	110.60
3	c	115	LEU	CB-CA-C	5.39	120.45	110.20
16	V	67	ASP	N-CA-CB	5.39	120.31	110.60
24	Q	169	ASP	CB-CG-OD1	-5.39	113.44	118.30
4	D	185	PRO	C-N-CA	5.39	135.18	121.70
22	S	345	TYR	CD1-CG-CD2	-5.39	111.97	117.90
25	R	334	ARG	NE-CZ-NH2	-5.39	117.60	120.30
29	I	291	ARG	NE-CZ-NH2	-5.39	117.60	120.30
14	n	144	TRP	CG-CD2-CE3	-5.39	129.05	133.90
4	D	170	THR	CA-CB-CG2	-5.39	104.86	112.40
7	G	48	PHE	CB-CA-C	-5.39	99.63	110.40
32	M	131	MET	CG-SD-CE	-5.38	91.58	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	k	59	TYR	CB-CG-CD2	-5.38	117.77	121.00
24	Q	13	ARG	NE-CZ-NH2	-5.38	117.61	120.30
12	5	216	ASP	CB-CG-OD1	5.38	123.14	118.30
18	X	133	SER	N-CA-CB	5.38	118.57	110.50
25	R	116	LYS	N-CA-CB	-5.38	100.91	110.60
10	j	81	ALA	N-CA-CB	5.38	117.63	110.10
13	m	99	ARG	NH1-CZ-NH2	5.38	125.32	119.40
14	n	49	TYR	CB-CG-CD2	-5.38	117.77	121.00
31	L	137	ARG	CD-NE-CZ	5.38	131.13	123.60
8	1	146	TYR	CB-CG-CD2	-5.38	117.77	121.00
20	Z	429	ASN	N-CA-C	-5.38	96.49	111.00
10	j	57	ALA	N-CA-CB	-5.38	102.58	110.10
12	l	245	TYR	CG-CD1-CE1	-5.37	117.00	121.30
12	5	121	ALA	N-CA-CB	5.37	117.62	110.10
26	U	180	ASP	CB-CG-OD2	5.37	123.14	118.30
26	U	233	PHE	CB-CG-CD1	5.37	124.56	120.80
31	L	357	ARG	NE-CZ-NH2	-5.37	117.61	120.30
31	L	404	ARG	N-CA-CB	-5.37	100.93	110.60
5	e	165	TYR	CB-CG-CD1	5.37	124.22	121.00
7	G	78	TYR	CB-CG-CD1	5.37	124.22	121.00
17	T	213	ASN	C-N-CA	5.37	135.13	121.70
11	k	165	VAL	CA-CB-CG2	-5.37	102.84	110.90
3	c	221	ASN	O-C-N	5.37	131.29	122.70
20	Z	301	THR	CA-CB-CG2	-5.37	104.88	112.40
22	S	144	LEU	N-CA-CB	5.37	121.14	110.40
23	P	260	VAL	CA-CB-CG1	-5.37	102.85	110.90
25	R	283	THR	CA-CB-CG2	-5.37	104.88	112.40
31	L	94	ASP	CB-CG-OD1	-5.37	113.47	118.30
21	N	477	SER	CB-CA-C	-5.37	99.90	110.10
7	G	22	PHE	CB-CG-CD2	5.37	124.56	120.80
11	4	145	ASP	O-C-N	-5.37	114.12	122.70
28	H	292	ARG	NE-CZ-NH2	5.37	122.98	120.30
29	I	386	ASP	CB-CG-OD1	5.37	123.13	118.30
5	e	185	ASN	N-CA-CB	5.36	120.25	110.60
2	B	187	ASP	N-CA-CB	5.36	120.25	110.60
21	N	788	TYR	CG-CD1-CE1	-5.36	117.01	121.30
24	Q	221	MET	CG-SD-CE	5.36	108.78	100.20
30	K	335	ASP	CB-CG-OD2	5.36	123.13	118.30
24	Q	407	ALA	N-CA-CB	5.36	117.61	110.10
26	U	47	ARG	NE-CZ-NH2	-5.36	117.62	120.30
32	M	93	ASP	N-CA-C	-5.36	96.53	111.00
13	m	41	TYR	CG-CD2-CE2	-5.36	117.01	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	112	TYR	CD1-CE1-CZ	5.36	124.62	119.80
33	J	271	THR	CA-CB-CG2	5.36	119.90	112.40
17	T	207	ALA	CB-CA-C	-5.36	102.06	110.10
28	H	202	GLU	N-CA-CB	5.36	120.24	110.60
14	n	141	ASN	N-CA-C	-5.36	96.54	111.00
3	C	226	TYR	CG-CD2-CE2	-5.36	117.02	121.30
23	P	295	SER	N-CA-CB	5.36	118.53	110.50
8	h	48	ASP	CB-CG-OD1	-5.35	113.48	118.30
6	F	212	SER	N-CA-CB	5.35	118.53	110.50
9	2	239	THR	CA-CB-CG2	-5.35	104.91	112.40
10	3	124	PHE	N-CA-CB	5.35	120.23	110.60
23	P	63	VAL	CA-CB-CG1	-5.35	102.88	110.90
9	i	225	ARG	NE-CZ-NH2	-5.35	117.63	120.30
5	E	85	ALA	CB-CA-C	-5.35	102.08	110.10
17	T	199	PHE	CB-CG-CD2	-5.35	117.06	120.80
31	L	255	TYR	CB-CG-CD1	5.35	124.21	121.00
32	M	284	ASP	CB-CG-OD2	-5.35	113.49	118.30
33	J	333	ARG	NE-CZ-NH1	-5.35	117.63	120.30
8	1	120	TYR	CG-CD1-CE1	-5.35	117.02	121.30
12	5	179	TYR	N-CA-C	-5.34	96.57	111.00
18	X	98	PHE	CD1-CE1-CZ	-5.34	113.69	120.10
6	f	171	TYR	CD1-CE1-CZ	5.34	124.61	119.80
20	Z	277	GLU	OE1-CD-OE2	5.34	129.71	123.30
24	Q	246	TYR	CG-CD2-CE2	-5.34	117.03	121.30
5	E	156	PHE	CZ-CE2-CD2	-5.34	113.69	120.10
14	n	68	ARG	NE-CZ-NH2	5.34	122.97	120.30
18	X	75	TRP	CZ3-CH2-CZ2	-5.34	115.19	121.60
22	S	84	ASP	N-CA-CB	5.34	120.21	110.60
2	b	96	SER	N-CA-CB	5.34	118.51	110.50
14	n	226	ARG	NE-CZ-NH2	-5.34	117.63	120.30
20	Z	903	MET	CG-SD-CE	-5.34	91.66	100.20
26	U	180	ASP	CB-CG-OD1	-5.34	113.50	118.30
8	1	96	TYR	CG-CD2-CE2	5.33	125.57	121.30
11	4	195	PHE	CG-CD2-CE2	-5.33	114.93	120.80
25	R	26	VAL	CA-CB-CG1	5.33	118.90	110.90
33	J	305	LEU	CB-CA-C	-5.33	100.07	110.20
12	l	97	ALA	N-CA-CB	5.33	117.56	110.10
13	m	168	TYR	CB-CG-CD1	5.33	124.20	121.00
5	E	163	THR	CA-CB-CG2	-5.33	104.94	112.40
27	O	284	GLU	CB-CG-CD	-5.33	99.81	114.20
22	S	118	PHE	CB-CG-CD2	-5.33	117.07	120.80
1	A	135	ARG	NE-CZ-NH2	-5.33	117.64	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	40	THR	N-CA-C	-5.33	96.61	111.00
13	6	75	ARG	NE-CZ-NH1	5.33	122.96	120.30
30	K	171	TYR	CZ-CE2-CD2	-5.33	115.01	119.80
32	M	357	ARG	NE-CZ-NH1	5.33	122.96	120.30
2	B	99	ARG	N-CA-CB	5.33	120.19	110.60
9	2	67	SER	O-C-N	-5.33	110.98	121.10
17	T	35	ILE	CA-CB-CG2	5.33	121.55	110.90
25	R	260	THR	CA-CB-CG2	-5.33	104.94	112.40
7	g	119	TYR	CD1-CE1-CZ	-5.32	115.01	119.80
12	5	222	ASP	CB-CG-OD2	-5.32	113.51	118.30
5	E	133	LEU	CB-CA-C	-5.32	100.09	110.20
10	j	181	SER	N-CA-CB	5.32	118.48	110.50
12	l	189	TYR	CD1-CG-CD2	5.32	123.75	117.90
9	2	104	ARG	NE-CZ-NH2	5.32	122.96	120.30
27	O	214	ALA	CB-CA-C	-5.32	102.12	110.10
4	D	202	VAL	CA-CB-CG2	5.32	118.88	110.90
18	X	11	ARG	NE-CZ-NH1	-5.32	117.64	120.30
1	A	89	ASP	CB-CG-OD1	-5.32	113.52	118.30
2	b	147	LEU	CB-CG-CD2	-5.32	101.96	111.00
12	5	186	THR	CA-CB-CG2	5.32	119.84	112.40
12	5	267	ASP	CB-CG-OD1	5.32	123.08	118.30
21	N	880	ARG	NE-CZ-NH1	5.32	122.96	120.30
30	K	329	LEU	N-CA-C	-5.32	96.65	111.00
22	S	54	TRP	CG-CD2-CE3	-5.31	129.12	133.90
22	S	211	ARG	NE-CZ-NH1	5.31	122.96	120.30
24	Q	398	TYR	CB-CG-CD2	-5.31	117.81	121.00
25	R	259	PHE	CB-CG-CD1	-5.31	117.08	120.80
26	U	93	TYR	CZ-CE2-CD2	5.31	124.58	119.80
22	S	183	LEU	N-CA-CB	5.31	121.02	110.40
14	n	197	ASP	CB-CG-OD1	-5.31	113.52	118.30
5	E	153	TYR	CZ-CE2-CD2	-5.31	115.02	119.80
19	Y	48	THR	N-CA-C	-5.31	96.66	111.00
16	V	197	TYR	CB-CG-CD1	-5.31	117.82	121.00
15	W	35	PHE	CB-CG-CD2	-5.31	117.09	120.80
22	S	269	GLU	CB-CA-C	-5.30	99.79	110.40
25	R	237	THR	CA-CB-OG1	5.30	120.14	109.00
29	I	114	ASP	CB-CG-OD2	5.30	123.07	118.30
3	C	146	TYR	CG-CD1-CE1	5.30	125.54	121.30
6	F	147	PHE	CB-CG-CD1	-5.30	117.09	120.80
14	7	124	TYR	CD1-CG-CD2	5.30	123.73	117.90
23	P	257	TRP	N-CA-CB	5.30	120.14	110.60
25	R	382	ASP	N-CA-C	-5.30	96.69	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	124	SER	N-CA-CB	5.30	118.45	110.50
9	i	152	TYR	CB-CA-C	5.30	121.00	110.40
21	N	322	ASP	CB-CG-OD1	5.30	123.07	118.30
13	6	46	ARG	CB-CA-C	-5.30	99.81	110.40
28	H	210	ASP	C-N-CA	5.30	134.94	121.70
6	f	31	GLN	C-N-CA	5.29	133.42	122.30
5	E	67	ILE	N-CA-C	-5.29	96.70	111.00
20	Z	130	GLY	CA-C-O	-5.29	111.07	120.60
20	Z	151	HIS	CB-CA-C	-5.29	99.82	110.40
20	Z	449	ALA	N-CA-CB	5.29	117.51	110.10
20	Z	619	ASP	CB-CG-OD1	5.29	123.06	118.30
20	Z	19	SER	N-CA-CB	5.29	118.44	110.50
21	N	455	MET	CA-CB-CG	5.29	122.29	113.30
11	4	17	SER	N-CA-CB	5.29	118.43	110.50
14	7	102	ASP	CB-CA-C	-5.29	99.82	110.40
26	U	293	GLU	OE1-CD-OE2	5.29	129.65	123.30
5	E	188	HIS	CA-CB-CG	5.29	122.59	113.60
10	3	183	TRP	CG-CD2-CE3	-5.29	129.14	133.90
13	6	68	ASP	CB-CG-OD2	-5.29	113.54	118.30
11	4	135	TYR	CZ-CE2-CD2	-5.28	115.04	119.80
14	7	144	TRP	CG-CD2-CE3	-5.28	129.15	133.90
28	H	152	ILE	CB-CA-C	5.28	122.17	111.60
14	n	102	ASP	CB-CG-OD2	-5.28	113.55	118.30
9	i	57	ASP	CB-CG-OD2	5.28	123.05	118.30
12	l	130	TRP	CG-CD2-CE3	-5.28	129.15	133.90
13	m	70	ASP	CB-CG-OD2	-5.28	113.55	118.30
5	E	42	THR	CA-CB-OG1	5.28	120.09	109.00
12	l	219	TYR	CB-CG-CD1	-5.28	117.83	121.00
22	S	317	HIS	CA-CB-CG	5.28	122.58	113.60
30	K	64	GLN	N-CA-CB	5.28	120.10	110.60
7	g	118	GLN	N-CA-CB	5.28	120.10	110.60
6	F	137	TYR	CG-CD1-CE1	-5.28	117.08	121.30
13	6	62	ALA	N-CA-CB	5.28	117.49	110.10
23	P	357	TYR	CB-CG-CD2	-5.28	117.83	121.00
28	H	235	PHE	CB-CG-CD2	-5.28	117.11	120.80
32	M	176	PRO	O-C-N	5.28	131.14	122.70
2	b	224	TYR	N-CA-CB	5.28	120.10	110.60
9	i	195	ASP	N-CA-CB	5.28	120.10	110.60
1	A	71	TYR	CB-CG-CD1	-5.28	117.83	121.00
10	3	176	ASP	CB-CG-OD2	5.28	123.05	118.30
17	T	149	ASP	CB-CG-OD2	-5.28	113.55	118.30
20	Z	187	SER	O-C-N	-5.28	114.26	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	307	TYR	CB-CG-CD1	5.28	124.17	121.00
31	L	326	ALA	N-CA-CB	5.28	117.49	110.10
32	M	267	PHE	CB-CG-CD1	-5.27	117.11	120.80
3	C	63	THR	CA-CB-CG2	-5.27	105.02	112.40
24	Q	335	PHE	N-CA-CB	5.27	120.09	110.60
22	S	473	ASP	CB-CG-OD2	-5.27	113.56	118.30
13	6	31	LEU	CB-CG-CD2	5.27	119.96	111.00
17	T	13	ILE	C-N-CA	5.27	134.87	121.70
20	Z	158	ALA	N-CA-CB	5.27	117.48	110.10
6	F	101	ARG	CG-CD-NE	-5.27	100.74	111.80
8	1	174	TRP	CG-CD1-NE1	-5.27	104.83	110.10
21	N	441	VAL	CA-CB-CG1	5.27	118.80	110.90
33	J	290	ILE	N-CA-C	-5.27	96.78	111.00
18	X	118	ASP	CB-CG-OD1	-5.26	113.56	118.30
27	O	310	PHE	CB-CG-CD2	-5.26	117.12	120.80
31	L	73	GLN	CA-CB-CG	-5.26	101.82	113.40
32	M	170	MET	CG-SD-CE	-5.26	91.78	100.20
3	c	9	ARG	NE-CZ-NH1	5.26	122.93	120.30
2	B	236	ARG	NE-CZ-NH1	5.26	122.93	120.30
16	V	57	PHE	O-C-N	5.26	131.12	122.70
20	Z	584	VAL	CA-CB-CG1	-5.26	103.01	110.90
29	I	204	HIS	CA-CB-CG	5.26	122.55	113.60
6	F	13	PHE	CB-CG-CD2	5.26	124.48	120.80
13	6	150	ALA	N-CA-CB	5.26	117.46	110.10
20	Z	731	GLY	C-N-CA	5.26	134.85	121.70
5	e	170	LYS	N-CA-CB	5.26	120.06	110.60
8	h	180	GLY	N-CA-C	-5.26	99.95	113.10
4	d	161	ALA	N-CA-CB	5.26	117.46	110.10
22	S	167	LEU	CB-CG-CD2	5.26	119.94	111.00
28	H	139	ASP	CB-CG-OD1	-5.26	113.57	118.30
28	H	343	PHE	CB-CG-CD2	-5.26	117.12	120.80
4	D	5	ASP	CB-CG-OD1	-5.25	113.57	118.30
7	G	15	PHE	CD1-CG-CD2	5.25	125.13	118.30
21	N	308	ASN	N-CA-C	-5.25	96.82	111.00
24	Q	420	ASN	N-CA-CB	5.25	120.06	110.60
28	H	310	GLU	OE1-CD-OE2	5.25	129.60	123.30
10	j	157	ASN	N-CA-CB	5.25	120.05	110.60
8	1	153	GLU	C-N-CA	5.25	134.83	121.70
20	Z	146	PHE	N-CA-CB	5.25	120.05	110.60
24	Q	306	TYR	CD1-CE1-CZ	5.25	124.53	119.80
6	F	179	PHE	CB-CG-CD1	5.25	124.47	120.80
13	6	225	TYR	CB-CG-CD2	-5.25	117.85	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	h	21	VAL	N-CA-C	-5.25	96.83	111.00
10	3	36	VAL	O-C-N	-5.25	114.30	122.70
20	Z	491	LEU	N-CA-CB	5.25	120.90	110.40
20	Z	798	ARG	NE-CZ-NH1	5.25	122.92	120.30
29	I	85	PHE	CG-CD1-CE1	-5.25	115.03	120.80
30	K	320	ARG	NE-CZ-NH1	-5.25	117.67	120.30
12	l	97	ALA	N-CA-C	-5.25	96.84	111.00
21	N	815	LYS	CA-CB-CG	5.25	124.94	113.40
6	F	76	GLY	N-CA-C	-5.24	99.99	113.10
10	3	46	TYR	CG-CD2-CE2	-5.24	117.11	121.30
14	7	159	PHE	CB-CG-CD1	5.24	124.47	120.80
19	Y	74	THR	CA-CB-OG1	5.24	120.00	109.00
27	O	166	ARG	NH1-CZ-NH2	-5.24	113.64	119.40
1	a	133	TYR	CG-CD2-CE2	5.24	125.49	121.30
14	n	40	THR	N-CA-CB	5.24	120.25	110.30
16	V	239	ALA	CB-CA-C	-5.24	102.24	110.10
27	O	327	LEU	N-CA-CB	5.24	120.88	110.40
1	a	221	ASN	CB-CA-C	-5.24	99.93	110.40
18	X	122	TYR	CD1-CE1-CZ	5.24	124.51	119.80
17	T	174	PHE	CB-CG-CD2	-5.24	117.14	120.80
23	P	40	LEU	CB-CG-CD2	5.24	119.90	111.00
25	R	408	ASP	C-N-CA	5.24	133.29	122.30
3	c	144	TYR	CG-CD2-CE2	5.23	125.49	121.30
23	P	282	HIS	O-C-N	-5.23	114.33	122.70
30	K	121	ARG	NE-CZ-NH2	-5.23	117.68	120.30
6	F	164	ARG	NH1-CZ-NH2	5.23	125.16	119.40
11	4	107	TYR	CB-CG-CD1	-5.23	117.86	121.00
29	I	268	PHE	CB-CG-CD1	5.23	124.46	120.80
3	c	109	GLU	N-CA-CB	5.23	120.01	110.60
6	f	45	VAL	CA-CB-CG2	5.23	118.75	110.90
28	H	184	GLU	N-CA-CB	5.23	120.02	110.60
28	H	169	GLU	OE1-CD-OE2	-5.23	117.03	123.30
26	U	266	THR	CA-CB-CG2	-5.22	105.08	112.40
27	O	250	TRP	CB-CG-CD2	5.22	133.39	126.60
12	l	226	GLU	C-N-CA	5.22	134.76	121.70
13	6	56	ASP	CB-CG-OD1	5.22	123.00	118.30
26	U	26	GLN	N-CA-CB	5.22	120.00	110.60
27	O	188	PHE	CB-CG-CD2	-5.22	117.14	120.80
28	H	112	SER	O-C-N	-5.22	114.34	122.70
17	T	230	ASN	N-CA-CB	5.22	120.00	110.60
20	Z	415	MET	CG-SD-CE	-5.22	91.85	100.20
22	S	188	TYR	CB-CG-CD1	5.22	124.13	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	117	THR	CA-CB-CG2	-5.22	105.09	112.40
3	c	158	THR	N-CA-CB	5.22	120.22	110.30
17	T	150	ARG	NE-CZ-NH2	-5.22	117.69	120.30
12	l	129	PHE	CD1-CE1-CZ	-5.22	113.84	120.10
30	K	128	ARG	NH1-CZ-NH2	5.22	125.14	119.40
15	W	180	LEU	N-CA-CB	5.22	120.83	110.40
22	S	54	TRP	CD2-CE2-CZ2	-5.22	116.04	122.30
32	M	170	MET	N-CA-CB	5.22	119.99	110.60
3	c	180	TYR	CB-CG-CD1	5.21	124.13	121.00
5	e	136	ARG	CG-CD-NE	-5.21	100.85	111.80
1	A	163	TYR	CG-CD2-CE2	5.21	125.47	121.30
21	N	348	PHE	CB-CG-CD1	-5.21	117.15	120.80
23	P	237	VAL	CA-CB-CG1	5.21	118.72	110.90
27	O	141	ASN	N-CA-CB	5.21	119.98	110.60
31	L	267	PHE	CB-CG-CD1	5.21	124.45	120.80
32	M	383	THR	N-CA-CB	5.21	120.21	110.30
2	B	226	GLY	CA-C-O	-5.21	111.22	120.60
18	X	34	GLU	N-CA-C	-5.21	96.93	111.00
21	N	475	ALA	CB-CA-C	-5.21	102.28	110.10
23	P	367	GLU	N-CA-CB	5.21	119.98	110.60
24	Q	84	TYR	CB-CG-CD2	-5.21	117.87	121.00
26	U	22	TYR	CB-CG-CD2	-5.21	117.87	121.00
21	N	242	PHE	CB-CG-CD2	5.21	124.45	120.80
1	a	55	SER	N-CA-CB	5.21	118.31	110.50
9	i	60	CYS	N-CA-C	-5.21	96.94	111.00
5	e	22	PHE	CB-CG-CD1	-5.21	117.16	120.80
7	G	188	SER	N-CA-CB	5.21	118.31	110.50
16	V	29	ILE	N-CA-C	-5.21	96.94	111.00
24	Q	211	PRO	N-CA-C	5.21	125.64	112.10
31	L	107	GLU	N-CA-C	-5.21	96.94	111.00
10	3	199	TYR	CG-CD2-CE2	-5.20	117.14	121.30
20	Z	503	ASP	CB-CG-OD1	-5.20	113.62	118.30
25	R	325	HIS	CA-CB-CG	-5.20	104.75	113.60
32	M	216	LYS	O-C-N	5.20	132.05	123.20
7	g	61	PRO	N-CD-CG	5.20	111.00	103.20
12	l	119	THR	CA-CB-CG2	-5.20	105.12	112.40
7	G	241	ASP	CB-CG-OD1	-5.20	113.62	118.30
8	1	131	LEU	N-CA-C	-5.20	96.96	111.00
13	6	182	TYR	CZ-CE2-CD2	-5.20	115.12	119.80
27	O	174	THR	CA-CB-CG2	-5.20	105.12	112.40
21	N	287	LEU	N-CA-CB	5.20	120.80	110.40
22	S	217	PHE	CB-CG-CD1	-5.20	117.16	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	39	VAL	O-C-N	-5.20	114.39	122.70
23	P	103	TYR	CB-CG-CD2	-5.20	117.88	121.00
28	H	306	ILE	CA-CB-CG1	5.20	120.87	111.00
22	S	52	TYR	CD1-CE1-CZ	-5.20	115.12	119.80
29	I	246	ARG	NE-CZ-NH2	-5.20	117.70	120.30
9	i	87	LEU	CB-CG-CD2	5.19	119.83	111.00
13	6	221	ARG	CD-NE-CZ	-5.19	116.33	123.60
21	N	364	LYS	CG-CD-CE	5.19	127.48	111.90
5	E	106	ASP	CB-CG-OD2	5.19	122.97	118.30
16	V	273	ARG	CD-NE-CZ	-5.19	116.33	123.60
5	e	166	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
3	C	163	ILE	CA-CB-CG1	5.19	120.86	111.00
30	K	242	PHE	CB-CG-CD1	-5.19	117.17	120.80
3	C	39	MET	CG-SD-CE	-5.19	91.90	100.20
21	N	208	ARG	CD-NE-CZ	5.19	130.86	123.60
28	H	273	ARG	NH1-CZ-NH2	-5.19	113.69	119.40
11	k	187	ASP	N-CA-CB	5.18	119.93	110.60
26	U	33	CYS	N-CA-CB	5.18	119.93	110.60
27	O	95	SER	CB-CA-C	-5.18	100.25	110.10
25	R	330	VAL	CA-CB-CG2	-5.18	103.13	110.90
33	J	10	ILE	C-N-CA	5.18	134.66	121.70
8	h	202	TYR	CB-CG-CD2	-5.18	117.89	121.00
10	3	21	VAL	CA-CB-CG1	-5.18	103.13	110.90
21	N	856	PHE	CB-CG-CD2	-5.18	117.17	120.80
16	V	173	THR	N-CA-CB	5.18	120.14	110.30
21	N	618	ARG	NH1-CZ-NH2	5.18	125.10	119.40
9	i	157	GLY	O-C-N	-5.18	114.41	122.70
14	n	57	ALA	CB-CA-C	-5.18	102.33	110.10
13	6	31	LEU	N-CA-C	-5.18	97.02	111.00
5	e	132	ARG	N-CA-CB	5.18	119.92	110.60
7	G	201	TYR	CB-CA-C	-5.18	100.05	110.40
23	P	225	VAL	CA-CB-CG1	5.18	118.67	110.90
24	Q	27	TYR	CB-CG-CD1	-5.18	117.89	121.00
28	H	303	ALA	CB-CA-C	5.18	117.86	110.10
6	F	225	TYR	N-CA-CB	5.17	119.91	110.60
12	5	83	PHE	CB-CG-CD1	-5.17	117.18	120.80
13	6	57	ASN	N-CA-CB	5.17	119.91	110.60
24	Q	377	LEU	N-CA-CB	5.17	120.75	110.40
29	I	422	ARG	NE-CZ-NH2	5.17	122.89	120.30
8	1	197	PHE	N-CA-CB	5.17	119.91	110.60
1	A	185	HIS	CA-CB-CG	-5.17	104.81	113.60
20	Z	404	ASP	CB-CG-OD1	-5.17	113.65	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	194	ARG	NE-CZ-NH2	-5.17	117.72	120.30
20	Z	869	ASP	CB-CG-OD1	-5.17	113.65	118.30
30	K	240	SER	N-CA-CB	5.17	118.25	110.50
31	L	181	ASP	CB-CG-OD1	5.17	122.95	118.30
29	I	265	ARG	NE-CZ-NH1	5.17	122.89	120.30
2	b	205	ASN	N-CA-CB	5.17	119.90	110.60
14	n	144	TRP	CB-CG-CD1	5.17	133.72	127.00
9	2	232	TYR	CG-CD1-CE1	-5.17	117.17	121.30
29	I	424	MET	C-N-CA	5.17	134.61	121.70
12	l	124	ALA	CB-CA-C	-5.17	102.35	110.10
15	W	182	TYR	CB-CG-CD2	5.16	124.10	121.00
22	S	160	ARG	CB-CG-CD	5.16	125.02	111.60
5	E	104	ASP	N-CA-CB	5.16	119.89	110.60
16	V	303	VAL	CA-CB-CG2	-5.16	103.16	110.90
20	Z	955	VAL	CB-CA-C	-5.16	101.59	111.40
24	Q	396	TRP	CE3-CZ3-CH2	-5.16	115.52	121.20
27	O	257	ALA	N-CA-CB	5.16	117.32	110.10
28	H	50	LYS	N-CA-CB	5.16	119.88	110.60
31	L	286	ILE	O-C-N	-5.16	114.43	123.20
8	h	151	PHE	CD1-CE1-CZ	-5.16	113.91	120.10
13	6	114	TYR	CB-CG-CD1	5.16	124.09	121.00
22	S	300	ALA	N-CA-CB	-5.16	102.88	110.10
24	Q	313	ASP	CB-CG-OD2	-5.15	113.66	118.30
1	a	166	TYR	CD1-CE1-CZ	-5.15	115.16	119.80
19	Y	32	ASP	C-N-CA	5.15	134.58	121.70
21	N	685	VAL	CA-CB-CG2	-5.15	103.17	110.90
23	P	305	THR	CA-CB-CG2	-5.15	105.19	112.40
1	a	247	ALA	N-CA-CB	5.15	117.31	110.10
6	F	192	ALA	N-CA-CB	5.15	117.31	110.10
7	G	242	PHE	CB-CG-CD1	5.15	124.41	120.80
28	H	394	LYS	O-C-N	-5.15	114.46	122.70
9	2	114	GLN	CG-CD-OE1	5.15	131.90	121.60
13	m	37	ASN	N-CA-CB	5.15	119.86	110.60
17	T	249	MET	CA-CB-CG	5.15	122.05	113.30
21	N	70	TYR	CB-CG-CD1	-5.15	117.91	121.00
28	H	420	ARG	NE-CZ-NH1	-5.15	117.73	120.30
5	e	204	LEU	CB-CG-CD2	-5.15	102.25	111.00
3	C	141	ASP	CB-CG-OD2	5.15	122.93	118.30
6	F	87	TYR	CZ-CE2-CD2	-5.15	115.17	119.80
21	N	203	ARG	N-CA-CB	-5.14	101.34	110.60
3	c	17	GLY	C-N-CA	5.14	134.56	121.70
6	F	38	LEU	N-CA-CB	5.14	120.68	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	308	ASN	N-CA-CB	5.14	119.85	110.60
21	N	721	ASP	CB-CG-OD2	5.14	122.93	118.30
20	Z	2	VAL	CG1-CB-CG2	5.14	119.12	110.90
7	G	55	THR	CA-CB-CG2	-5.14	105.21	112.40
27	O	298	GLU	CG-CD-OE1	-5.14	108.02	118.30
13	6	47	TYR	CG-CD1-CE1	-5.14	117.19	121.30
13	6	130	VAL	CG1-CB-CG2	-5.14	102.68	110.90
21	N	609	LEU	CB-CG-CD2	5.14	119.73	111.00
28	H	260	ALA	CB-CA-C	-5.14	102.39	110.10
33	J	20	LYS	CA-C-N	5.14	131.48	117.10
6	f	212	SER	N-CA-C	-5.13	97.14	111.00
7	g	8	TYR	CG-CD1-CE1	-5.13	117.19	121.30
1	A	182	LEU	CB-CG-CD2	5.13	119.73	111.00
8	1	161	VAL	CA-CB-CG2	-5.13	103.20	110.90
28	H	311	ILE	O-C-N	-5.13	114.48	122.70
9	2	211	LYS	CB-CA-C	-5.13	100.13	110.40
29	I	340	ARG	CA-C-N	5.13	131.47	117.10
10	3	183	TRP	CG-CD1-NE1	-5.13	104.97	110.10
12	l	78	THR	CA-CB-CG2	-5.13	105.22	112.40
13	6	141	ARG	NE-CZ-NH1	5.13	122.86	120.30
24	Q	163	ARG	NE-CZ-NH1	-5.13	117.73	120.30
4	d	148	TYR	N-CA-CB	5.12	119.83	110.60
11	4	23	ARG	NH1-CZ-NH2	-5.12	113.76	119.40
21	N	839	ARG	N-CA-C	-5.12	97.16	111.00
21	N	99	GLU	N-CA-C	-5.12	97.17	111.00
21	N	482	ALA	CB-CA-C	-5.12	102.41	110.10
13	6	157	PHE	CB-CG-CD2	-5.12	117.22	120.80
14	7	162	TYR	CD1-CE1-CZ	-5.12	115.19	119.80
20	Z	886	VAL	CA-CB-CG1	-5.12	103.22	110.90
28	H	243	PRO	N-CA-CB	5.12	109.45	103.30
9	i	34	GLY	N-CA-C	-5.12	100.30	113.10
21	N	179	THR	CA-CB-CG2	-5.12	105.23	112.40
27	O	196	LEU	CB-CG-CD1	-5.12	102.30	111.00
11	k	43	LEU	CB-CG-CD1	-5.12	102.30	111.00
14	n	195	GLU	OE1-CD-OE2	5.12	129.44	123.30
2	b	228	PRO	N-CD-CG	5.12	110.87	103.20
10	j	185	ALA	N-CA-CB	5.12	117.26	110.10
16	V	219	GLU	OE1-CD-OE2	5.12	129.44	123.30
21	N	879	SER	CB-CA-C	-5.12	100.38	110.10
17	T	193	THR	O-C-N	5.11	130.88	122.70
24	Q	116	PHE	CB-CG-CD2	-5.11	117.22	120.80
29	I	137	ASP	N-CA-CB	5.11	119.81	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	198	TYR	CD1-CE1-CZ	-5.11	115.20	119.80
31	L	264	ARG	NE-CZ-NH1	5.11	122.86	120.30
33	J	44	LEU	CB-CG-CD1	5.11	119.69	111.00
33	J	211	ILE	CA-CB-CG1	5.11	120.71	111.00
8	h	24	GLY	N-CA-C	-5.11	100.32	113.10
3	C	25	ALA	N-CA-CB	-5.11	102.94	110.10
20	Z	336	SER	N-CA-CB	5.11	118.17	110.50
33	J	120	TYR	N-CA-CB	5.11	119.80	110.60
13	m	113	TYR	CB-CG-CD2	5.11	124.06	121.00
22	S	346	TYR	CD1-CE1-CZ	5.11	124.40	119.80
25	R	204	TRP	CD1-NE1-CE2	-5.11	104.40	109.00
3	C	97	ASN	N-CA-CB	5.11	119.80	110.60
12	5	133	TRP	CZ3-CH2-CZ2	5.11	127.73	121.60
24	Q	373	VAL	CA-CB-CG1	5.11	118.56	110.90
31	L	117	TYR	CB-CG-CD2	-5.11	117.94	121.00
15	W	100	HIS	CB-CA-C	-5.11	100.19	110.40
32	M	342	ARG	NE-CZ-NH1	-5.11	117.75	120.30
9	i	67	SER	N-CA-CB	5.10	118.16	110.50
17	T	179	ASP	CB-CG-OD2	-5.10	113.71	118.30
20	Z	55	ARG	NE-CZ-NH2	-5.10	117.75	120.30
29	I	241	SER	N-CA-CB	5.10	118.16	110.50
25	R	233	ASP	O-C-N	5.10	130.86	122.70
11	4	104	ILE	N-CA-C	-5.10	97.23	111.00
15	W	15	TYR	CG-CD1-CE1	-5.10	117.22	121.30
22	S	408	CYS	CB-CA-C	-5.10	100.20	110.40
29	I	163	ASP	CB-CG-OD2	5.10	122.89	118.30
13	m	47	TYR	CB-CG-CD2	-5.10	117.94	121.00
1	A	186	PHE	CG-CD1-CE1	-5.10	115.19	120.80
16	V	228	TYR	CD1-CE1-CZ	-5.10	115.21	119.80
21	N	96	GLN	C-N-CA	5.10	134.44	121.70
1	a	234	PHE	CB-CG-CD1	-5.10	117.23	120.80
18	X	100	TRP	NE1-CE2-CD2	5.10	112.40	107.30
22	S	65	ASN	O-C-N	5.10	130.85	122.70
31	L	348	GLU	OE1-CD-OE2	5.10	129.41	123.30
9	2	90	SER	N-CA-CB	5.09	118.14	110.50
10	3	14	ALA	N-CA-CB	5.09	117.23	110.10
32	M	393	ALA	N-CA-CB	5.09	117.23	110.10
5	e	93	ARG	NE-CZ-NH2	-5.09	117.75	120.30
22	S	183	LEU	CB-CG-CD1	-5.09	102.34	111.00
27	O	393	VAL	CA-CB-CG2	-5.09	103.26	110.90
13	6	193	ARG	CD-NE-CZ	5.09	130.73	123.60
20	Z	625	THR	CA-C-N	5.09	131.35	117.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	349	PHE	CB-CA-C	-5.09	100.22	110.40
1	a	184	ASN	N-CA-CB	5.09	119.76	110.60
6	f	34	VAL	CG1-CB-CG2	5.09	119.04	110.90
14	n	257	ASP	CB-CG-OD1	5.09	122.88	118.30
1	A	163	TYR	CZ-CE2-CD2	-5.09	115.22	119.80
20	Z	533	VAL	CG1-CB-CG2	-5.09	102.75	110.90
2	b	130	PHE	CG-CD2-CE2	-5.09	115.20	120.80
22	S	240	ASP	CB-CG-OD2	5.09	122.88	118.30
32	M	96	ASN	N-CA-CB	5.09	119.76	110.60
5	e	248	ALA	N-CA-CB	5.09	117.22	110.10
8	h	78	GLN	CB-CA-C	-5.09	100.23	110.40
13	m	114	TYR	CZ-CE2-CD2	5.09	124.38	119.80
2	B	5	TYR	CB-CG-CD1	5.08	124.05	121.00
20	Z	19	SER	N-CA-C	-5.08	97.27	111.00
8	1	72	LEU	CB-CA-C	-5.08	100.54	110.20
12	5	117	LEU	CA-C-N	-5.08	106.03	116.20
22	S	184	TRP	CB-CG-CD2	-5.08	119.99	126.60
27	O	106	PHE	CD1-CG-CD2	-5.08	111.69	118.30
1	A	111	ASP	CB-CG-OD2	-5.08	113.73	118.30
1	A	115	ASP	CB-CG-OD2	5.08	122.87	118.30
20	Z	52	LEU	CB-CG-CD1	5.08	119.64	111.00
27	O	355	PRO	N-CD-CG	5.08	110.82	103.20
26	U	82	LYS	CA-C-O	-5.08	109.43	120.10
10	j	193	ASP	CB-CG-OD1	5.08	122.87	118.30
6	F	104	ALA	N-CA-CB	5.08	117.21	110.10
13	6	68	ASP	CB-CG-OD1	5.08	122.87	118.30
15	W	24	THR	CA-CB-CG2	-5.08	105.29	112.40
20	Z	968	ASP	N-CA-C	-5.08	97.29	111.00
26	U	202	SER	N-CA-CB	5.08	118.12	110.50
27	O	147	ARG	CB-CA-C	5.08	120.56	110.40
33	J	172	GLU	CB-CA-C	5.08	120.56	110.40
32	M	433	TYR	CG-CD2-CE2	5.08	125.36	121.30
31	L	193	LEU	CB-CG-CD2	5.08	119.63	111.00
4	d	215	VAL	CB-CA-C	5.07	121.04	111.40
1	A	49	ASP	CB-CG-OD1	-5.07	113.73	118.30
9	2	56	ALA	CB-CA-C	-5.07	102.49	110.10
21	N	208	ARG	NE-CZ-NH1	5.07	122.84	120.30
14	7	68	ARG	NE-CZ-NH1	5.07	122.84	120.30
20	Z	868	ASN	CB-CA-C	-5.07	100.26	110.40
11	k	46	PHE	CB-CG-CD2	-5.07	117.25	120.80
22	S	58	LYS	CB-CG-CD	5.07	124.78	111.60
26	U	110	PHE	N-CA-CB	5.07	119.72	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	442	ASP	CB-CG-OD1	5.07	122.86	118.30
16	V	228	TYR	CB-CG-CD1	5.07	124.04	121.00
20	Z	553	ARG	CB-CA-C	-5.07	100.26	110.40
22	S	481	TYR	CG-CD2-CE2	-5.07	117.25	121.30
23	P	30	ASN	CB-CA-C	-5.07	100.27	110.40
23	P	211	PRO	O-C-N	5.07	130.81	122.70
29	I	345	ASP	CB-CG-OD2	-5.07	113.74	118.30
32	M	315	PHE	N-CA-CB	5.07	119.72	110.60
11	k	130	TYR	N-CA-CB	5.07	119.72	110.60
31	L	325	MET	C-N-CA	5.06	134.36	121.70
8	h	13	MET	CG-SD-CE	5.06	108.30	100.20
1	A	233	PHE	CG-CD1-CE1	-5.06	115.23	120.80
2	B	53	SER	N-CA-C	-5.06	97.33	111.00
7	G	20	ARG	NE-CZ-NH1	5.06	122.83	120.30
22	S	141	LEU	CB-CG-CD1	-5.06	102.39	111.00
27	O	383	LYS	N-CA-CB	5.06	119.71	110.60
21	N	888	ASP	CB-CG-OD1	-5.06	113.75	118.30
20	Z	153	TYR	CG-CD1-CE1	-5.06	117.25	121.30
20	Z	846	PHE	N-CA-C	-5.06	97.34	111.00
22	S	88	PHE	CB-CG-CD1	5.06	124.34	120.80
10	j	188	TYR	CB-CG-CD1	-5.06	117.97	121.00
18	X	75	TRP	CB-CG-CD2	-5.06	120.02	126.60
20	Z	312	TYR	CA-CB-CG	-5.06	103.79	113.40
30	K	392	LEU	CB-CA-C	5.06	119.81	110.20
6	f	18	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
25	R	398	ALA	N-CA-CB	5.05	117.17	110.10
28	H	205	ASP	CB-CG-OD2	5.05	122.85	118.30
30	K	376	ASP	CB-CG-OD1	-5.05	113.75	118.30
32	M	275	PRO	N-CD-CG	5.05	110.78	103.20
6	F	24	TYR	CG-CD2-CE2	-5.05	117.26	121.30
21	N	185	ILE	CB-CG1-CD1	5.05	128.05	113.90
8	h	35	ILE	N-CA-C	-5.05	97.36	111.00
10	3	183	TRP	CD1-NE1-CE2	5.05	113.55	109.00
20	Z	774	ARG	N-CA-CB	5.05	119.69	110.60
20	Z	888	LEU	N-CA-CB	5.05	120.50	110.40
22	S	196	ARG	CG-CD-NE	-5.05	101.19	111.80
32	M	170	MET	CB-CA-C	-5.05	100.30	110.40
25	R	299	SER	CB-CA-C	5.05	119.69	110.10
27	O	190	TYR	CB-CG-CD1	5.05	124.03	121.00
1	a	214	LEU	N-CA-CB	5.05	120.50	110.40
7	G	40	ILE	N-CA-C	-5.05	97.37	111.00
12	5	226	GLU	CA-CB-CG	5.05	124.50	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	6	TYR	CD1-CE1-CZ	5.04	124.34	119.80
13	6	196	PHE	CB-CG-CD1	5.04	124.33	120.80
8	1	111	TYR	CG-CD1-CE1	-5.04	117.27	121.30
13	6	79	SER	N-CA-CB	5.04	118.06	110.50
20	Z	629	VAL	CG1-CB-CG2	5.04	118.97	110.90
31	L	255	TYR	CZ-CE2-CD2	5.04	124.34	119.80
11	k	45	SER	N-CA-CB	5.04	118.06	110.50
1	A	243	GLU	N-CA-CB	5.04	119.67	110.60
2	B	235	PHE	CB-CG-CD1	5.04	124.33	120.80
5	E	105	GLU	N-CA-C	-5.04	97.39	111.00
6	F	123	TYR	CG-CD1-CE1	-5.04	117.27	121.30
12	5	133	TRP	CB-CG-CD1	5.04	133.55	127.00
14	7	261	TYR	CG-CD2-CE2	-5.04	117.27	121.30
27	O	111	SER	N-CA-CB	5.04	118.06	110.50
27	O	195	TYR	CG-CD2-CE2	-5.04	117.27	121.30
9	i	225	ARG	CA-CB-CG	5.04	124.48	113.40
5	E	226	ASP	CB-CG-OD1	-5.04	113.77	118.30
11	4	59	TYR	CB-CG-CD2	5.04	124.02	121.00
5	e	143	LEU	CB-CG-CD2	5.03	119.56	111.00
11	k	57	ALA	N-CA-CB	5.03	117.15	110.10
22	S	470	GLN	O-C-N	-5.03	114.65	122.70
28	H	138	GLU	N-CA-CB	5.03	119.66	110.60
33	J	320	SER	O-C-N	5.03	130.75	122.70
11	4	30	ASP	CB-CG-OD2	-5.03	113.77	118.30
11	k	53	THR	CA-CB-CG2	-5.03	105.36	112.40
8	1	81	THR	CA-CB-CG2	-5.03	105.36	112.40
14	7	213	ALA	CB-CA-C	-5.03	102.56	110.10
30	K	299	LEU	CB-CA-C	5.03	119.76	110.20
7	g	201	TYR	CD1-CE1-CZ	-5.03	115.27	119.80
9	i	174	ASP	CB-CG-OD2	-5.03	113.77	118.30
4	D	160	SER	N-CA-CB	5.03	118.04	110.50
8	h	113	ASP	CB-CG-OD2	5.03	122.83	118.30
14	n	253	ASP	CB-CG-OD2	5.03	122.83	118.30
4	D	226	SER	N-CA-CB	5.03	118.04	110.50
6	F	39	ARG	CA-CB-CG	5.03	124.46	113.40
2	b	156	TYR	CG-CD2-CE2	-5.03	117.28	121.30
2	b	159	TRP	N-CA-CB	5.03	119.64	110.60
3	C	71	ASP	CB-CG-OD2	5.03	122.82	118.30
11	4	59	TYR	CG-CD1-CE1	5.03	125.32	121.30
21	N	232	LEU	N-CA-CB	5.03	120.45	110.40
27	O	81	TYR	CB-CG-CD2	-5.03	117.98	121.00
4	d	204	GLN	N-CA-CB	5.02	119.64	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	k	104	ILE	N-CA-C	-5.02	97.43	111.00
1	A	71	TYR	CD1-CG-CD2	5.02	123.43	117.90
1	a	65	ASP	CB-CG-OD2	-5.02	113.78	118.30
1	a	163	TYR	N-CA-CB	5.02	119.64	110.60
8	1	79	TYR	CZ-CE2-CD2	5.02	124.32	119.80
18	X	98	PHE	CB-CG-CD1	5.02	124.32	120.80
20	Z	608	TYR	CG-CD2-CE2	-5.02	117.28	121.30
28	H	194	SER	O-C-N	-5.02	114.67	122.70
4	D	109	LEU	CB-CG-CD2	-5.02	102.46	111.00
10	3	31	SER	CB-CA-C	-5.02	100.56	110.10
21	N	488	CYS	O-C-N	5.02	130.73	122.70
28	H	155	PHE	CB-CA-C	-5.02	100.36	110.40
31	L	214	PRO	N-CA-CB	5.02	109.33	103.30
2	b	81	ASP	CB-CG-OD2	-5.02	113.78	118.30
4	D	213	THR	CA-CB-CG2	5.02	119.43	112.40
22	S	413	LEU	N-CA-C	-5.02	97.45	111.00
2	b	137	ALA	CB-CA-C	-5.02	102.57	110.10
7	G	52	LYS	N-CA-CB	5.02	119.63	110.60
10	3	122	ALA	N-CA-CB	5.02	117.12	110.10
26	U	248	ASP	CB-CA-C	-5.02	100.36	110.40
31	L	177	GLU	N-CA-CB	5.02	119.63	110.60
4	D	233	VAL	CA-CB-CG2	-5.01	103.38	110.90
6	F	225	TYR	CG-CD1-CE1	-5.01	117.29	121.30
32	M	386	PHE	N-CA-CB	5.01	119.63	110.60
7	g	93	ARG	NE-CZ-NH1	5.01	122.81	120.30
9	i	104	ARG	NE-CZ-NH1	5.01	122.81	120.30
3	C	208	TYR	CB-CG-CD2	-5.01	117.99	121.00
14	7	164	ASN	N-CA-CB	5.01	119.62	110.60
3	c	15	PRO	N-CA-CB	5.01	109.31	103.30
10	j	198	ARG	NE-CZ-NH1	5.01	122.81	120.30
7	G	9	ASP	N-CA-CB	5.01	119.62	110.60
24	Q	129	LYS	N-CA-CB	5.01	119.62	110.60
25	R	338	TYR	CB-CG-CD1	-5.01	117.99	121.00
5	E	53	ARG	NE-CZ-NH1	5.01	122.81	120.30
10	3	162	ASP	CA-CB-CG	-5.01	102.38	113.40
28	H	460	THR	CA-C-N	-5.01	106.18	117.20
8	h	127	SER	N-CA-C	-5.01	97.48	111.00
22	S	275	TYR	CG-CD2-CE2	5.01	125.31	121.30
12	l	152	ALA	CB-CA-C	5.01	117.61	110.10
1	A	137	LEU	CB-CG-CD1	-5.01	102.49	111.00
21	N	322	ASP	CB-CA-C	-5.01	100.39	110.40
28	H	234	ARG	NE-CZ-NH1	5.01	122.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	896	PHE	CG-CD2-CE2	5.00	126.31	120.80
22	S	239	ARG	CB-CG-CD	5.00	124.61	111.60
27	O	228	TYR	CG-CD2-CE2	-5.00	117.30	121.30
4	d	160	SER	CB-CA-C	-5.00	100.59	110.10
1	A	218	PHE	CB-CG-CD1	5.00	124.30	120.80
13	6	133	PHE	CB-CG-CD1	5.00	124.30	120.80
20	Z	783	VAL	CA-CB-CG2	-5.00	103.39	110.90
4	d	172	ARG	NH1-CZ-NH2	-5.00	113.90	119.40
5	E	192	THR	O-C-N	5.00	130.70	122.70
9	2	109	LEU	CB-CG-CD2	5.00	119.50	111.00
11	4	130	TYR	CD1-CG-CD2	5.00	123.40	117.90
21	N	412	TYR	CZ-CE2-CD2	5.00	124.30	119.80
31	L	220	LEU	CB-CG-CD2	5.00	119.50	111.00
32	M	218	ALA	N-CA-C	-5.00	97.50	111.00
32	M	233	ARG	NE-CZ-NH2	-5.00	117.80	120.30

There are no chirality outliers.

All (353) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	111	TYR	Sidechain
8	1	17	PHE	Sidechain
8	1	198	TYR	Sidechain
8	1	202	TYR	Sidechain
8	1	34	TYR	Sidechain
8	1	79	TYR	Sidechain
9	2	101	ARG	Sidechain
9	2	104	ARG	Sidechain
9	2	117	PHE	Sidechain
9	2	215	TYR	Sidechain
9	2	225	ARG	Sidechain
9	2	236	ARG	Sidechain
10	3	154	TYR	Sidechain
10	3	177	ARG	Sidechain
10	3	28	ARG	Sidechain
10	3	50	PHE	Sidechain
10	3	69	TYR	Sidechain
11	4	121	TYR	Sidechain
11	4	147	HIS	Sidechain
11	4	176	PHE	Sidechain
11	4	23	ARG	Sidechain
11	4	70	ARG	Sidechain

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Mol	Chain	Res	Type	Group
11	4	73	TYR	Sidechain
11	4	95	ARG	Sidechain
12	5	179	TYR	Sidechain
12	5	202	PHE	Sidechain
12	5	210	PHE	Sidechain
12	5	242	ARG	Sidechain
13	6	13	TYR	Sidechain
13	6	131	TYR	Sidechain
13	6	182	TYR	Sidechain
13	6	221	ARG	Sidechain
13	6	225	TYR	Sidechain
13	6	41	TYR	Sidechain
13	6	83	TYR	Sidechain
14	7	124	TYR	Sidechain
14	7	126	PHE	Sidechain
14	7	194	ARG	Sidechain
14	7	226	ARG	Sidechain
14	7	261	TYR	Sidechain
14	7	49	TYR	Sidechain
1	A	105	ARG	Sidechain
1	A	106	TYR	Sidechain
1	A	11	GLY	Peptide
1	A	12	TYR	Peptide,Sidechain
1	A	131	ARG	Sidechain
1	A	186	PHE	Sidechain
1	A	30	TYR	Sidechain
1	A	46	ARG	Sidechain
2	B	101	TYR	Sidechain
2	B	156	TYR	Sidechain
2	B	204	PHE	Sidechain
2	B	23	TYR	Sidechain
2	B	235	PHE	Sidechain
2	B	236	ARG	Sidechain
2	B	4	ARG	Sidechain
2	B	75	TYR	Sidechain
3	C	149	TYR	Sidechain
3	C	230	PHE	Sidechain
4	D	108	TYR	Sidechain
4	D	120	TYR	Sidechain
4	D	127	ARG	Sidechain
4	D	166	ARG	Sidechain
4	D	232	TYR	Sidechain

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Mol	Chain	Res	Type	Group
4	D	48	ARG	Sidechain
4	D	83	ARG	Sidechain
5	E	136	ARG	Sidechain
5	E	166	ARG	Sidechain
5	E	167	TYR	Sidechain
5	E	53	ARG	Sidechain
5	E	8	TYR	Sidechain
6	F	123	TYR	Sidechain
6	F	128	TYR	Sidechain
6	F	137	TYR	Sidechain
6	F	174	ARG	Sidechain
6	F	225	TYR	Sidechain
6	F	4	ASN	Peptide
6	F	82	ARG	Sidechain
6	F	94	TYR	Sidechain
7	G	242	PHE	Sidechain
28	H	145	TYR	Sidechain
28	H	181	TYR	Sidechain
28	H	208	TYR	Sidechain
28	H	266	ARG	Sidechain
28	H	283	TYR	Sidechain
28	H	292	ARG	Sidechain
28	H	331	ARG	Sidechain
28	H	344	ASP	Peptide
28	H	377	PHE	Sidechain
28	H	403	ARG	Sidechain
28	H	435	ARG	Sidechain
28	H	72	SER	Peptide
28	H	95	HIS	Sidechain
29	I	222	TYR	Sidechain
29	I	245	LEU	Peptide
29	I	246	ARG	Peptide
29	I	316	PHE	Sidechain
29	I	339	ILE	Peptide
29	I	340	ARG	Peptide
29	I	342	GLY	Peptide
29	I	345	ASP	Peptide
29	I	350	PHE	Sidechain
29	I	426	ASN	Peptide
29	I	64	ARG	Sidechain
33	J	116	ARG	Sidechain
33	J	210	PHE	Peptide,Sidechain

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Mol	Chain	Res	Type	Group
33	J	231	ARG	Sidechain
33	J	238	ARG	Sidechain
33	J	260	GLY	Peptide
33	J	282	PHE	Peptide
33	J	309	ARG	Peptide,Sidechain
33	J	333	ARG	Sidechain
33	J	344	ARG	Sidechain
33	J	368	TYR	Sidechain
33	J	373	ARG	Sidechain
33	J	42	ARG	Sidechain
33	J	56	ARG	Sidechain
33	J	63	ARG	Sidechain
33	J	94	TYR	Sidechain
30	K	128	ARG	Sidechain
30	K	233	ALA	Peptide
30	K	234	PHE	Peptide
30	K	236	ARG	Peptide
30	K	252	ARG	Sidechain
30	K	259	ARG	Sidechain
30	K	281	ARG	Sidechain
30	K	303	MET	Peptide
30	K	329	LEU	Peptide
30	K	330	ARG	Sidechain
30	K	332	GLY	Peptide
30	K	333	ARG	Peptide
30	K	411	TYR	Sidechain
30	K	412	ALA	Peptide
30	K	427	TYR	Sidechain
30	K	58	TYR	Sidechain
30	K	67	TYR	Sidechain
30	K	77	ARG	Sidechain
31	L	126	ARG	Sidechain
31	L	161	ARG	Sidechain
31	L	191	ARG	Sidechain
31	L	221	TYR	Sidechain
31	L	243	PHE	Sidechain
31	L	255	TYR	Sidechain
31	L	269	TYR	Sidechain
31	L	290	ARG	Sidechain
31	L	312	MET	Peptide
31	L	314	GLY	Peptide
31	L	315	PHE	Peptide

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Mol	Chain	Res	Type	Group
31	L	316	ASP	Peptide
31	L	338	LEU	Peptide
31	L	339	ARG	Peptide,Sidechain
31	L	342	ARG	Peptide
31	L	386	PHE	Sidechain
31	L	407	ARG	Sidechain
31	L	62	ARG	Sidechain
31	L	77	ARG	Sidechain
31	L	78	ARG	Sidechain
32	M	172	VAL	Peptide
32	M	213	ARG	Sidechain
32	M	267	PHE	Sidechain
32	M	292	ASP	Mainchain
32	M	342	ARG	Sidechain
32	M	381	ARG	Sidechain
32	M	425	ARG	Sidechain
21	N	109	TYR	Sidechain
21	N	188	TYR	Sidechain
21	N	222	TYR	Sidechain
21	N	242	PHE	Sidechain
21	N	340	HIS	Sidechain
21	N	422	TYR	Sidechain
21	N	463	TYR	Sidechain
21	N	471	TYR	Sidechain
21	N	504	TYR	Sidechain
21	N	559	TYR	Sidechain
21	N	70	TYR	Sidechain
21	N	739	PHE	Sidechain
21	N	743	PHE	Sidechain
21	N	776	TYR	Sidechain
21	N	777	ALA	Peptide
21	N	813	ARG	Sidechain
21	N	861	TYR	Sidechain
21	N	88	ARG	Sidechain
21	N	881	TYR	Sidechain
21	N	889	ARG	Sidechain
21	N	896	PHE	Sidechain
27	O	137	TYR	Sidechain
27	O	178	TYR	Sidechain
27	O	33	TYR	Sidechain
27	O	62	TYR	Sidechain
27	O	98	TYR	Sidechain

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Mol	Chain	Res	Type	Group
23	P	193	TYR	Sidechain
23	P	213	TYR	Sidechain
23	P	220	TYR	Sidechain
23	P	221	TYR	Sidechain
23	P	230	HIS	Sidechain
23	P	232	ARG	Sidechain
23	P	234	TYR	Sidechain
23	P	3	ARG	Sidechain
23	P	318	TYR	Sidechain
23	P	356	TYR	Sidechain
23	P	364	ARG	Sidechain
24	Q	116	PHE	Sidechain
24	Q	145	HIS	Sidechain
24	Q	146	TYR	Sidechain
24	Q	20	TYR	Sidechain
24	Q	209	TYR	Sidechain
24	Q	243	PHE	Sidechain
24	Q	246	TYR	Sidechain
24	Q	27	TYR	Sidechain
24	Q	286	TYR	Sidechain
24	Q	294	ARG	Sidechain
24	Q	306	TYR	Sidechain
24	Q	332	ARG	Sidechain
24	Q	339	TYR	Sidechain
24	Q	400	TYR	Sidechain
25	R	140	TYR	Sidechain
25	R	179	PHE	Sidechain
25	R	181	TYR	Sidechain
25	R	207	ARG	Sidechain
25	R	210	TYR	Sidechain
25	R	246	TYR	Sidechain
25	R	297	TYR	Sidechain
25	R	304	TYR	Sidechain
25	R	321	TYR	Sidechain
25	R	338	TYR	Sidechain
25	R	345	TYR	Sidechain
25	R	400	TYR	Sidechain
25	R	70	TYR	Peptide
22	S	119	TYR	Sidechain
22	S	145	PHE	Sidechain
22	S	185	PHE	Sidechain
22	S	239	ARG	Sidechain

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Mol	Chain	Res	Type	Group
22	S	259	TYR	Sidechain
22	S	346	TYR	Sidechain
22	S	377	TYR	Sidechain
22	S	399	TYR	Sidechain
22	S	421	TYR	Sidechain
22	S	467	PHE	Sidechain
22	S	82	TYR	Sidechain
17	T	186	ARG	Sidechain
17	T	234	TYR	Sidechain
17	T	251	HIS	Peptide
26	U	137	TYR	Sidechain
26	U	254	ARG	Sidechain
26	U	288	PHE	Sidechain
26	U	72	TYR	Sidechain
26	U	93	TYR	Sidechain
16	V	100	ARG	Sidechain
16	V	20	ARG	Sidechain
16	V	251	TYR	Sidechain
16	V	273	ARG	Sidechain
16	V	28	TYR	Sidechain
16	V	61	TYR	Sidechain
15	W	148	GLU	Mainchain
15	W	163	ASN	Peptide
15	W	179	ARG	Sidechain
15	W	23	ARG	Sidechain
18	X	17	TYR	Sidechain
18	X	22	ARG	Sidechain
18	X	27	ILE	Peptide
18	X	96	ARG	Sidechain
19	Y	84	TYR	Sidechain
20	Z	103	TYR	Sidechain
20	Z	136	ARG	Sidechain
20	Z	138	ARG	Sidechain
20	Z	195	PHE	Sidechain
20	Z	210	TYR	Sidechain
20	Z	236	PHE	Sidechain
20	Z	323	TYR	Sidechain
20	Z	341	TYR	Sidechain
20	Z	394	TYR	Sidechain
20	Z	441	TYR	Sidechain
20	Z	477	TYR	Sidechain
20	Z	55	ARG	Sidechain

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Mol	Chain	Res	Type	Group
20	Z	608	TYR	Sidechain
20	Z	766	HIS	Sidechain
20	Z	902	TYR	Sidechain
1	a	106	TYR	Sidechain
1	a	11	GLY	Peptide
1	a	12	TYR	Peptide,Sidechain
1	a	135	ARG	Sidechain
1	a	14	ARG	Sidechain
1	a	166	TYR	Sidechain
1	a	19	PHE	Sidechain
2	b	128	ARG	Sidechain
2	b	224	TYR	Sidechain
2	b	4	ARG	Sidechain
2	b	6	SER	Peptide
2	b	99	ARG	Sidechain
3	c	113	ARG	Sidechain
3	c	114	ARG	Sidechain
3	c	129	ARG	Peptide
3	c	144	TYR	Sidechain
3	c	180	TYR	Sidechain
3	c	20	TYR	Sidechain
3	c	9	ARG	Sidechain
4	d	111	ARG	Sidechain
4	d	120	TYR	Sidechain
4	d	172	ARG	Sidechain
4	d	174	PHE	Sidechain
4	d	232	TYR	Sidechain
4	d	29	ARG	Sidechain
5	e	156	PHE	Sidechain
5	e	231	TYR	Sidechain
5	e	72	ARG	Sidechain
6	f	126	ARG	Sidechain
6	f	128	TYR	Sidechain
6	f	137	TYR	Sidechain
6	f	171	TYR	Sidechain
6	f	18	ARG	Peptide
6	f	4	ASN	Peptide
6	f	59	TYR	Sidechain
6	f	6	TYR	Sidechain
7	g	112	PHE	Sidechain
7	g	132	PHE	Sidechain
8	h	133	TYR	Sidechain

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Mol	Chain	Res	Type	Group
8	h	183	ARG	Sidechain
8	h	198	TYR	Sidechain
8	h	70	TYR	Sidechain
8	h	75	TYR	Sidechain
9	i	119	TYR	Sidechain
9	i	126	TYR	Sidechain
9	i	152	TYR	Sidechain
9	i	215	TYR	Sidechain
10	j	203	ARG	Sidechain
10	j	28	ARG	Sidechain
10	j	40	PHE	Sidechain
10	j	46	TYR	Sidechain
10	j	99	ARG	Sidechain
11	k	107	TYR	Sidechain
11	k	171	ARG	Sidechain
11	k	195	PHE	Sidechain
11	k	59	TYR	Sidechain
11	k	85	ARG	Sidechain
12	l	139	ARG	Sidechain
12	l	148	ARG	Sidechain
12	l	212	TYR	Sidechain
12	l	230	TYR	Sidechain
12	l	245	TYR	Sidechain
12	l	272	PHE	Sidechain
13	m	103	HIS	Sidechain
13	m	111	PHE	Sidechain
13	m	13	TYR	Sidechain
13	m	41	TYR	Sidechain
14	n	109	TYR	Sidechain
14	n	261	TYR	Sidechain
14	n	63	TYR	Sidechain
14	n	74	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	242/244 (99%)	223 (92%)	17 (7%)	2 (1%)	19	60
1	a	242/244 (99%)	230 (95%)	8 (3%)	4 (2%)	9	42
2	B	246/248 (99%)	226 (92%)	19 (8%)	1 (0%)	34	72
2	b	246/248 (99%)	231 (94%)	12 (5%)	3 (1%)	13	50
3	C	239/241 (99%)	231 (97%)	6 (2%)	2 (1%)	19	60
3	c	239/241 (99%)	226 (95%)	11 (5%)	2 (1%)	19	60
4	D	236/252 (94%)	221 (94%)	14 (6%)	1 (0%)	34	72
4	d	250/252 (99%)	237 (95%)	10 (4%)	3 (1%)	13	50
5	E	243/245 (99%)	228 (94%)	13 (5%)	2 (1%)	19	60
5	e	243/245 (99%)	225 (93%)	17 (7%)	1 (0%)	34	72
6	F	230/232 (99%)	214 (93%)	16 (7%)	0	100	100
6	f	230/232 (99%)	217 (94%)	13 (6%)	0	100	100
7	G	243/245 (99%)	226 (93%)	15 (6%)	2 (1%)	19	60
7	g	243/245 (99%)	228 (94%)	10 (4%)	5 (2%)	7	36
8	1	194/196 (99%)	183 (94%)	9 (5%)	2 (1%)	15	54
8	h	194/196 (99%)	187 (96%)	5 (3%)	2 (1%)	15	54
9	2	224/226 (99%)	213 (95%)	10 (4%)	1 (0%)	34	72
9	i	224/226 (99%)	209 (93%)	13 (6%)	2 (1%)	17	56
10	3	202/204 (99%)	192 (95%)	7 (4%)	3 (2%)	10	45
10	j	202/204 (99%)	186 (92%)	15 (7%)	1 (0%)	29	69
11	4	193/195 (99%)	180 (93%)	9 (5%)	4 (2%)	7	36
11	k	193/195 (99%)	177 (92%)	12 (6%)	4 (2%)	7	36
12	5	210/212 (99%)	199 (95%)	8 (4%)	3 (1%)	11	46
12	l	210/212 (99%)	200 (95%)	9 (4%)	1 (0%)	29	69
13	6	220/222 (99%)	205 (93%)	12 (6%)	3 (1%)	11	46

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
13	m	220/222 (99%)	204 (93%)	14 (6%)	2 (1%)	17 56
14	7	227/232 (98%)	211 (93%)	14 (6%)	2 (1%)	17 56
14	n	230/232 (99%)	213 (93%)	15 (6%)	2 (1%)	17 56
15	W	195/197 (99%)	180 (92%)	11 (6%)	4 (2%)	7 36
16	V	287/289 (99%)	261 (91%)	16 (6%)	10 (4%)	3 25
17	T	264/266 (99%)	247 (94%)	11 (4%)	6 (2%)	6 34
18	X	125/127 (98%)	101 (81%)	19 (15%)	5 (4%)	3 23
19	Y	87/89 (98%)	73 (84%)	11 (13%)	3 (3%)	3 26
20	Z	902/970 (93%)	805 (89%)	72 (8%)	25 (3%)	5 30
21	N	920/922 (100%)	853 (93%)	52 (6%)	15 (2%)	9 43
22	S	473/475 (100%)	441 (93%)	21 (4%)	11 (2%)	6 34
23	P	438/440 (100%)	418 (95%)	13 (3%)	7 (2%)	9 43
24	Q	432/434 (100%)	398 (92%)	21 (5%)	13 (3%)	4 28
25	R	403/405 (100%)	378 (94%)	20 (5%)	5 (1%)	13 50
26	U	302/304 (99%)	282 (93%)	16 (5%)	4 (1%)	12 48
27	O	386/388 (100%)	368 (95%)	15 (4%)	3 (1%)	19 60
28	H	424/426 (100%)	376 (89%)	36 (8%)	12 (3%)	5 30
29	I	383/385 (100%)	344 (90%)	25 (6%)	14 (4%)	3 24
30	K	392/394 (100%)	344 (88%)	36 (9%)	12 (3%)	4 27
31	L	386/388 (100%)	352 (91%)	25 (6%)	9 (2%)	6 34
32	M	419/421 (100%)	384 (92%)	24 (6%)	11 (3%)	5 31
33	J	403/405 (100%)	360 (89%)	27 (7%)	16 (4%)	3 23
All	All	13936/14113 (99%)	12887 (92%)	804 (6%)	245 (2%)	12 40

All (245) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	13	ASP
2	b	6	SER
2	b	53	SER
7	g	209	GLU
8	h	127	SER
13	m	138	SER
1	A	13	ASP

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Mol	Chain	Res	Type
10	3	40	PHE
15	W	149	GLN
16	V	47	MET
16	V	171	ARG
16	V	185	ILE
17	T	173	GLU
18	X	29	VAL
20	Z	85	VAL
20	Z	802	ASP
21	N	17	GLN
22	S	84	ASP
23	P	46	THR
23	P	86	HIS
24	Q	384	LYS
25	R	72	VAL
25	R	146	ASP
25	R	245	SER
26	U	5	HIS
26	U	42	ASN
27	O	243	VAL
28	H	112	SER
28	H	136	ALA
29	I	317	ASP
29	I	340	ARG
29	I	371	LEU
30	K	37	ASN
30	K	334	LEU
30	K	425	ASP
31	L	290	ARG
31	L	316	ASP
32	M	318	ASP
33	J	211	ILE
1	a	60	PRO
4	d	204	GLN
9	i	200	SER
7	G	9	ASP
7	G	209	GLU
8	1	40	THR
11	4	152	MET
12	5	286	ILE
13	6	138	SER
14	7	110	ASP

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Mol	Chain	Res	Type
16	V	175	SER
16	V	271	VAL
17	T	97	SER
18	X	106	SER
20	Z	57	LYS
20	Z	82	MET
20	Z	205	LEU
20	Z	825	ALA
20	Z	899	GLN
21	N	123	PHE
21	N	175	ASP
21	N	473	ASP
21	N	634	LEU
21	N	832	HIS
21	N	855	GLU
22	S	47	THR
22	S	150	LYS
22	S	433	GLU
23	P	130	ILE
24	Q	44	ALA
24	Q	68	MET
24	Q	170	ASP
24	Q	189	ARG
24	Q	286	TYR
24	Q	386	PHE
24	Q	387	TYR
25	R	280	ILE
26	U	160	THR
28	H	128	ASN
29	I	344	ILE
31	L	340	PRO
33	J	72	VAL
33	J	212	ARG
33	J	249	GLU
33	J	312	ARG
33	J	335	MET
1	a	11	GLY
5	e	73	HIS
7	g	9	ASP
12	l	183	GLU
14	n	262	GLY
3	C	183	ASP

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Mol	Chain	Res	Type
4	D	204	GLN
8	1	41	ASP
10	3	182	GLY
10	3	184	GLY
12	5	98	GLY
16	V	262	THR
16	V	272	GLY
17	T	137	GLU
18	X	105	ASN
20	Z	578	GLY
20	Z	920	GLY
20	Z	947	GLY
20	Z	957	LEU
21	N	395	ALA
21	N	757	THR
21	N	831	GLU
21	N	842	ASN
21	N	862	SER
22	S	100	HIS
23	P	89	LEU
23	P	272	PRO
24	Q	126	LYS
24	Q	211	PRO
24	Q	230	LYS
24	Q	253	ASN
24	Q	353	PRO
25	R	182	ASN
27	O	70	TYR
28	H	381	ASP
28	H	401	GLY
29	I	115	ASP
29	I	216	PRO
29	I	298	GLY
29	I	339	ILE
30	K	231	LYS
30	K	236	ARG
30	K	308	GLN
30	K	417	THR
31	L	101	ILE
31	L	177	GLU
31	L	282	GLU
32	M	17	GLU

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Mol	Chain	Res	Type
32	M	109	ASP
32	M	114	GLY
33	J	119	SER
33	J	263	GLY
3	c	7	ASP
7	g	73	HIS
10	j	116	SER
11	k	72	ASP
11	k	73	TYR
13	m	208	ASP
1	A	11	GLY
5	E	130	GLU
11	4	2	ASP
12	5	183	GLU
13	6	27	ASP
13	6	173	ASN
16	V	61	TYR
17	T	251	HIS
20	Z	65	GLU
20	Z	80	SER
20	Z	143	VAL
20	Z	233	LEU
20	Z	377	ALA
20	Z	770	GLU
20	Z	870	ALA
20	Z	932	ALA
20	Z	940	GLY
21	N	712	ASN
21	N	765	ASP
23	P	255	ALA
26	U	30	ASN
28	H	126	ASN
28	H	190	ARG
28	H	314	VAL
29	I	116	ASP
29	I	163	ASP
29	I	290	LYS
29	I	372	SER
29	I	426	ASN
30	K	49	PHE
30	K	284	ALA
31	L	317	ASN

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Mol	Chain	Res	Type
31	L	343	LEU
32	M	240	ASN
32	M	352	PRO
33	J	275	LEU
33	J	284	THR
11	k	2	ASP
11	k	132	ALA
3	C	184	MET
11	4	73	TYR
14	7	111	ASN
15	W	144	PHE
16	V	72	PRO
16	V	184	ASN
18	X	21	SER
18	X	24	CYS
19	Y	43	TRP
20	Z	25	PRO
20	Z	309	GLN
20	Z	376	SER
20	Z	513	ALA
21	N	88	ARG
22	S	83	PRO
22	S	97	THR
22	S	126	LYS
22	S	153	GLU
23	P	372	THR
28	H	303	ALA
29	I	427	LYS
30	K	330	ARG
31	L	178	ILE
32	M	91	ILE
32	M	173	ASP
32	M	287	GLY
32	M	384	ASP
32	M	433	TYR
33	J	218	LEU
33	J	261	SER
33	J	373	ARG
33	J	398	ILE
1	a	10	ALA
4	d	103	PRO
7	g	131	PRO

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Mol	Chain	Res	Type
7	g	187	LEU
9	i	249	ILE
14	n	43	SER
5	E	73	HIS
9	2	120	GLN
15	W	180	LEU
15	W	190	ILE
17	T	117	ASN
17	T	257	THR
19	Y	44	ALA
19	Y	49	ILE
22	S	44	THR
27	O	225	ASP
28	H	145	TYR
33	J	341	ILE
28	H	152	ILE
28	H	345	PRO
3	c	129	ARG
20	Z	254	PRO
22	S	115	PRO
2	b	129	PRO
4	d	185	PRO
8	h	123	PRO
2	B	53	SER
30	K	314	VAL
11	4	173	PRO
33	J	10	ILE
30	K	274	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	207/207 (100%)	194 (94%)	13 (6%)	18 43
1	a	207/207 (100%)	198 (96%)	9 (4%)	29 53
2	B	207/207 (100%)	196 (95%)	11 (5%)	22 47

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	b	207/207 (100%)	202 (98%)	5 (2%)	49	69
3	C	201/201 (100%)	194 (96%)	7 (4%)	36	59
3	c	201/201 (100%)	194 (96%)	7 (4%)	36	59
4	D	210/224 (94%)	205 (98%)	5 (2%)	49	69
4	d	224/224 (100%)	211 (94%)	13 (6%)	20	45
5	E	201/201 (100%)	197 (98%)	4 (2%)	55	74
5	e	201/201 (100%)	195 (97%)	6 (3%)	41	63
6	F	191/191 (100%)	187 (98%)	4 (2%)	53	72
6	f	191/191 (100%)	183 (96%)	8 (4%)	30	54
7	G	202/202 (100%)	199 (98%)	3 (2%)	65	80
7	g	202/202 (100%)	193 (96%)	9 (4%)	27	52
8	1	162/162 (100%)	158 (98%)	4 (2%)	47	68
8	h	162/162 (100%)	157 (97%)	5 (3%)	40	62
9	2	185/185 (100%)	177 (96%)	8 (4%)	29	53
9	i	185/185 (100%)	179 (97%)	6 (3%)	39	62
10	3	172/172 (100%)	169 (98%)	3 (2%)	60	78
10	j	172/172 (100%)	167 (97%)	5 (3%)	42	64
11	4	173/173 (100%)	161 (93%)	12 (7%)	15	40
11	k	173/173 (100%)	171 (99%)	2 (1%)	71	84
12	5	169/169 (100%)	161 (95%)	8 (5%)	26	51
12	l	169/169 (100%)	166 (98%)	3 (2%)	59	77
13	6	185/185 (100%)	180 (97%)	5 (3%)	44	65
13	m	185/185 (100%)	179 (97%)	6 (3%)	39	62
14	7	195/198 (98%)	194 (100%)	1 (0%)	88	93
14	n	198/198 (100%)	190 (96%)	8 (4%)	31	55
15	W	171/171 (100%)	167 (98%)	4 (2%)	50	70
16	V	253/253 (100%)	245 (97%)	8 (3%)	39	62
17	T	249/249 (100%)	241 (97%)	8 (3%)	39	62
18	X	116/116 (100%)	111 (96%)	5 (4%)	29	53
19	Y	81/81 (100%)	78 (96%)	3 (4%)	34	58
20	Z	773/828 (93%)	747 (97%)	26 (3%)	37	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	N	776/776 (100%)	758 (98%)	18 (2%)	50	70
22	S	447/447 (100%)	437 (98%)	10 (2%)	52	71
23	P	412/412 (100%)	404 (98%)	8 (2%)	57	75
24	Q	391/391 (100%)	384 (98%)	7 (2%)	59	77
25	R	356/356 (100%)	341 (96%)	15 (4%)	30	54
26	U	277/277 (100%)	271 (98%)	6 (2%)	52	71
27	O	363/363 (100%)	350 (96%)	13 (4%)	35	59
28	H	361/361 (100%)	347 (96%)	14 (4%)	32	56
29	I	342/342 (100%)	333 (97%)	9 (3%)	46	66
30	K	346/346 (100%)	335 (97%)	11 (3%)	39	62
31	L	332/332 (100%)	321 (97%)	11 (3%)	38	61
32	M	364/364 (100%)	346 (95%)	18 (5%)	25	50
33	J	352/352 (100%)	342 (97%)	10 (3%)	43	65
All	All	12099/12171 (99%)	11715 (97%)	384 (3%)	42	62

All (384) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	16	ILE
1	a	38	THR
1	a	114	CYS
1	a	120	ARG
1	a	126	GLN
1	a	195	ASN
1	a	219	SER
1	a	232	LYS
1	a	240	ASN
2	b	35	LEU
2	b	97	TYR
2	b	168	SER
2	b	178	ARG
2	b	194	LEU
3	c	12	ILE
3	c	21	GLN
3	c	66	LEU
3	c	133	VAL
3	c	158	THR

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Mol	Chain	Res	Type
3	c	202	ASP
3	c	213	PHE
4	d	5	ASP
4	d	10	ILE
4	d	14	ASP
4	d	24	LEU
4	d	40	ASN
4	d	46	CYS
4	d	58	ARG
4	d	71	VAL
4	d	81	ASP
4	d	106	VAL
4	d	139	ASP
4	d	146	LYS
4	d	180	ASP
5	e	9	ASP
5	e	43	LYS
5	e	88	MET
5	e	104	ASP
5	e	113	THR
5	e	222	ILE
6	f	38	LEU
6	f	52	ASN
6	f	72	LEU
6	f	123	TYR
6	f	130	VAL
6	f	150	SER
6	f	153	VAL
6	f	219	ASP
7	g	9	ASP
7	g	21	ASN
7	g	36	THR
7	g	52	LYS
7	g	107	ILE
7	g	150	MET
7	g	212	PHE
7	g	218	TRP
7	g	224	THR
8	h	13	MET
8	h	130	LYS
8	h	152	ARG
8	h	153	GLU

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Mol	Chain	Res	Type
8	h	158	GLU
9	i	54	ILE
9	i	109	LEU
9	i	196	LEU
9	i	227	GLU
9	i	228	LYS
9	i	236	ARG
10	j	13	VAL
10	j	74	TYR
10	j	82	ILE
10	j	156	PRO
10	j	193	ASP
11	k	120	ASP
11	k	186	LYS
12	l	79	LEU
12	l	106	VAL
12	l	276	LYS
13	m	15	ASP
13	m	99	ARG
13	m	100	ASN
13	m	115	VAL
13	m	122	LEU
13	m	136	VAL
14	n	63	TYR
14	n	102	ASP
14	n	106	GLU
14	n	112	PRO
14	n	137	ARG
14	n	197	ASP
14	n	230	LEU
14	n	245	LEU
1	A	13	ASP
1	A	16	ILE
1	A	61	ASP
1	A	65	ASP
1	A	86	PRO
1	A	87	ILE
1	A	92	ASN
1	A	126	GLN
1	A	130	GLN
1	A	139	VAL
1	A	205	PHE

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Mol	Chain	Res	Type
1	A	220	LYS
1	A	232	LYS
2	B	33	THR
2	B	35	LEU
2	B	43	VAL
2	B	60	THR
2	B	66	LEU
2	B	74	VAL
2	B	81	ASP
2	B	194	LEU
2	B	205	ASN
2	B	225	THR
2	B	233	PRO
3	C	52	VAL
3	C	66	LEU
3	C	123	THR
3	C	165	VAL
3	C	168	ASN
3	C	213	PHE
3	C	222	ASP
4	D	24	LEU
4	D	46	CYS
4	D	58	ARG
4	D	106	VAL
4	D	142	ASP
5	E	9	ASP
5	E	43	LYS
5	E	71	ASP
5	E	72	ARG
6	F	38	LEU
6	F	72	LEU
6	F	79	PRO
6	F	80	ASP
7	G	114	ASP
7	G	123	HIS
7	G	218	TRP
8	1	48	ASP
8	1	85	GLU
8	1	135	ILE
8	1	166	HIS
9	2	54	ILE
9	2	67	SER

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Mol	Chain	Res	Type
9	2	105	VAL
9	2	132	VAL
9	2	161	LEU
9	2	173	GLN
9	2	200	SER
9	2	236	ARG
10	3	26	ASP
10	3	147	PHE
10	3	196	VAL
11	4	22	THR
11	4	30	ASP
11	4	58	GLU
11	4	61	GLN
11	4	78	GLN
11	4	101	ASN
11	4	126	VAL
11	4	141	PHE
11	4	145	ASP
11	4	168	LEU
11	4	186	LYS
11	4	193	ASP
12	5	79	LEU
12	5	109	VAL
12	5	133	TRP
12	5	161	LEU
12	5	179	TYR
12	5	212	TYR
12	5	222	ASP
12	5	250	VAL
13	6	26	GLU
13	6	31	LEU
13	6	106	TYR
13	6	216	THR
13	6	217	LYS
14	7	39	VAL
15	W	14	GLU
15	W	59	PRO
15	W	140	ASP
15	W	173	THR
16	V	32	ILE
16	V	58	VAL
16	V	76	THR

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Mol	Chain	Res	Type
16	V	140	VAL
16	V	223	SER
16	V	232	GLU
16	V	262	THR
16	V	283	THR
17	T	44	LEU
17	T	84	GLN
17	T	90	PHE
17	T	94	HIS
17	T	96	LEU
17	T	107	SER
17	T	147	LYS
17	T	150	ARG
18	X	11	ARG
18	X	67	ILE
18	X	68	LEU
18	X	76	VAL
18	X	98	PHE
19	Y	29	LEU
19	Y	38	PHE
19	Y	62	GLU
20	Z	61	SER
20	Z	104	ASP
20	Z	146	PHE
20	Z	191	SER
20	Z	293	MET
20	Z	323	TYR
20	Z	411	LYS
20	Z	490	ILE
20	Z	517	ASP
20	Z	534	PHE
20	Z	566	LEU
20	Z	609	THR
20	Z	617	ILE
20	Z	722	ASP
20	Z	756	MET
20	Z	761	PHE
20	Z	764	LEU
20	Z	776	VAL
20	Z	817	LEU
20	Z	824	ASN
20	Z	834	LEU

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Mol	Chain	Res	Type
20	Z	842	GLN
20	Z	850	LEU
20	Z	865	ASP
20	Z	913	ILE
20	Z	945	ILE
21	N	45	ASP
21	N	72	LEU
21	N	124	TYR
21	N	143	LYS
21	N	175	ASP
21	N	245	LEU
21	N	282	TYR
21	N	297	ASP
21	N	301	THR
21	N	326	SER
21	N	366	THR
21	N	546	LEU
21	N	738	GLN
21	N	774	ASN
21	N	784	TYR
21	N	809	ARG
21	N	829	LYS
21	N	891	VAL
22	S	49	ASP
22	S	72	GLU
22	S	101	LYS
22	S	180	ASN
22	S	290	ASN
22	S	291	GLU
22	S	405	ARG
22	S	455	GLU
22	S	475	TYR
22	S	490	ASN
23	P	1	MET
23	P	3	ARG
23	P	14	SER
23	P	176	LYS
23	P	228	SER
23	P	235	LEU
23	P	309	MET
23	P	396	PRO
24	Q	73	LYS

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Mol	Chain	Res	Type
24	Q	130	ARG
24	Q	170	ASP
24	Q	198	LEU
24	Q	211	PRO
24	Q	221	MET
24	Q	241	GLU
25	R	37	LYS
25	R	63	TYR
25	R	94	PHE
25	R	134	TRP
25	R	183	ASP
25	R	199	GLU
25	R	212	THR
25	R	229	LYS
25	R	239	THR
25	R	245	SER
25	R	274	PRO
25	R	282	THR
25	R	333	MET
25	R	359	VAL
25	R	394	ASP
26	U	5	HIS
26	U	116	ASN
26	U	142	GLN
26	U	236	LEU
26	U	239	LEU
26	U	244	ASP
27	O	25	LEU
27	O	34	GLU
27	O	39	PHE
27	O	58	ARG
27	O	62	TYR
27	O	70	TYR
27	O	71	ASP
27	O	128	LEU
27	O	225	ASP
27	O	272	VAL
27	O	289	GLN
27	O	291	ILE
27	O	348	VAL
28	H	52	THR
28	H	72	SER

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Mol	Chain	Res	Type
28	H	74	THR
28	H	186	PRO
28	H	203	LYS
28	H	274	VAL
28	H	333	MET
28	H	343	PHE
28	H	357	ARG
28	H	375	VAL
28	H	381	ASP
28	H	394	LYS
28	H	399	GLU
28	H	409	ARG
29	I	67	ASP
29	I	214	LYS
29	I	216	PRO
29	I	225	PRO
29	I	314	ASP
29	I	333	THR
29	I	346	ARG
29	I	408	ARG
29	I	423	VAL
30	K	64	GLN
30	K	67	TYR
30	K	121	ARG
30	K	137	VAL
30	K	169	VAL
30	K	251	PRO
30	K	302	GLN
30	K	311	ASN
30	K	333	ARG
30	K	358	SER
30	K	400	TYR
31	L	86	LYS
31	L	109	MET
31	L	131	VAL
31	L	148	LEU
31	L	177	GLU
31	L	187	THR
31	L	269	TYR
31	L	333	LEU
31	L	339	ARG
31	L	365	THR

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Mol	Chain	Res	Type
31	L	415	LEU
32	M	18	LEU
32	M	66	LYS
32	M	119	VAL
32	M	124	ARG
32	M	134	LEU
32	M	158	THR
32	M	179	THR
32	M	182	ASP
32	M	200	PRO
32	M	205	ASP
32	M	244	LEU
32	M	284	ASP
32	M	305	MET
32	M	331	ASP
32	M	352	PRO
32	M	371	ASP
32	M	421	GLU
32	M	433	TYR
33	J	68	PRO
33	J	81	ASP
33	J	105	LYS
33	J	218	LEU
33	J	233	LEU
33	J	249	GLU
33	J	251	ASP
33	J	257	ARG
33	J	288	ILE
33	J	373	ARG

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (135) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	126	GLN
1	a	130	GLN
1	a	175	GLN
1	a	195	ASN
2	b	30	GLN
2	b	180	ASN
2	b	218	ASN
4	d	117	GLN
4	d	178	ASN

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Mol	Chain	Res	Type
4	d	230	ASN
4	d	253	ASN
5	e	108	ASN
5	e	215	ASN
6	f	43	HIS
7	g	43	ASN
7	g	64	ASN
7	g	144	ASN
7	g	147	HIS
8	h	47	HIS
8	h	150	ASN
8	h	170	GLN
10	j	8	ASN
11	k	63	ASN
11	k	101	ASN
12	l	128	GLN
13	m	9	GLN
13	m	100	ASN
13	m	103	HIS
14	n	36	GLN
14	n	51	ASN
14	n	158	GLN
14	n	246	GLN
1	A	92	ASN
1	A	175	GLN
1	A	193	HIS
1	A	209	HIS
2	B	143	ASN
2	B	180	ASN
3	C	156	ASN
4	D	16	HIS
4	D	178	ASN
4	D	204	GLN
5	E	147	HIS
5	E	233	ASN
6	F	21	GLN
6	F	117	GLN
6	F	199	GLN
7	G	43	ASN
7	G	68	GLN
7	G	87	HIS
7	G	127	ASN

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Mol	Chain	Res	Type
9	2	201	ASN
10	3	48	HIS
10	3	72	ASN
10	3	113	ASN
10	3	169	GLN
10	3	173	ASN
11	4	55	GLN
11	4	133	HIS
12	5	128	GLN
12	5	254	HIS
12	5	263	HIS
13	6	205	GLN
14	7	153	GLN
14	7	182	HIS
14	7	185	ASN
15	W	92	GLN
15	W	106	GLN
15	W	108	GLN
16	V	176	ASN
16	V	291	ASN
17	T	118	ASN
17	T	123	HIS
17	T	236	ASN
18	X	18	ASN
18	X	105	ASN
19	Y	63	ASN
19	Y	89	GLN
20	Z	132	HIS
20	Z	151	HIS
20	Z	275	GLN
20	Z	405	ASN
20	Z	427	GLN
20	Z	502	ASN
20	Z	763	HIS
20	Z	769	ASN
20	Z	871	HIS
20	Z	897	HIS
21	N	71	ASN
21	N	506	GLN
21	N	674	GLN
21	N	690	HIS
21	N	747	HIS

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Mol	Chain	Res	Type
21	N	859	ASN
22	S	19	HIS
22	S	290	ASN
22	S	335	GLN
22	S	472	HIS
22	S	490	ASN
23	P	30	ASN
23	P	88	GLN
23	P	278	ASN
23	P	342	GLN
24	Q	106	GLN
24	Q	145	HIS
24	Q	147	GLN
24	Q	178	HIS
24	Q	213	GLN
24	Q	420	ASN
25	R	136	ASN
25	R	208	ASN
25	R	340	GLN
25	R	397	ASN
25	R	401	HIS
26	U	26	GLN
26	U	230	GLN
27	O	107	GLN
27	O	236	HIS
27	O	389	GLN
28	H	148	ASN
28	H	387	ASN
28	H	392	HIS
29	I	117	HIS
29	I	266	GLN
29	I	329	ASN
29	I	365	HIS
30	K	98	GLN
31	L	273	HIS
31	L	364	HIS
32	M	74	GLN
32	M	143	ASN
32	M	240	ASN
33	J	269	GLN
33	J	376	HIS
33	J	394	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	ADP	L	501	35	24,29,29	1.44	4 (16%)	29,45,45	1.93	5 (17%)
34	ATP	I	501	35	26,33,33	1.51	4 (15%)	31,52,52	3.01	8 (25%)
34	ATP	K	501	35	26,33,33	1.16	3 (11%)	31,52,52	2.27	8 (25%)
34	ATP	J	501	35	26,33,33	1.71	5 (19%)	31,52,52	2.69	5 (16%)
36	ADP	M	501	35	24,29,29	1.16	3 (12%)	29,45,45	1.77	4 (13%)
34	ATP	H	501	35	26,33,33	1.73	7 (26%)	31,52,52	2.66	8 (25%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ADP	L	501	35	-	3/12/32/32	0/3/3/3
34	ATP	I	501	35	-	3/18/38/38	0/3/3/3

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

All (26) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	J	501	ATP	C3'-C4'	-4.31	1.42	1.53
34	H	501	ATP	O4'-C4'	4.30	1.54	1.45
34	I	501	ATP	C8-N7	-4.30	1.27	1.34
34	J	501	ATP	C8-N7	-3.64	1.28	1.34
36	L	501	ADP	C8-N7	-3.49	1.28	1.34
34	J	501	ATP	C2-N3	3.49	1.37	1.32
34	J	501	ATP	C4-N3	-3.45	1.30	1.35
36	L	501	ADP	C2'-C1'	-3.23	1.48	1.53
34	I	501	ATP	O4'-C4'	-3.17	1.37	1.45
34	I	501	ATP	C3'-C4'	2.76	1.60	1.53
36	L	501	ADP	C3'-C4'	-2.72	1.46	1.53
34	H	501	ATP	C8-N7	-2.70	1.29	1.34
34	H	501	ATP	C2-N3	2.64	1.36	1.32
36	M	501	ADP	C2-N3	2.58	1.36	1.32
36	L	501	ADP	C2-N1	2.56	1.38	1.33
34	H	501	ATP	PG-O1G	2.44	1.58	1.50
34	K	501	ATP	O2'-C2'	-2.44	1.37	1.43
34	K	501	ATP	O3'-C3'	2.34	1.48	1.43
34	J	501	ATP	C5-C4	-2.23	1.35	1.40
36	M	501	ADP	C5-C4	2.22	1.46	1.40
34	H	501	ATP	O4'-C1'	-2.22	1.38	1.41
34	K	501	ATP	C2-N1	-2.20	1.29	1.33
34	H	501	ATP	C2'-C1'	2.16	1.57	1.53
34	H	501	ATP	C6-C5	-2.15	1.35	1.43
36	M	501	ADP	PA-O5'	2.03	1.67	1.59
34	I	501	ATP	PA-O2A	-2.01	1.45	1.55

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	I	501	ATP	PB-O3B-PG	10.00	167.13	132.83
34	H	501	ATP	PB-O3B-PG	8.96	163.57	132.83
34	J	501	ATP	PA-O3A-PB	8.16	160.83	132.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	H	501	ATP	PA-O3A-PB	7.37	158.11	132.83
34	I	501	ATP	C1'-N9-C4	7.09	139.09	126.64
34	I	501	ATP	PA-O3A-PB	6.76	156.02	132.83
34	K	501	ATP	PA-O3A-PB	6.50	155.12	132.83
34	J	501	ATP	PB-O3B-PG	6.49	155.10	132.83
34	J	501	ATP	N6-C6-N1	6.41	131.89	118.57
36	L	501	ADP	PA-O3A-PB	6.35	154.62	132.83
34	I	501	ATP	N6-C6-N1	5.80	130.60	118.57
34	J	501	ATP	C5-C6-N6	-5.73	111.65	120.35
34	K	501	ATP	PB-O3B-PG	5.46	151.55	132.83
34	K	501	ATP	N6-C6-N1	5.05	129.06	118.57
36	M	501	ADP	PA-O3A-PB	4.91	149.69	132.83
34	H	501	ATP	N6-C6-N1	4.71	128.36	118.57
34	H	501	ATP	C5-C6-N6	-4.29	113.83	120.35
36	M	501	ADP	N6-C6-N1	4.20	127.30	118.57
36	L	501	ADP	C5-C6-N6	-4.05	114.19	120.35
36	L	501	ADP	N6-C6-N1	3.93	126.72	118.57
34	K	501	ATP	C5-C6-N6	-3.66	114.79	120.35
34	I	501	ATP	C5-C6-N1	-3.38	112.69	120.35
36	L	501	ADP	C2-N1-C6	-3.16	113.36	118.75
36	L	501	ADP	C1'-N9-C4	2.92	131.77	126.64
36	M	501	ADP	C5-C6-N1	-2.77	114.07	120.35
34	I	501	ATP	C2-N1-C6	2.73	123.43	118.75
34	J	501	ATP	O4'-C1'-C2'	-2.54	103.22	106.93
34	K	501	ATP	C4-C5-N7	-2.53	106.76	109.40
34	H	501	ATP	O5'-C5'-C4'	2.51	117.62	108.99
34	I	501	ATP	C5-C6-N6	-2.48	116.58	120.35
34	H	501	ATP	O4'-C1'-C2'	2.40	110.43	106.93
34	I	501	ATP	O4'-C4'-C3'	-2.30	100.57	105.11
34	K	501	ATP	C1'-N9-C4	-2.27	122.64	126.64
34	H	501	ATP	O3G-PG-O2G	2.24	116.19	107.64
36	M	501	ADP	C3'-C2'-C1'	2.24	104.35	100.98
34	K	501	ATP	C2-N1-C6	-2.20	115.00	118.75
34	H	501	ATP	O4'-C4'-C3'	-2.12	100.91	105.11
34	K	501	ATP	O3G-PG-O2G	2.07	115.56	107.64

There are no chirality outliers.

All (20) torsion outliers are listed below:

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

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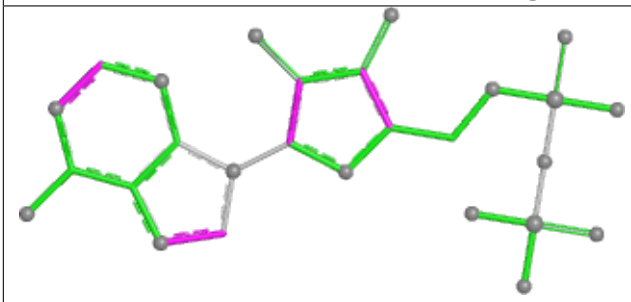
Mol	Chain	Res	Type	Atoms
34	K	501	ATP	C5'-O5'-PA-O1A
34	K	501	ATP	C5'-O5'-PA-O2A
34	J	501	ATP	C5'-O5'-PA-O1A
34	J	501	ATP	C5'-O5'-PA-O2A
36	L	501	ADP	C5'-O5'-PA-O2A
36	L	501	ADP	C5'-O5'-PA-O3A
36	M	501	ADP	PA-O3A-PB-O2B
36	M	501	ADP	PA-O3A-PB-O3B
36	M	501	ADP	C5'-O5'-PA-O2A
36	M	501	ADP	C5'-O5'-PA-O3A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

There are no ring outliers.

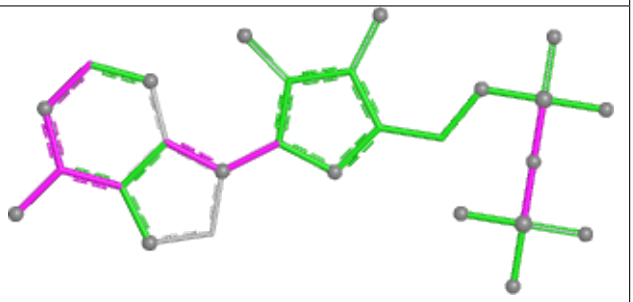
No monomer is involved in short contacts.

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

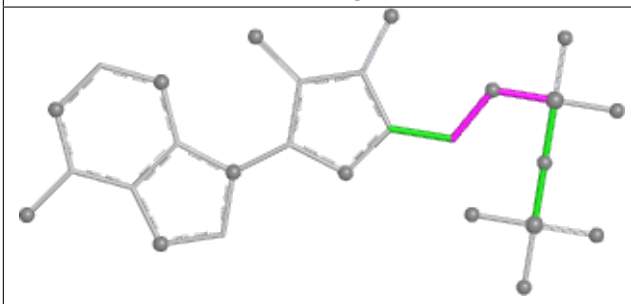
Ligand ADP L 501



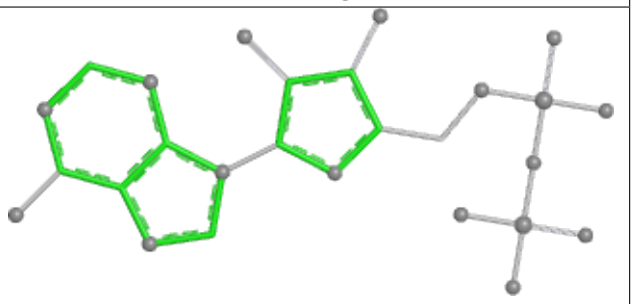
Bond lengths



Bond angles

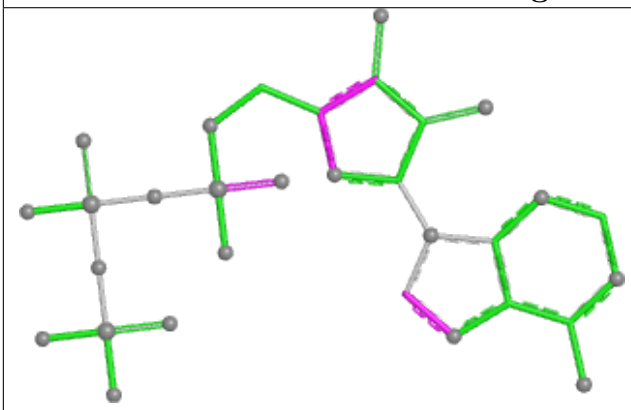


Torsions

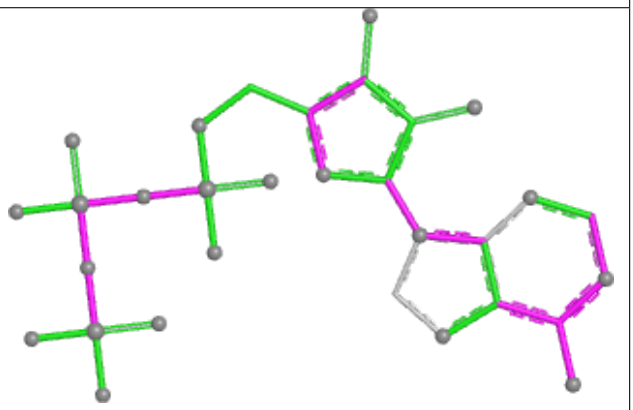


Rings

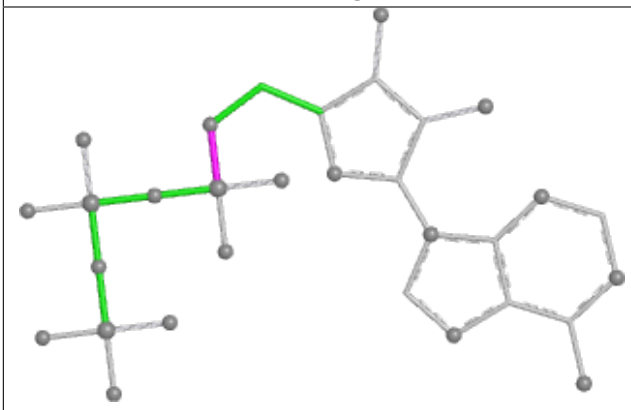
Ligand ATP I 501



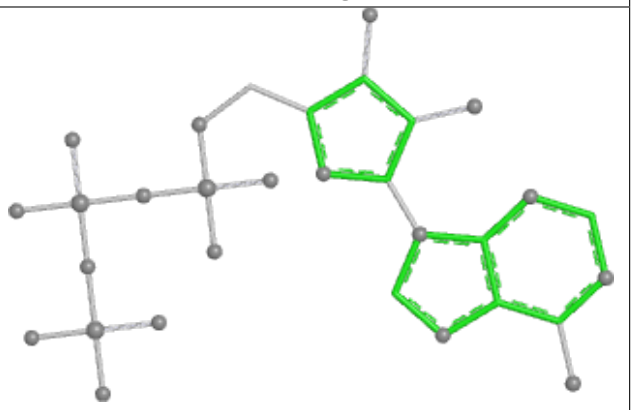
Bond lengths



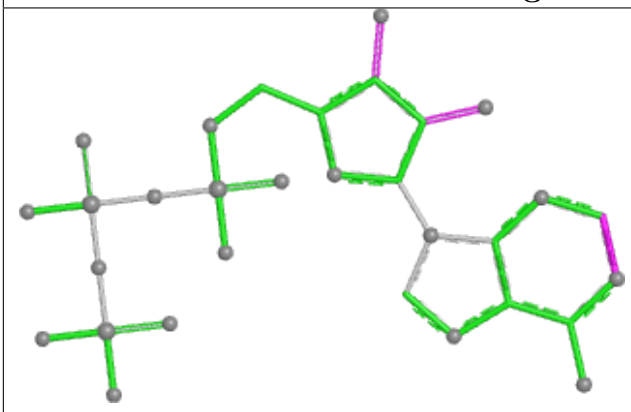
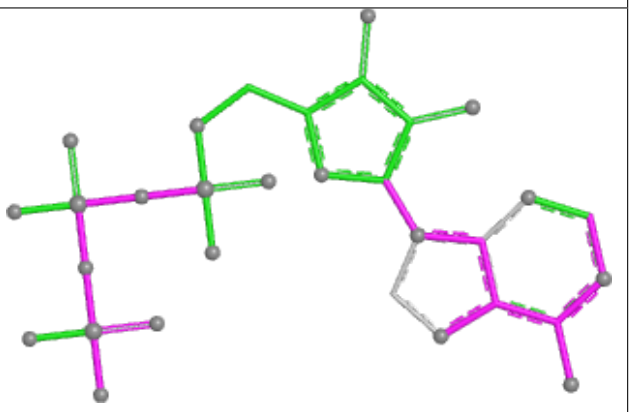
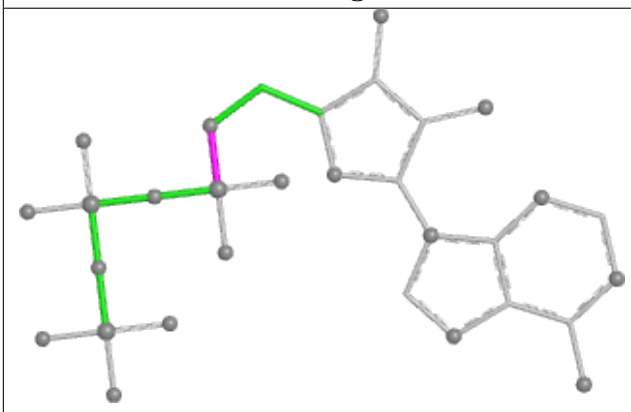
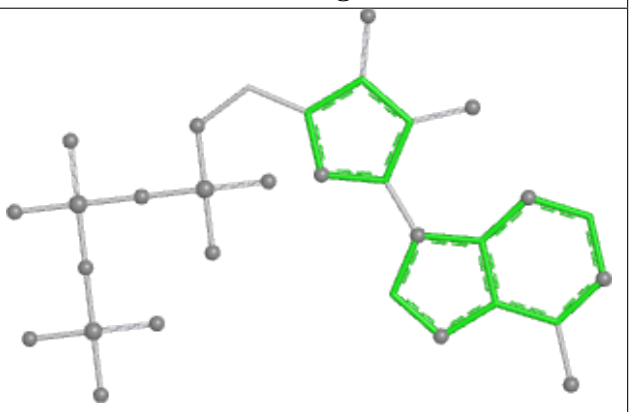
Bond angles

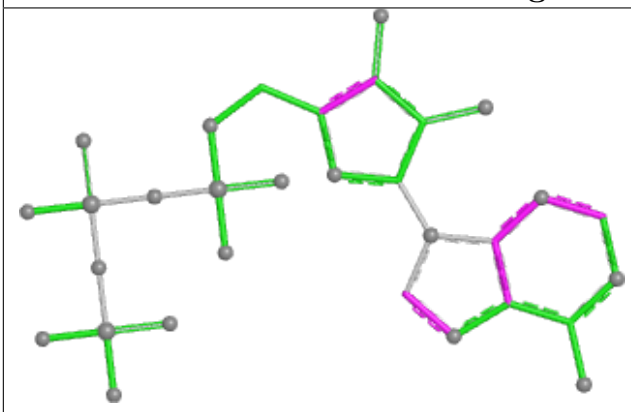
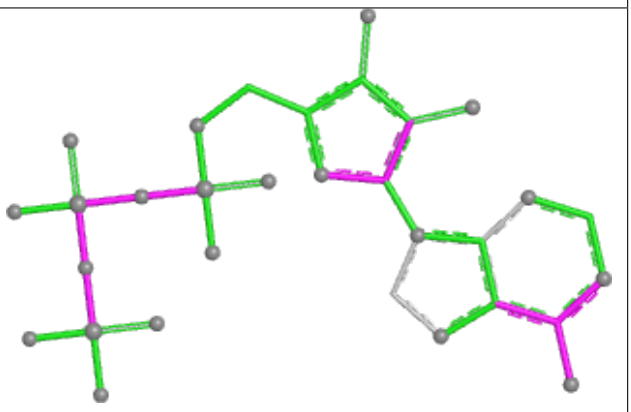
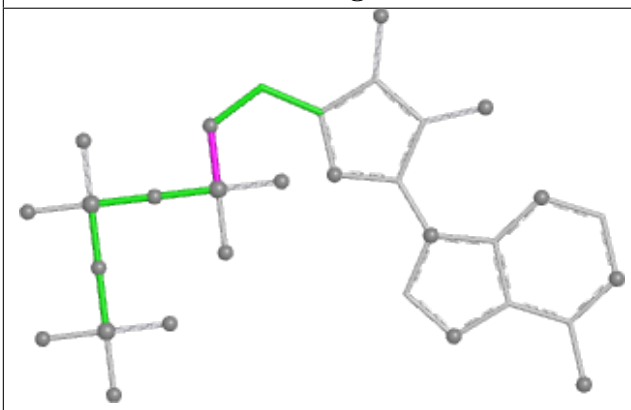
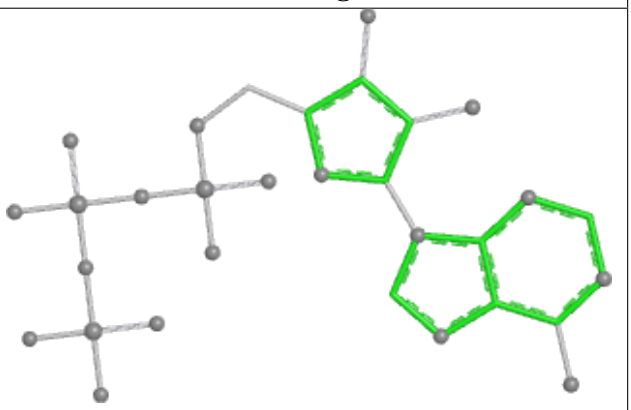


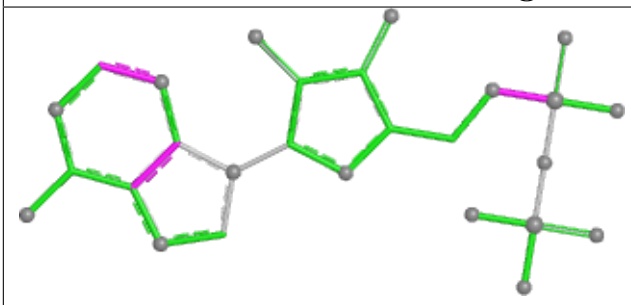
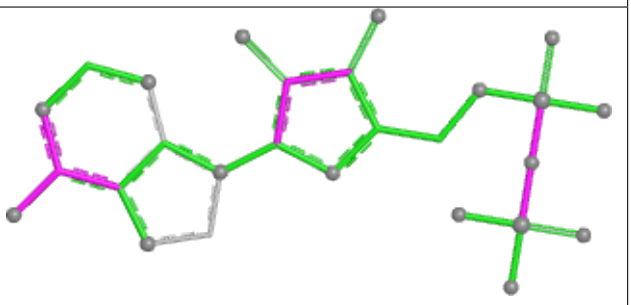
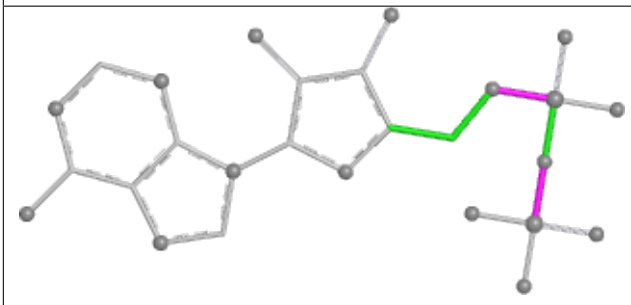
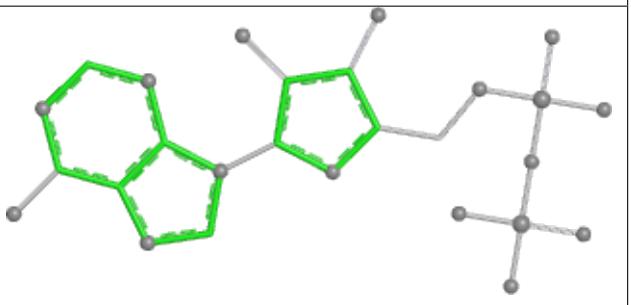
Torsions

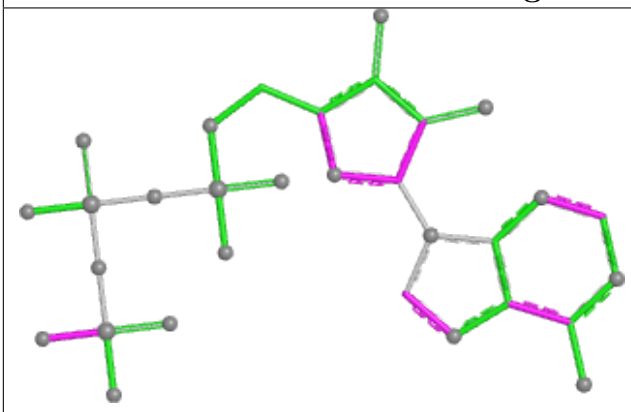
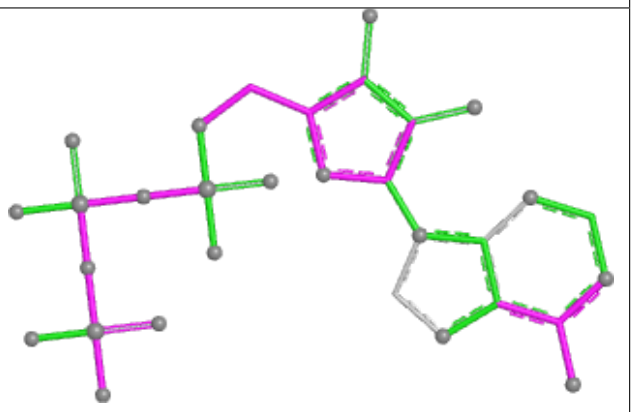
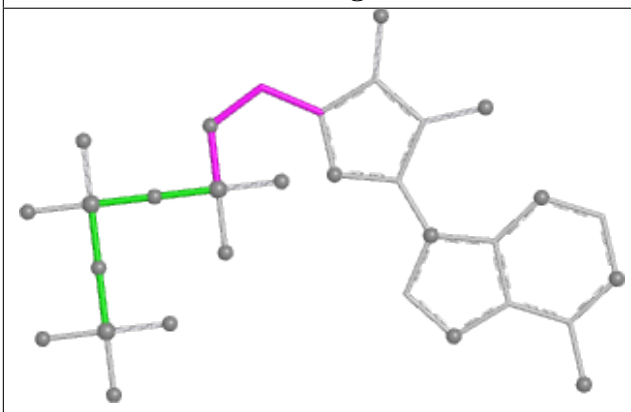
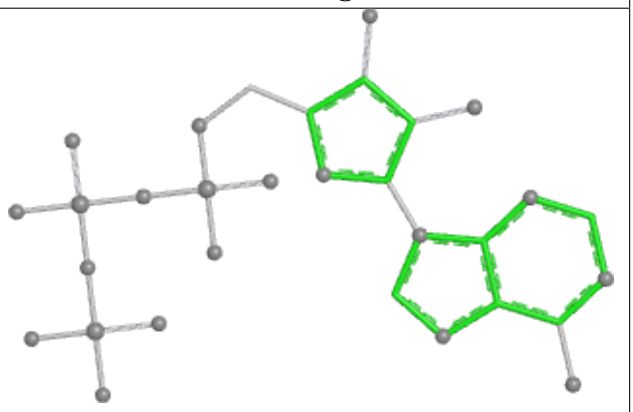


Rings

Ligand ATP K 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP J 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP M 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP H 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.

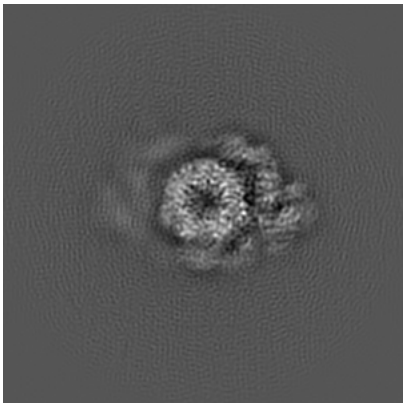
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4324. These allow visual inspection of the internal detail of the map and identification of artifacts.

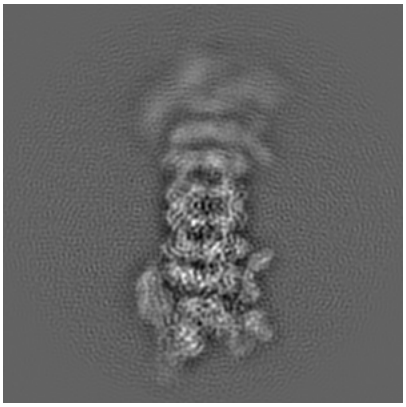
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

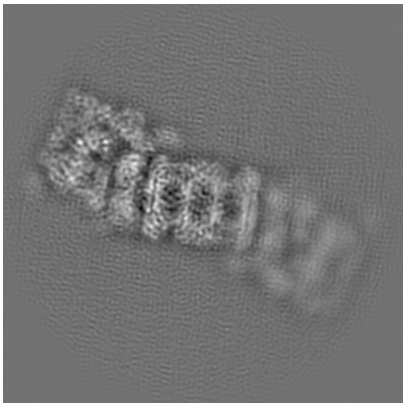
6.1.1 Primary map



X



Y

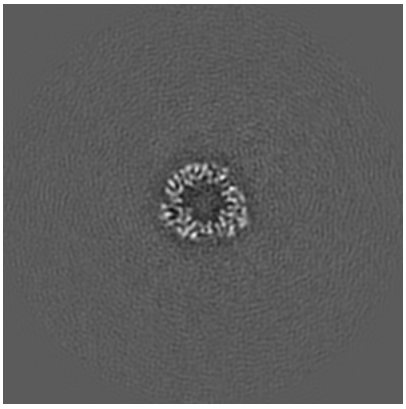


Z

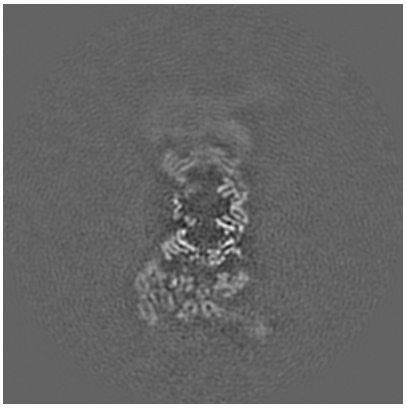
The images above show the map projected in three orthogonal directions.

6.2 Central slices

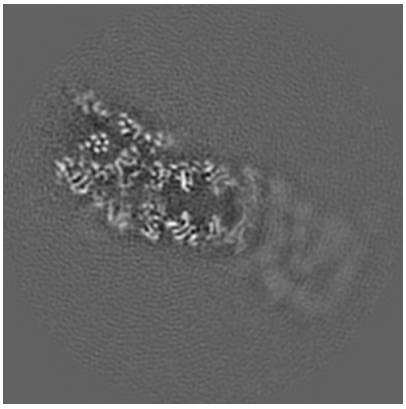
6.2.1 Primary map



X Index: 192



Y Index: 192

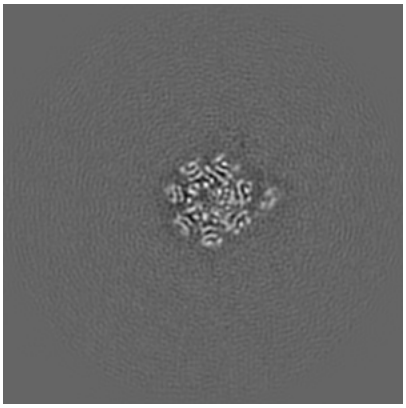


Z Index: 192

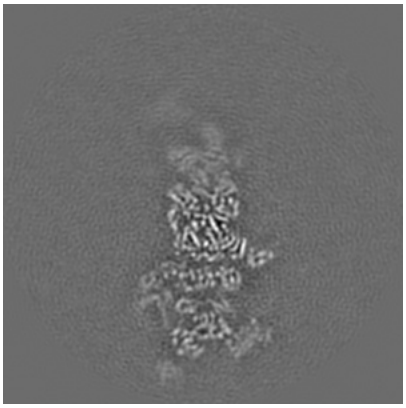
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

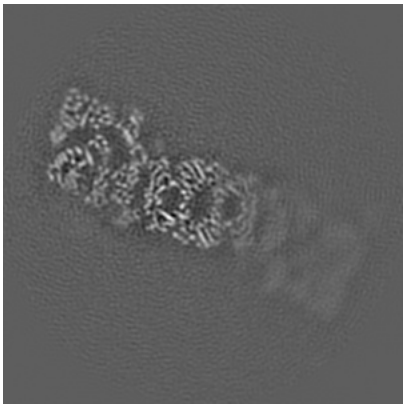
6.3.1 Primary map



X Index: 150



Y Index: 213



Z Index: 181

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

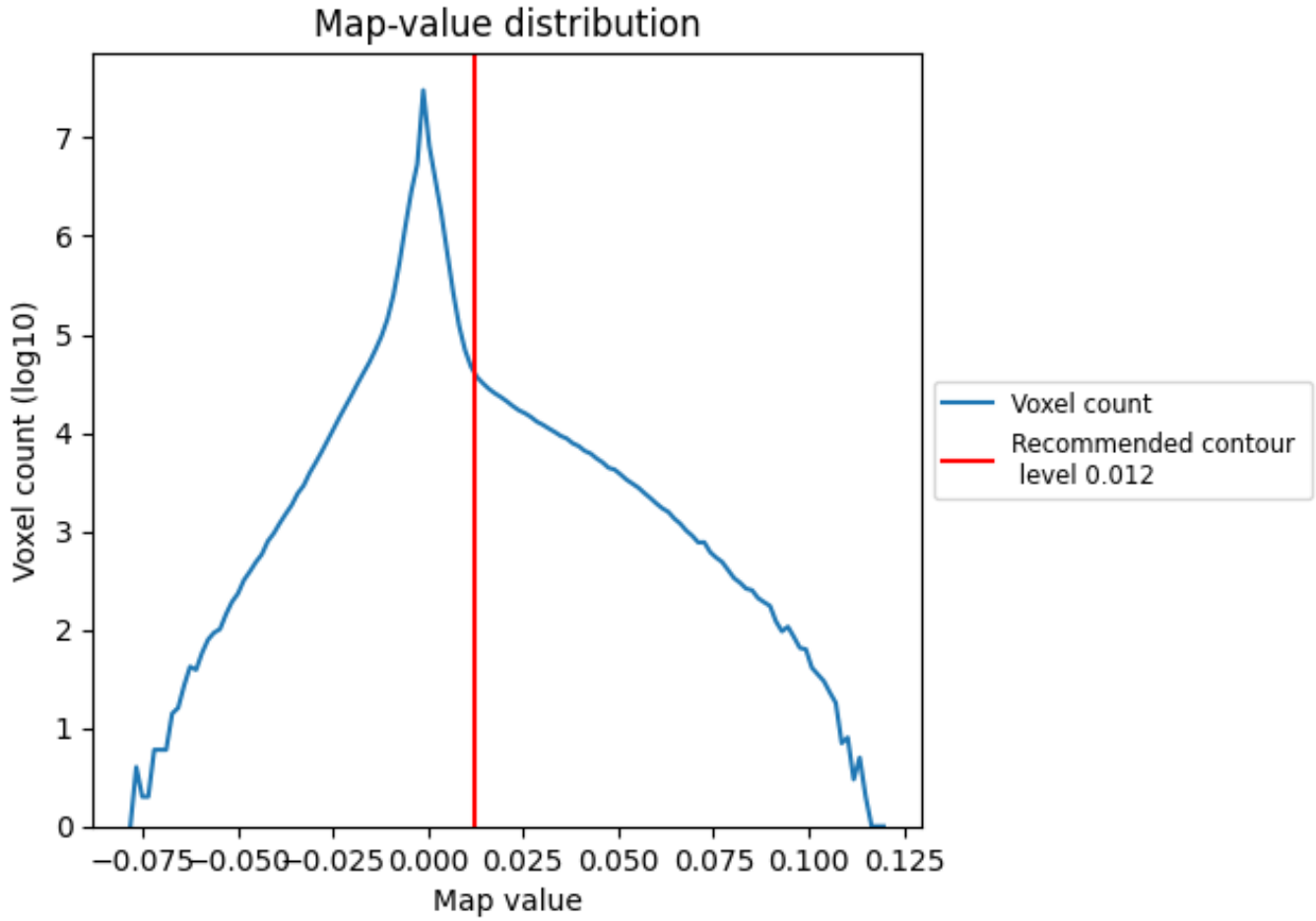
6.5 Mask visualisation (i)

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

7 Map analysis

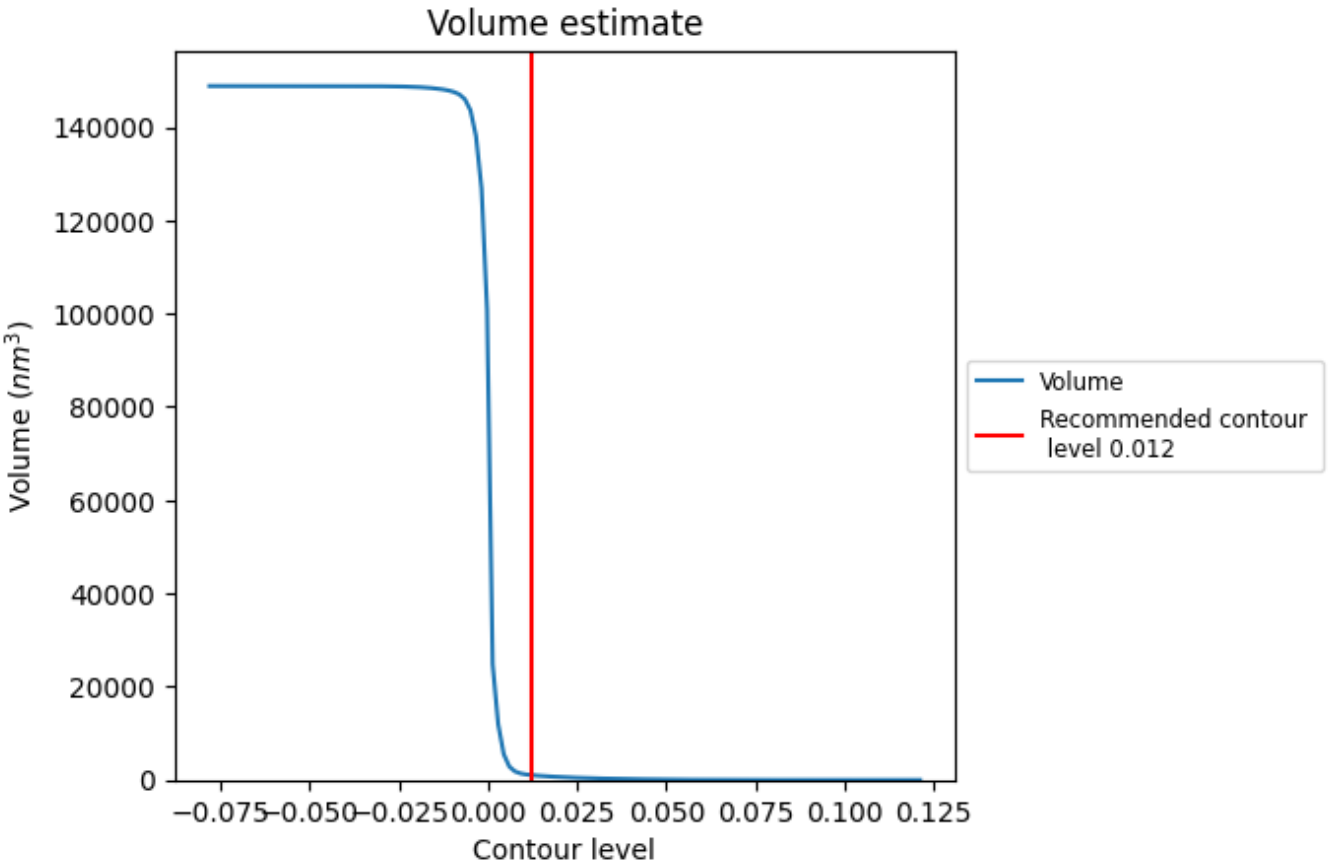
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

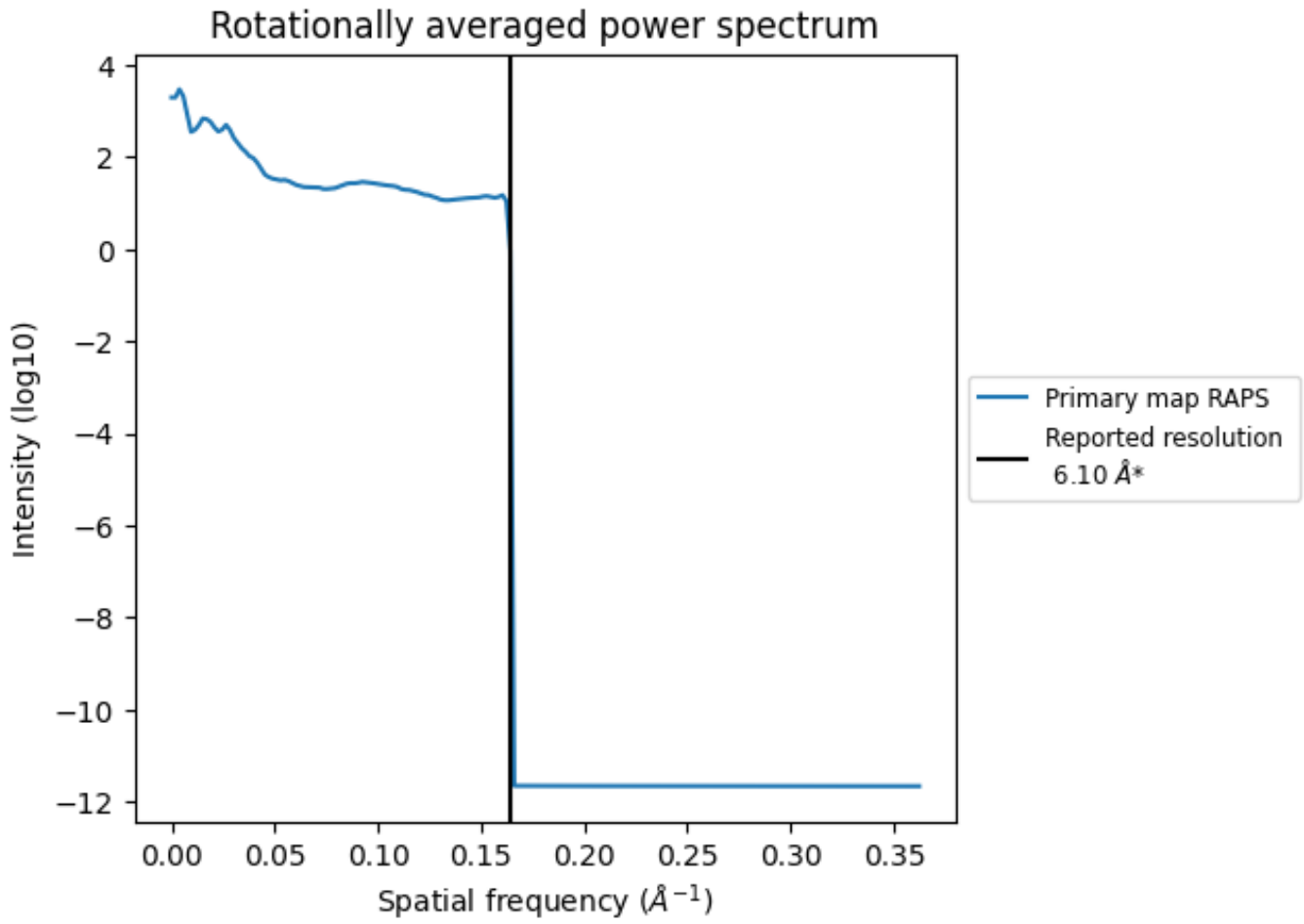
7.2 Volume estimate



The volume at the recommended contour level is 1059 nm^3; this corresponds to an approximate mass of 957 kDa.

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

7.3 Rotationally averaged power spectrum (i)



*Reported resolution corresponds to spatial frequency of 0.164 Å^{-1}

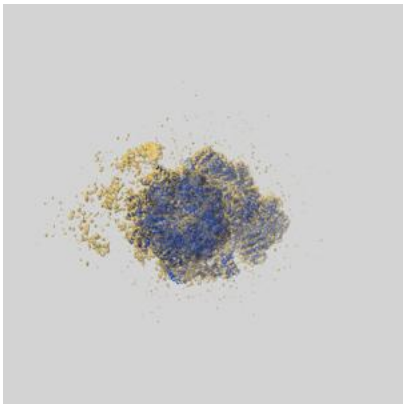
8 Fourier-Shell correlation

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

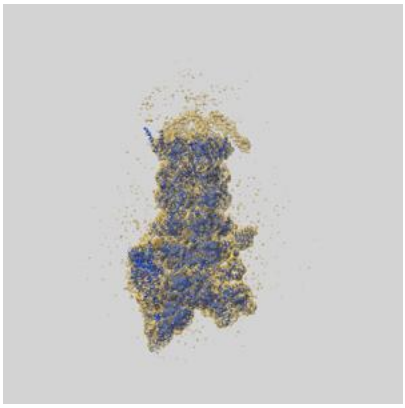
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4324 and PDB model 6FVY. Per-residue inclusion information can be found in section 3 on page 13.

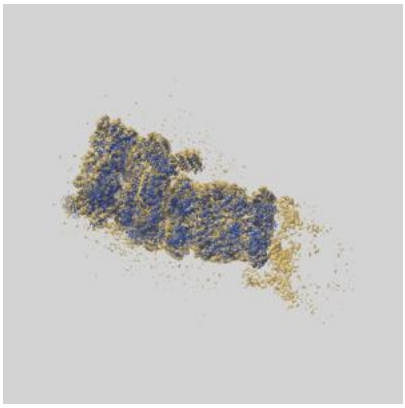
9.1 Map-model overlay



X



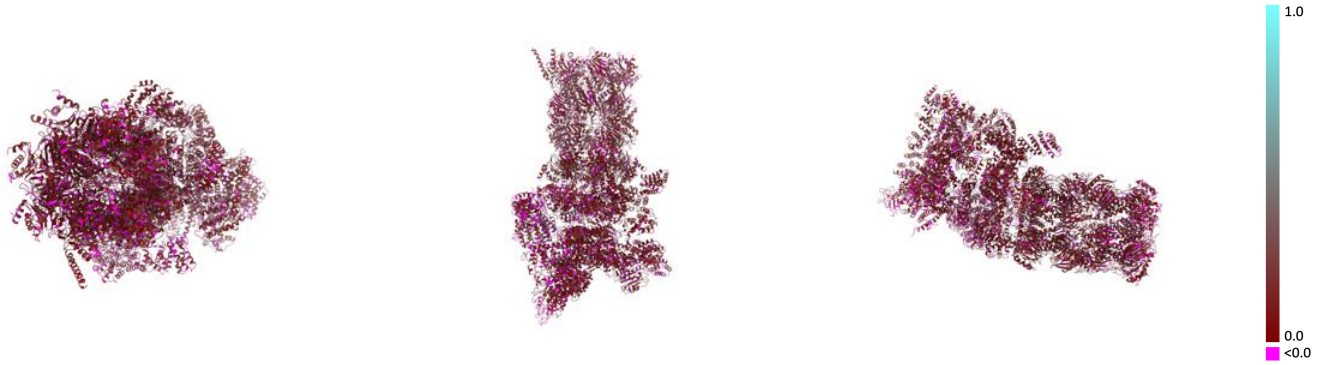
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

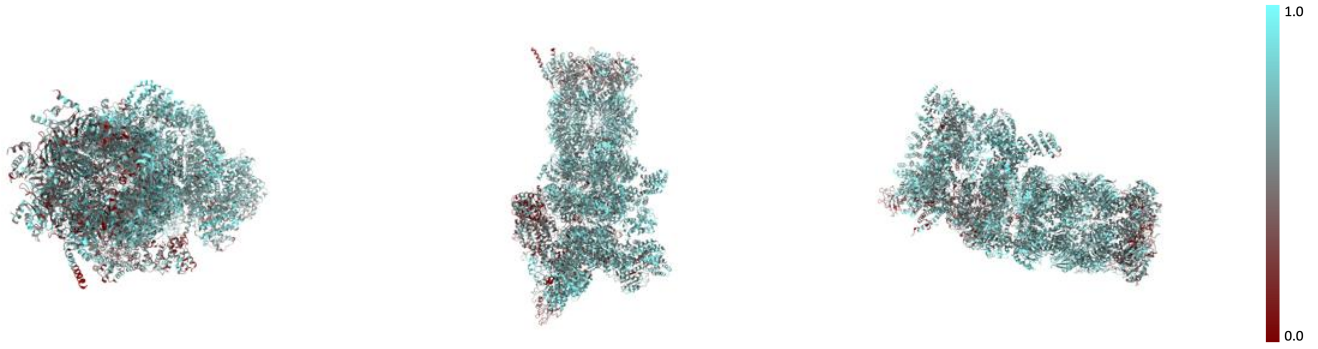
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

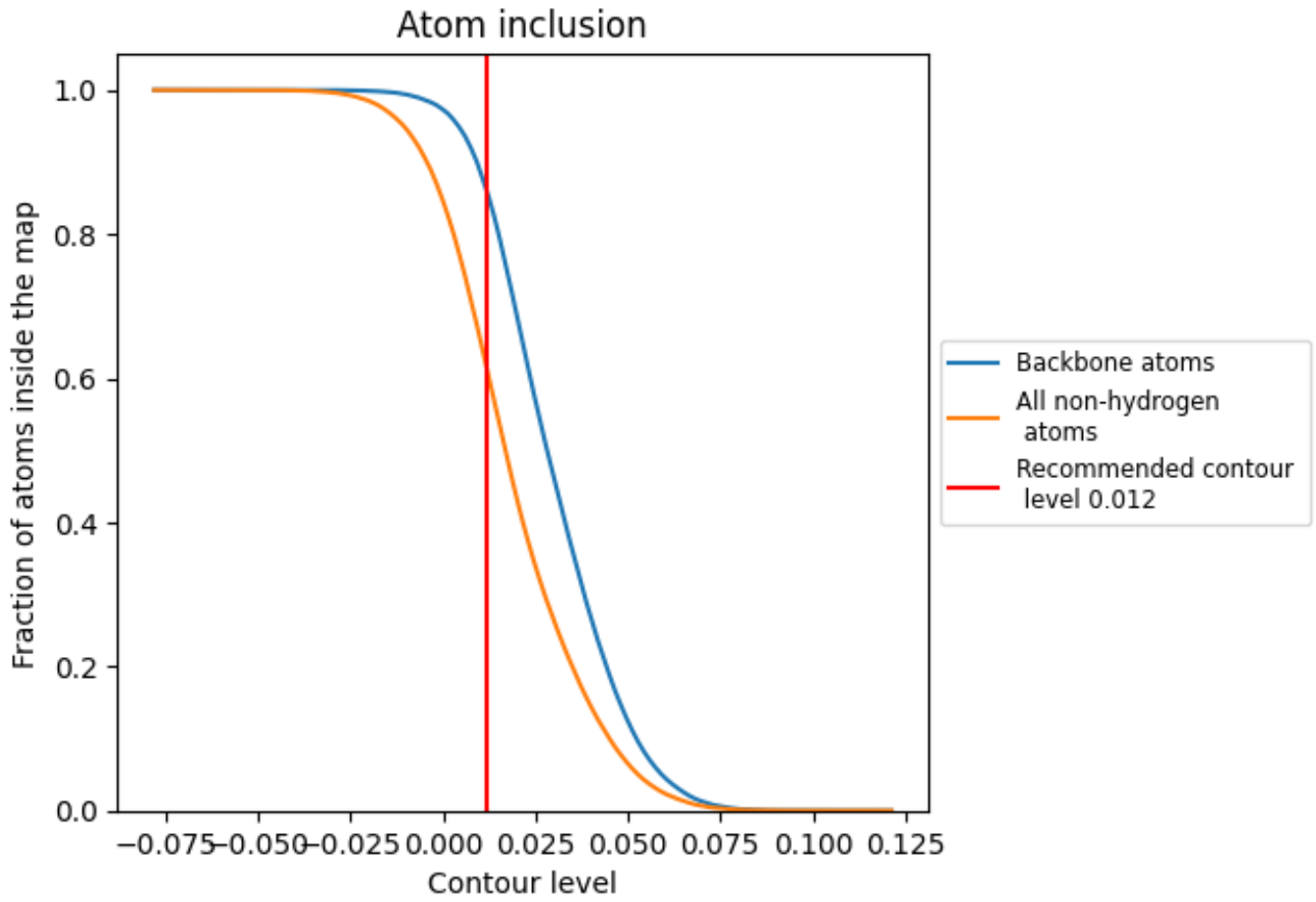
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 61% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6091	0.1360
1	0.7008	0.1640
2	0.6932	0.1730
3	0.6645	0.1570
4	0.6926	0.1590
5	0.7234	0.1650
6	0.7033	0.1680
7	0.7079	0.1630
A	0.6790	0.1610
B	0.6834	0.1720
C	0.6732	0.1650
D	0.6820	0.1620
E	0.6753	0.1630
F	0.7082	0.1770
G	0.6997	0.1750
H	0.5330	0.1100
I	0.5801	0.1360
J	0.5708	0.1200
K	0.6119	0.1380
L	0.6345	0.1470
M	0.5816	0.1220
N	0.6427	0.1420
O	0.6703	0.1350
P	0.7317	0.1450
Q	0.6909	0.1360
R	0.6857	0.1350
S	0.6051	0.1280
T	0.6298	0.1350
U	0.5988	0.1340
V	0.6323	0.1410
W	0.5697	0.1240
X	0.2032	0.0430
Y	0.4440	0.0820
Z	0.4329	0.0710
a	0.4873	0.1350

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Chain	Atom inclusion	Q-score
b	0.4727	0.1430
c	0.4802	0.1220
d	0.4357	0.1190
e	0.4645	0.1210
f	0.5034	0.1260
g	0.4960	0.1360
h	0.6718	0.1370
i	0.6478	0.1460
j	0.6517	0.1450
k	0.6344	0.1410
l	0.6737	0.1520
m	0.6585	0.1460
n	0.6588	0.1530