Full wwPDB EM Validation Report ⓘ

Nov 20, 2022 – 12:58 am GMT

PDB ID	:	6FVT
EMDB ID	:	EMD-3534
Title	:	26S proteasome, s1 state
Authors	:	Eisele, M.R.; Reed, R.G.; Rudack, T.; Schweitzer, A.; Beck, F.; Nagy, I.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Tomko, R.J.; Sakata, E.
Deposited on	:	2018-03-05
Resolution	:	4.10 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:

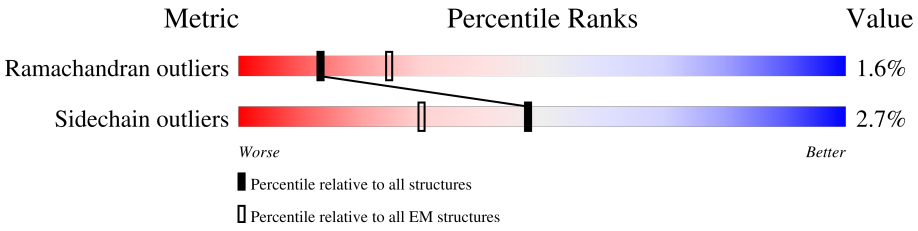
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 4.10 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	241	81% 17%
1	a	241	78% 18%
2	B	249	75% 24%
2	b	249	79% 18%
3	C	244	77% 19% 5%
3	c	244	79% 19%
4	D	251	67% 23% 6%
4	d	251	80% 16%
5	E	244	80% 16%

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Mol	Chain	Length	Quality of chain
5	e	244	81% 17%
6	F	231	75% 21%
6	f	231	80% 17%
7	G	245	80% 18%
7	g	245	78% 20%
8	1	196	77% 19% 5%
8	h	196	76% 20%
9	2	226	83% 15%
9	i	226	81% 18%
10	3	204	80% 18%
10	j	204	78% 19%
11	4	195	74% 22% 5%
11	k	195	75% 23%
12	5	212	75% 24%
12	l	212	75% 23%
13	6	222	73% 24%
13	m	222	73% 24%
14	7	232	75% 20%
14	n	232	71% 27%
15	W	197	90% 80% 18%
16	V	289	50% 81% 18%
17	T	266	76% 79% 18%
18	X	127	100% 76% 21%
19	Y	89	75% 76% 22%
20	Z	970	86% 73% 18% 7%

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Mol	Chain	Length	Quality of chain
21	N	922	84% 80% 18%
22	S	475	64% 79% 18%
23	P	440	21% 82% 15%
24	Q	434	18% 76% 21%
25	R	405	36% 76% 21%
26	U	304	59% 85% 14%
27	O	388	62% 79% 19%
28	H	426	25% 76% 21%
29	I	385	20% 78% 19%
30	K	394	21% 81% 16%
31	L	388	23% 79% 19%
32	M	421	25% 78% 20%
33	J	405	32% 80% 18%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 110541 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
1	a	241	Total	C	N	O	S	0	0
			1908	1214	320	366	8		
1	A	241	Total	C	N	O	S	0	0
			1908	1214	320	366	8		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
3	c	244	Total	C	N	O	S	0	0
			1905	1201	321	380	3		
3	C	244	Total	C	N	O	S	0	0
			1905	1201	321	380	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	d	251	Total	C	N	O	S	0	0
			1982	1235	350	393	4		
4	D	237	Total	C	N	O	S	0	0
			1859	1164	325	366	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	e	244	Total	C	N	O	S	0	0
			1883	1176	316	384	7		
5	E	244	Total	C	N	O	S	0	0
			1883	1176	316	384	7		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	g	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		

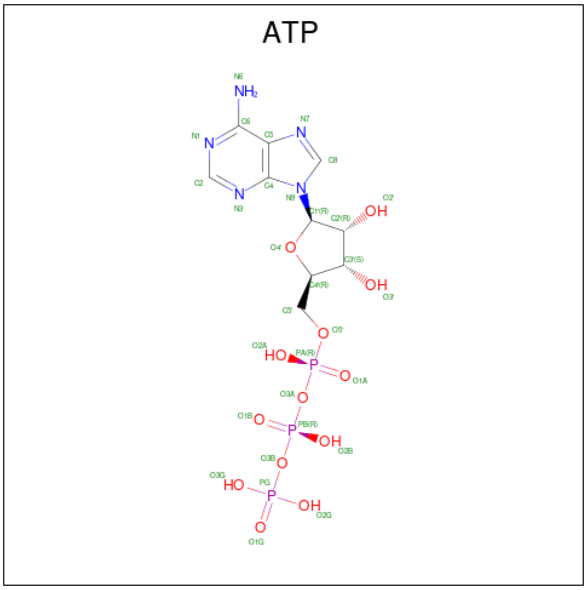
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

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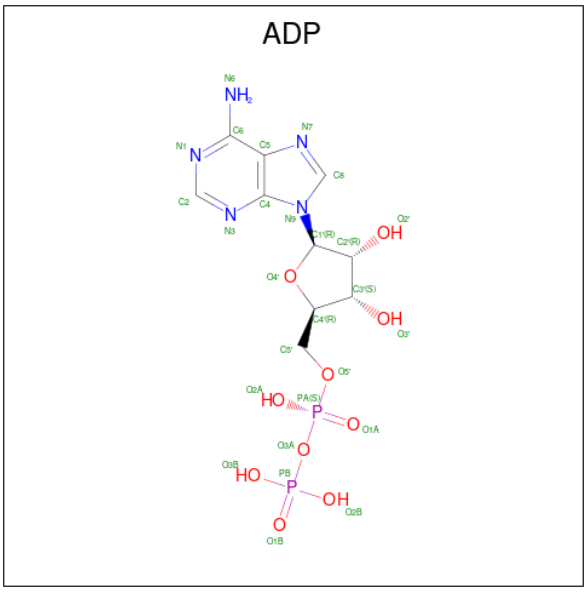
Mol	Chain	Residues	Atoms					AltConf
34	I	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	K	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	L	1	Total	C	N	O	P	0
			31	10	5	13	3	
34	M	1	Total	C	N	O	P	0
			31	10	5	13	3	

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

Mol	Chain	Residues	Atoms		AltConf
35	H	2	Total	Mg	0
			2	2	
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	J	1	Total	Mg	0
			1	1	

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



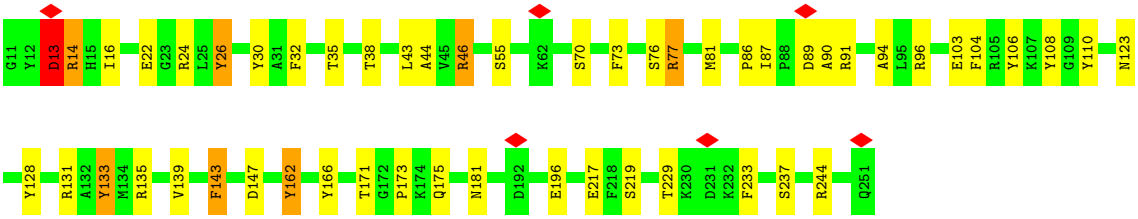
Mol	Chain	Residues	Atoms					AltConf
36	J	1	Total	C	N	O	P	0
			27	10	5	10	2	

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.

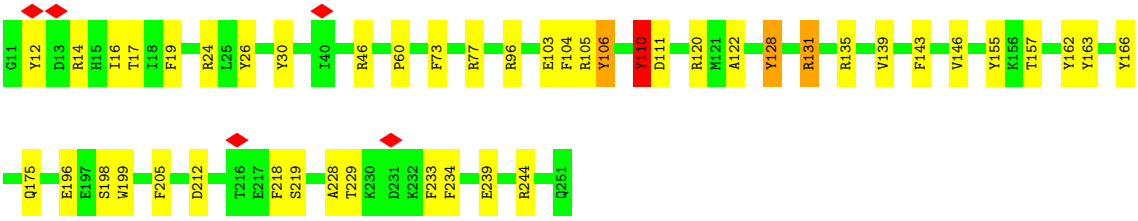
• Molecule 1: Proteasome subunit alpha type-1

Chain a:



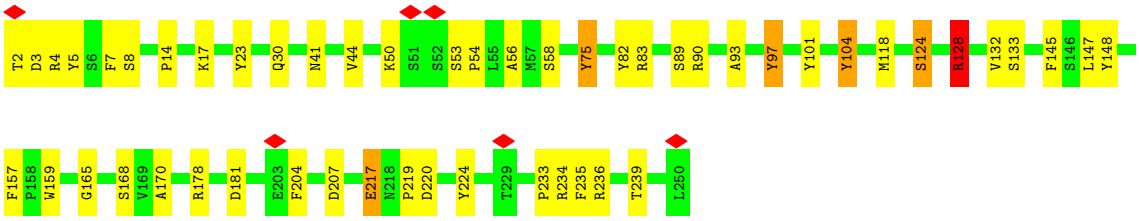
• Molecule 1: Proteasome subunit alpha type-1

Chain A:



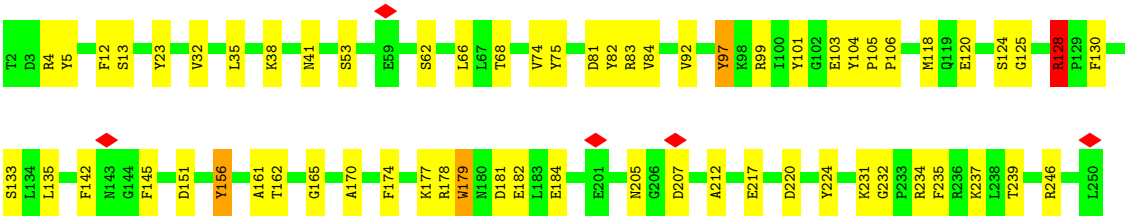
• Molecule 2: Proteasome subunit alpha type-2

Chain b:

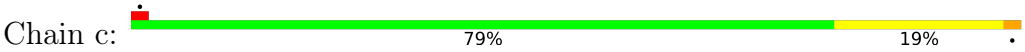


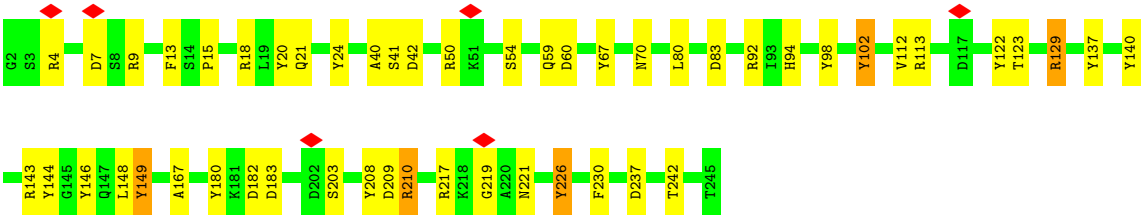
• Molecule 2: Proteasome subunit alpha type-2

Chain B:

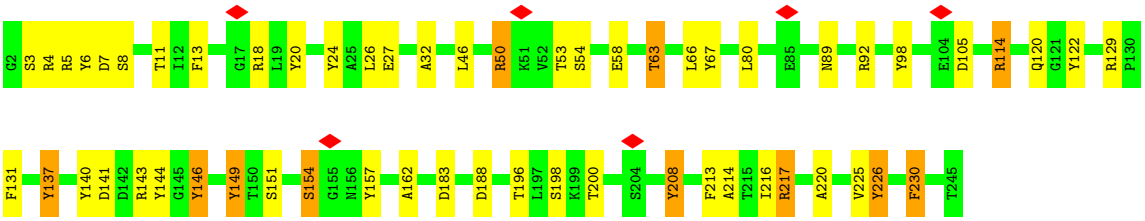


• Molecule 3: Proteasome subunit alpha type-3

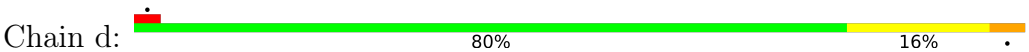


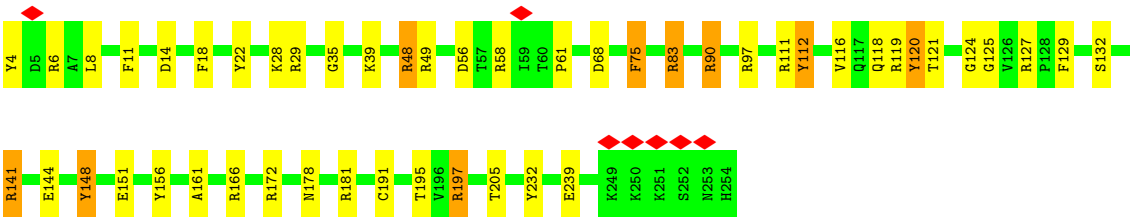


• Molecule 3: Proteasome subunit alpha type-3

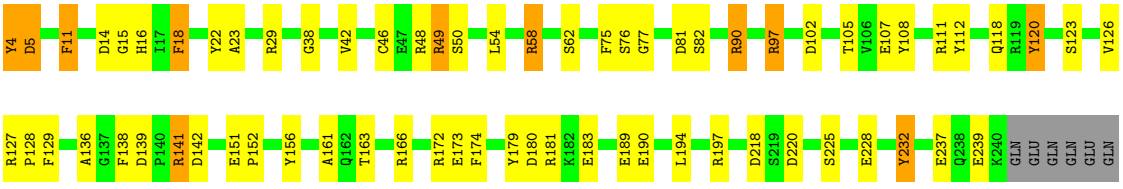


• Molecule 4: Proteasome subunit alpha type-4



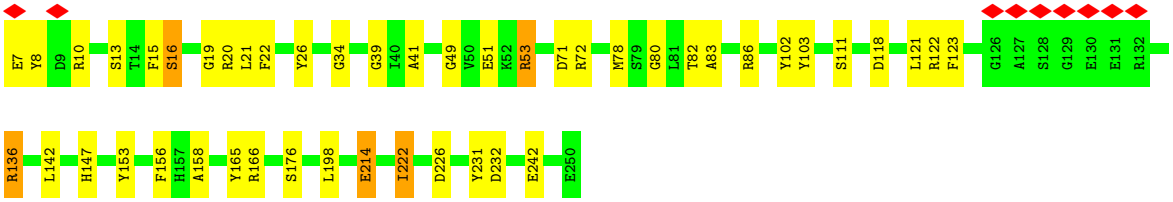


• Molecule 4: Proteasome subunit alpha type-4



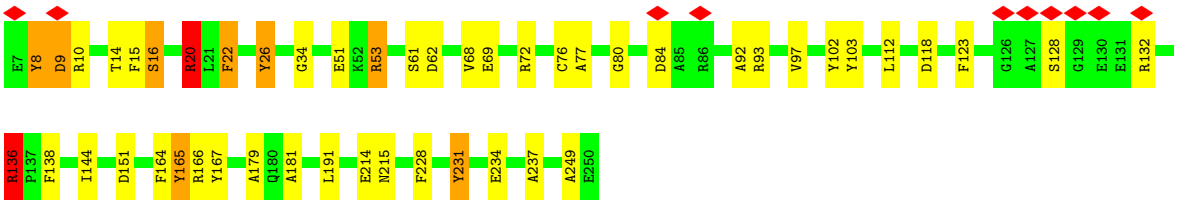
• Molecule 5: Proteasome subunit alpha type-5

Chain e:



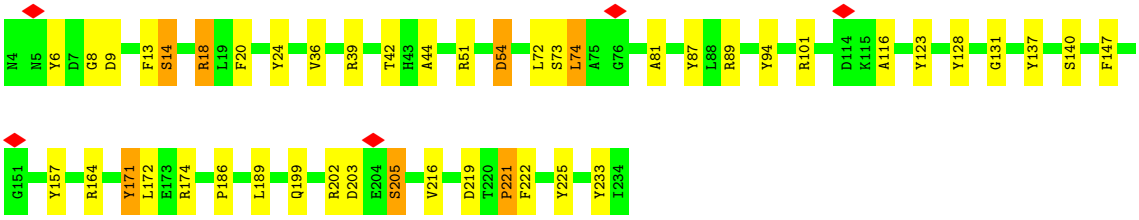
• Molecule 5: Proteasome subunit alpha type-5

Chain E:



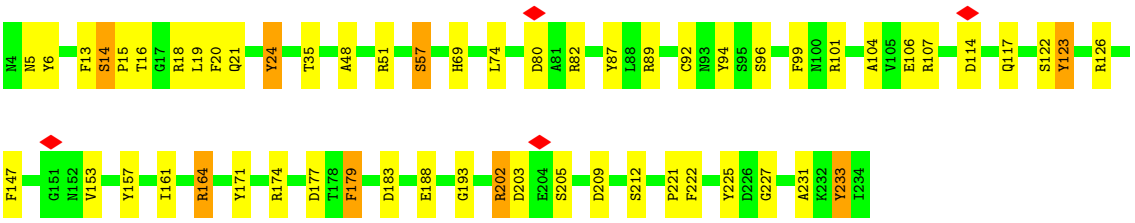
• Molecule 6: Proteasome subunit alpha type-6

Chain f:



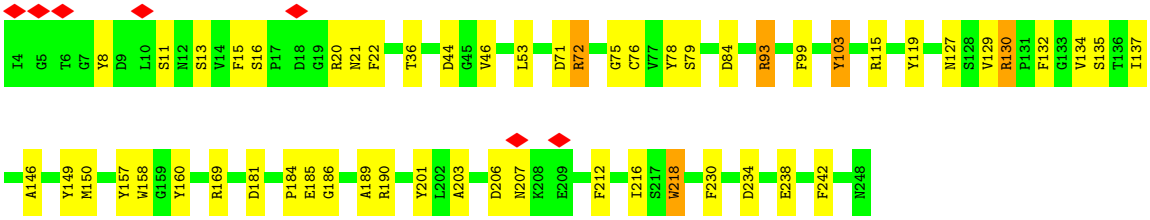
• Molecule 6: Proteasome subunit alpha type-6

Chain F:

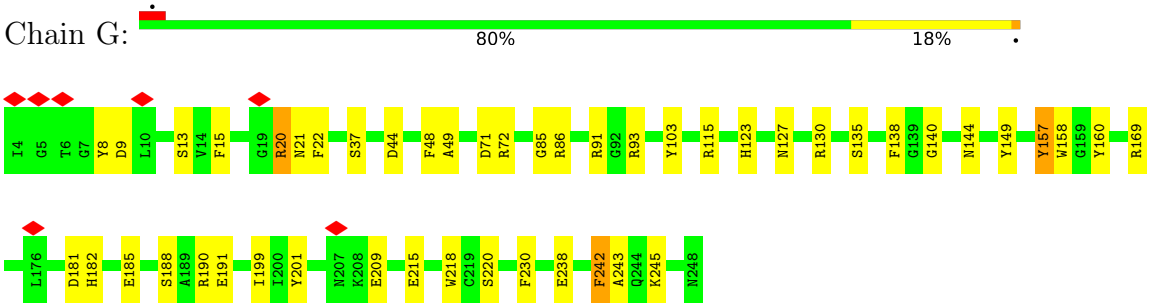


• Molecule 7: Probable proteasome subunit alpha type-7

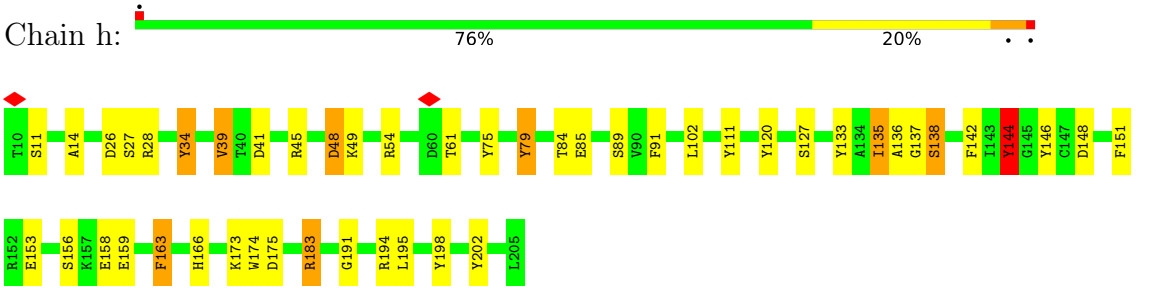
Chain g:



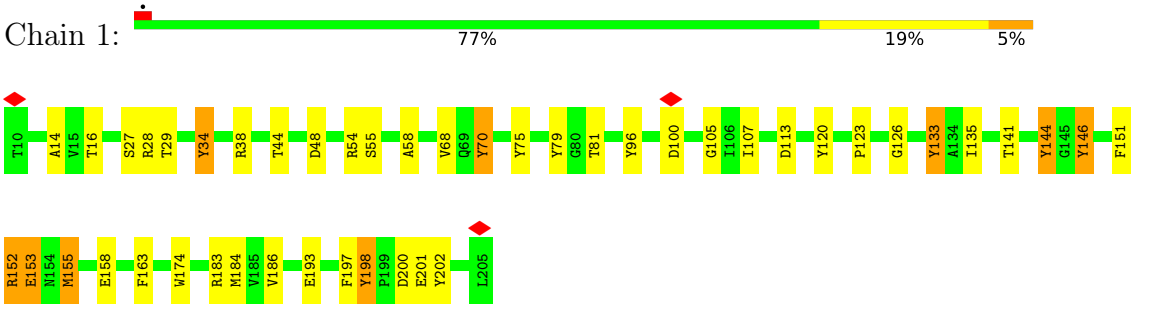
• Molecule 7: Probable proteasome subunit alpha type-7



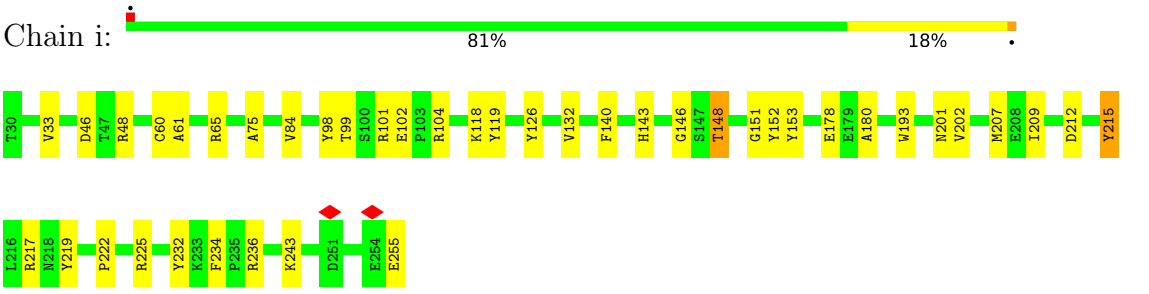
• Molecule 8: Proteasome subunit beta type-1



• Molecule 8: Proteasome subunit beta type-1

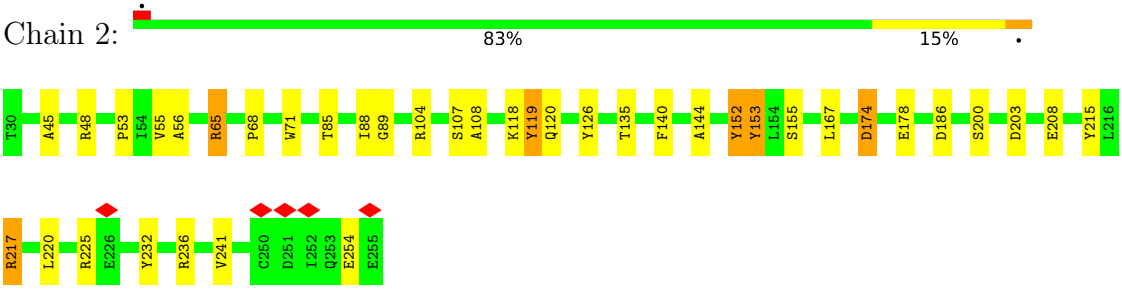


• Molecule 9: Proteasome subunit beta type-2



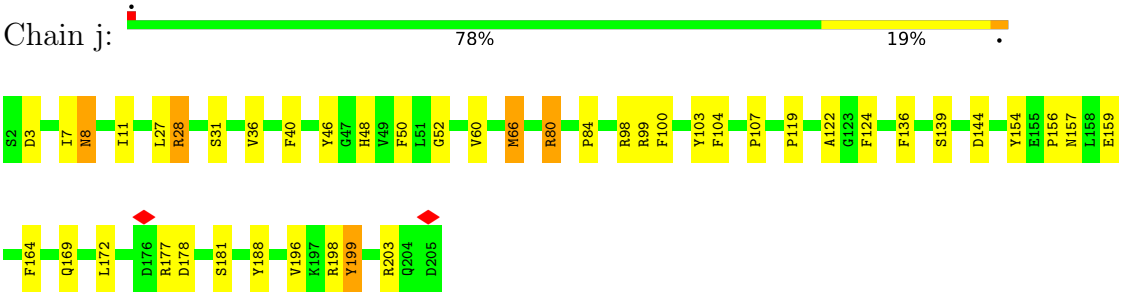
• Molecule 9: Proteasome subunit beta type-2

Chain 2:



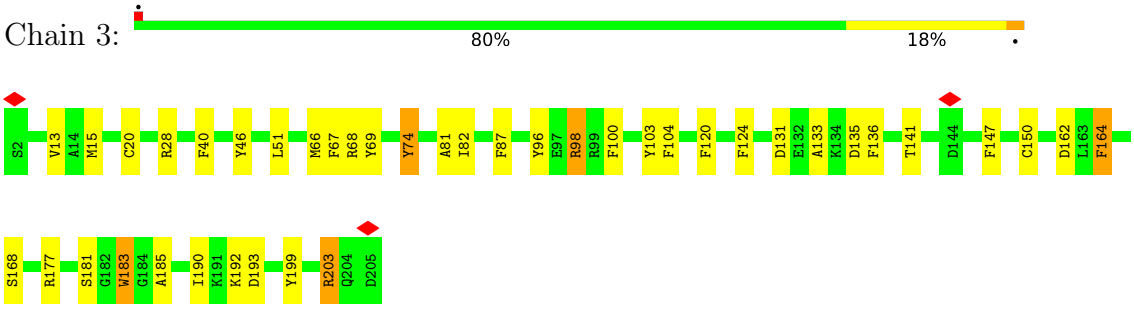
• Molecule 10: Proteasome subunit beta type-3

Chain j:



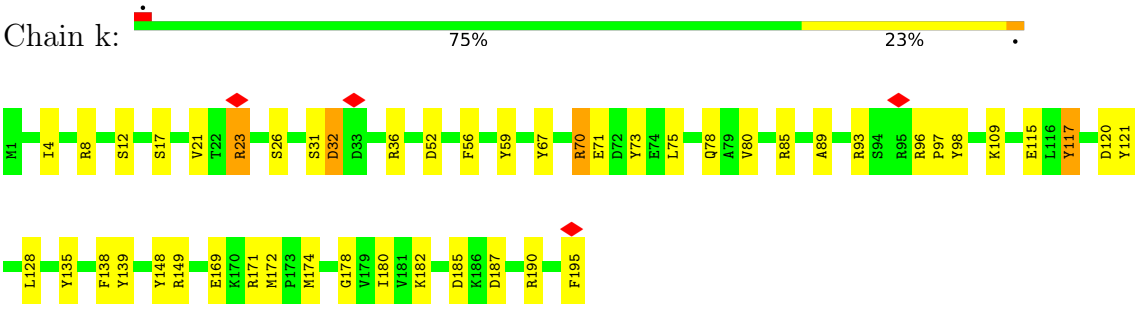
• Molecule 10: Proteasome subunit beta type-3

Chain 3:



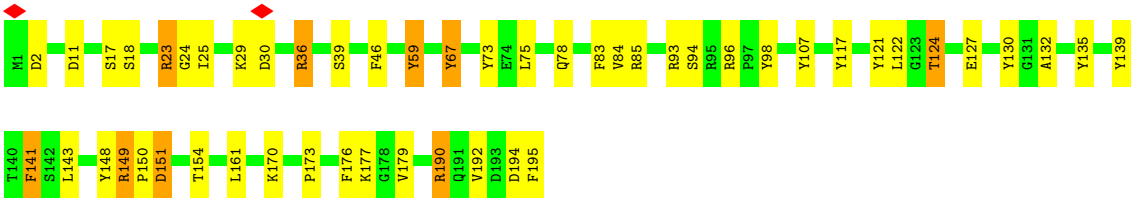
• Molecule 11: Proteasome subunit beta type-4

Chain k:

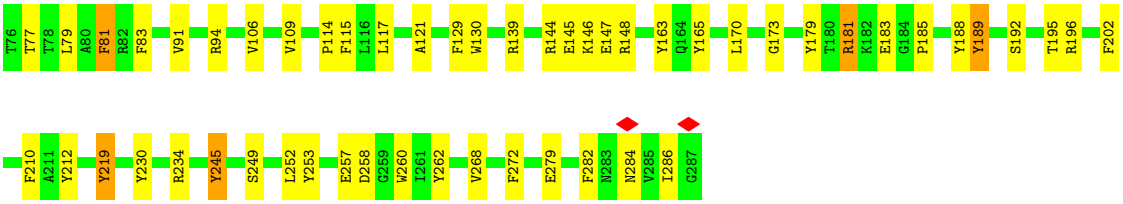


• Molecule 11: Proteasome subunit beta type-4

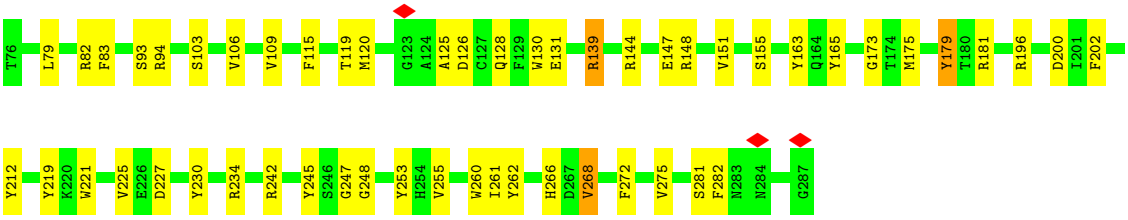
Chain 4:



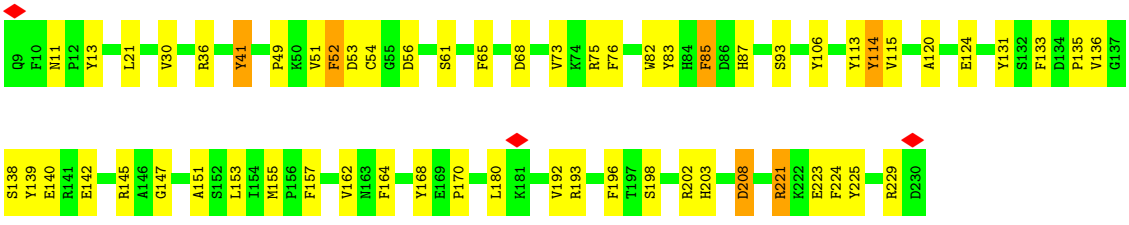
• Molecule 12: Proteasome subunit beta type-5



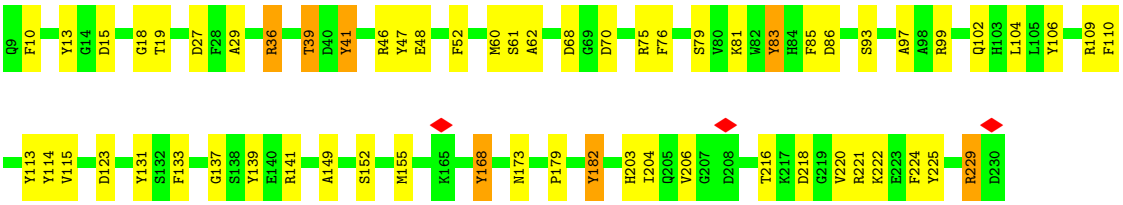
• Molecule 12: Proteasome subunit beta type-5



• Molecule 13: Proteasome subunit beta type-6

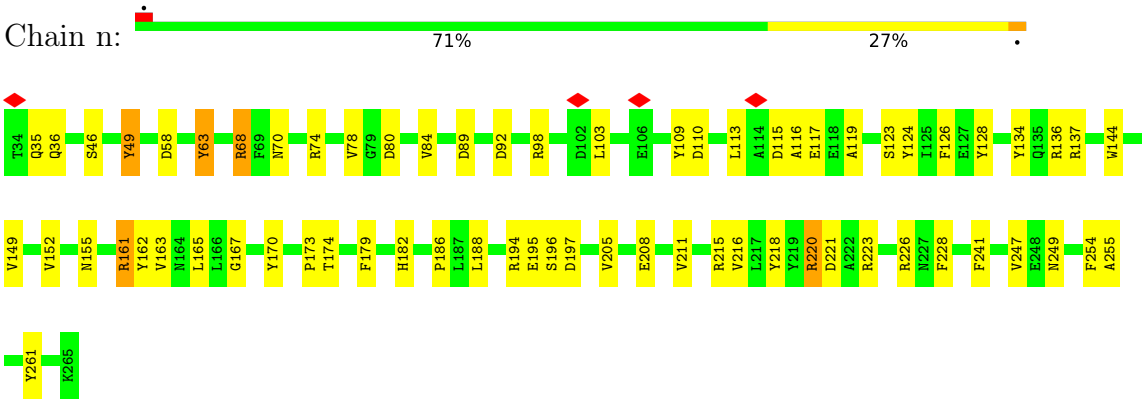


• Molecule 13: Proteasome subunit beta type-6



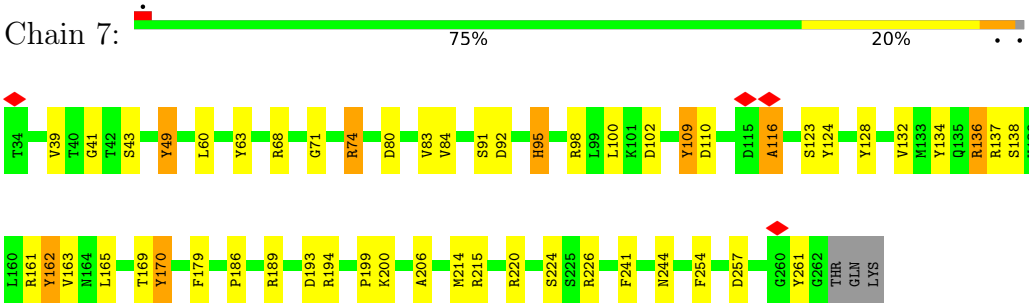
• Molecule 14: Proteasome subunit beta type-7

Chain n:



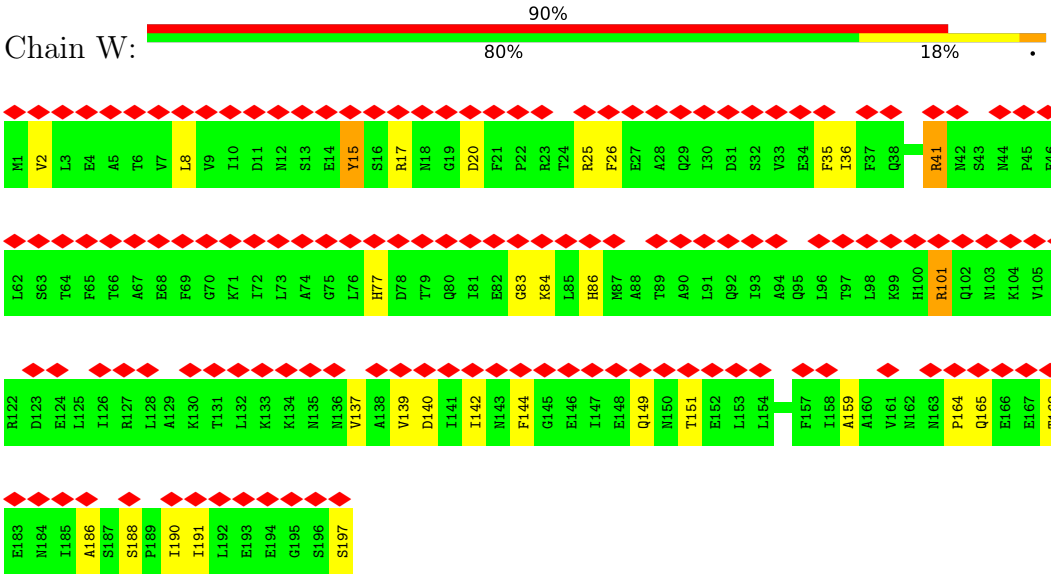
• Molecule 14: Proteasome subunit beta type-7

Chain 7:



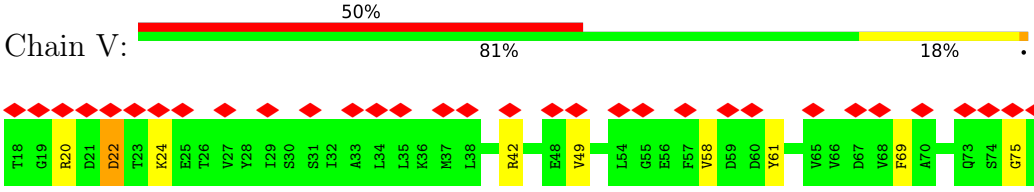
• Molecule 15: 26S proteasome regulatory subunit RPN10

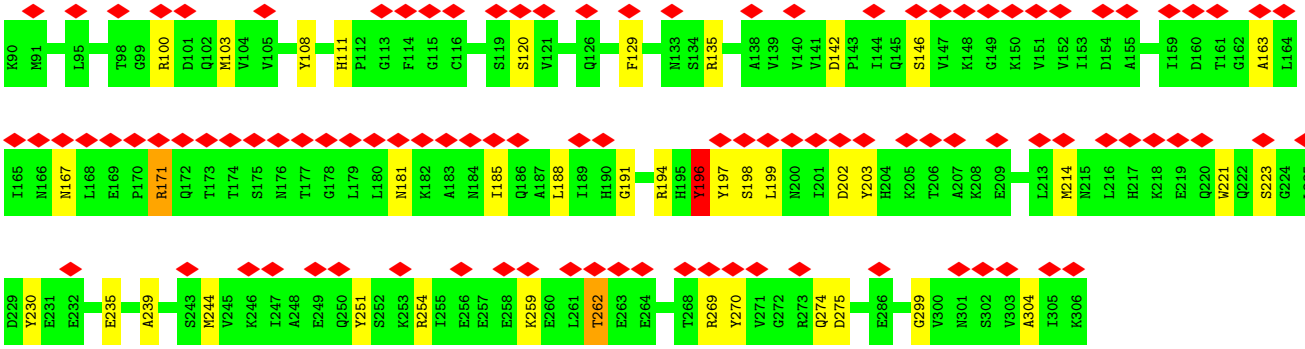
Chain W:



• Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

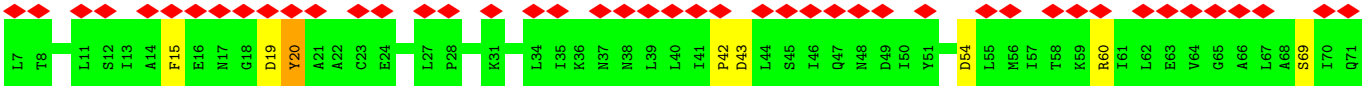
Chain V:

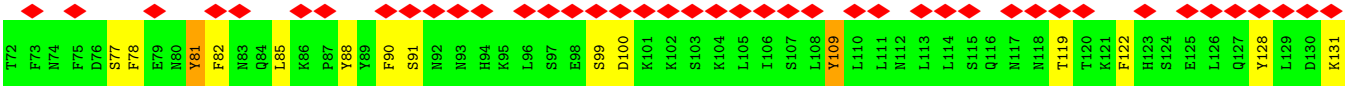


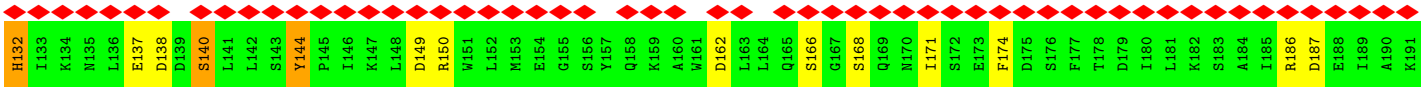


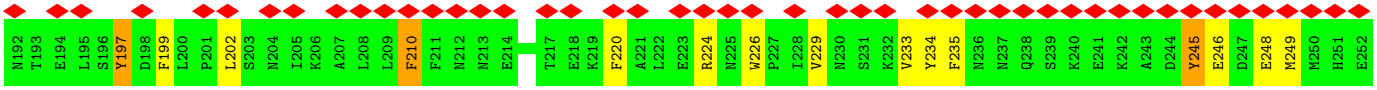
• Molecule 17: 26S proteasome regulatory subunit RPN12

Chain T:



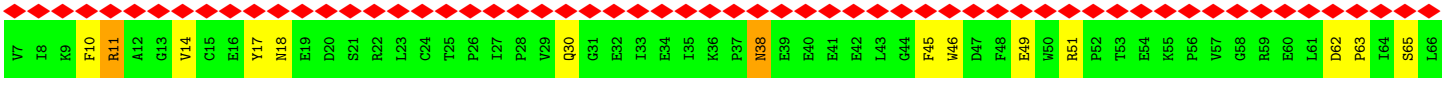


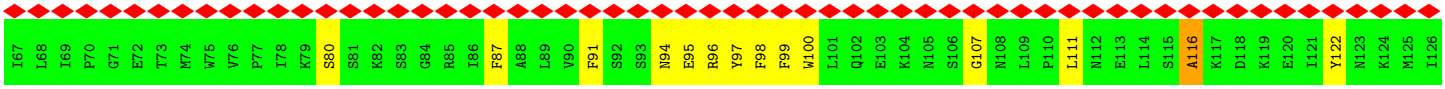


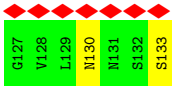


• Molecule 18: 26S proteasome regulatory subunit RPN13

Chain X:

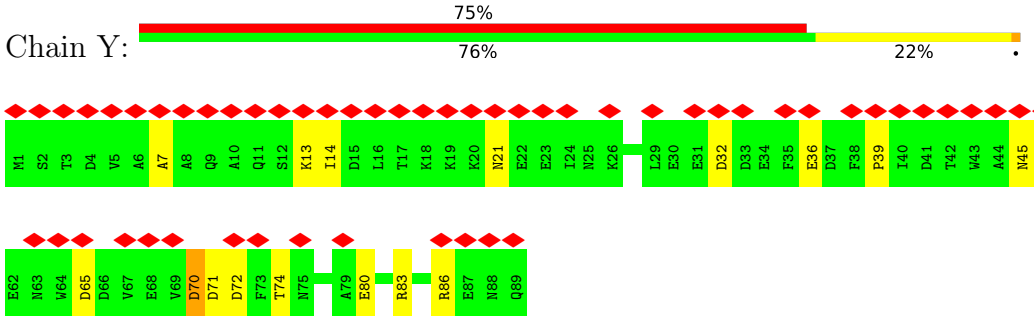






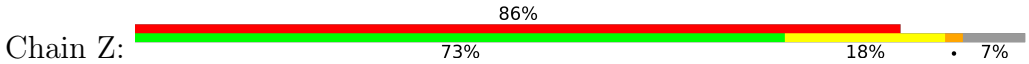
• Molecule 19: 26S proteasome complex subunit SEM1

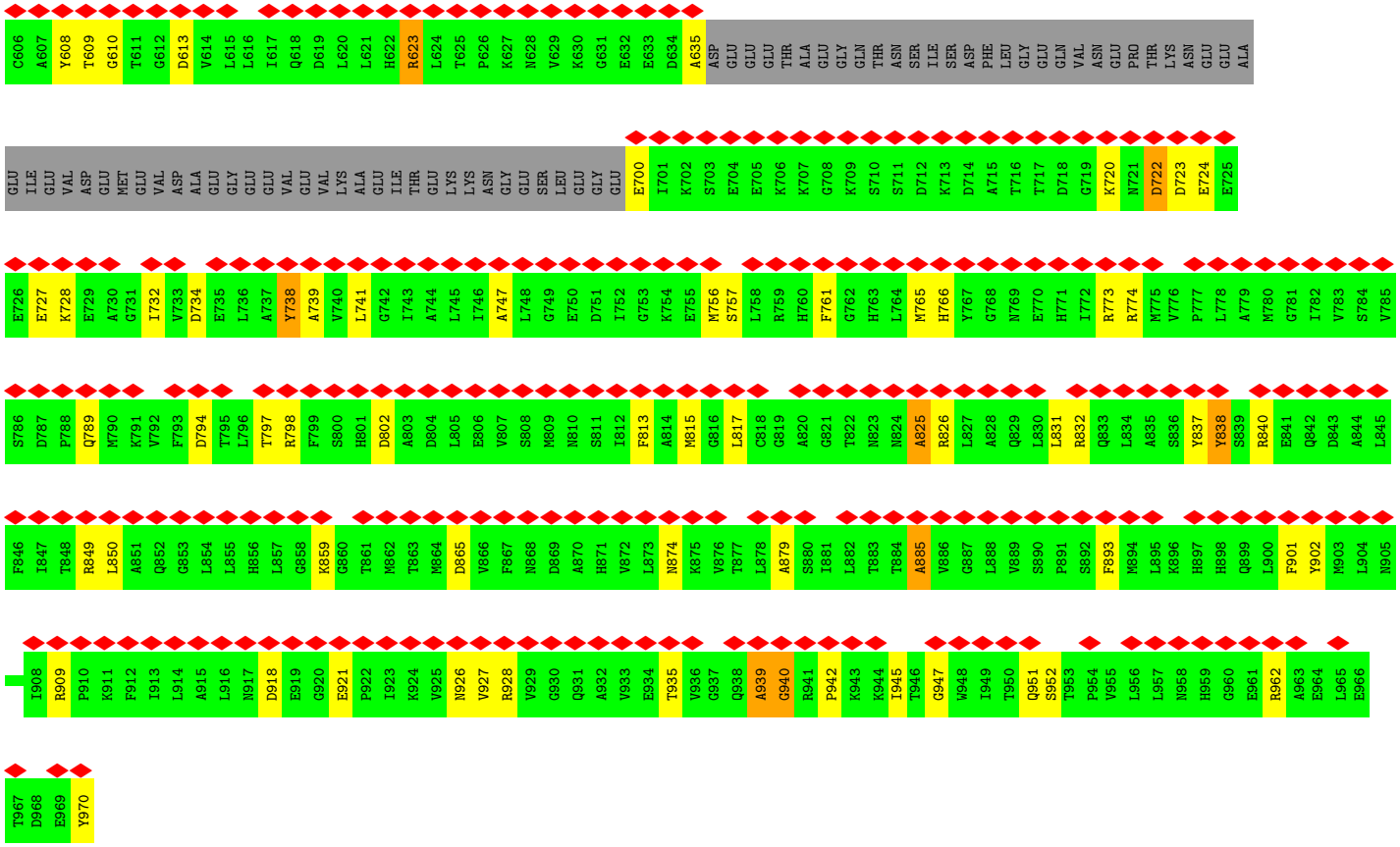
Chain Y:



• Molecule 20: 26S proteasome regulatory subunit RPN1

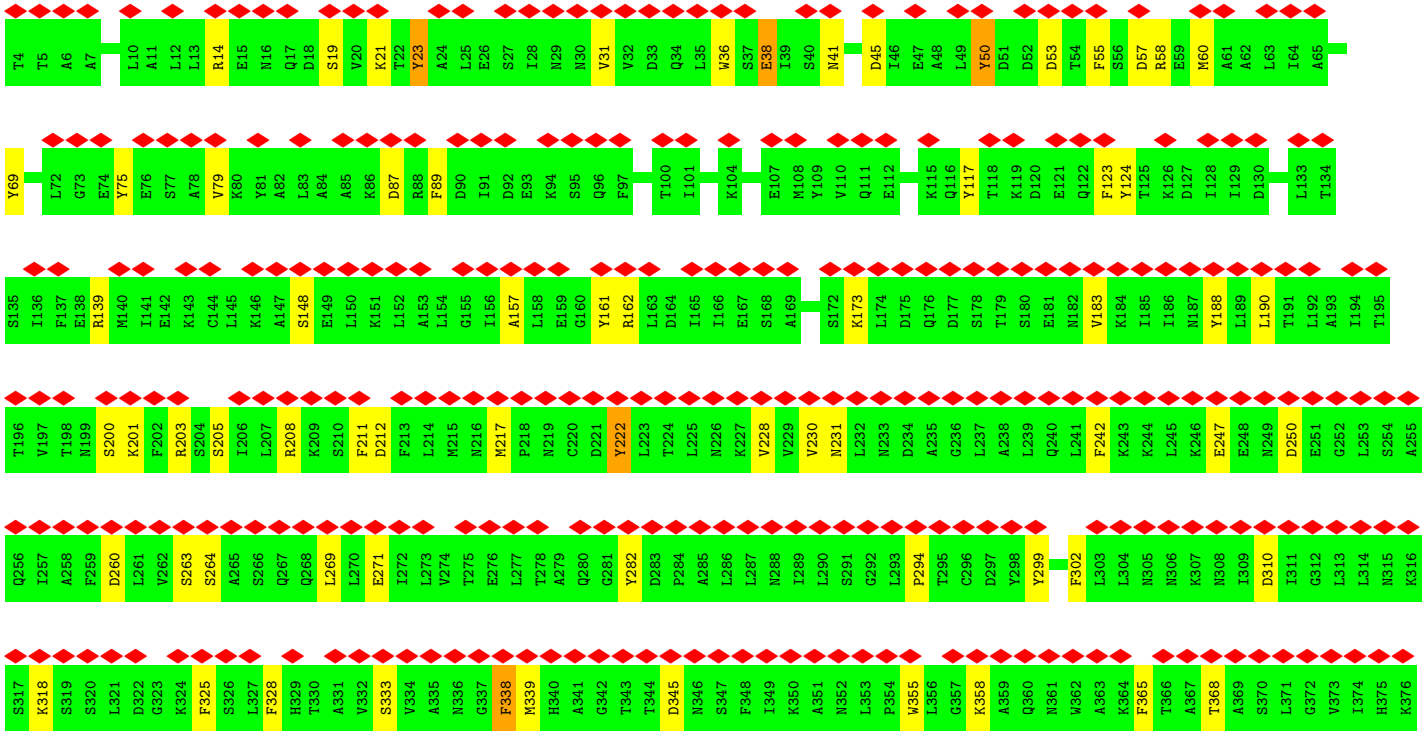
Chain Z:

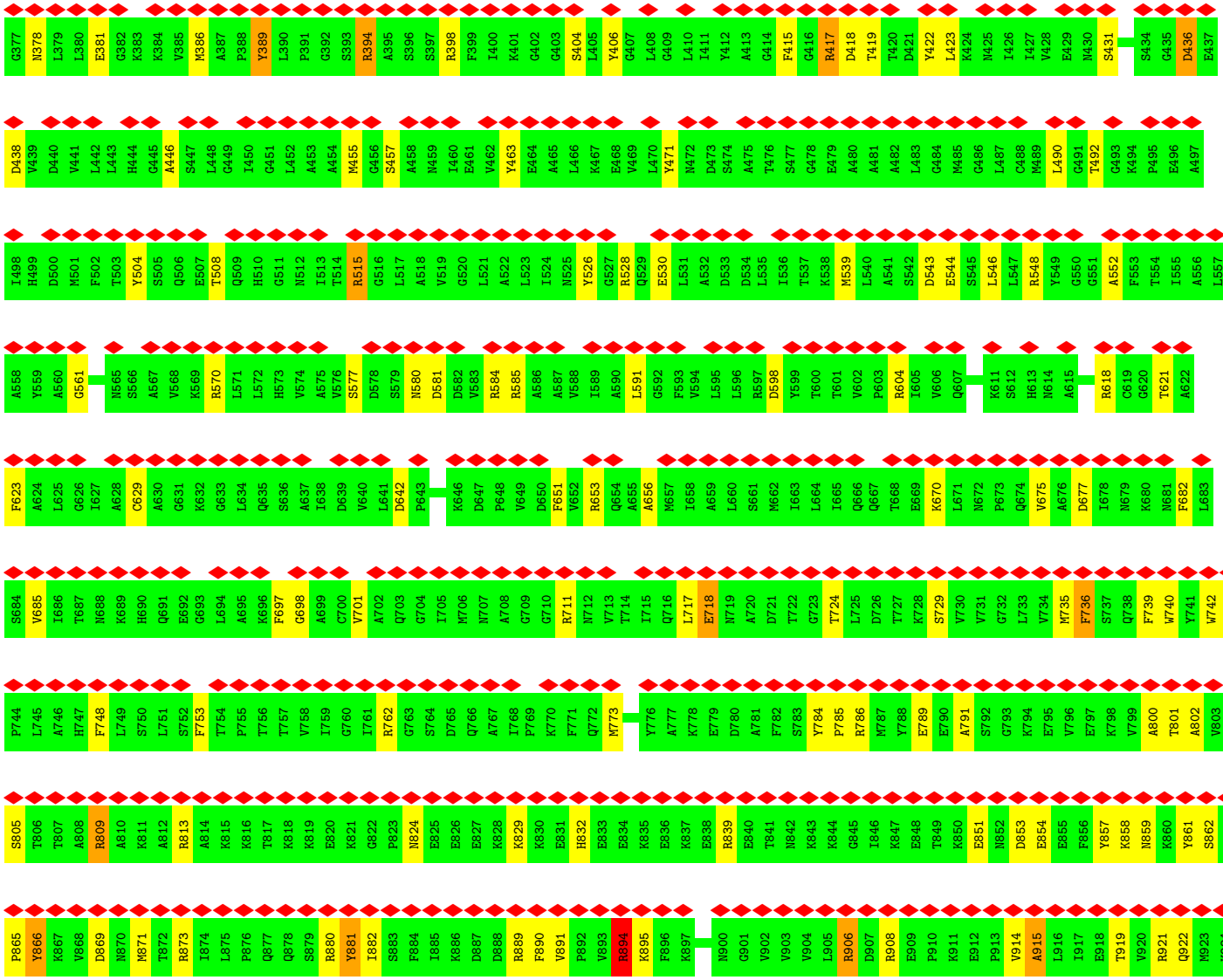




• Molecule 21: 26S proteasome regulatory subunit RPN2

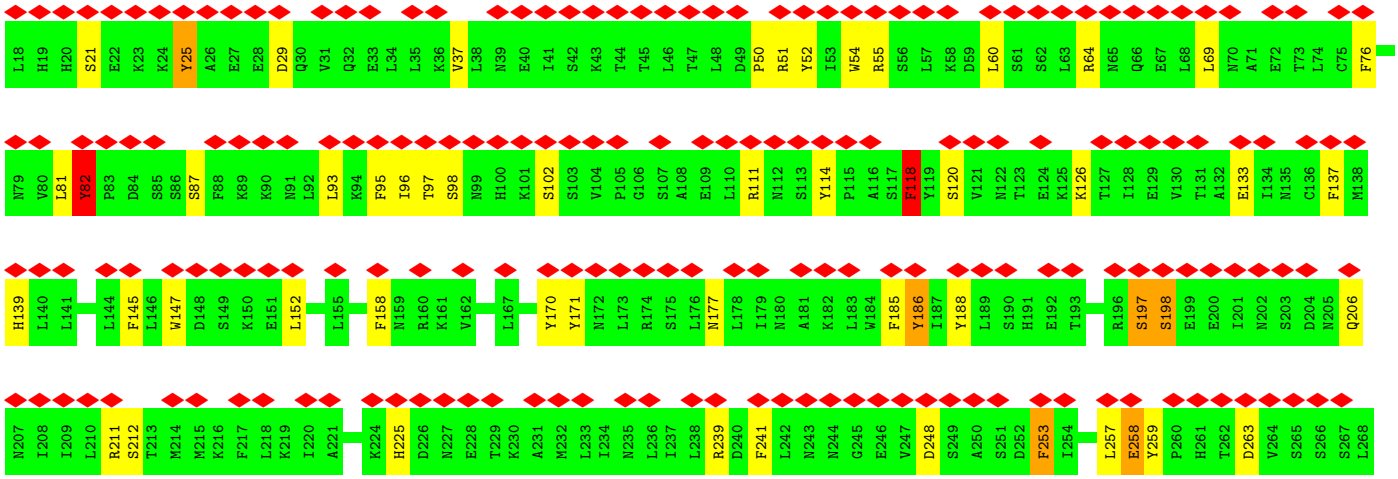
Chain N:

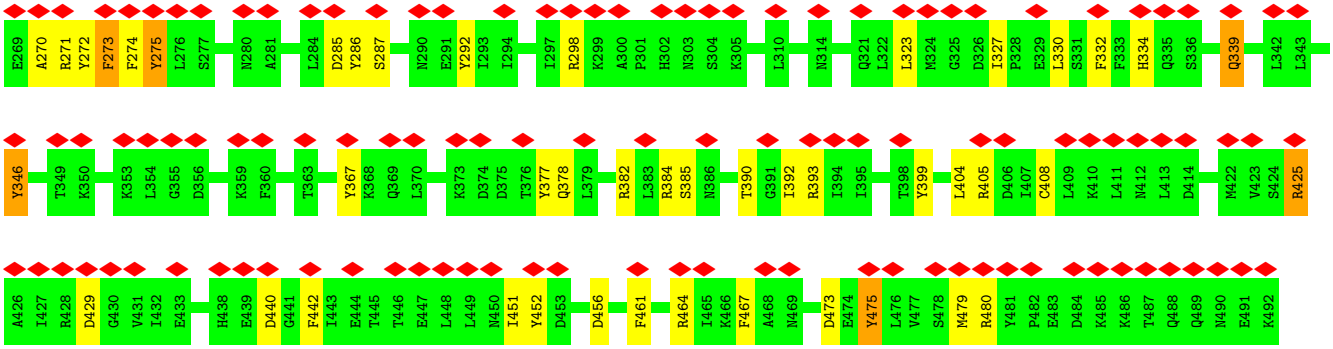




• Molecule 22: 26S proteasome regulatory subunit RPN3

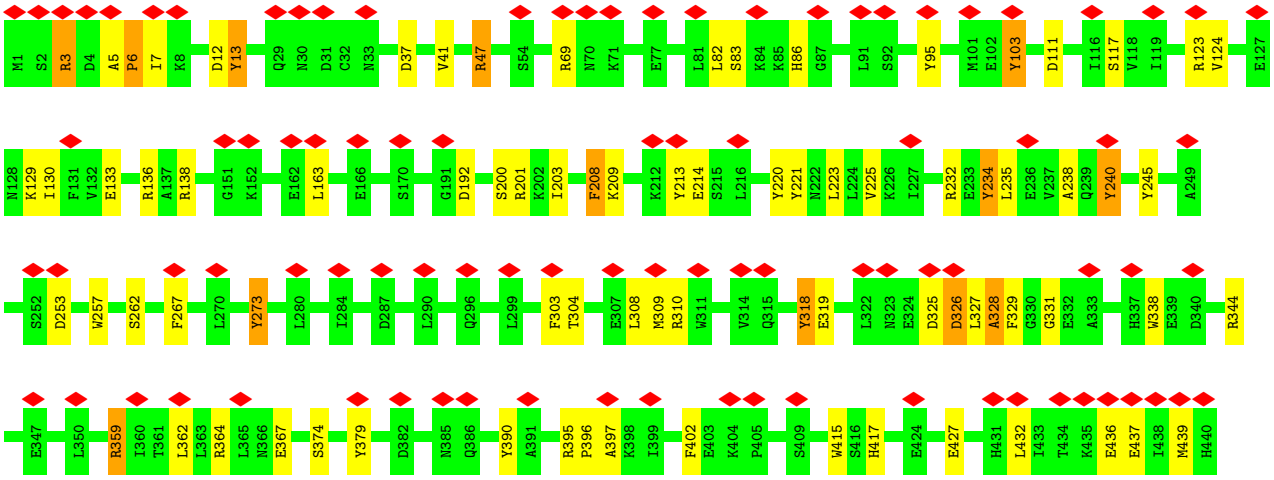
Chain S:





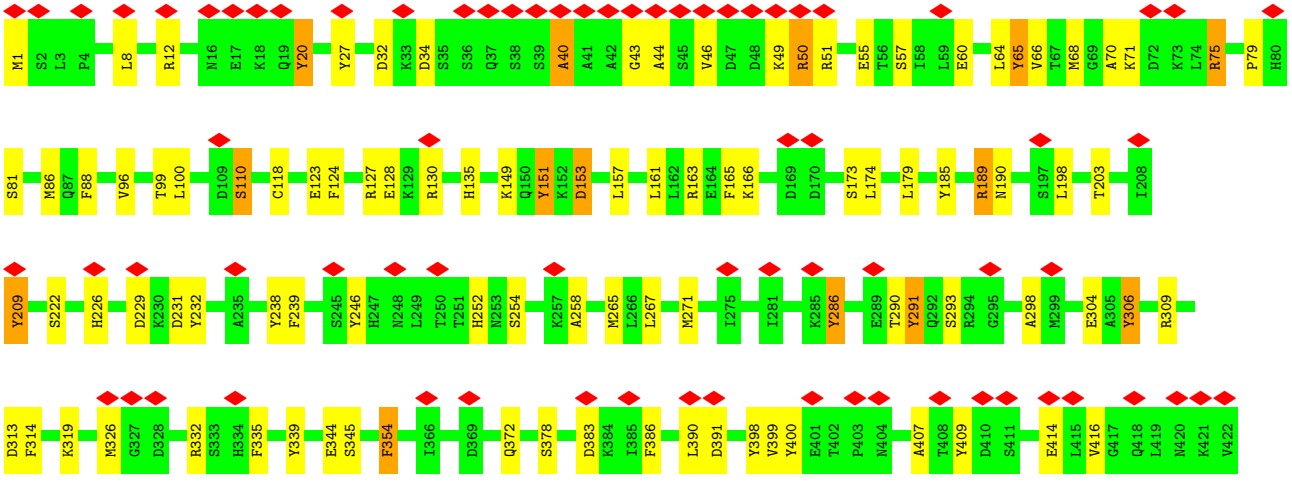
• Molecule 23: 26S proteasome regulatory subunit RPN5

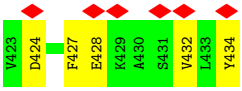
Chain P:



• Molecule 24: 26S proteasome regulatory subunit RPN6

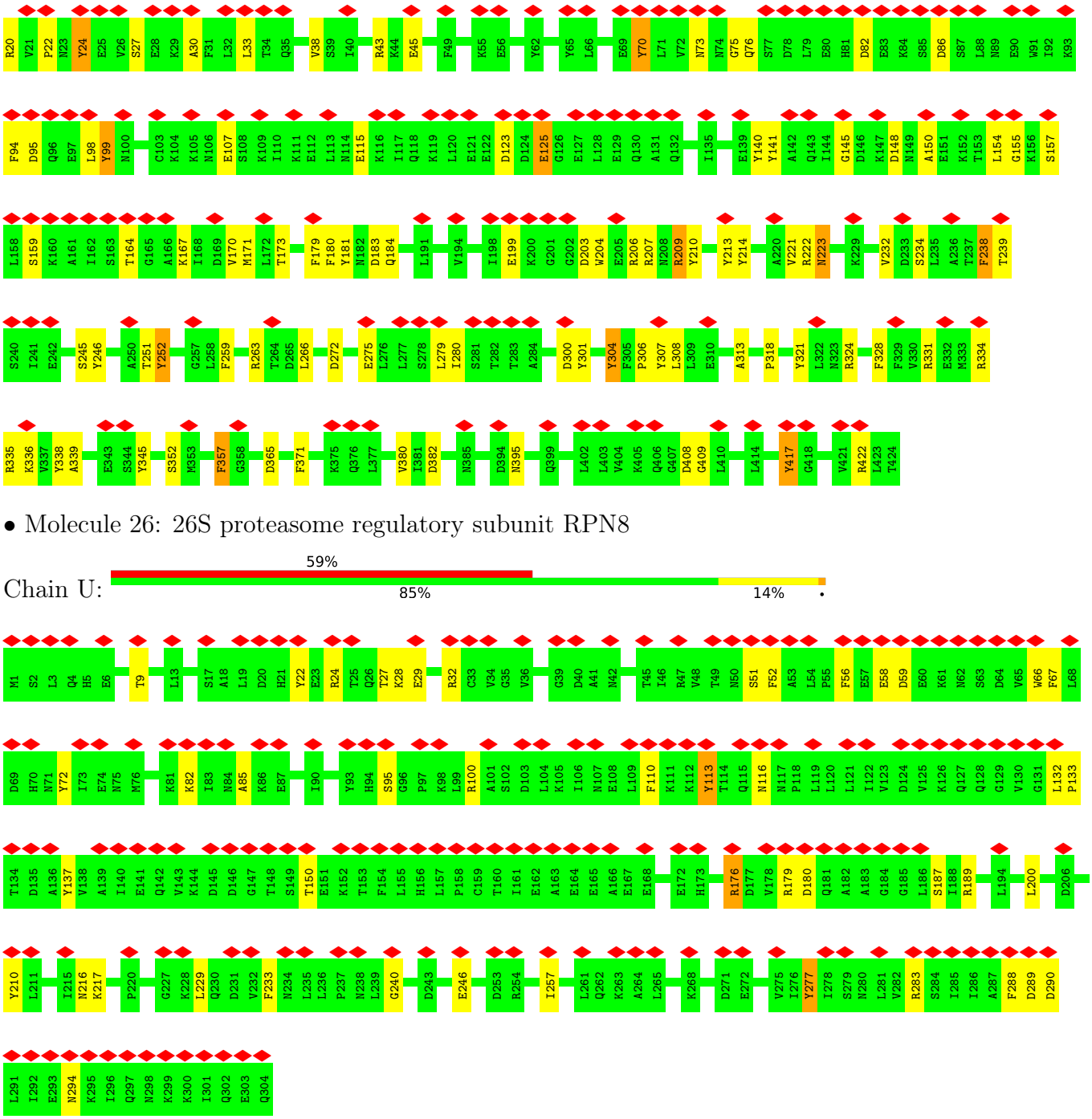
Chain Q:





• Molecule 25: 26S proteasome regulatory subunit RPN7

Chain R:

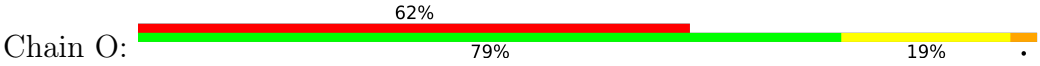


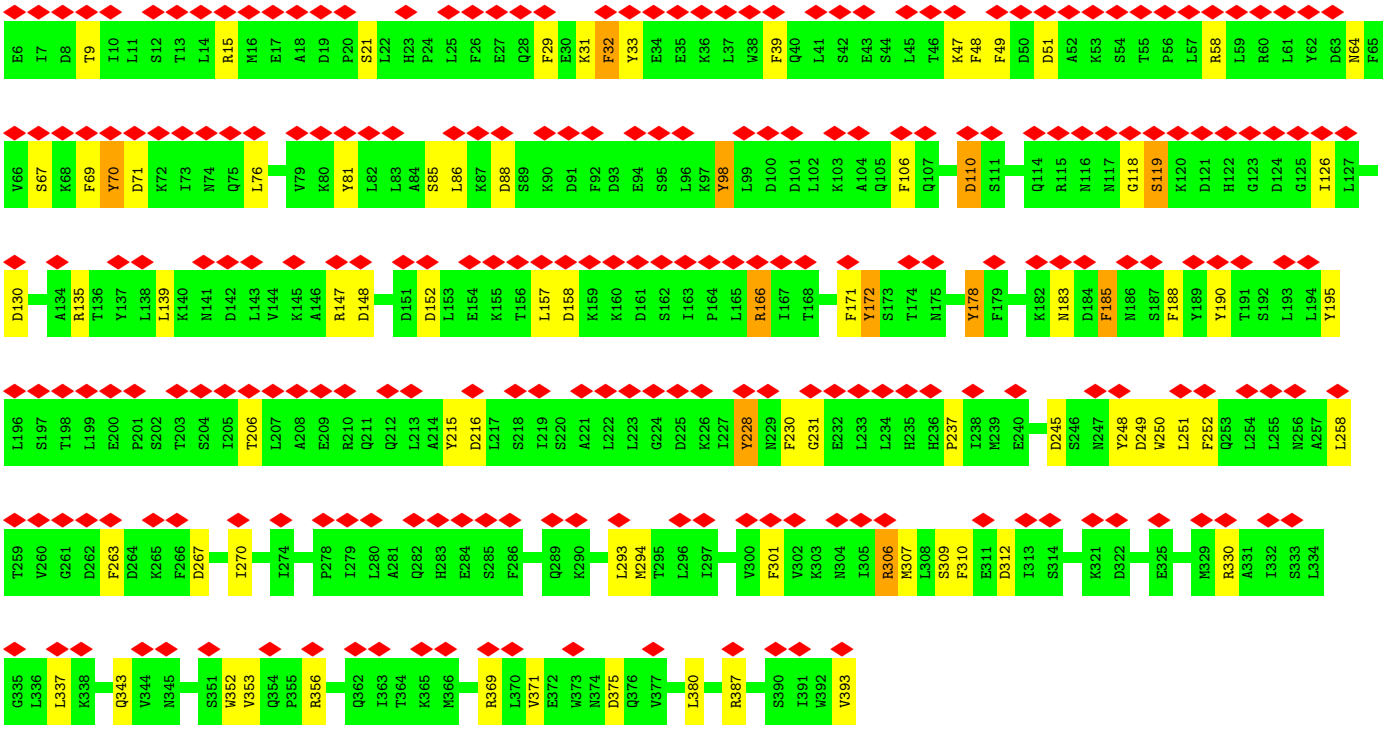
• Molecule 26: 26S proteasome regulatory subunit RPN8

Chain U:

• Molecule 27: 26S proteasome regulatory subunit RPN9

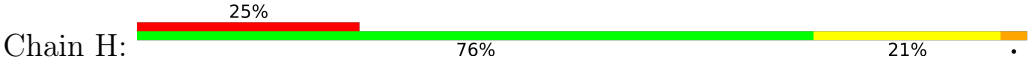
Chain O:

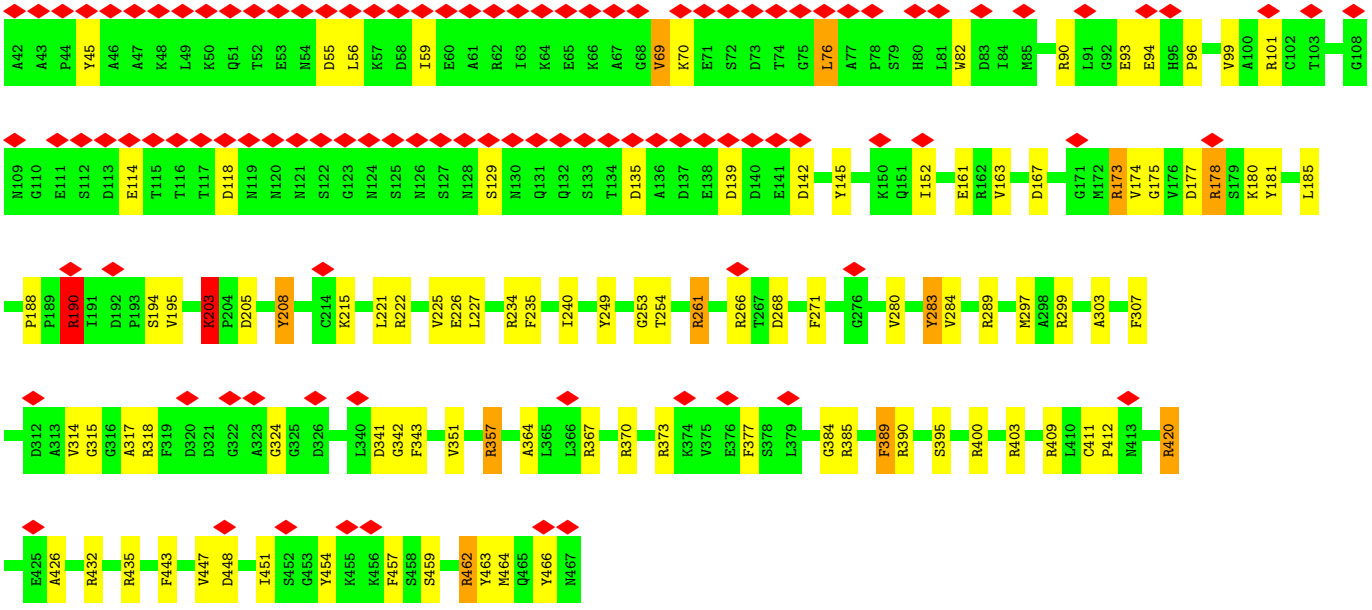




• Molecule 28: 26S proteasome regulatory subunit 7 homolog

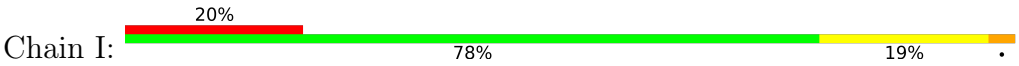
Chain H:

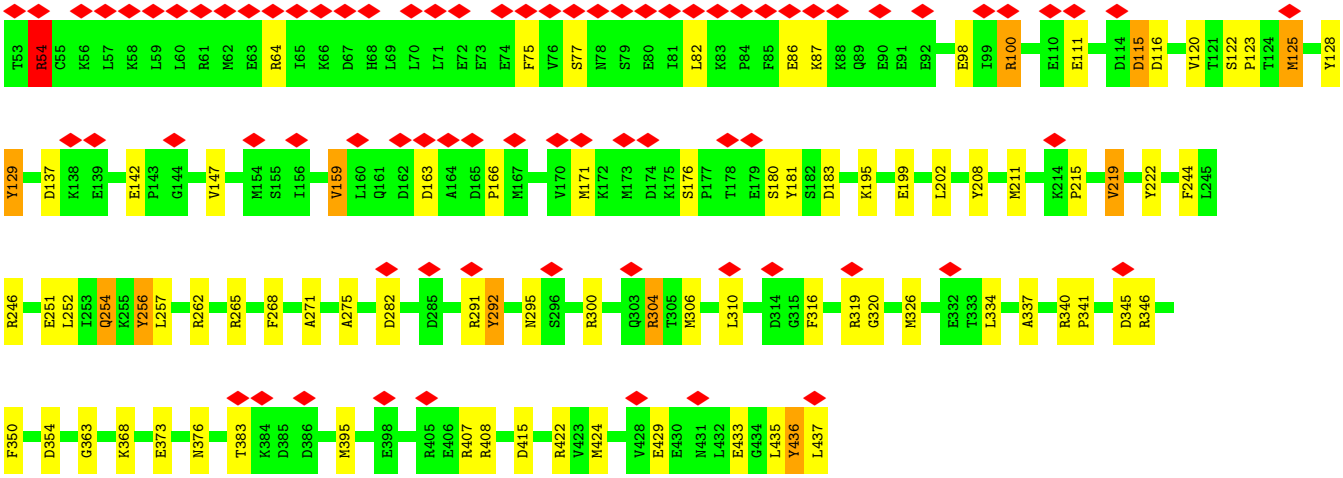




• Molecule 29: 26S proteasome regulatory subunit 4 homolog

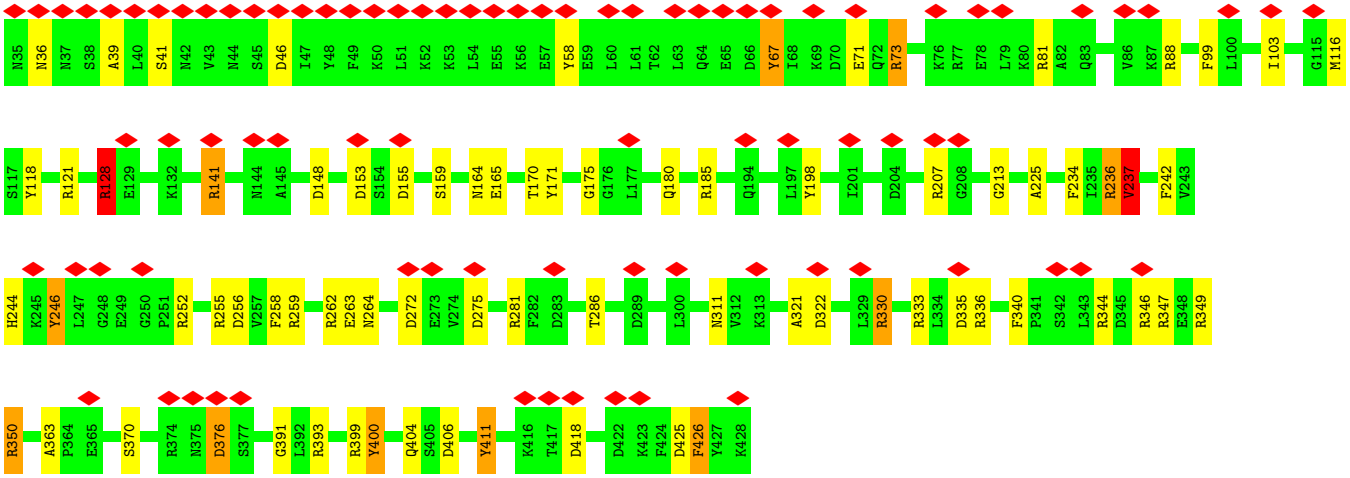
Chain I:





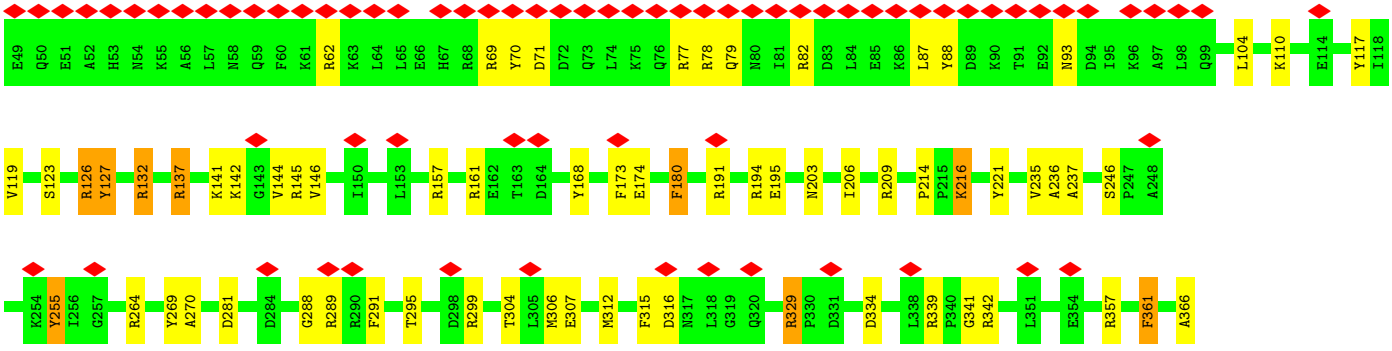
• Molecule 30: 26S proteasome regulatory subunit 6B homolog

Chain K:

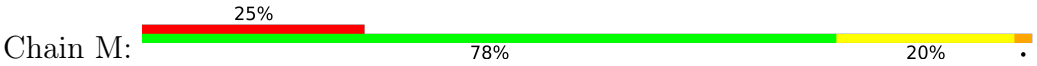


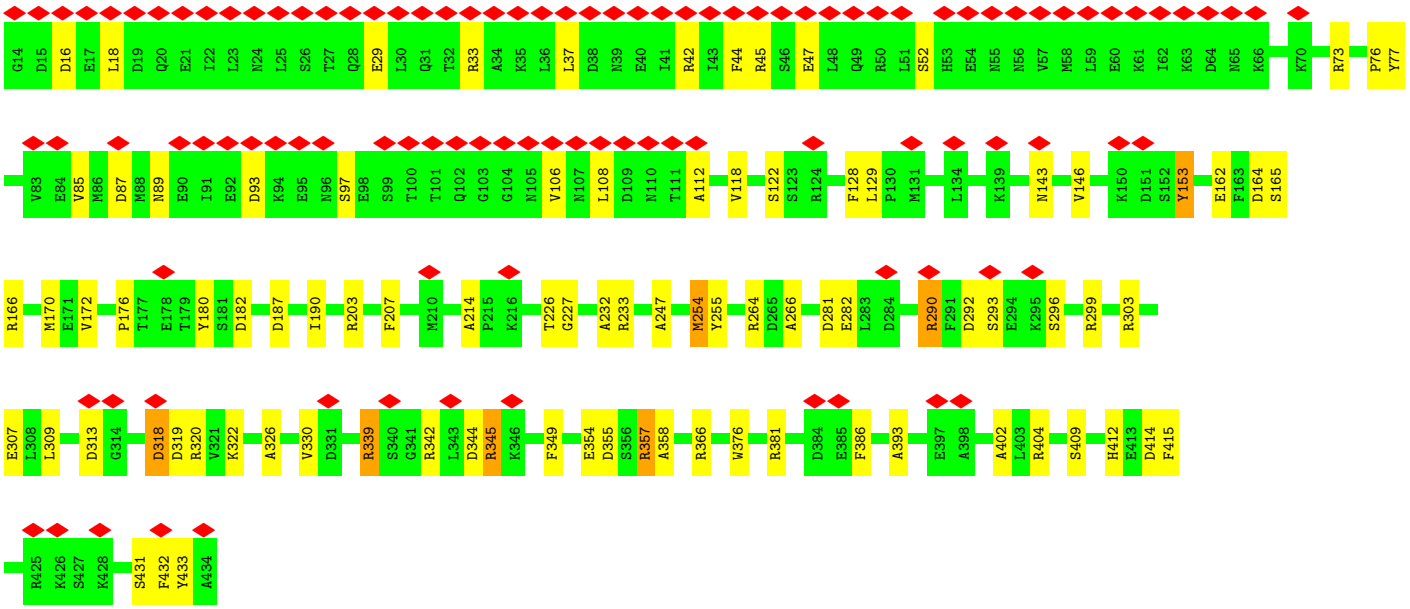
• Molecule 31: 26S proteasome subunit RPT4

Chain L:

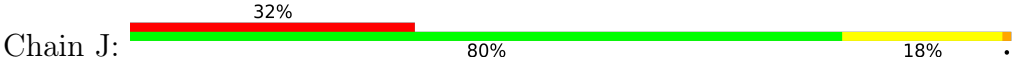


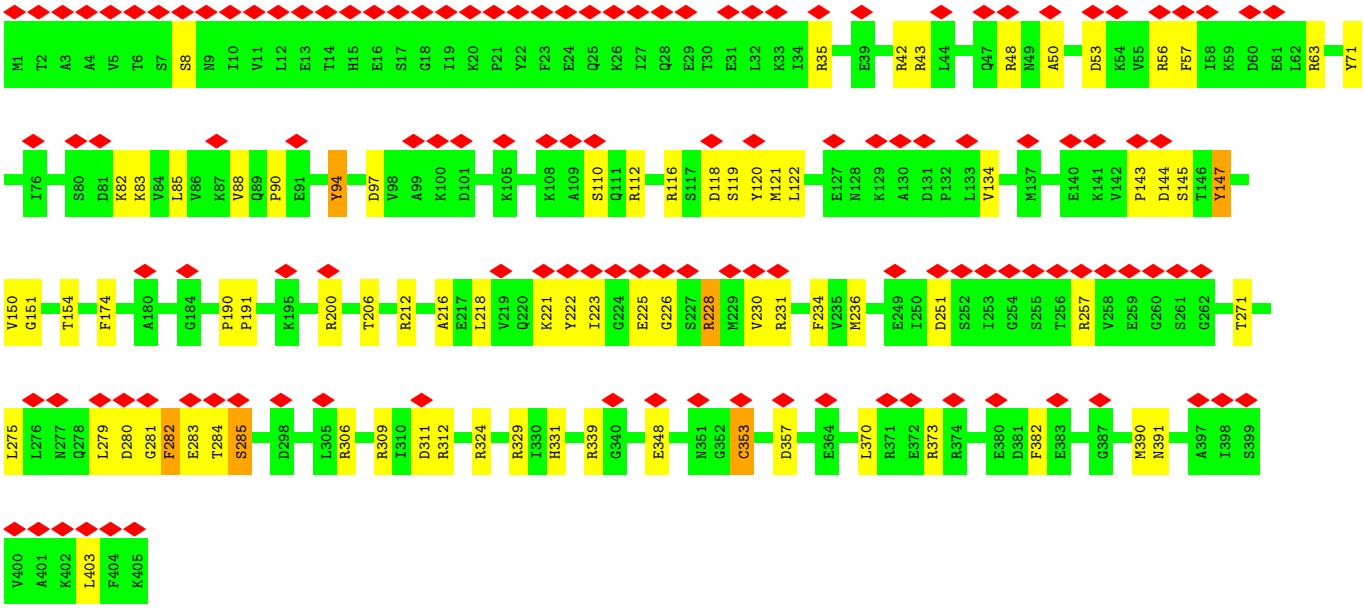
• Molecule 32: 26S proteasome regulatory subunit 6A





• Molecule 33: 26S proteasome regulatory subunit 8 homolog





4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	286500	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	45	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.211	Depositor
Minimum map value	-0.133	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.02	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.74	13/1946 (0.7%)	1.91	43/2634 (1.6%)
1	a	1.71	19/1946 (1.0%)	1.95	47/2634 (1.8%)
2	B	1.71	21/1944 (1.1%)	2.06	57/2632 (2.2%)
2	b	1.77	22/1944 (1.1%)	1.92	40/2632 (1.5%)
3	C	1.73	11/1935 (0.6%)	2.05	71/2618 (2.7%)
3	c	1.73	25/1935 (1.3%)	1.93	47/2618 (1.8%)
4	D	1.79	27/1888 (1.4%)	2.06	55/2557 (2.2%)
4	d	1.73	21/2012 (1.0%)	1.98	48/2718 (1.8%)
5	E	1.67	9/1909 (0.5%)	1.93	43/2571 (1.7%)
5	e	1.71	15/1909 (0.8%)	1.99	46/2571 (1.8%)
6	F	1.74	20/1800 (1.1%)	1.94	42/2433 (1.7%)
6	f	1.71	9/1800 (0.5%)	2.03	43/2433 (1.8%)
7	G	1.71	18/1945 (0.9%)	1.89	38/2625 (1.4%)
7	g	1.75	21/1945 (1.1%)	1.89	41/2625 (1.6%)
8	1	1.75	18/1541 (1.2%)	1.88	39/2087 (1.9%)
8	h	1.73	16/1541 (1.0%)	2.04	39/2087 (1.9%)
9	2	1.71	17/1751 (1.0%)	1.88	37/2373 (1.6%)
9	i	1.78	17/1751 (1.0%)	1.91	36/2373 (1.5%)
10	3	1.73	7/1611 (0.4%)	1.90	36/2174 (1.7%)
10	j	1.75	15/1611 (0.9%)	1.82	33/2174 (1.5%)
11	4	1.77	19/1590 (1.2%)	2.00	49/2142 (2.3%)
11	k	1.72	10/1590 (0.6%)	1.97	43/2142 (2.0%)
12	5	1.72	13/1681 (0.8%)	2.02	53/2274 (2.3%)
12	l	1.79	18/1681 (1.1%)	1.94	46/2274 (2.0%)
13	6	1.78	21/1795 (1.2%)	2.05	55/2420 (2.3%)
13	m	1.75	22/1795 (1.2%)	1.99	52/2420 (2.1%)
14	7	1.78	18/1821 (1.0%)	2.02	53/2470 (2.1%)
14	n	1.80	26/1847 (1.4%)	1.99	49/2503 (2.0%)
15	W	1.67	8/1558 (0.5%)	1.86	36/2111 (1.7%)
16	V	1.73	17/2309 (0.7%)	1.94	48/3115 (1.5%)
17	T	1.68	18/2236 (0.8%)	1.96	49/3017 (1.6%)
18	X	1.76	8/1059 (0.8%)	1.91	18/1432 (1.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	Y	1.65	4/741 (0.5%)	1.92	16/1000 (1.6%)
20	Z	1.68	66/7123 (0.9%)	1.91	150/9645 (1.6%)
21	N	1.69	56/7273 (0.8%)	1.90	164/9822 (1.7%)
22	S	1.73	31/3967 (0.8%)	1.92	88/5355 (1.6%)
23	P	1.68	29/3664 (0.8%)	1.87	72/4940 (1.5%)
24	Q	1.71	31/3556 (0.9%)	1.99	94/4787 (2.0%)
25	R	1.72	31/3314 (0.9%)	1.98	85/4469 (1.9%)
26	U	1.62	13/2461 (0.5%)	1.78	32/3327 (1.0%)
27	O	1.69	20/3247 (0.6%)	1.95	71/4380 (1.6%)
28	H	1.73	29/3363 (0.9%)	1.97	86/4532 (1.9%)
29	I	1.70	26/3061 (0.8%)	1.97	82/4121 (2.0%)
30	K	1.74	36/3156 (1.1%)	1.93	61/4261 (1.4%)
31	L	1.74	31/3129 (1.0%)	1.99	70/4204 (1.7%)
32	M	1.72	31/3323 (0.9%)	1.89	69/4478 (1.5%)
33	J	1.70	25/3212 (0.8%)	1.90	62/4316 (1.4%)
All	All	1.72	998/112216 (0.9%)	1.94	2634/151526 (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	7
1	a	0	8
2	B	0	4
2	b	0	3
3	C	0	10
3	c	0	8
4	D	0	10
4	d	0	10
5	E	0	7
5	e	0	1
6	F	0	14
6	f	0	7
7	G	0	7
7	g	0	8
8	1	0	8
8	h	0	6
9	2	0	5
9	i	0	2
10	3	0	7

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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	9
13	m	0	6
14	7	0	9
14	n	0	5
15	W	0	4
16	V	0	2
17	T	0	8
18	X	0	3
20	Z	0	15
21	N	0	16
22	S	0	13
23	P	0	8
24	Q	0	12
25	R	0	10
26	U	0	6
27	O	0	9
28	H	0	14
29	I	0	8
30	K	0	15
31	L	0	7
32	M	0	5
33	J	0	4
All	All	0	347

All (998) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	349	ARG	CD-NE	9.92	1.63	1.46
21	N	457	SER	CA-CB	9.49	1.67	1.52
18	X	100	TRP	NE1-CE2	9.34	1.49	1.37
14	7	161	ARG	CD-NE	8.97	1.61	1.46
29	I	128	TYR	CG-CD1	8.88	1.50	1.39
19	Y	36	GLU	CG-CD	8.85	1.65	1.51
32	M	299	ARG	NE-CZ	8.76	1.44	1.33
33	J	312	ARG	NE-CZ	8.72	1.44	1.33
1	A	163	TYR	CE2-CZ	8.61	1.49	1.38
27	O	48	PHE	CG-CD2	8.59	1.51	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	304	TYR	CE1-CZ	8.54	1.49	1.38
26	U	176	ARG	CZ-NH2	8.52	1.44	1.33
25	R	43	ARG	CZ-NH2	8.43	1.44	1.33
12	l	144	ARG	CD-NE	8.33	1.60	1.46
21	N	851	GLU	CB-CG	8.31	1.68	1.52
23	P	437	GLU	CG-CD	8.30	1.64	1.51
2	b	8	SER	CA-CB	8.24	1.65	1.52
21	N	355	TRP	NE1-CE2	8.16	1.48	1.37
10	3	46	TYR	CG-CD1	8.14	1.49	1.39
20	Z	165	TYR	CB-CG	-8.06	1.39	1.51
11	k	12	SER	CA-CB	8.03	1.65	1.52
32	M	264	ARG	NE-CZ	8.00	1.43	1.33
33	J	285	SER	CA-CB	8.00	1.65	1.52
26	U	187	SER	CA-CB	7.98	1.65	1.52
11	k	148	TYR	CG-CD1	7.98	1.49	1.39
12	l	212	TYR	CZ-OH	7.90	1.51	1.37
32	M	404	ARG	NE-CZ	7.88	1.43	1.33
6	f	18	ARG	CZ-NH1	7.87	1.43	1.33
16	V	171	ARG	CD-NE	7.78	1.59	1.46
16	V	203	TYR	CE2-CZ	7.78	1.48	1.38
9	i	236	ARG	CD-NE	7.76	1.59	1.46
2	B	178	ARG	NE-CZ	7.74	1.43	1.33
27	O	85	SER	CA-CB	7.73	1.64	1.52
6	f	24	TYR	CE1-CZ	7.71	1.48	1.38
30	K	349	ARG	CZ-NH2	7.68	1.43	1.33
28	H	173	ARG	NE-CZ	7.67	1.43	1.33
20	Z	134	SER	CA-CB	7.65	1.64	1.52
1	A	14	ARG	CZ-NH1	7.62	1.43	1.33
9	2	48	ARG	CD-NE	7.59	1.59	1.46
5	e	86	ARG	NE-CZ	7.58	1.43	1.33
13	6	131	TYR	CE2-CZ	7.57	1.48	1.38
14	n	74	ARG	NE-CZ	7.57	1.42	1.33
31	L	264	ARG	NE-CZ	7.56	1.42	1.33
25	R	155	GLY	CA-C	-7.51	1.39	1.51
14	n	63	TYR	CG-CD1	7.50	1.49	1.39
33	J	312	ARG	CZ-NH2	7.50	1.42	1.33
10	3	28	ARG	CD-NE	7.50	1.59	1.46
13	6	149	ALA	N-CA	-7.49	1.31	1.46
25	R	324	ARG	CD-NE	7.49	1.59	1.46
2	B	179	TRP	CD2-CE3	-7.49	1.29	1.40
12	5	225	VAL	CB-CG2	7.48	1.68	1.52
20	Z	58	GLU	CD-OE2	7.47	1.33	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	D	181	ARG	CD-NE	7.47	1.59	1.46
9	2	89	GLY	N-CA	7.47	1.57	1.46
1	a	244	ARG	CD-NE	7.46	1.59	1.46
22	S	480	ARG	NE-CZ	7.44	1.42	1.33
6	F	6	TYR	CB-CG	-7.42	1.40	1.51
21	N	205	SER	CA-CB	7.42	1.64	1.52
30	K	330	ARG	NE-CZ	7.42	1.42	1.33
2	b	157	PHE	CB-CG	-7.41	1.38	1.51
32	M	355	ASP	N-CA	-7.39	1.31	1.46
30	K	399	ARG	CZ-NH2	7.37	1.42	1.33
22	S	475	TYR	CA-CB	7.34	1.70	1.53
14	n	49	TYR	CG-CD1	7.34	1.48	1.39
7	G	85	GLY	N-CA	-7.34	1.35	1.46
8	1	201	GLU	CB-CG	7.32	1.66	1.52
10	j	103	TYR	CG-CD2	7.24	1.48	1.39
12	5	234	ARG	NE-CZ	7.24	1.42	1.33
20	Z	826	ARG	CZ-NH2	7.23	1.42	1.33
29	I	54	ARG	NE-CZ	7.22	1.42	1.33
14	n	208	GLU	CD-OE2	7.21	1.33	1.25
25	R	24	TYR	CB-CG	7.20	1.62	1.51
33	J	119	SER	CA-CB	7.19	1.63	1.52
11	4	127	GLU	CG-CD	7.19	1.62	1.51
21	N	577	SER	CA-CB	7.17	1.63	1.52
20	Z	370	SER	CA-CB	7.16	1.63	1.52
15	W	60	ARG	NE-CZ	7.14	1.42	1.33
1	A	143	PHE	CG-CD1	7.14	1.49	1.38
3	c	129	ARG	CZ-NH2	7.13	1.42	1.33
2	B	234	ARG	NE-CZ	7.11	1.42	1.33
31	L	400	PHE	CG-CD2	7.06	1.49	1.38
10	3	168	SER	CB-OG	7.06	1.51	1.42
14	7	136	ARG	CZ-NH1	7.05	1.42	1.33
14	7	49	TYR	CG-CD2	7.05	1.48	1.39
21	N	786	ARG	NE-CZ	7.04	1.42	1.33
20	Z	441	TYR	CG-CD2	7.04	1.48	1.39
28	H	249	TYR	CZ-OH	7.04	1.49	1.37
29	I	300	ARG	CD-NE	7.04	1.58	1.46
13	m	36	ARG	NE-CZ	7.03	1.42	1.33
7	G	149	TYR	CB-CG	-7.02	1.41	1.51
3	c	50	ARG	CZ-NH2	6.99	1.42	1.33
22	S	25	TYR	CE2-CZ	6.99	1.47	1.38
5	E	26	TYR	CG-CD2	6.99	1.48	1.39
8	1	27	SER	CA-CB	6.97	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	102	GLU	CD-OE1	6.94	1.33	1.25
9	2	236	ARG	NE-CZ	6.94	1.42	1.33
14	7	215	ARG	CZ-NH2	6.94	1.42	1.33
4	D	237	GLU	CG-CD	6.93	1.62	1.51
19	Y	61	GLU	CD-OE1	6.91	1.33	1.25
22	S	287	SER	CB-OG	6.91	1.51	1.42
7	g	169	ARG	CZ-NH1	6.90	1.42	1.33
6	F	123	TYR	CG-CD2	6.90	1.48	1.39
22	S	50	PRO	N-CD	-6.88	1.38	1.47
24	Q	189	ARG	CZ-NH1	6.88	1.42	1.33
33	J	191	PRO	N-CD	-6.86	1.38	1.47
31	L	366	ALA	CA-CB	6.84	1.66	1.52
7	g	75	GLY	CA-C	-6.84	1.41	1.51
10	j	98	ARG	NE-CZ	6.84	1.42	1.33
24	Q	378	SER	CB-OG	6.84	1.51	1.42
6	F	174	ARG	NE-CZ	6.81	1.42	1.33
7	G	130	ARG	CZ-NH2	6.81	1.41	1.33
6	F	51	ARG	CZ-NH2	6.80	1.41	1.33
12	l	145	GLU	CD-OE2	6.80	1.33	1.25
17	T	197	TYR	CG-CD1	-6.80	1.30	1.39
23	P	232	ARG	CZ-NH1	6.78	1.41	1.33
21	N	19	SER	CA-CB	6.77	1.63	1.52
23	P	415	TRP	NE1-CE2	6.77	1.46	1.37
2	b	58	SER	CA-CB	6.76	1.63	1.52
22	S	51	ARG	NE-CZ	6.76	1.41	1.33
13	6	79	SER	CB-OG	-6.76	1.33	1.42
25	R	222	ARG	CD-NE	6.74	1.57	1.46
30	K	67	TYR	CG-CD2	6.74	1.48	1.39
12	l	165	TYR	CD1-CE1	6.73	1.49	1.39
14	7	220	ARG	NE-CZ	6.73	1.41	1.33
3	C	5	ARG	NE-CZ	6.72	1.41	1.33
29	I	291	ARG	CZ-NH1	6.72	1.41	1.33
21	N	394	ARG	CZ-NH1	6.71	1.41	1.33
12	5	179	TYR	CZ-OH	6.70	1.49	1.37
24	Q	163	ARG	NE-CZ	6.69	1.41	1.33
32	M	357	ARG	NE-CZ	6.68	1.41	1.33
9	2	48	ARG	CZ-NH2	6.68	1.41	1.33
12	l	245	TYR	CG-CD2	6.68	1.47	1.39
1	A	105	ARG	CZ-NH2	6.67	1.41	1.33
8	1	38	ARG	CD-NE	6.66	1.57	1.46
20	Z	244	ARG	CZ-NH2	6.65	1.41	1.33
25	R	352	SER	CA-CB	6.65	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	122	SER	CA-CB	6.65	1.62	1.52
8	h	158	GLU	CD-OE2	6.65	1.32	1.25
30	K	81	ARG	NE-CZ	6.64	1.41	1.33
4	D	197	ARG	CZ-NH1	6.64	1.41	1.33
8	h	45	ARG	CZ-NH2	6.63	1.41	1.33
22	S	384	ARG	NE-CZ	6.63	1.41	1.33
25	R	159	SER	CA-CB	6.62	1.62	1.52
31	L	407	ARG	CZ-NH2	6.62	1.41	1.33
31	L	289	ARG	CD-NE	6.61	1.57	1.46
9	i	126	TYR	CZ-OH	6.59	1.49	1.37
20	Z	497	PHE	CE1-CZ	6.59	1.49	1.37
5	e	242	GLU	CD-OE2	6.58	1.32	1.25
4	D	107	GLU	CD-OE2	6.58	1.32	1.25
24	Q	20	TYR	CB-CG	-6.58	1.41	1.51
6	f	39	ARG	CD-NE	6.58	1.57	1.46
6	f	131	GLY	N-CA	-6.58	1.36	1.46
3	c	4	ARG	NE-CZ	6.57	1.41	1.33
25	R	334	ARG	CD-NE	6.57	1.57	1.46
33	J	43	ARG	CZ-NH1	6.57	1.41	1.33
5	e	39	GLY	CA-C	-6.56	1.41	1.51
3	c	15	PRO	N-CD	-6.56	1.38	1.47
3	c	210	ARG	CZ-NH2	6.56	1.41	1.33
4	D	123	SER	CA-CB	6.56	1.62	1.52
8	h	120	TYR	CZ-OH	6.56	1.49	1.37
22	S	480	ARG	CD-NE	6.53	1.57	1.46
20	Z	428	TRP	CB-CG	6.53	1.62	1.50
21	N	310	ASP	N-CA	-6.52	1.33	1.46
31	L	168	TYR	CD1-CE1	6.52	1.49	1.39
14	n	128	TYR	CB-CG	-6.52	1.41	1.51
14	7	137	ARG	CZ-NH1	6.51	1.41	1.33
14	n	70	ASN	CB-CG	6.50	1.66	1.51
22	S	367	TYR	CE1-CZ	6.50	1.47	1.38
21	N	623	PHE	CE2-CZ	6.50	1.49	1.37
28	H	454	TYR	CG-CD1	6.50	1.47	1.39
4	d	112	TYR	CE1-CZ	6.49	1.47	1.38
10	j	159	GLU	CG-CD	6.48	1.61	1.51
20	Z	486	SER	CA-CB	6.46	1.62	1.52
6	F	24	TYR	CZ-OH	6.46	1.48	1.37
26	U	100	ARG	CZ-NH1	6.45	1.41	1.33
13	6	99	ARG	CZ-NH1	6.44	1.41	1.33
20	Z	446	GLU	CG-CD	6.44	1.61	1.51
7	g	16	SER	CA-CB	6.44	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	P	138	ARG	CZ-NH2	6.44	1.41	1.33
7	G	190	ARG	CD-NE	6.43	1.57	1.46
17	T	166	SER	CA-CB	6.43	1.62	1.52
17	T	99	SER	CA-CB	6.43	1.62	1.52
25	R	207	ARG	NE-CZ	6.43	1.41	1.33
23	P	319	GLU	CG-CD	6.42	1.61	1.51
3	C	208	TYR	CG-CD2	6.41	1.47	1.39
3	C	213	PHE	CG-CD2	6.41	1.48	1.38
28	H	403	ARG	CZ-NH1	6.40	1.41	1.33
14	n	220	ARG	NE-CZ	6.40	1.41	1.33
16	V	251	TYR	CG-CD1	6.40	1.47	1.39
7	g	201	TYR	CB-CG	6.39	1.61	1.51
20	Z	773	ARG	CZ-NH2	6.39	1.41	1.33
27	O	215	TYR	CG-CD1	6.38	1.47	1.39
2	b	204	PHE	CG-CD2	6.38	1.48	1.38
14	n	137	ARG	CZ-NH1	6.37	1.41	1.33
7	G	123	HIS	CB-CG	-6.36	1.38	1.50
11	k	149	ARG	CZ-NH2	6.36	1.41	1.33
14	n	136	ARG	CD-NE	6.36	1.57	1.46
14	n	98	ARG	CZ-NH2	6.36	1.41	1.33
31	L	341	GLY	CA-C	-6.36	1.41	1.51
11	4	67	TYR	CG-CD2	6.35	1.47	1.39
14	n	161	ARG	CZ-NH1	6.35	1.41	1.33
21	N	294	PRO	N-CD	6.35	1.56	1.47
8	1	183	ARG	CZ-NH1	6.35	1.41	1.33
27	O	166	ARG	NE-CZ	6.35	1.41	1.33
2	B	97	TYR	CE2-CZ	6.34	1.46	1.38
2	b	178	ARG	CZ-NH2	6.34	1.41	1.33
32	M	227	GLY	CA-C	-6.34	1.41	1.51
12	l	148	ARG	NE-CZ	6.34	1.41	1.33
21	N	854	GLU	CG-CD	6.34	1.61	1.51
25	R	207	ARG	CD-NE	6.33	1.57	1.46
32	M	433	TYR	CG-CD1	6.32	1.47	1.39
12	l	253	TYR	CD1-CE1	6.32	1.48	1.39
12	l	245	TYR	CE1-CZ	6.32	1.46	1.38
12	l	139	ARG	NE-CZ	6.31	1.41	1.33
7	G	238	GLU	CD-OE1	6.31	1.32	1.25
29	I	180	SER	CA-CB	6.30	1.62	1.52
22	S	382	ARG	NE-CZ	6.29	1.41	1.33
32	M	299	ARG	CD-NE	6.29	1.57	1.46
13	6	18	GLY	CA-C	-6.28	1.41	1.51
6	F	106	GLU	CD-OE1	6.28	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	138	ARG	NE-CZ	6.28	1.41	1.33
26	U	210	TYR	CE2-CZ	6.28	1.46	1.38
13	6	47	TYR	CD1-CE1	6.28	1.48	1.39
2	B	125	GLY	CA-C	-6.28	1.41	1.51
20	Z	826	ARG	NE-CZ	6.27	1.41	1.33
29	I	129	TYR	CG-CD2	6.27	1.47	1.39
28	H	101	ARG	NE-CZ	6.27	1.41	1.33
6	f	221	PRO	N-CD	-6.26	1.39	1.47
33	J	309	ARG	NE-CZ	6.26	1.41	1.33
10	j	122	ALA	CA-CB	6.26	1.65	1.52
29	I	129	TYR	CZ-OH	6.25	1.48	1.37
14	7	189	ARG	CZ-NH2	6.25	1.41	1.33
15	W	25	ARG	CD-NE	6.25	1.57	1.46
15	W	41	ARG	NE-CZ	6.25	1.41	1.33
16	V	135	ARG	CD-NE	6.24	1.57	1.46
20	Z	940	GLY	N-CA	-6.24	1.36	1.46
16	V	223	SER	CA-CB	6.24	1.62	1.52
21	N	69	TYR	CG-CD2	6.24	1.47	1.39
25	R	213	TYR	CG-CD2	6.24	1.47	1.39
3	c	59	GLN	N-CA	-6.24	1.33	1.46
4	D	58	ARG	CZ-NH2	6.24	1.41	1.33
8	1	144	TYR	CG-CD1	6.23	1.47	1.39
32	M	339	ARG	NE-CZ	6.23	1.41	1.33
24	Q	304	GLU	CD-OE1	-6.22	1.18	1.25
31	L	289	ARG	NE-CZ	6.21	1.41	1.33
1	A	120	ARG	CZ-NH1	6.20	1.41	1.33
5	e	72	ARG	CZ-NH2	6.20	1.41	1.33
33	J	231	ARG	CZ-NH1	6.20	1.41	1.33
5	e	122	ARG	NE-CZ	6.19	1.41	1.33
1	A	77	ARG	CD-NE	6.19	1.56	1.46
27	O	15	ARG	CZ-NH2	6.18	1.41	1.33
16	V	230	TYR	CD1-CE1	-6.18	1.30	1.39
8	1	96	TYR	CE1-CZ	6.17	1.46	1.38
20	Z	217	GLU	CG-CD	6.17	1.61	1.51
4	D	120	TYR	CE1-CZ	6.17	1.46	1.38
20	Z	210	TYR	CE2-CZ	6.17	1.46	1.38
3	c	217	ARG	CZ-NH1	6.17	1.41	1.33
31	L	78	ARG	CZ-NH2	6.17	1.41	1.33
22	S	327	ILE	C-N	6.16	1.46	1.34
25	R	140	TYR	CE2-CZ	6.16	1.46	1.38
21	N	809	ARG	NE-CZ	6.15	1.41	1.33
8	1	158	GLU	N-CA	-6.15	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	77	TYR	CG-CD1	6.15	1.47	1.39
3	c	54	SER	CA-CB	6.15	1.62	1.52
10	3	98	ARG	NE-CZ	6.14	1.41	1.33
11	4	24	GLY	N-CA	-6.14	1.36	1.46
20	Z	248	TYR	CE2-CZ	6.14	1.46	1.38
10	j	188	TYR	CG-CD1	6.13	1.47	1.39
13	6	99	ARG	NE-CZ	6.13	1.41	1.33
29	I	340	ARG	CZ-NH2	6.13	1.41	1.33
4	d	125	GLY	N-CA	-6.13	1.36	1.46
8	h	91	PHE	CG-CD1	6.13	1.48	1.38
18	X	133	SER	CA-CB	6.13	1.62	1.52
21	N	697	PHE	CB-CG	-6.12	1.41	1.51
20	Z	952	SER	CA-CB	6.12	1.62	1.52
16	V	191	GLY	CA-C	-6.12	1.42	1.51
1	A	198	SER	CA-CB	6.12	1.62	1.52
1	A	46	ARG	CZ-NH2	6.11	1.41	1.33
6	F	6	TYR	CG-CD2	6.11	1.47	1.39
33	J	306	ARG	CD-NE	6.11	1.56	1.46
5	E	10	ARG	NE-CZ	6.11	1.41	1.33
12	l	94	ARG	CZ-NH1	6.10	1.41	1.33
21	N	908	ARG	CZ-NH2	6.10	1.41	1.33
24	Q	232	TYR	CD1-CE1	6.10	1.48	1.39
17	T	174	PHE	CG-CD2	6.09	1.47	1.38
22	S	440	ASP	C-N	6.09	1.44	1.33
12	l	262	TYR	CE1-CZ	6.09	1.46	1.38
22	S	197	SER	CA-CB	6.09	1.62	1.52
22	S	292	TYR	CE2-CZ	6.09	1.46	1.38
7	g	130	ARG	CZ-NH1	6.09	1.41	1.33
11	k	23	ARG	CZ-NH1	6.09	1.41	1.33
30	K	252	ARG	CD-NE	6.09	1.56	1.46
30	K	330	ARG	CZ-NH2	6.08	1.41	1.33
2	B	128	ARG	CZ-NH2	6.08	1.41	1.33
10	j	8	ASN	C-N	6.07	1.44	1.33
16	V	202	ASP	N-CA	-6.06	1.34	1.46
33	J	222	TYR	CE1-CZ	6.06	1.46	1.38
21	N	740	TRP	NE1-CE2	6.05	1.45	1.37
4	D	108	TYR	CG-CD2	6.05	1.47	1.39
24	Q	60	GLU	CB-CG	6.04	1.63	1.52
22	S	21	SER	CA-CB	6.04	1.62	1.52
5	e	19	GLY	CA-C	-6.04	1.42	1.51
23	P	232	ARG	CZ-NH2	6.04	1.41	1.33
12	5	247	GLY	CA-C	-6.04	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	M	255	TYR	CB-CG	-6.04	1.42	1.51
11	4	149	ARG	NE-CZ	6.03	1.40	1.33
5	E	61	SER	CA-CB	-6.03	1.44	1.52
23	P	220	TYR	CZ-OH	6.02	1.48	1.37
24	Q	185	TYR	CG-CD1	6.02	1.47	1.39
10	j	181	SER	N-CA	-6.02	1.34	1.46
21	N	338	PHE	CB-CG	6.02	1.61	1.51
33	J	226	GLY	CA-C	-6.02	1.42	1.51
9	2	65	ARG	CD-NE	6.01	1.56	1.46
32	M	322	LYS	N-CA	-6.01	1.34	1.46
24	Q	12	ARG	CZ-NH1	6.01	1.40	1.33
16	V	254	ARG	CZ-NH2	6.01	1.40	1.33
16	V	198	SER	CA-CB	6.00	1.61	1.52
24	Q	407	ALA	CA-CB	5.99	1.65	1.52
23	P	221	TYR	CD2-CE2	5.99	1.48	1.39
8	h	163	PHE	CG-CD2	5.99	1.47	1.38
2	b	44	VAL	CA-CB	-5.99	1.42	1.54
2	B	182	GLU	CD-OE1	5.98	1.32	1.25
20	Z	426	TYR	CG-CD2	5.98	1.47	1.39
13	m	203	HIS	CB-CG	-5.98	1.39	1.50
21	N	200	SER	CA-CB	5.98	1.61	1.52
13	6	85	PHE	CE1-CZ	5.97	1.48	1.37
30	K	128	ARG	NE-CZ	5.97	1.40	1.33
5	E	62	ASP	N-CA	-5.96	1.34	1.46
32	M	29	GLU	CB-CG	5.96	1.63	1.52
10	j	139	SER	CA-CB	5.96	1.61	1.52
1	a	217	GLU	CD-OE1	5.95	1.32	1.25
8	h	153	GLU	CG-CD	5.95	1.60	1.51
25	R	24	TYR	CE1-CZ	5.95	1.46	1.38
25	R	409	GLY	N-CA	-5.95	1.37	1.46
14	n	123	SER	CA-CB	5.95	1.61	1.52
11	4	85	ARG	CD-NE	5.95	1.56	1.46
25	R	324	ARG	CZ-NH2	5.95	1.40	1.33
23	P	3	ARG	CD-NE	5.94	1.56	1.46
8	h	144	TYR	CG-CD1	5.94	1.46	1.39
4	D	228	GLU	CB-CG	5.93	1.63	1.52
32	M	47	GLU	CD-OE2	5.93	1.32	1.25
8	1	55	SER	CA-CB	5.92	1.61	1.52
4	d	111	ARG	CZ-NH1	5.92	1.40	1.33
25	R	145	GLY	CA-C	5.92	1.61	1.51
20	Z	927	VAL	CA-CB	-5.91	1.42	1.54
33	J	283	GLU	CD-OE2	-5.90	1.19	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	313	ALA	CA-CB	5.90	1.64	1.52
9	i	217	ARG	CD-NE	5.90	1.56	1.46
6	F	193	GLY	N-CA	-5.89	1.37	1.46
30	K	333	ARG	CD-NE	5.89	1.56	1.46
24	Q	293	SER	CA-CB	5.88	1.61	1.52
3	c	143	ARG	CD-NE	5.88	1.56	1.46
8	1	201	GLU	CD-OE2	5.88	1.32	1.25
3	c	92	ARG	CZ-NH2	5.88	1.40	1.33
30	K	281	ARG	CZ-NH2	5.88	1.40	1.33
2	b	97	TYR	CE2-CZ	5.87	1.46	1.38
5	e	231	TYR	CG-CD2	5.87	1.46	1.39
2	b	159	TRP	NE1-CE2	5.87	1.45	1.37
13	6	106	TYR	CZ-OH	5.87	1.47	1.37
20	Z	96	TYR	CG-CD2	5.87	1.46	1.39
4	d	29	ARG	CD-NE	5.87	1.56	1.46
32	M	77	TYR	CE1-CZ	5.86	1.46	1.38
3	c	140	TYR	CE1-CZ	5.86	1.46	1.38
2	B	5	TYR	CE1-CZ	5.85	1.46	1.38
22	S	385	SER	CA-CB	5.84	1.61	1.52
31	L	357	ARG	CZ-NH2	5.84	1.40	1.33
31	L	195	GLU	CD-OE2	-5.84	1.19	1.25
18	X	122	TYR	CD1-CE1	5.84	1.48	1.39
22	S	177	ASN	CB-CG	5.84	1.64	1.51
27	O	310	PHE	C-N	5.84	1.47	1.34
13	m	193	ARG	CZ-NH2	5.84	1.40	1.33
17	T	266	TYR	CG-CD2	5.83	1.46	1.39
28	H	261	ARG	NE-CZ	5.83	1.40	1.33
27	O	21	SER	CA-CB	5.83	1.61	1.52
26	U	240	GLY	CA-C	-5.83	1.42	1.51
5	E	132	ARG	NE-CZ	5.83	1.40	1.33
6	F	16	THR	C-N	5.83	1.43	1.33
23	P	390	TYR	CB-CG	5.82	1.60	1.51
24	Q	81	SER	CB-OG	5.82	1.49	1.42
21	N	38	GLU	CB-CG	5.82	1.63	1.52
13	m	41	TYR	CG-CD2	5.82	1.46	1.39
22	S	133	GLU	CD-OE2	5.82	1.32	1.25
11	4	121	TYR	CE1-CZ	5.81	1.46	1.38
28	H	222	ARG	NE-CZ	5.81	1.40	1.33
4	D	120	TYR	CG-CD1	5.81	1.46	1.39
27	O	250	TRP	CB-CG	5.81	1.60	1.50
29	I	422	ARG	CZ-NH2	5.80	1.40	1.33
20	Z	161	ILE	C-N	5.79	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	698	GLY	CA-C	-5.79	1.42	1.51
11	k	115	GLU	CD-OE2	5.79	1.32	1.25
20	Z	928	ARG	CZ-NH1	5.79	1.40	1.33
28	H	432	ARG	NE-CZ	5.79	1.40	1.33
17	T	128	TYR	CD2-CE2	5.78	1.48	1.39
28	H	435	ARG	CZ-NH1	5.78	1.40	1.33
12	l	234	ARG	CZ-NH1	5.78	1.40	1.33
3	C	217	ARG	CZ-NH1	5.78	1.40	1.33
7	G	20	ARG	CZ-NH2	5.78	1.40	1.33
5	E	34	GLY	CA-C	-5.78	1.42	1.51
33	J	200	ARG	CZ-NH2	5.78	1.40	1.33
14	n	247	VAL	CB-CG1	5.77	1.65	1.52
27	O	178	TYR	CE1-CZ	5.77	1.46	1.38
10	j	199	TYR	CE1-CZ	5.77	1.46	1.38
27	O	118	GLY	N-CA	-5.77	1.37	1.46
29	I	208	TYR	CG-CD1	5.77	1.46	1.39
32	M	42	ARG	CZ-NH1	5.77	1.40	1.33
21	N	471	TYR	CG-CD1	5.77	1.46	1.39
23	P	344	ARG	NE-CZ	5.77	1.40	1.33
24	Q	75	ARG	CZ-NH1	5.77	1.40	1.33
6	F	231	ALA	N-CA	5.76	1.57	1.46
23	P	253	ASP	CB-CG	5.76	1.63	1.51
24	Q	65	TYR	CG-CD2	5.76	1.46	1.39
5	e	7	GLU	CD-OE1	5.76	1.31	1.25
3	c	18	ARG	NE-CZ	5.75	1.40	1.33
13	m	145	ARG	CD-NE	5.75	1.56	1.46
20	Z	4	GLU	CG-CD	5.75	1.60	1.51
30	K	242	PHE	CG-CD1	5.75	1.47	1.38
16	V	270	TYR	CE2-CZ	5.75	1.46	1.38
23	P	223	LEU	N-CA	-5.74	1.34	1.46
25	R	27	SER	CA-CB	-5.74	1.44	1.52
30	K	350	ARG	NE-CZ	5.74	1.40	1.33
29	I	300	ARG	NE-CZ	5.74	1.40	1.33
32	M	255	TYR	CE2-CZ	5.74	1.46	1.38
28	H	451	ILE	CA-CB	-5.73	1.41	1.54
23	P	262	SER	CA-CB	5.73	1.61	1.52
32	M	166	ARG	NE-CZ	5.73	1.40	1.33
11	4	73	TYR	N-CA	-5.73	1.34	1.46
23	P	427	GLU	CG-CD	5.73	1.60	1.51
5	e	166	ARG	CD-NE	5.72	1.56	1.46
28	H	93	GLU	CB-CG	5.72	1.63	1.52
3	C	3	SER	CA-CB	5.72	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	f	101	ARG	CD-NE	5.72	1.56	1.46
3	c	203	SER	CA-CB	5.72	1.61	1.52
14	n	161	ARG	CD-NE	5.71	1.56	1.46
20	Z	248	TYR	CG-CD1	5.71	1.46	1.39
32	M	318	ASP	CA-CB	5.71	1.66	1.53
28	H	466	TYR	CG-CD2	5.71	1.46	1.39
6	F	96	SER	CB-OG	5.71	1.49	1.42
29	I	251	GLU	CD-OE1	5.71	1.31	1.25
11	4	173	PRO	N-CD	-5.70	1.39	1.47
1	a	14	ARG	NE-CZ	5.70	1.40	1.33
23	P	367	GLU	CD-OE2	5.70	1.31	1.25
24	Q	390	LEU	CA-CB	5.70	1.66	1.53
9	i	48	ARG	CZ-NH1	5.69	1.40	1.33
8	h	166	HIS	CB-CG	5.69	1.60	1.50
20	Z	951	GLN	CA-CB	5.69	1.66	1.53
21	N	515	ARG	CD-NE	5.68	1.56	1.46
31	L	137	ARG	CZ-NH1	5.68	1.40	1.33
6	F	122	SER	CA-CB	5.68	1.61	1.52
20	Z	551	LEU	N-CA	-5.68	1.34	1.46
4	D	141	ARG	CZ-NH1	5.68	1.40	1.33
2	b	75	TYR	CE2-CZ	5.67	1.46	1.38
18	X	11	ARG	NE-CZ	5.67	1.40	1.33
7	g	190	ARG	NE-CZ	5.67	1.40	1.33
9	2	215	TYR	CG-CD1	5.67	1.46	1.39
23	P	364	ARG	CZ-NH2	5.67	1.40	1.33
4	d	48	ARG	NE-CZ	5.67	1.40	1.33
16	V	221	TRP	NE1-CE2	5.67	1.45	1.37
23	P	117	SER	CA-CB	5.66	1.61	1.52
3	C	92	ARG	CZ-NH2	5.66	1.40	1.33
20	Z	962	ARG	NE-CZ	5.66	1.40	1.33
26	U	110	PHE	CG-CD2	5.66	1.47	1.38
14	7	241	PHE	CG-CD1	5.66	1.47	1.38
8	1	81	THR	N-CA	-5.66	1.35	1.46
14	7	261	TYR	CE1-CZ	5.65	1.45	1.38
20	Z	97	PRO	N-CD	-5.65	1.40	1.47
30	K	185	ARG	CZ-NH2	5.65	1.40	1.33
7	g	79	SER	CA-CB	5.65	1.61	1.52
30	K	255	ARG	CZ-NH1	5.65	1.40	1.33
7	G	37	SER	CB-OG	5.65	1.49	1.42
2	b	82	TYR	CZ-OH	5.64	1.47	1.37
8	1	146	TYR	CG-CD1	5.64	1.46	1.39
2	B	83	ARG	CZ-NH1	5.64	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	346	ARG	CZ-NH1	5.64	1.40	1.33
15	W	137	VAL	N-CA	-5.64	1.35	1.46
10	j	203	ARG	CD-NE	5.64	1.56	1.46
7	G	135	SER	CA-CB	5.64	1.61	1.52
27	O	147	ARG	NE-CZ	5.64	1.40	1.33
29	I	123	PRO	CA-C	-5.64	1.41	1.52
13	m	225	TYR	CB-CG	5.63	1.60	1.51
14	n	226	ARG	NE-CZ	5.63	1.40	1.33
13	6	110	PHE	CB-CG	5.63	1.60	1.51
25	R	417	TYR	CD1-CE1	5.63	1.47	1.39
30	K	207	ARG	CZ-NH2	5.63	1.40	1.33
13	m	75	ARG	CZ-NH1	5.63	1.40	1.33
25	R	306	PRO	N-CD	-5.63	1.40	1.47
20	Z	477	TYR	CE1-CZ	5.63	1.45	1.38
25	R	234	SER	CB-OG	-5.63	1.34	1.42
4	D	97	ARG	CZ-NH2	5.62	1.40	1.33
10	j	198	ARG	NE-CZ	5.62	1.40	1.33
17	T	69	SER	CA-CB	5.62	1.61	1.52
30	K	171	TYR	CE2-CZ	5.62	1.45	1.38
1	A	219	SER	CA-CB	5.62	1.61	1.52
9	i	178	GLU	CD-OE1	5.62	1.31	1.25
30	K	244	HIS	CB-CG	-5.62	1.40	1.50
4	d	141	ARG	CZ-NH1	5.61	1.40	1.33
14	n	186	PRO	N-CD	-5.61	1.40	1.47
7	g	135	SER	CA-CB	5.61	1.61	1.52
23	P	133	GLU	N-CA	-5.61	1.35	1.46
4	d	151	GLU	CD-OE1	5.61	1.31	1.25
28	H	390	ARG	CZ-NH1	5.61	1.40	1.33
9	i	140	PHE	CG-CD1	5.60	1.47	1.38
22	S	55	ARG	CZ-NH1	5.60	1.40	1.33
25	R	422	ARG	CZ-NH1	5.60	1.40	1.33
8	h	28	ARG	NE-CZ	5.60	1.40	1.33
4	D	38	GLY	CA-C	-5.59	1.42	1.51
4	d	61	PRO	N-CA	-5.59	1.37	1.47
21	N	124	TYR	CE2-CZ	5.59	1.45	1.38
3	C	198	SER	CA-CB	5.59	1.61	1.52
17	T	60	ARG	NE-CZ	5.59	1.40	1.33
29	I	98	GLU	CB-CG	5.59	1.62	1.52
13	6	46	ARG	NE-CZ	5.58	1.40	1.33
20	Z	574	TYR	CE1-CZ	5.58	1.45	1.38
9	i	152	TYR	CG-CD2	5.58	1.46	1.39
33	J	228	ARG	CD-NE	5.58	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	6	ARG	CD-NE	5.58	1.55	1.46
4	D	75	PHE	CG-CD2	5.58	1.47	1.38
11	4	96	ARG	CZ-NH2	5.58	1.40	1.33
27	O	356	ARG	CZ-NH2	5.58	1.40	1.33
31	L	214	PRO	N-CD	-5.58	1.40	1.47
28	H	173	ARG	CZ-NH2	5.57	1.40	1.33
28	H	462	ARG	CZ-NH2	5.57	1.40	1.33
24	Q	12	ARG	NE-CZ	5.57	1.40	1.33
33	J	94	TYR	CG-CD1	5.57	1.46	1.39
9	i	232	TYR	CE1-CZ	5.57	1.45	1.38
21	N	921	ARG	NE-CZ	5.57	1.40	1.33
31	L	339	ARG	NE-CZ	5.57	1.40	1.33
3	c	219	GLY	CA-C	-5.57	1.43	1.51
23	P	200	SER	CB-OG	-5.57	1.35	1.42
5	e	16	SER	CA-CB	5.56	1.61	1.52
15	W	179	ARG	CZ-NH1	5.56	1.40	1.33
20	Z	22	LYS	CA-CB	5.56	1.66	1.53
27	O	380	LEU	C-N	5.56	1.43	1.33
8	1	54	ARG	CD-NE	5.56	1.55	1.46
29	I	176	SER	CA-CB	5.55	1.61	1.52
11	k	56	PHE	CE2-CZ	5.55	1.47	1.37
4	d	172	ARG	NE-CZ	5.54	1.40	1.33
26	U	100	ARG	CD-NE	5.54	1.55	1.46
12	l	183	GLU	CB-CG	5.54	1.62	1.52
31	L	342	ARG	NE-CZ	5.54	1.40	1.33
4	d	97	ARG	NE-CZ	5.54	1.40	1.33
30	K	399	ARG	NE-CZ	5.54	1.40	1.33
33	J	145	SER	CA-CB	-5.54	1.44	1.52
21	N	584	ARG	NE-CZ	5.54	1.40	1.33
23	P	338	TRP	NE1-CE2	5.54	1.44	1.37
4	D	76	SER	N-CA	-5.53	1.35	1.46
14	7	137	ARG	NE-CZ	5.53	1.40	1.33
9	2	254	GLU	CA-CB	5.53	1.66	1.53
4	D	183	GLU	CD-OE1	5.53	1.31	1.25
14	7	254	PHE	CB-CG	5.53	1.60	1.51
17	T	150	ARG	CD-NE	5.53	1.55	1.46
31	L	209	ARG	CZ-NH1	5.52	1.40	1.33
18	X	91	PHE	CE1-CZ	5.52	1.47	1.37
8	h	191	GLY	CA-C	-5.52	1.43	1.51
12	5	151	VAL	CB-CG2	5.52	1.64	1.52
14	n	188	LEU	C-N	5.51	1.46	1.34
30	K	41	SER	CA-CB	5.51	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	96	VAL	CB-CG2	5.51	1.64	1.52
25	R	157	SER	CA-CB	5.51	1.61	1.52
13	m	229	ARG	CZ-NH1	5.51	1.40	1.33
14	n	173	PRO	N-CD	-5.51	1.40	1.47
13	m	198	SER	CA-CB	5.51	1.61	1.52
26	U	52	PHE	CG-CD1	5.51	1.47	1.38
28	H	299	ARG	CD-NE	5.51	1.55	1.46
17	T	42	PRO	CA-C	5.50	1.63	1.52
10	j	80	ARG	CZ-NH2	5.50	1.40	1.33
15	W	36	ILE	N-CA	-5.50	1.35	1.46
24	Q	55	GLU	CD-OE2	5.50	1.31	1.25
7	g	132	PHE	CG-CD2	5.50	1.47	1.38
7	G	242	PHE	CB-CG	5.50	1.60	1.51
7	g	238	GLU	CD-OE2	5.50	1.31	1.25
8	1	38	ARG	CZ-NH2	5.49	1.40	1.33
11	4	117	TYR	CG-CD2	5.49	1.46	1.39
3	c	113	ARG	CD-NE	5.49	1.55	1.46
9	i	225	ARG	CZ-NH2	5.49	1.40	1.33
4	d	124	GLY	CA-C	-5.49	1.43	1.51
31	L	142	LYS	CA-CB	5.49	1.66	1.53
12	5	163	TYR	CE1-CZ	5.49	1.45	1.38
17	T	15	PHE	CG-CD1	5.49	1.47	1.38
22	S	273	PHE	CB-CG	-5.49	1.42	1.51
24	Q	344	GLU	CG-CD	5.49	1.60	1.51
24	Q	57	SER	CA-CB	5.48	1.61	1.52
14	7	91	SER	CB-OG	-5.48	1.35	1.42
20	Z	298	PHE	CG-CD1	5.48	1.47	1.38
3	C	27	GLU	CB-CG	5.48	1.62	1.52
23	P	123	ARG	CD-NE	5.48	1.55	1.46
21	N	417	ARG	CZ-NH1	5.47	1.40	1.33
13	m	75	ARG	CD-NE	5.47	1.55	1.46
1	a	135	ARG	CD-NE	5.47	1.55	1.46
20	Z	942	PRO	CA-CB	-5.47	1.42	1.53
14	n	167	GLY	CA-C	-5.47	1.43	1.51
30	K	165	GLU	CD-OE1	5.47	1.31	1.25
9	i	217	ARG	CZ-NH2	5.46	1.40	1.33
2	B	217	GLU	CG-CD	5.46	1.60	1.51
18	X	49	GLU	CG-CD	5.46	1.60	1.51
28	H	384	GLY	CA-C	-5.46	1.43	1.51
5	e	214	GLU	CD-OE2	5.46	1.31	1.25
4	d	197	ARG	CZ-NH1	5.46	1.40	1.33
31	L	145	ARG	CZ-NH1	5.46	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	128	ARG	NE-CZ	5.45	1.40	1.33
2	B	4	ARG	NE-CZ	5.45	1.40	1.33
8	h	54	ARG	CZ-NH1	5.45	1.40	1.33
23	P	234	TYR	CG-CD2	5.45	1.46	1.39
32	M	412	HIS	CB-CG	5.45	1.59	1.50
8	1	34	TYR	CZ-OH	5.45	1.47	1.37
12	l	183	GLU	CG-CD	5.45	1.60	1.51
20	Z	96	TYR	CB-CG	5.45	1.59	1.51
30	K	67	TYR	CZ-OH	5.44	1.47	1.37
4	d	144	GLU	CD-OE1	5.44	1.31	1.25
21	N	753	PHE	CG-CD2	5.44	1.47	1.38
28	H	411	CYS	CB-SG	-5.44	1.73	1.81
13	m	140	GLU	N-CA	-5.43	1.35	1.46
28	H	373	ARG	NE-CZ	5.43	1.40	1.33
30	K	344	ARG	CD-NE	5.43	1.55	1.46
33	J	373	ARG	CZ-NH2	5.43	1.40	1.33
20	Z	389	PHE	CG-CD2	5.43	1.46	1.38
22	S	87	SER	CA-CB	5.43	1.61	1.52
5	E	103	TYR	CE2-CZ	5.42	1.45	1.38
30	K	281	ARG	NE-CZ	5.42	1.40	1.33
1	a	128	TYR	CG-CD2	5.42	1.46	1.39
3	c	242	THR	C-N	5.42	1.42	1.33
9	2	200	SER	CB-OG	-5.42	1.35	1.42
21	N	742	TRP	CG-CD1	-5.42	1.29	1.36
7	G	182	HIS	CB-CG	5.42	1.59	1.50
32	M	307	GLU	CG-CD	5.42	1.60	1.51
15	W	159	ALA	CA-CB	5.41	1.63	1.52
29	I	166	PRO	N-CD	-5.41	1.40	1.47
9	2	236	ARG	CZ-NH1	5.41	1.40	1.33
12	5	94	ARG	CZ-NH2	5.41	1.40	1.33
14	n	46	SER	CA-CB	5.40	1.61	1.52
32	M	282	GLU	CD-OE1	-5.40	1.19	1.25
2	B	145	PHE	CG-CD1	5.40	1.46	1.38
28	H	181	TYR	CE1-CZ	5.40	1.45	1.38
11	4	130	TYR	CD1-CE1	5.40	1.47	1.39
21	N	271	GLU	CG-CD	5.40	1.60	1.51
26	U	216	ASN	CA-CB	5.40	1.67	1.53
26	U	277	TYR	CB-CG	5.40	1.59	1.51
2	B	184	GLU	N-CA	-5.39	1.35	1.46
21	N	718	GLU	CD-OE1	5.39	1.31	1.25
11	4	93	ARG	CD-NE	5.39	1.55	1.46
20	Z	623	ARG	CD-NE	5.39	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Q	414	GLU	CD-OE1	5.39	1.31	1.25
31	L	137	ARG	CZ-NH2	5.39	1.40	1.33
25	R	75	GLY	CA-C	-5.39	1.43	1.51
2	b	217	GLU	CD-OE1	5.39	1.31	1.25
14	n	68	ARG	CD-NE	5.39	1.55	1.46
20	Z	592	GLU	CD-OE2	5.39	1.31	1.25
32	M	153	TYR	CE1-CZ	5.39	1.45	1.38
6	F	179	PHE	CG-CD2	5.39	1.46	1.38
7	g	201	TYR	CZ-OH	5.39	1.47	1.37
12	5	155	SER	CA-CB	5.39	1.61	1.52
1	a	38	THR	N-CA	-5.38	1.35	1.46
3	c	40	ALA	CA-CB	5.38	1.63	1.52
3	c	9	ARG	NE-CZ	5.38	1.40	1.33
4	D	141	ARG	NE-CZ	5.38	1.40	1.33
31	L	71	ASP	N-CA	-5.38	1.35	1.46
13	6	218	ASP	CA-CB	5.37	1.65	1.53
13	6	225	TYR	CZ-OH	5.37	1.47	1.37
29	I	199	GLU	CD-OE2	5.37	1.31	1.25
9	i	65	ARG	CZ-NH1	5.37	1.40	1.33
22	S	120	SER	CA-C	-5.37	1.39	1.52
17	T	246	GLU	CB-CG	5.37	1.62	1.52
13	m	131	TYR	CZ-OH	5.36	1.47	1.37
24	Q	345	SER	CB-OG	5.36	1.49	1.42
28	H	400	ARG	CZ-NH2	5.36	1.40	1.33
30	K	263	GLU	CG-CD	5.36	1.59	1.51
20	Z	909	ARG	CZ-NH1	5.36	1.40	1.33
13	6	41	TYR	CE2-CZ	5.35	1.45	1.38
20	Z	610	GLY	N-CA	-5.35	1.38	1.46
16	V	221	TRP	CD2-CE3	-5.35	1.32	1.40
21	N	584	ARG	CD-NE	5.35	1.55	1.46
30	K	71	GLU	CD-OE2	5.34	1.31	1.25
7	g	72	ARG	NE-CZ	5.34	1.40	1.33
4	d	191	CYS	CB-SG	5.34	1.91	1.82
21	N	544	GLU	CD-OE1	5.34	1.31	1.25
25	R	263	ARG	CZ-NH2	5.34	1.40	1.33
7	g	158	TRP	CG-CD1	5.34	1.44	1.36
12	5	247	GLY	C-N	5.34	1.42	1.33
20	Z	287	ARG	CZ-NH1	5.34	1.40	1.33
21	N	813	ARG	CZ-NH2	5.34	1.40	1.33
24	Q	151	TYR	CG-CD1	5.34	1.46	1.39
33	J	231	ARG	CD-NE	5.34	1.55	1.46
2	B	53	SER	CA-CB	5.33	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	a	77	ARG	CD-NE	5.32	1.55	1.46
6	F	57	SER	CA-CB	5.32	1.60	1.52
20	Z	174	GLU	CD-OE1	5.32	1.31	1.25
2	b	157	PHE	CG-CD2	5.32	1.46	1.38
2	B	13	SER	CA-CB	5.32	1.60	1.52
21	N	866	TYR	CG-CD1	5.32	1.46	1.39
31	L	79	GLN	N-CA	-5.32	1.35	1.46
12	l	188	TYR	CE1-CZ	5.32	1.45	1.38
2	b	82	TYR	CG-CD1	5.31	1.46	1.39
3	C	220	ALA	CA-CB	5.31	1.63	1.52
10	j	40	PHE	CG-CD1	5.31	1.46	1.38
23	P	103	TYR	CA-CB	5.31	1.65	1.53
8	1	120	TYR	CZ-OH	5.31	1.46	1.37
1	a	43	LEU	C-N	5.30	1.46	1.34
21	N	389	TYR	CG-CD1	5.30	1.46	1.39
25	R	252	TYR	CB-CG	5.30	1.59	1.51
29	I	129	TYR	CE1-CZ	5.30	1.45	1.38
5	e	166	ARG	CZ-NH1	5.30	1.40	1.33
33	J	339	ARG	CZ-NH1	5.30	1.40	1.33
21	N	247	GLU	CA-CB	5.30	1.65	1.53
33	J	329	ARG	CD-NE	5.30	1.55	1.46
4	D	108	TYR	CE1-CZ	5.30	1.45	1.38
27	O	188	PHE	CG-CD1	5.30	1.46	1.38
7	g	115	ARG	NE-CZ	5.29	1.40	1.33
13	m	93	SER	CA-CB	5.29	1.60	1.52
30	K	426	PHE	CE1-CZ	5.29	1.47	1.37
7	g	20	ARG	CZ-NH1	5.29	1.40	1.33
20	Z	64	TYR	CD1-CE1	5.29	1.47	1.39
22	S	186	TYR	CD2-CE2	5.29	1.47	1.39
29	I	265	ARG	NE-CZ	5.29	1.40	1.33
14	7	224	SER	CA-CB	5.29	1.60	1.52
28	H	94	GLU	CG-CD	5.28	1.59	1.51
5	e	103	TYR	CB-CG	-5.28	1.43	1.51
7	G	209	GLU	CG-CD	5.28	1.59	1.51
6	F	164	ARG	CD-NE	5.28	1.55	1.46
22	S	147	TRP	CZ3-CH2	5.28	1.48	1.40
4	d	90	ARG	CZ-NH1	5.28	1.40	1.33
9	2	107	SER	CA-CB	5.28	1.60	1.52
33	J	56	ARG	CD-NE	5.28	1.55	1.46
17	T	15	PHE	CE1-CZ	5.28	1.47	1.37
23	P	83	SER	CA-CB	5.28	1.60	1.52
33	J	228	ARG	NE-CZ	5.28	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	94	SER	CB-OG	5.28	1.49	1.42
8	h	137	GLY	CA-C	-5.27	1.43	1.51
2	B	104	TYR	CB-CG	-5.27	1.43	1.51
7	G	130	ARG	CZ-NH1	5.27	1.40	1.33
21	N	75	TYR	CG-CD1	5.27	1.46	1.39
4	D	22	TYR	CG-CD1	5.27	1.46	1.39
11	k	97	PRO	CA-CB	5.27	1.64	1.53
2	B	82	TYR	CG-CD2	5.27	1.46	1.39
25	R	107	GLU	CG-CD	5.26	1.59	1.51
29	I	211	MET	C-N	5.26	1.42	1.33
1	a	162	TYR	CG-CD1	5.26	1.46	1.39
2	b	30	GLN	C-N	5.26	1.42	1.33
28	H	409	ARG	CZ-NH2	5.26	1.39	1.33
12	5	148	ARG	NE-CZ	5.26	1.39	1.33
13	6	221	ARG	CD-NE	5.26	1.55	1.46
20	Z	153	TYR	CG-CD1	5.26	1.46	1.39
27	O	185	PHE	CA-CB	5.26	1.65	1.53
30	K	336	ARG	CZ-NH2	5.26	1.39	1.33
21	N	701	VAL	CB-CG2	5.25	1.63	1.52
4	d	49	ARG	NE-CZ	5.25	1.39	1.33
21	N	117	TYR	CE2-CZ	5.25	1.45	1.38
20	Z	8	LYS	CA-CB	5.25	1.65	1.53
1	a	237	SER	CA-CB	5.25	1.60	1.52
11	4	23	ARG	NE-CZ	5.25	1.39	1.33
27	O	263	PHE	CB-CG	-5.25	1.42	1.51
8	1	28	ARG	CZ-NH2	5.25	1.39	1.33
13	6	133	PHE	CG-CD2	5.25	1.46	1.38
1	a	103	GLU	CG-CD	5.25	1.59	1.51
3	C	144	TYR	CZ-OH	5.25	1.46	1.37
30	K	36	ASN	CA-CB	5.24	1.66	1.53
20	Z	774	ARG	CZ-NH1	5.24	1.39	1.33
21	N	14	ARG	CZ-NH1	5.24	1.39	1.33
21	N	162	ARG	NE-CZ	5.24	1.39	1.33
14	n	124	TYR	CG-CD2	5.23	1.46	1.39
11	4	67	TYR	CZ-OH	5.23	1.46	1.37
20	Z	700	GLU	CG-CD	5.23	1.59	1.51
12	l	81	PHE	CG-CD2	5.23	1.46	1.38
9	2	65	ARG	N-CA	-5.23	1.35	1.46
14	7	124	TYR	CG-CD2	5.23	1.46	1.39
1	A	205	PHE	CG-CD2	5.23	1.46	1.38
23	P	318	TYR	CZ-OH	5.23	1.46	1.37
13	m	113	TYR	CE1-CZ	5.23	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	149	TYR	CZ-OH	5.22	1.46	1.37
13	6	229	ARG	NE-CZ	5.22	1.39	1.33
17	T	186	ARG	NE-CZ	5.22	1.39	1.33
7	g	93	ARG	NE-CZ	5.22	1.39	1.33
9	2	155	SER	CA-CB	5.22	1.60	1.52
24	Q	51	ARG	NE-CZ	5.22	1.39	1.33
9	i	193	TRP	CB-CG	5.22	1.59	1.50
21	N	358	LYS	C-N	5.22	1.46	1.34
7	G	215	GLU	CD-OE1	5.22	1.31	1.25
13	6	206	VAL	N-CA	-5.22	1.35	1.46
16	V	75	GLY	CA-C	-5.22	1.43	1.51
11	k	139	TYR	CG-CD2	5.21	1.46	1.39
21	N	50	TYR	CG-CD1	5.21	1.46	1.39
22	S	258	GLU	CD-OE2	5.21	1.31	1.25
7	G	160	TYR	CD2-CE2	5.21	1.47	1.39
31	L	123	SER	CA-CB	5.21	1.60	1.52
19	Y	39	PRO	CA-CB	-5.21	1.43	1.53
4	D	77	GLY	N-CA	-5.20	1.38	1.46
11	4	190	ARG	NE-CZ	5.20	1.39	1.33
26	U	95	SER	CA-CB	5.20	1.60	1.52
21	N	264	SER	N-CA	-5.20	1.35	1.46
26	U	32	ARG	NE-CZ	5.20	1.39	1.33
32	M	313	ASP	C-N	5.20	1.42	1.33
31	L	401	PHE	CB-CG	-5.20	1.42	1.51
4	d	166	ARG	NE-CZ	5.20	1.39	1.33
24	Q	314	PHE	CE2-CZ	5.20	1.47	1.37
5	e	153	TYR	CE1-CZ	5.20	1.45	1.38
9	i	101	ARG	CB-CG	5.20	1.66	1.52
6	f	140	SER	CA-CB	5.19	1.60	1.52
31	L	191	ARG	NE-CZ	5.19	1.39	1.33
3	c	41	SER	CA-CB	5.19	1.60	1.52
4	D	156	TYR	CE2-CZ	5.19	1.45	1.38
27	O	301	PHE	CB-CG	-5.19	1.42	1.51
29	I	292	TYR	CG-CD2	5.19	1.45	1.39
14	n	78	VAL	C-N	5.19	1.42	1.33
22	S	212	SER	CA-CB	5.19	1.60	1.52
2	B	165	GLY	N-CA	-5.18	1.38	1.46
14	7	220	ARG	CZ-NH1	5.18	1.39	1.33
2	b	41	ASN	CB-CG	5.18	1.62	1.51
1	a	32	PHE	CG-CD1	5.18	1.46	1.38
11	k	135	TYR	CZ-OH	5.18	1.46	1.37
14	7	68	ARG	NE-CZ	5.18	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	2	120	GLN	C-N	5.18	1.42	1.33
22	S	98	SER	CA-CB	5.18	1.60	1.52
30	K	393	ARG	CZ-NH2	5.18	1.39	1.33
1	a	133	TYR	CB-CG	5.17	1.59	1.51
3	c	20	TYR	CE1-CZ	5.17	1.45	1.38
7	g	242	PHE	CG-CD2	5.17	1.46	1.38
23	P	359	ARG	CZ-NH2	5.17	1.39	1.33
5	e	51	GLU	CD-OE1	5.17	1.31	1.25
5	E	166	ARG	NE-CZ	5.17	1.39	1.33
17	T	137	GLU	CD-OE1	5.17	1.31	1.25
20	Z	468	GLU	CD-OE1	-5.17	1.20	1.25
25	R	45	GLU	CD-OE1	5.17	1.31	1.25
8	h	159	GLU	CD-OE2	5.17	1.31	1.25
10	j	169	GLN	CG-CD	5.17	1.62	1.51
32	M	52	SER	CA-CB	5.17	1.60	1.52
9	i	104	ARG	NE-CZ	5.16	1.39	1.33
9	i	255	GLU	CG-CD	5.16	1.59	1.51
31	L	137	ARG	CD-NE	5.16	1.55	1.46
6	F	225	TYR	CZ-OH	5.16	1.46	1.37
11	4	83	PHE	CG-CD2	5.16	1.46	1.38
20	Z	64	TYR	CZ-OH	5.16	1.46	1.37
16	V	120	SER	CA-CB	5.16	1.60	1.52
21	N	585	ARG	NE-CZ	5.16	1.39	1.33
2	b	5	TYR	CG-CD2	5.16	1.45	1.39
7	g	99	PHE	CG-CD2	5.16	1.46	1.38
6	f	24	TYR	CB-CG	5.15	1.59	1.51
6	F	205	SER	CB-OG	5.15	1.49	1.42
4	d	111	ARG	CD-NE	5.15	1.55	1.46
4	D	4	TYR	CE2-CZ	5.15	1.45	1.38
20	Z	440	LEU	C-N	5.15	1.45	1.34
4	d	161	ALA	N-CA	-5.15	1.36	1.46
30	K	159	SER	CA-CB	5.15	1.60	1.52
8	1	174	TRP	CZ3-CH2	5.14	1.48	1.40
30	K	121	ARG	CD-NE	5.14	1.55	1.46
2	B	38	LYS	CA-CB	5.14	1.65	1.53
24	Q	398	TYR	CE2-CZ	5.14	1.45	1.38
4	D	108	TYR	CE2-CZ	5.14	1.45	1.38
20	Z	849	ARG	CZ-NH1	5.14	1.39	1.33
29	I	363	GLY	CA-C	-5.14	1.43	1.51
3	c	7	ASP	CA-CB	5.14	1.65	1.53
20	Z	341	TYR	CE1-CZ	5.14	1.45	1.38
1	A	19	PHE	CE2-CZ	5.14	1.47	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	n	194	ARG	NE-CZ	5.13	1.39	1.33
20	Z	41	GLU	CD-OE2	-5.13	1.20	1.25
20	Z	832	ARG	CZ-NH1	5.13	1.39	1.33
20	Z	124	MET	CG-SD	5.13	1.94	1.81
11	4	85	ARG	CZ-NH2	5.13	1.39	1.33
13	m	170	PRO	CA-CB	5.13	1.63	1.53
6	F	227	GLY	CA-C	-5.12	1.43	1.51
9	2	215	TYR	CD1-CE1	5.12	1.47	1.39
31	L	78	ARG	CD-NE	5.12	1.55	1.46
20	Z	623	ARG	CZ-NH2	5.12	1.39	1.33
3	c	143	ARG	NE-CZ	5.12	1.39	1.33
18	X	96	ARG	CZ-NH2	5.12	1.39	1.33
21	N	670	LYS	CA-CB	5.12	1.65	1.53
28	H	395	SER	CA-CB	5.12	1.60	1.52
13	m	114	TYR	CE1-CZ	5.12	1.45	1.38
7	G	8	TYR	CD1-CE1	5.12	1.47	1.39
13	m	147	GLY	C-N	5.12	1.42	1.33
9	i	119	TYR	CG-CD2	5.12	1.45	1.39
28	H	114	GLU	CG-CD	5.12	1.59	1.51
33	J	212	ARG	CD-NE	5.12	1.55	1.46
27	O	393	VAL	CA-CB	-5.11	1.44	1.54
7	G	188	SER	N-CA	-5.11	1.36	1.46
3	c	113	ARG	CZ-NH1	5.11	1.39	1.33
9	2	53	PRO	CA-C	-5.11	1.42	1.52
23	P	273	TYR	CB-CG	-5.11	1.44	1.51
29	I	350	PHE	CG-CD1	5.11	1.46	1.38
32	M	354	GLU	CG-CD	5.11	1.59	1.51
28	H	351	VAL	CB-CG2	5.11	1.63	1.52
12	5	261	ILE	N-CA	-5.10	1.36	1.46
21	N	561	GLY	CA-C	-5.10	1.43	1.51
26	U	66	TRP	CZ2-CH2	5.10	1.47	1.37
30	K	128	ARG	CZ-NH2	5.10	1.39	1.33
20	Z	147	GLU	CG-CD	5.10	1.59	1.51
30	K	259	ARG	NE-CZ	5.10	1.39	1.33
2	B	205	ASN	CB-CG	5.09	1.62	1.51
27	O	387	ARG	CD-NE	5.09	1.55	1.46
20	Z	394	TYR	CB-CG	5.09	1.59	1.51
31	L	173	PHE	CG-CD1	5.09	1.46	1.38
6	F	164	ARG	NE-CZ	5.09	1.39	1.33
19	Y	86	ARG	NE-CZ	5.09	1.39	1.33
31	L	246	SER	CA-CB	5.09	1.60	1.52
2	b	165	GLY	CA-C	-5.09	1.43	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	103	TYR	CE2-CZ	5.09	1.45	1.38
21	N	881	TYR	CG-CD2	5.09	1.45	1.39
4	D	239	GLU	CD-OE2	-5.09	1.20	1.25
20	Z	272	TYR	CG-CD1	5.09	1.45	1.39
21	N	880	ARG	CZ-NH2	5.09	1.39	1.33
13	m	142	GLU	CD-OE1	5.09	1.31	1.25
1	A	96	ARG	CZ-NH2	5.09	1.39	1.33
24	Q	55	GLU	CG-CD	5.09	1.59	1.51
29	I	262	ARG	CZ-NH2	5.08	1.39	1.33
22	S	405	ARG	N-CA	-5.08	1.36	1.46
12	5	196	ARG	NE-CZ	5.08	1.39	1.33
23	P	402	PHE	CG-CD1	5.08	1.46	1.38
16	V	163	ALA	CA-CB	5.08	1.63	1.52
8	h	183	ARG	NE-CZ	5.08	1.39	1.33
13	6	36	ARG	CA-CB	5.08	1.65	1.53
27	O	166	ARG	CZ-NH1	5.08	1.39	1.33
12	l	268	VAL	C-N	5.07	1.42	1.33
13	m	145	ARG	CZ-NH2	5.07	1.39	1.33
4	D	151	GLU	CG-CD	5.07	1.59	1.51
33	J	174	PHE	CG-CD1	5.07	1.46	1.38
4	D	128	PRO	N-CD	-5.07	1.40	1.47
1	a	70	SER	CB-OG	5.07	1.48	1.42
32	M	176	PRO	N-CD	-5.07	1.40	1.47
30	K	58	TYR	CE1-CZ	5.07	1.45	1.38
2	b	159	TRP	CD2-CE3	-5.07	1.32	1.40
9	2	225	ARG	NE-CZ	5.07	1.39	1.33
31	L	168	TYR	CG-CD1	-5.07	1.32	1.39
6	f	73	SER	CA-CB	5.07	1.60	1.52
12	l	130	TRP	CZ3-CH2	5.07	1.48	1.40
6	F	233	TYR	CZ-OH	5.07	1.46	1.37
12	5	234	ARG	CD-NE	5.07	1.55	1.46
10	3	28	ARG	NE-CZ	5.06	1.39	1.33
10	3	164	PHE	CE2-CZ	5.06	1.47	1.37
21	N	889	ARG	CZ-NH2	5.06	1.39	1.33
2	b	50	LYS	CA-CB	5.06	1.65	1.53
3	C	66	LEU	CA-C	-5.06	1.39	1.52
10	3	69	TYR	CZ-OH	5.06	1.46	1.37
15	W	15	TYR	CB-CG	5.06	1.59	1.51
22	S	408	CYS	CB-SG	5.06	1.90	1.82
25	R	275	GLU	CA-CB	5.06	1.65	1.53
1	a	131	ARG	CZ-NH2	5.06	1.39	1.33
9	2	208	GLU	CG-CD	5.06	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	H	318	ARG	NE-CZ	5.06	1.39	1.33
18	X	46	TRP	CD2-CE2	-5.06	1.35	1.41
24	Q	50	ARG	CZ-NH1	5.06	1.39	1.33
7	g	103	TYR	CG-CD1	5.06	1.45	1.39
17	T	88	TYR	CE1-CZ	5.06	1.45	1.38
20	Z	757	SER	CA-CB	5.06	1.60	1.52
16	V	299	GLY	N-CA	-5.05	1.38	1.46
24	Q	309	ARG	N-CA	-5.05	1.36	1.46
2	b	7	PHE	CG-CD1	5.05	1.46	1.38
13	m	223	GLU	CG-CD	5.05	1.59	1.51
4	D	76	SER	CA-CB	5.05	1.60	1.52
31	L	412	PRO	CA-C	-5.05	1.42	1.52
21	N	58	ARG	NE-CZ	5.05	1.39	1.33
24	Q	286	TYR	CG-CD2	5.04	1.45	1.39
32	M	207	PHE	CG-CD1	5.04	1.46	1.38
2	b	236	ARG	CZ-NH1	5.04	1.39	1.33
13	6	179	PRO	CA-CB	5.04	1.63	1.53
20	Z	592	GLU	CA-C	-5.04	1.39	1.52
21	N	203	ARG	CZ-NH1	5.04	1.39	1.33
21	N	398	ARG	CD-NE	5.04	1.55	1.46
1	A	155	TYR	CZ-OH	5.04	1.46	1.37
25	R	304	TYR	CG-CD2	5.04	1.45	1.39
20	Z	454	GLY	CA-C	5.04	1.59	1.51
11	k	80	VAL	CA-C	-5.04	1.39	1.52
1	a	22	GLU	C-N	5.04	1.42	1.33
5	E	128	SER	CA-CB	5.04	1.60	1.52
1	a	233	PHE	CA-C	-5.03	1.39	1.52
22	S	346	TYR	CA-CB	5.03	1.65	1.53
29	I	98	GLU	CD-OE1	5.03	1.31	1.25
2	B	234	ARG	CZ-NH1	5.03	1.39	1.33
21	N	333	SER	C-N	5.03	1.45	1.34
28	H	283	TYR	CE1-CZ	5.03	1.45	1.38
1	a	77	ARG	CZ-NH2	5.03	1.39	1.33
21	N	431	SER	CA-CB	5.03	1.60	1.52
33	J	282	PHE	CB-CG	5.03	1.59	1.51
8	h	138	SER	C-N	5.03	1.42	1.33
14	n	215	ARG	CA-CB	-5.03	1.42	1.53
11	4	179	VAL	CB-CG2	5.03	1.63	1.52
29	I	340	ARG	CZ-NH1	5.03	1.39	1.33
32	M	404	ARG	CD-NE	5.03	1.54	1.46
31	L	146	VAL	CA-CB	-5.02	1.44	1.54
17	T	186	ARG	CZ-NH2	5.02	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	c	122	TYR	CE2-CZ	5.02	1.45	1.38
7	g	186	GLY	N-CA	-5.02	1.38	1.46
13	6	93	SER	CB-OG	5.02	1.48	1.42
20	Z	186	GLY	CA-C	-5.02	1.43	1.51
22	S	118	PHE	CE2-CZ	5.02	1.46	1.37
8	h	11	SER	CA-CB	5.02	1.60	1.52
14	n	103	LEU	N-CA	-5.02	1.36	1.46
17	T	81	TYR	CE2-CZ	5.02	1.45	1.38
7	g	242	PHE	CE1-CZ	5.02	1.46	1.37
20	Z	575	MET	CG-SD	5.01	1.94	1.81
14	7	71	GLY	CA-C	-5.01	1.43	1.51
10	j	164	PHE	CG-CD1	5.01	1.46	1.38
8	1	193	GLU	CD-OE1	5.01	1.31	1.25
32	M	165	SER	N-CA	-5.01	1.36	1.46
4	d	58	ARG	CD-NE	5.01	1.54	1.46
14	7	84	VAL	C-N	5.01	1.42	1.33
13	m	131	TYR	CG-CD2	5.01	1.45	1.39
28	H	463	TYR	CG-CD1	5.01	1.45	1.39
24	Q	335	PHE	N-CA	5.00	1.56	1.46
1	a	55	SER	CA-CB	5.00	1.60	1.52
3	c	21	GLN	CG-CD	5.00	1.62	1.51
13	m	124	GLU	CG-CD	5.00	1.59	1.51

All (2634) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	174	ARG	NE-CZ-NH1	21.23	130.91	120.30
31	L	168	TYR	CB-CG-CD1	-20.07	108.96	121.00
6	f	174	ARG	NE-CZ-NH2	-19.19	110.70	120.30
3	c	210	ARG	NE-CZ-NH2	-18.85	110.87	120.30
23	P	240	TYR	CB-CG-CD2	-18.61	109.83	121.00
25	R	209	ARG	NE-CZ-NH2	-18.33	111.13	120.30
25	R	246	TYR	CB-CG-CD2	-18.29	110.03	121.00
23	P	240	TYR	CB-CG-CD1	18.16	131.90	121.00
22	S	382	ARG	NE-CZ-NH2	-17.70	111.45	120.30
13	6	109	ARG	NE-CZ-NH2	-17.38	111.61	120.30
1	A	96	ARG	NE-CZ-NH2	-17.04	111.78	120.30
31	L	194	ARG	NE-CZ-NH1	16.66	128.63	120.30
24	Q	398	TYR	CB-CG-CD1	-16.66	111.00	121.00
2	B	101	TYR	CB-CG-CD1	16.62	130.97	121.00
3	c	210	ARG	NE-CZ-NH1	16.52	128.56	120.30
5	e	122	ARG	NE-CZ-NH2	-16.47	112.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	124	TYR	CB-CG-CD1	16.39	130.84	121.00
17	T	197	TYR	CB-CG-CD1	16.37	130.82	121.00
25	R	246	TYR	CB-CG-CD1	16.17	130.70	121.00
4	D	11	PHE	CB-CG-CD1	15.87	131.91	120.80
27	O	98	TYR	CB-CG-CD2	-15.80	111.52	121.00
3	c	180	TYR	CB-CG-CD1	15.75	130.45	121.00
17	T	150	ARG	NE-CZ-NH2	-15.54	112.53	120.30
13	6	41	TYR	CB-CG-CD2	15.23	130.14	121.00
3	C	20	TYR	CB-CG-CD2	-15.23	111.86	121.00
24	Q	434	TYR	CB-CG-CD2	-15.21	111.87	121.00
17	T	197	TYR	CB-CG-CD2	-14.99	112.00	121.00
29	I	75	PHE	CB-CG-CD2	14.97	131.28	120.80
17	T	234	TYR	CB-CG-CD1	-14.92	112.05	121.00
33	J	324	ARG	NE-CZ-NH1	14.91	127.75	120.30
22	S	82	TYR	CB-CG-CD2	-14.90	112.06	121.00
24	Q	163	ARG	NE-CZ-NH1	14.90	127.75	120.30
12	5	94	ARG	NE-CZ-NH1	14.90	127.75	120.30
24	Q	163	ARG	NE-CZ-NH2	-14.81	112.89	120.30
28	H	400	ARG	NE-CZ-NH1	14.78	127.69	120.30
31	L	168	TYR	CB-CG-CD2	14.72	129.83	121.00
6	f	89	ARG	NE-CZ-NH2	-14.72	112.94	120.30
33	J	200	ARG	NE-CZ-NH2	-14.69	112.96	120.30
29	I	346	ARG	NE-CZ-NH1	14.56	127.58	120.30
21	N	394	ARG	NE-CZ-NH2	14.47	127.54	120.30
20	Z	136	ARG	NE-CZ-NH2	-14.36	113.12	120.30
21	N	584	ARG	NE-CZ-NH1	14.29	127.44	120.30
27	O	98	TYR	CB-CG-CD1	14.11	129.46	121.00
3	C	24	TYR	CB-CG-CD2	-14.05	112.57	121.00
25	R	43	ARG	NE-CZ-NH1	14.05	127.33	120.30
16	V	194	ARG	NE-CZ-NH2	-14.03	113.28	120.30
29	I	304	ARG	NE-CZ-NH1	13.98	127.29	120.30
24	Q	409	TYR	CB-CG-CD1	13.96	129.38	121.00
30	K	330	ARG	NE-CZ-NH2	-13.93	113.33	120.30
27	O	310	PHE	CB-CG-CD2	-13.88	111.09	120.80
5	e	86	ARG	NE-CZ-NH1	-13.79	113.41	120.30
31	L	392	ARG	NE-CZ-NH2	-13.78	113.41	120.30
23	P	390	TYR	CB-CG-CD1	13.70	129.22	121.00
24	Q	165	PHE	CB-CG-CD1	13.68	130.38	120.80
27	O	106	PHE	CB-CG-CD1	13.68	130.37	120.80
24	Q	165	PHE	CB-CG-CD2	-13.62	111.26	120.80
20	Z	155	ARG	NE-CZ-NH1	13.56	127.08	120.30
22	S	271	ARG	NE-CZ-NH2	-13.55	113.53	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	20	ARG	NE-CZ-NH2	-13.54	113.53	120.30
4	D	120	TYR	CB-CG-CD2	-13.47	112.92	121.00
9	i	215	TYR	CB-CG-CD2	-13.40	112.96	121.00
33	J	147	TYR	CB-CG-CD1	13.24	128.94	121.00
2	B	23	TYR	CB-CG-CD2	-13.14	113.12	121.00
14	n	109	TYR	CB-CG-CD1	13.12	128.87	121.00
2	B	97	TYR	CB-CG-CD1	-13.05	113.17	121.00
11	k	96	ARG	NE-CZ-NH1	13.05	126.83	120.30
1	a	110	TYR	CB-CG-CD2	-13.00	113.20	121.00
4	D	18	PHE	CB-CG-CD1	-12.97	111.72	120.80
4	d	83	ARG	NE-CZ-NH2	12.96	126.78	120.30
17	T	234	TYR	CB-CG-CD2	12.87	128.72	121.00
29	I	75	PHE	CB-CG-CD1	-12.87	111.79	120.80
14	n	162	TYR	CB-CG-CD2	-12.85	113.29	121.00
9	i	217	ARG	NE-CZ-NH1	12.80	126.70	120.30
2	B	82	TYR	CB-CG-CD2	-12.71	113.37	121.00
32	M	281	ASP	CB-CG-OD2	-12.61	106.95	118.30
6	f	128	TYR	CB-CG-CD2	-12.56	113.47	121.00
5	e	72	ARG	NE-CZ-NH1	12.52	126.56	120.30
11	4	190	ARG	NE-CZ-NH2	-12.51	114.04	120.30
4	d	48	ARG	NE-CZ-NH1	12.51	126.55	120.30
4	d	48	ARG	NE-CZ-NH2	-12.43	114.08	120.30
14	7	170	TYR	CB-CG-CD2	12.43	128.46	121.00
4	D	166	ARG	NE-CZ-NH1	-12.40	114.10	120.30
8	h	198	TYR	CB-CG-CD2	-12.37	113.58	121.00
2	B	101	TYR	CB-CG-CD2	-12.37	113.58	121.00
25	R	334	ARG	NE-CZ-NH2	-12.36	114.12	120.30
28	H	385	ARG	NE-CZ-NH2	12.32	126.46	120.30
16	V	194	ARG	NE-CZ-NH1	12.31	126.46	120.30
24	Q	65	TYR	CB-CG-CD2	-12.31	113.62	121.00
4	d	141	ARG	NE-CZ-NH1	12.29	126.45	120.30
6	F	202	ARG	NE-CZ-NH2	12.29	126.44	120.30
3	C	20	TYR	CB-CG-CD1	12.28	128.37	121.00
31	L	137	ARG	NE-CZ-NH2	-12.26	114.17	120.30
24	Q	12	ARG	NE-CZ-NH1	-12.24	114.18	120.30
27	O	178	TYR	CB-CG-CD2	-12.24	113.66	121.00
5	e	72	ARG	NE-CZ-NH2	-12.23	114.18	120.30
30	K	349	ARG	NE-CZ-NH1	12.22	126.41	120.30
16	V	42	ARG	NE-CZ-NH1	-12.19	114.20	120.30
22	S	55	ARG	NE-CZ-NH2	-12.18	114.21	120.30
12	5	234	ARG	NE-CZ-NH2	-12.14	114.23	120.30
12	l	179	TYR	CB-CG-CD1	12.12	128.27	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	101	TYR	CB-CG-CD1	-12.06	113.76	121.00
20	Z	893	PHE	CB-CG-CD1	12.06	129.24	120.80
27	O	106	PHE	CB-CG-CD2	-12.05	112.36	120.80
23	P	201	ARG	NE-CZ-NH1	11.98	126.29	120.30
1	a	244	ARG	NE-CZ-NH2	-11.94	114.33	120.30
4	d	172	ARG	NE-CZ-NH1	11.92	126.26	120.30
32	M	73	ARG	NE-CZ-NH2	11.92	126.26	120.30
8	h	194	ARG	NE-CZ-NH2	-11.85	114.38	120.30
21	N	618	ARG	NE-CZ-NH2	-11.84	114.38	120.30
23	P	390	TYR	CB-CG-CD2	-11.84	113.90	121.00
28	H	261	ARG	NE-CZ-NH1	-11.82	114.39	120.30
1	a	166	TYR	CB-CG-CD2	-11.81	113.91	121.00
29	I	100	ARG	NE-CZ-NH2	-11.80	114.40	120.30
4	D	120	TYR	CB-CG-CD1	11.79	128.08	121.00
6	F	82	ARG	NE-CZ-NH1	11.76	126.18	120.30
32	M	299	ARG	NE-CZ-NH2	-11.73	114.43	120.30
7	G	201	TYR	CB-CG-CD2	-11.71	113.97	121.00
8	h	198	TYR	CB-CG-CD1	11.65	127.99	121.00
30	K	73	ARG	NE-CZ-NH1	11.64	126.12	120.30
1	a	128	TYR	CB-CG-CD1	11.62	127.97	121.00
23	P	69	ARG	NE-CZ-NH2	-11.61	114.50	120.30
14	n	179	PHE	CB-CG-CD1	11.60	128.92	120.80
14	7	226	ARG	NE-CZ-NH2	-11.57	114.52	120.30
28	H	283	TYR	CB-CG-CD1	-11.56	114.06	121.00
5	E	166	ARG	NE-CZ-NH2	-11.55	114.52	120.30
3	C	149	TYR	CB-CG-CD1	-11.55	114.07	121.00
32	M	77	TYR	CB-CG-CD1	-11.53	114.08	121.00
27	O	70	TYR	CB-CG-CD2	-11.52	114.09	121.00
14	7	189	ARG	NE-CZ-NH1	11.51	126.06	120.30
32	M	164	ASP	CB-CG-OD2	-11.51	107.94	118.30
5	E	136	ARG	NE-CZ-NH1	11.50	126.05	120.30
11	4	148	TYR	CB-CG-CD1	-11.50	114.10	121.00
9	2	215	TYR	CB-CG-CD1	-11.49	114.11	121.00
3	C	98	TYR	CB-CG-CD2	-11.46	114.12	121.00
12	5	202	PHE	CB-CG-CD1	11.45	128.81	120.80
3	c	67	TYR	CB-CG-CD1	-11.43	114.14	121.00
5	e	165	TYR	CB-CG-CD2	-11.41	114.16	121.00
20	Z	497	PHE	CB-CG-CD2	11.40	128.78	120.80
30	K	185	ARG	NE-CZ-NH1	11.38	125.99	120.30
25	R	334	ARG	NE-CZ-NH1	11.37	125.98	120.30
14	n	49	TYR	CB-CG-CD2	-11.35	114.19	121.00
4	d	120	TYR	CB-CG-CD2	-11.35	114.19	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	350	PHE	CB-CG-CD2	-11.33	112.87	120.80
28	H	178	ARG	NE-CZ-NH2	-11.30	114.65	120.30
2	b	235	PHE	CB-CG-CD1	-11.28	112.91	120.80
14	n	124	TYR	CB-CG-CD2	-11.26	114.24	121.00
21	N	124	TYR	CB-CG-CD2	11.25	127.75	121.00
11	k	8	ARG	NE-CZ-NH2	-11.23	114.68	120.30
21	N	528	ARG	NE-CZ-NH1	11.23	125.92	120.30
25	R	338	TYR	CB-CG-CD2	-11.23	114.26	121.00
8	h	120	TYR	CB-CG-CD2	-11.20	114.28	121.00
20	Z	394	TYR	CB-CG-CD1	-11.20	114.28	121.00
1	a	96	ARG	NE-CZ-NH1	11.20	125.90	120.30
2	B	5	TYR	CB-CG-CD1	-11.19	114.28	121.00
10	3	40	PHE	CB-CG-CD1	-11.19	112.97	120.80
2	b	82	TYR	CB-CG-CD1	-11.19	114.29	121.00
20	Z	840	ARG	NE-CZ-NH2	-11.18	114.71	120.30
31	L	291	PHE	CB-CG-CD2	-11.18	112.98	120.80
20	Z	553	ARG	NE-CZ-NH1	11.17	125.89	120.30
8	h	133	TYR	CB-CG-CD2	11.15	127.69	121.00
13	m	106	TYR	CB-CG-CD2	11.11	127.66	121.00
4	D	49	ARG	NE-CZ-NH2	11.11	125.85	120.30
17	T	82	PHE	CB-CG-CD1	11.09	128.56	120.80
22	S	239	ARG	NE-CZ-NH2	-11.07	114.77	120.30
30	K	349	ARG	NE-CZ-NH2	-11.07	114.77	120.30
22	S	239	ARG	NE-CZ-NH1	11.06	125.83	120.30
1	A	128	TYR	CB-CG-CD1	11.02	127.61	121.00
20	Z	193	PHE	CB-CG-CD1	11.02	128.51	120.80
22	S	253	PHE	CB-CG-CD2	-11.02	113.09	120.80
16	V	196	TYR	CB-CG-CD1	10.95	127.57	121.00
16	V	108	TYR	CB-CG-CD2	-10.95	114.43	121.00
30	K	426	PHE	CB-CG-CD1	-10.93	113.15	120.80
21	N	618	ARG	NE-CZ-NH1	10.93	125.77	120.30
24	Q	434	TYR	CB-CG-CD1	10.93	127.56	121.00
33	J	231	ARG	NE-CZ-NH1	-10.93	114.84	120.30
8	h	45	ARG	NE-CZ-NH1	10.93	125.76	120.30
4	d	156	TYR	CB-CG-CD1	10.83	127.50	121.00
27	O	310	PHE	CB-CG-CD1	10.79	128.35	120.80
21	N	398	ARG	NE-CZ-NH2	-10.79	114.91	120.30
33	J	97	ASP	CB-CG-OD2	10.78	128.00	118.30
30	K	185	ARG	NE-CZ-NH2	-10.77	114.91	120.30
11	4	36	ARG	NE-CZ-NH2	-10.77	114.92	120.30
11	4	23	ARG	NE-CZ-NH1	-10.75	114.92	120.30
31	L	357	ARG	NE-CZ-NH2	-10.75	114.92	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	194	ARG	NE-CZ-NH2	-10.74	114.93	120.30
20	Z	298	PHE	CB-CG-CD1	10.73	128.31	120.80
24	Q	232	TYR	CB-CG-CD1	-10.72	114.57	121.00
21	N	471	TYR	CB-CG-CD1	-10.72	114.57	121.00
28	H	90	ARG	NE-CZ-NH1	10.71	125.65	120.30
24	Q	209	TYR	CB-CG-CD1	10.70	127.42	121.00
6	F	174	ARG	NE-CZ-NH2	-10.69	114.96	120.30
12	l	202	PHE	CB-CG-CD2	-10.66	113.33	120.80
9	2	48	ARG	NE-CZ-NH2	-10.64	114.98	120.30
20	Z	385	PHE	CB-CG-CD1	10.64	128.25	120.80
11	4	190	ARG	NE-CZ-NH1	10.58	125.59	120.30
5	e	26	TYR	CB-CG-CD2	-10.54	114.67	121.00
4	D	22	TYR	CB-CG-CD1	10.54	127.32	121.00
20	Z	172	ASP	CB-CG-OD2	-10.54	108.82	118.30
32	M	164	ASP	CB-CG-OD1	10.52	127.77	118.30
14	7	128	TYR	CB-CG-CD2	-10.50	114.70	121.00
33	J	231	ARG	NE-CZ-NH2	10.49	125.55	120.30
21	N	682	PHE	CB-CG-CD1	10.49	128.14	120.80
3	c	4	ARG	NE-CZ-NH1	10.48	125.54	120.30
23	P	379	TYR	CB-CG-CD1	-10.48	114.71	121.00
7	g	201	TYR	CB-CG-CD2	-10.47	114.72	121.00
2	b	83	ARG	NE-CZ-NH1	10.43	125.52	120.30
6	F	99	PHE	CB-CG-CD2	10.41	128.09	120.80
13	m	202	ARG	NE-CZ-NH2	-10.40	115.10	120.30
25	R	263	ARG	NE-CZ-NH2	-10.40	115.10	120.30
22	S	377	TYR	CB-CG-CD2	10.37	127.22	121.00
24	Q	65	TYR	CB-CG-CD1	10.36	127.22	121.00
28	H	173	ARG	NE-CZ-NH1	-10.34	115.13	120.30
18	X	98	PHE	CB-CG-CD2	10.34	128.04	120.80
20	Z	623	ARG	NE-CZ-NH2	-10.33	115.13	120.30
26	U	32	ARG	NE-CZ-NH1	10.33	125.47	120.30
11	4	195	PHE	CB-CG-CD2	-10.32	113.57	120.80
6	f	202	ARG	NE-CZ-NH2	-10.32	115.14	120.30
22	S	298	ARG	NE-CZ-NH1	10.32	125.46	120.30
11	k	70	ARG	NE-CZ-NH2	-10.30	115.15	120.30
20	Z	840	ARG	NE-CZ-NH1	10.29	125.45	120.30
18	X	11	ARG	NE-CZ-NH2	-10.29	115.15	120.30
11	k	174	MET	CG-SD-CE	-10.28	83.75	100.20
22	S	271	ARG	NE-CZ-NH1	10.27	125.44	120.30
22	S	95	PHE	CB-CG-CD1	10.26	127.98	120.80
17	T	266	TYR	CB-CG-CD1	10.25	127.15	121.00
2	B	124	SER	N-CA-CB	10.23	125.84	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	82	ARG	NE-CZ-NH1	-10.22	115.19	120.30
14	7	241	PHE	CB-CG-CD2	-10.20	113.66	120.80
20	Z	165	TYR	CB-CG-CD1	10.19	127.12	121.00
22	S	286	TYR	CB-CG-CD2	-10.18	114.89	121.00
31	L	299	ARG	NE-CZ-NH1	10.17	125.39	120.30
2	B	23	TYR	CB-CG-CD1	10.16	127.09	121.00
1	a	110	TYR	CG-CD2-CE2	-10.15	113.18	121.30
24	Q	409	TYR	CB-CG-CD2	-10.13	114.92	121.00
21	N	548	ARG	NE-CZ-NH1	10.11	125.35	120.30
16	V	42	ARG	NE-CZ-NH2	10.10	125.35	120.30
28	H	385	ARG	NE-CZ-NH1	-10.06	115.27	120.30
8	h	133	TYR	CB-CG-CD1	-10.06	114.96	121.00
21	N	417	ARG	NE-CZ-NH2	10.04	125.32	120.30
4	D	172	ARG	NE-CZ-NH1	10.01	125.31	120.30
25	R	307	TYR	CB-CG-CD2	-10.00	115.00	121.00
33	J	311	ASP	CB-CG-OD1	9.99	127.29	118.30
23	P	201	ARG	NE-CZ-NH2	-9.99	115.31	120.30
23	P	395	ARG	NE-CZ-NH1	9.98	125.29	120.30
6	F	123	TYR	CB-CG-CD1	-9.95	115.03	121.00
29	I	422	ARG	NE-CZ-NH2	-9.95	115.33	120.30
6	f	171	TYR	CB-CG-CD2	-9.93	115.04	121.00
27	O	70	TYR	CB-CG-CD1	9.92	126.95	121.00
30	K	346	ARG	NE-CZ-NH1	-9.92	115.34	120.30
23	P	208	PHE	CB-CG-CD1	9.91	127.73	120.80
8	1	120	TYR	CB-CG-CD2	-9.90	115.06	121.00
21	N	325	PHE	CB-CG-CD2	-9.90	113.87	120.80
13	6	46	ARG	NE-CZ-NH1	-9.89	115.35	120.30
4	d	172	ARG	NE-CZ-NH2	-9.88	115.36	120.30
15	W	26	PHE	CB-CG-CD2	9.87	127.70	120.80
27	O	356	ARG	NE-CZ-NH2	-9.86	115.37	120.30
20	Z	497	PHE	CB-CG-CD1	-9.85	113.91	120.80
9	2	232	TYR	CB-CG-CD2	-9.83	115.10	121.00
3	C	217	ARG	NE-CZ-NH1	9.82	125.21	120.30
24	Q	306	TYR	CB-CG-CD2	-9.81	115.11	121.00
11	k	93	ARG	NE-CZ-NH1	9.80	125.20	120.30
21	N	211	PHE	CB-CG-CD1	9.79	127.65	120.80
21	N	894	ARG	NE-CZ-NH1	9.79	125.19	120.30
1	A	12	TYR	CB-CG-CD2	-9.77	115.14	121.00
4	D	112	TYR	CB-CG-CD1	9.76	126.86	121.00
5	E	166	ARG	NE-CZ-NH1	9.76	125.18	120.30
23	P	221	TYR	CB-CG-CD1	-9.74	115.16	121.00
12	5	200	ASP	CB-CG-OD2	-9.71	109.56	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	249	ASP	CB-CG-OD1	9.69	127.02	118.30
3	C	131	PHE	CB-CG-CD1	9.68	127.58	120.80
14	7	226	ARG	NE-CZ-NH1	9.68	125.14	120.30
20	Z	441	TYR	CB-CG-CD2	9.68	126.81	121.00
8	1	202	TYR	CB-CG-CD1	9.67	126.81	121.00
28	H	420	ARG	NE-CZ-NH2	-9.67	115.46	120.30
4	d	4	TYR	CB-CG-CD1	9.65	126.79	121.00
27	O	69	PHE	CB-CG-CD1	9.65	127.56	120.80
33	J	324	ARG	NE-CZ-NH2	-9.65	115.48	120.30
15	W	179	ARG	NE-CZ-NH1	9.64	125.12	120.30
3	C	67	TYR	CB-CG-CD2	-9.63	115.22	121.00
31	L	289	ARG	NE-CZ-NH2	-9.62	115.49	120.30
21	N	188	TYR	CB-CG-CD2	-9.60	115.24	121.00
8	1	146	TYR	CB-CG-CD2	-9.60	115.24	121.00
1	A	128	TYR	CB-CG-CD2	-9.58	115.25	121.00
21	N	585	ARG	NE-CZ-NH2	-9.58	115.51	120.30
5	e	123	PHE	CB-CG-CD2	-9.58	114.10	120.80
6	f	128	TYR	CB-CG-CD1	9.57	126.74	121.00
13	6	149	ALA	CB-CA-C	-9.56	95.75	110.10
14	n	109	TYR	CB-CG-CD2	-9.55	115.27	121.00
21	N	604	ARG	NE-CZ-NH2	-9.55	115.52	120.30
27	O	110	ASP	CB-CG-OD1	9.55	126.90	118.30
15	W	113	PHE	CB-CG-CD2	-9.54	114.12	120.80
1	A	96	ARG	NE-CZ-NH1	9.52	125.06	120.30
6	f	164	ARG	NE-CZ-NH1	9.51	125.06	120.30
30	K	128	ARG	NE-CZ-NH2	-9.51	115.55	120.30
9	2	119	TYR	CB-CG-CD2	-9.50	115.30	121.00
22	S	55	ARG	NE-CZ-NH1	9.50	125.05	120.30
13	6	15	ASP	CB-CG-OD2	-9.50	109.75	118.30
19	Y	86	ARG	NE-CZ-NH2	9.49	125.05	120.30
13	6	109	ARG	NE-CZ-NH1	9.48	125.04	120.30
21	N	786	ARG	NE-CZ-NH2	-9.44	115.58	120.30
12	5	179	TYR	CB-CG-CD2	-9.41	115.35	121.00
24	Q	51	ARG	NE-CZ-NH2	9.39	125.00	120.30
33	J	212	ARG	NE-CZ-NH2	-9.38	115.61	120.30
26	U	233	PHE	CB-CG-CD1	-9.38	114.23	120.80
14	7	179	PHE	CB-CG-CD1	9.38	127.36	120.80
8	h	26	ASP	CB-CG-OD1	9.37	126.73	118.30
15	W	57	ALA	N-CA-CB	9.37	123.22	110.10
4	D	172	ARG	NE-CZ-NH2	-9.36	115.62	120.30
12	5	200	ASP	CB-CG-OD1	9.36	126.72	118.30
22	S	473	ASP	CB-CG-OD1	9.34	126.71	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	i	65	ARG	NE-CZ-NH2	9.33	124.97	120.30
28	H	101	ARG	NE-CZ-NH2	-9.31	115.64	120.30
1	a	26	TYR	CB-CG-CD2	-9.27	115.44	121.00
9	i	217	ARG	NE-CZ-NH2	-9.27	115.67	120.30
8	h	26	ASP	CB-CG-OD2	-9.26	109.96	118.30
13	6	110	PHE	CB-CG-CD1	-9.25	114.33	120.80
1	A	12	TYR	CB-CG-CD1	9.24	126.54	121.00
29	I	222	TYR	CB-CG-CD2	9.23	126.54	121.00
30	K	399	ARG	NE-CZ-NH1	9.22	124.91	120.30
16	V	108	TYR	CB-CG-CD1	9.22	126.53	121.00
20	Z	441	TYR	CB-CG-CD1	-9.22	115.47	121.00
16	V	100	ARG	NE-CZ-NH2	-9.21	115.70	120.30
14	n	226	ARG	NE-CZ-NH1	9.20	124.90	120.30
23	P	329	PHE	CB-CG-CD2	-9.20	114.36	120.80
3	C	122	TYR	CB-CG-CD1	9.16	126.50	121.00
14	7	241	PHE	CB-CG-CD1	9.14	127.20	120.80
21	N	139	ARG	NE-CZ-NH1	9.14	124.87	120.30
5	e	232	ASP	CB-CG-OD2	-9.13	110.08	118.30
22	S	382	ARG	NE-CZ-NH1	9.13	124.86	120.30
21	N	422	TYR	CB-CG-CD2	9.12	126.47	121.00
24	Q	32	ASP	CB-CG-OD1	9.12	126.51	118.30
23	P	439	MET	CG-SD-CE	-9.11	85.62	100.20
14	7	128	TYR	CB-CG-CD1	9.11	126.46	121.00
20	Z	193	PHE	CB-CG-CD2	-9.10	114.43	120.80
32	M	357	ARG	NE-CZ-NH1	-9.09	115.75	120.30
4	D	11	PHE	CB-CG-CD2	-9.09	114.44	120.80
21	N	839	ARG	NE-CZ-NH1	9.09	124.84	120.30
16	V	171	ARG	NE-CZ-NH1	9.09	124.84	120.30
14	n	68	ARG	NE-CZ-NH2	-9.08	115.76	120.30
31	L	88	TYR	CB-CG-CD2	-9.07	115.56	121.00
6	F	89	ARG	NE-CZ-NH2	9.07	124.83	120.30
10	3	68	ARG	NE-CZ-NH2	-9.06	115.77	120.30
14	n	228	PHE	CB-CG-CD1	9.05	127.14	120.80
13	m	225	TYR	CB-CG-CD2	-9.04	115.58	121.00
1	a	30	TYR	CB-CG-CD1	9.04	126.42	121.00
1	a	166	TYR	CB-CG-CD1	9.04	126.42	121.00
31	L	291	PHE	CB-CG-CD1	9.02	127.11	120.80
11	4	121	TYR	CB-CG-CD1	-9.02	115.59	121.00
30	K	234	PHE	CB-CG-CD1	-9.02	114.49	120.80
21	N	906	ARG	NE-CZ-NH2	-9.01	115.79	120.30
20	Z	939	ALA	N-CA-CB	8.99	122.69	110.10
26	U	56	PHE	CB-CG-CD1	8.99	127.10	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	196	TYR	CB-CG-CD2	-8.98	115.61	121.00
4	D	232	TYR	CB-CG-CD2	-8.98	115.61	121.00
14	n	223	ARG	NE-CZ-NH2	-8.97	115.81	120.30
20	Z	358	TYR	CB-CG-CD2	-8.97	115.62	121.00
20	Z	608	TYR	CB-CG-CD2	-8.97	115.62	121.00
2	B	82	TYR	CB-CG-CD1	8.96	126.38	121.00
8	1	14	ALA	N-CA-CB	8.96	122.65	110.10
27	O	369	ARG	NE-CZ-NH2	-8.95	115.82	120.30
11	4	83	PHE	CB-CG-CD2	-8.95	114.54	120.80
5	e	86	ARG	NH1-CZ-NH2	8.94	129.24	119.40
31	L	264	ARG	NE-CZ-NH2	-8.93	115.84	120.30
22	S	185	PHE	CB-CG-CD2	-8.91	114.56	120.80
8	h	148	ASP	CB-CG-OD1	8.91	126.31	118.30
21	N	148	SER	N-CA-CB	8.91	123.86	110.50
5	E	103	TYR	CB-CG-CD1	-8.89	115.67	121.00
20	Z	165	TYR	CB-CG-CD2	-8.89	115.67	121.00
11	k	73	TYR	CB-CG-CD2	8.89	126.33	121.00
3	C	98	TYR	CB-CG-CD1	8.88	126.33	121.00
8	1	96	TYR	CB-CG-CD2	-8.88	115.67	121.00
22	S	473	ASP	CB-CG-OD2	-8.88	110.31	118.30
10	j	99	ARG	NE-CZ-NH1	8.88	124.74	120.30
24	Q	400	TYR	CB-CG-CD1	8.87	126.32	121.00
7	G	201	TYR	CB-CG-CD1	8.87	126.32	121.00
25	R	141	TYR	CB-CG-CD2	-8.86	115.68	121.00
28	H	289	ARG	NE-CZ-NH1	8.86	124.73	120.30
21	N	604	ARG	NE-CZ-NH1	8.86	124.73	120.30
14	7	179	PHE	CB-CG-CD2	-8.86	114.60	120.80
9	i	119	TYR	CB-CG-CD1	8.85	126.31	121.00
15	W	25	ARG	NE-CZ-NH2	-8.84	115.88	120.30
30	K	234	PHE	CB-CG-CD2	8.83	126.98	120.80
11	4	59	TYR	CB-CG-CD1	8.81	126.29	121.00
21	N	386	MET	CG-SD-CE	-8.80	86.11	100.20
33	J	234	PHE	CB-CG-CD2	8.80	126.96	120.80
11	k	8	ARG	NE-CZ-NH1	8.80	124.70	120.30
24	Q	391	ASP	CB-CG-OD2	8.80	126.22	118.30
13	6	139	TYR	CB-CG-CD1	-8.78	115.73	121.00
13	m	106	TYR	CB-CG-CD1	-8.76	115.74	121.00
20	Z	513	ALA	CB-CA-C	8.76	123.23	110.10
28	H	370	ARG	NE-CZ-NH2	8.76	124.68	120.30
12	l	139	ARG	NE-CZ-NH2	-8.74	115.93	120.30
2	b	104	TYR	CB-CG-CD2	-8.72	115.77	121.00
25	R	331	ARG	NE-CZ-NH2	8.72	124.66	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	338	TYR	CB-CG-CD1	8.72	126.23	121.00
27	O	69	PHE	CB-CG-CD2	-8.72	114.69	120.80
27	O	306	ARG	NE-CZ-NH2	-8.71	115.94	120.30
29	I	265	ARG	NE-CZ-NH1	-8.72	115.94	120.30
1	a	77	ARG	NE-CZ-NH1	8.71	124.66	120.30
7	g	72	ARG	NE-CZ-NH1	8.71	124.66	120.30
16	V	171	ARG	NE-CZ-NH2	-8.71	115.95	120.30
7	G	20	ARG	NE-CZ-NH2	-8.71	115.95	120.30
2	B	174	PHE	CB-CG-CD2	8.70	126.89	120.80
21	N	455	MET	CG-SD-CE	-8.69	86.30	100.20
1	a	77	ARG	NE-CZ-NH2	-8.69	115.96	120.30
5	E	92	ALA	N-CA-CB	8.68	122.25	110.10
5	E	53	ARG	NE-CZ-NH2	-8.64	115.98	120.30
17	T	20	TYR	CB-CG-CD1	-8.63	115.82	121.00
27	O	228	TYR	CG-CD2-CE2	-8.63	114.40	121.30
20	Z	813	PHE	CB-CG-CD1	8.62	126.84	120.80
24	Q	339	TYR	CB-CG-CD1	8.62	126.17	121.00
7	G	181	ASP	CB-CG-OD1	8.61	126.05	118.30
13	6	224	PHE	CB-CG-CD1	-8.61	114.77	120.80
29	I	304	ARG	NE-CZ-NH2	-8.60	116.00	120.30
24	Q	189	ARG	NE-CZ-NH1	-8.60	116.00	120.30
20	Z	838	TYR	CG-CD1-CE1	-8.59	114.43	121.30
22	S	259	TYR	CB-CG-CD1	-8.59	115.84	121.00
7	G	242	PHE	CB-CG-CD2	-8.59	114.79	120.80
8	h	39	VAL	CA-CB-CG1	-8.59	98.02	110.90
4	d	197	ARG	NE-CZ-NH2	-8.58	116.01	120.30
21	N	889	ARG	NE-CZ-NH2	8.58	124.59	120.30
20	Z	385	PHE	CB-CG-CD2	-8.56	114.81	120.80
14	n	98	ARG	NE-CZ-NH1	8.54	124.57	120.30
22	S	480	ARG	NE-CZ-NH1	-8.53	116.03	120.30
6	F	174	ARG	NE-CZ-NH1	8.53	124.56	120.30
1	A	73	PHE	CB-CG-CD1	-8.51	114.84	120.80
13	m	68	ASP	CB-CG-OD2	-8.51	110.64	118.30
31	L	180	PHE	CB-CG-CD1	8.51	126.75	120.80
24	Q	383	ASP	CB-CG-OD1	-8.50	110.65	118.30
5	e	53	ARG	NE-CZ-NH1	8.50	124.55	120.30
8	1	151	PHE	CB-CG-CD1	-8.49	114.85	120.80
27	O	88	ASP	CB-CG-OD1	8.49	125.94	118.30
29	I	319	ARG	NE-CZ-NH1	8.49	124.55	120.30
20	Z	522	THR	CA-CB-CG2	-8.47	100.54	112.40
24	Q	239	PHE	CB-CG-CD1	-8.47	114.87	120.80
7	G	15	PHE	CB-CG-CD2	-8.46	114.88	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	174	PHE	CB-CG-CD2	8.46	126.72	120.80
32	M	339	ARG	NE-CZ-NH2	-8.46	116.07	120.30
21	N	548	ARG	NE-CZ-NH2	-8.46	116.07	120.30
33	J	234	PHE	CB-CG-CD1	-8.45	114.88	120.80
31	L	316	ASP	CB-CG-OD2	8.45	125.91	118.30
20	Z	323	TYR	CB-CG-CD2	8.45	126.07	121.00
10	3	203	ARG	NE-CZ-NH2	-8.45	116.08	120.30
5	E	136	ARG	NE-CZ-NH2	-8.45	116.08	120.30
20	Z	413	ASP	CB-CG-OD2	-8.44	110.70	118.30
6	f	14	SER	N-CA-CB	8.44	123.16	110.50
25	R	345	TYR	CB-CG-CD1	8.43	126.06	121.00
8	1	16	THR	CA-CB-CG2	-8.43	100.60	112.40
17	T	122	PHE	CB-CG-CD1	-8.43	114.90	120.80
22	S	332	PHE	CB-CG-CD1	8.43	126.70	120.80
22	S	248	ASP	CB-CG-OD1	8.43	125.88	118.30
14	7	136	ARG	NE-CZ-NH1	8.43	124.51	120.30
32	M	33	ARG	NE-CZ-NH2	-8.42	116.09	120.30
8	1	70	TYR	CB-CG-CD2	8.41	126.05	121.00
23	P	310	ARG	NE-CZ-NH2	8.41	124.51	120.30
1	A	234	PHE	CB-CG-CD1	-8.41	114.91	120.80
25	R	382	ASP	CB-CG-OD1	-8.41	110.73	118.30
27	O	81	TYR	CB-CG-CD1	-8.41	115.96	121.00
13	m	83	TYR	CB-CG-CD2	-8.40	115.96	121.00
5	E	102	TYR	CB-CG-CD1	8.40	126.04	121.00
3	C	4	ARG	NE-CZ-NH2	8.39	124.50	120.30
13	6	46	ARG	NE-CZ-NH2	8.37	124.49	120.30
21	N	325	PHE	CB-CG-CD1	8.37	126.66	120.80
6	F	14	SER	N-CA-CB	8.37	123.05	110.50
31	L	78	ARG	NE-CZ-NH1	8.36	124.48	120.30
7	g	84	ASP	CB-CG-OD2	-8.35	110.78	118.30
2	B	5	TYR	CB-CG-CD2	8.35	126.01	121.00
8	1	202	TYR	CB-CG-CD2	-8.35	115.99	121.00
17	T	162	ASP	CB-CG-OD2	-8.35	110.79	118.30
16	V	275	ASP	CB-CG-OD1	8.34	125.81	118.30
4	d	127	ARG	NE-CZ-NH1	8.33	124.47	120.30
13	m	139	TYR	CB-CG-CD1	-8.33	116.00	121.00
28	H	420	ARG	NE-CZ-NH1	8.32	124.46	120.30
31	L	413	ASP	CB-CG-OD2	-8.32	110.81	118.30
14	n	179	PHE	CB-CG-CD2	-8.31	114.98	120.80
16	V	20	ARG	NE-CZ-NH1	-8.30	116.15	120.30
24	Q	75	ARG	NE-CZ-NH1	8.30	124.45	120.30
33	J	71	TYR	CB-CG-CD1	-8.30	116.02	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	202	PHE	CB-CG-CD2	-8.30	114.99	120.80
21	N	394	ARG	NE-CZ-NH1	-8.29	116.15	120.30
13	m	41	TYR	CB-CG-CD2	8.29	125.97	121.00
28	H	454	TYR	CB-CG-CD2	-8.28	116.03	121.00
5	e	10	ARG	NE-CZ-NH2	-8.28	116.16	120.30
9	2	140	PHE	CB-CG-CD1	-8.27	115.01	120.80
27	O	245	ASP	CB-CG-OD1	-8.27	110.86	118.30
31	L	78	ARG	NE-CZ-NH2	-8.27	116.16	120.30
7	G	157	TYR	CG-CD1-CE1	8.27	127.91	121.30
22	S	170	TYR	CB-CG-CD1	8.27	125.96	121.00
22	S	158	PHE	CB-CG-CD1	-8.26	115.02	120.80
15	W	144	PHE	CB-CG-CD2	-8.26	115.02	120.80
29	I	436	TYR	CB-CG-CD1	-8.26	116.04	121.00
22	S	198	SER	N-CA-CB	8.26	122.89	110.50
31	L	329	ARG	NE-CZ-NH2	8.26	124.43	120.30
7	G	242	PHE	CB-CG-CD1	8.25	126.58	120.80
21	N	735	MET	CG-SD-CE	-8.25	87.00	100.20
11	4	107	TYR	CB-CG-CD2	-8.24	116.05	121.00
20	Z	928	ARG	NE-CZ-NH1	8.24	124.42	120.30
14	7	98	ARG	NE-CZ-NH1	8.24	124.42	120.30
29	I	407	ARG	NE-CZ-NH2	-8.24	116.18	120.30
11	k	32	ASP	CB-CG-OD2	8.22	125.70	118.30
14	7	189	ARG	NE-CZ-NH2	-8.22	116.19	120.30
20	Z	59	ASP	CB-CG-OD2	-8.21	110.91	118.30
22	S	292	TYR	CB-CG-CD1	-8.21	116.07	121.00
24	Q	332	ARG	NE-CZ-NH2	-8.21	116.20	120.30
31	L	82	ARG	NE-CZ-NH1	8.21	124.40	120.30
4	D	179	TYR	CB-CG-CD1	-8.21	116.08	121.00
29	I	350	PHE	CB-CG-CD1	8.20	126.54	120.80
1	A	73	PHE	CB-CG-CD2	8.19	126.54	120.80
21	N	260	ASP	CB-CG-OD2	8.19	125.67	118.30
7	g	181	ASP	CB-CG-OD2	8.18	125.67	118.30
7	g	130	ARG	NE-CZ-NH1	8.18	124.39	120.30
25	R	304	TYR	CB-CG-CD2	-8.18	116.09	121.00
28	H	318	ARG	NE-CZ-NH2	-8.18	116.21	120.30
2	b	83	ARG	NE-CZ-NH2	-8.17	116.21	120.30
9	2	108	ALA	N-CA-CB	8.17	121.54	110.10
10	j	99	ARG	NE-CZ-NH2	-8.17	116.22	120.30
16	V	69	PHE	CB-CG-CD2	8.16	126.52	120.80
22	S	29	ASP	CB-CG-OD2	-8.15	110.97	118.30
12	5	165	TYR	CB-CG-CD1	8.15	125.89	121.00
4	d	120	TYR	CB-CG-CD1	8.14	125.88	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	408	ARG	NE-CZ-NH1	8.13	124.37	120.30
11	4	130	TYR	CG-CD2-CE2	-8.13	114.79	121.30
21	N	302	PHE	CB-CG-CD2	-8.13	115.11	120.80
23	P	379	TYR	CB-CG-CD2	8.13	125.88	121.00
26	U	289	ASP	CB-CG-OD1	-8.13	110.99	118.30
20	Z	283	ALA	N-CA-CB	8.13	121.48	110.10
3	C	140	TYR	CB-CG-CD1	-8.12	116.13	121.00
14	n	58	ASP	CB-CG-OD1	8.11	125.60	118.30
29	I	268	PHE	CB-CG-CD1	-8.11	115.12	120.80
32	M	381	ARG	NE-CZ-NH1	8.10	124.35	120.30
21	N	58	ARG	NE-CZ-NH2	8.10	124.35	120.30
30	K	406	ASP	CB-CG-OD1	-8.09	111.02	118.30
28	H	432	ARG	NE-CZ-NH1	-8.09	116.25	120.30
5	E	138	PHE	CB-CG-CD2	-8.09	115.14	120.80
14	7	194	ARG	NE-CZ-NH2	-8.07	116.27	120.30
27	O	33	TYR	CB-CG-CD1	8.07	125.84	121.00
18	X	45	PHE	CB-CG-CD2	8.07	126.45	120.80
26	U	113	TYR	CG-CD1-CE1	-8.07	114.85	121.30
17	T	210	PHE	CB-CG-CD1	-8.05	115.16	120.80
19	Y	71	ASP	CB-CG-OD1	-8.05	111.05	118.30
21	N	406	TYR	CB-CG-CD1	8.05	125.83	121.00
8	h	48	ASP	CB-CG-OD2	-8.04	111.07	118.30
16	V	142	ASP	CB-CG-OD2	8.04	125.53	118.30
14	7	261	TYR	CG-CD1-CE1	8.02	127.72	121.30
7	g	146	ALA	N-CA-CB	8.02	121.32	110.10
31	L	339	ARG	NE-CZ-NH1	-8.01	116.30	120.30
20	Z	172	ASP	CB-CG-OD1	8.00	125.50	118.30
26	U	189	ARG	NE-CZ-NH1	8.00	124.30	120.30
14	7	261	TYR	CB-CG-CD2	8.00	125.80	121.00
2	b	101	TYR	CB-CG-CD2	7.99	125.80	121.00
4	d	68	ASP	CB-CG-OD1	-7.99	111.11	118.30
17	T	82	PHE	CG-CD2-CE2	7.98	129.58	120.80
9	i	207	MET	CG-SD-CE	-7.96	87.46	100.20
32	M	73	ARG	NE-CZ-NH1	-7.96	116.32	120.30
6	f	157	TYR	CB-CG-CD1	-7.96	116.22	121.00
11	k	89	ALA	N-CA-CB	7.95	121.23	110.10
2	b	234	ARG	NE-CZ-NH1	-7.95	116.33	120.30
8	h	14	ALA	N-CA-CB	7.95	121.23	110.10
6	F	20	PHE	CB-CG-CD2	-7.95	115.24	120.80
28	H	403	ARG	NE-CZ-NH2	-7.95	116.33	120.30
3	c	113	ARG	NE-CZ-NH2	7.93	124.27	120.30
11	k	121	TYR	CB-CG-CD2	-7.93	116.24	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	471	TYR	CB-CG-CD2	7.93	125.76	121.00
11	k	139	TYR	CB-CG-CD1	7.92	125.75	121.00
20	Z	80	SER	N-CA-CB	7.92	122.38	110.50
8	1	38	ARG	NE-CZ-NH2	-7.92	116.34	120.30
20	Z	813	PHE	CB-CG-CD2	-7.91	115.26	120.80
13	6	29	ALA	N-CA-CB	7.90	121.16	110.10
11	k	85	ARG	NE-CZ-NH2	7.90	124.25	120.30
20	Z	319	THR	CA-CB-CG2	-7.90	101.34	112.40
1	a	244	ARG	NE-CZ-NH1	7.89	124.24	120.30
12	5	262	TYR	CB-CG-CD2	-7.88	116.27	121.00
10	3	199	TYR	CB-CG-CD1	-7.88	116.27	121.00
24	Q	127	ARG	NE-CZ-NH2	-7.88	116.36	120.30
27	O	158	ASP	CB-CG-OD1	-7.88	111.21	118.30
4	D	90	ARG	NE-CZ-NH2	-7.88	116.36	120.30
31	L	315	PHE	CB-CG-CD2	-7.88	115.29	120.80
29	I	120	VAL	CA-CB-CG1	-7.86	99.10	110.90
5	E	102	TYR	CB-CG-CD2	-7.86	116.28	121.00
3	C	122	TYR	CB-CG-CD2	-7.86	116.28	121.00
7	g	201	TYR	CB-CG-CD1	7.86	125.72	121.00
26	U	22	TYR	CB-CG-CD2	-7.85	116.29	121.00
11	4	135	TYR	CB-CG-CD1	-7.85	116.29	121.00
19	Y	70	ASP	CB-CG-OD1	-7.85	111.23	118.30
20	Z	825	ALA	N-CA-CB	7.85	121.09	110.10
13	m	82	TRP	CB-CG-CD2	-7.84	116.41	126.60
10	3	193	ASP	CB-CG-OD2	-7.84	111.24	118.30
7	G	157	TYR	CD1-CE1-CZ	-7.84	112.75	119.80
1	a	94	ALA	N-CA-CB	7.83	121.07	110.10
24	Q	110	SER	N-CA-CB	7.83	122.25	110.50
3	C	140	TYR	CB-CG-CD2	7.83	125.70	121.00
20	Z	918	ASP	CB-CG-OD1	-7.83	111.26	118.30
32	M	247	ALA	CB-CA-C	7.81	121.82	110.10
20	Z	553	ARG	NE-CZ-NH2	-7.81	116.39	120.30
20	Z	739	ALA	N-CA-CB	7.81	121.04	110.10
29	I	436	TYR	CG-CD1-CE1	-7.81	115.05	121.30
21	N	801	THR	CA-CB-CG2	-7.80	101.47	112.40
2	B	83	ARG	NE-CZ-NH1	-7.80	116.40	120.30
22	S	145	PHE	CB-CG-CD2	7.80	126.26	120.80
22	S	285	ASP	CB-CG-OD1	7.79	125.31	118.30
23	P	395	ARG	NH1-CZ-NH2	-7.79	110.83	119.40
21	N	881	TYR	CB-CG-CD1	-7.77	116.34	121.00
14	n	98	ARG	NE-CZ-NH2	-7.77	116.42	120.30
21	N	417	ARG	NE-CZ-NH1	-7.76	116.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	209	TYR	CB-CG-CD2	-7.75	116.35	121.00
13	m	85	PHE	CB-CG-CD2	-7.74	115.38	120.80
12	l	144	ARG	NE-CZ-NH2	-7.74	116.43	120.30
30	K	121	ARG	NE-CZ-NH1	7.73	124.17	120.30
2	b	128	ARG	NE-CZ-NH2	7.72	124.16	120.30
15	W	17	ARG	NE-CZ-NH1	7.72	124.16	120.30
21	N	117	TYR	CB-CG-CD2	-7.72	116.37	121.00
30	K	246	TYR	CB-CG-CD2	-7.71	116.37	121.00
1	a	110	TYR	CG-CD1-CE1	-7.70	115.14	121.30
28	H	373	ARG	NE-CZ-NH2	-7.70	116.45	120.30
32	M	118	VAL	CA-CB-CG2	-7.70	99.36	110.90
9	2	126	TYR	CG-CD2-CE2	-7.69	115.14	121.30
12	l	245	TYR	CB-CG-CD1	-7.69	116.39	121.00
8	1	70	TYR	CB-CG-CD1	-7.68	116.39	121.00
6	f	87	TYR	CB-CG-CD2	-7.68	116.39	121.00
21	N	328	PHE	CB-CG-CD1	7.67	126.17	120.80
21	N	805	SER	N-CA-CB	7.67	122.00	110.50
18	X	96	ARG	NE-CZ-NH1	7.67	124.13	120.30
17	T	267	ALA	N-CA-CB	7.66	120.83	110.10
24	Q	267	LEU	CB-CG-CD1	7.66	124.02	111.00
11	4	83	PHE	CB-CG-CD1	7.65	126.16	120.80
32	M	339	ARG	NE-CZ-NH1	7.64	124.12	120.30
25	R	300	ASP	CB-CG-OD1	7.64	125.17	118.30
20	Z	794	ASP	CB-CG-OD1	-7.63	111.43	118.30
3	c	129	ARG	NE-CZ-NH2	-7.63	116.48	120.30
15	W	35	PHE	CB-CG-CD2	7.62	126.14	120.80
21	N	398	ARG	NE-CZ-NH1	7.62	124.11	120.30
6	f	9	ASP	CB-CG-OD2	7.61	125.15	118.30
9	i	119	TYR	CB-CG-CD2	-7.61	116.43	121.00
22	S	405	ARG	NE-CZ-NH1	7.61	124.11	120.30
10	j	199	TYR	CB-CG-CD2	-7.61	116.44	121.00
27	O	39	PHE	CB-CG-CD2	-7.60	115.48	120.80
24	Q	20	TYR	CB-CG-CD1	-7.60	116.44	121.00
14	n	58	ASP	CB-CG-OD2	-7.60	111.46	118.30
9	2	85	THR	CA-CB-CG2	-7.60	101.76	112.40
1	A	162	TYR	CG-CD2-CE2	-7.60	115.22	121.30
16	V	197	TYR	CB-CG-CD1	7.59	125.56	121.00
9	i	126	TYR	CB-CG-CD2	7.59	125.56	121.00
7	g	20	ARG	NE-CZ-NH1	7.59	124.09	120.30
4	d	127	ARG	NE-CZ-NH2	-7.59	116.51	120.30
22	S	346	TYR	CB-CG-CD2	-7.59	116.45	121.00
9	i	99	THR	CA-CB-CG2	-7.58	101.79	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	D	108	TYR	CD1-CE1-CZ	7.57	126.61	119.80
8	h	151	PHE	CB-CG-CD1	7.57	126.10	120.80
4	D	129	PHE	CG-CD2-CE2	7.57	129.13	120.80
24	Q	416	VAL	CA-CB-CG2	-7.57	99.54	110.90
27	O	371	VAL	CA-CB-CG2	-7.56	99.56	110.90
13	6	41	TYR	CG-CD2-CE2	7.56	127.35	121.30
13	m	224	PHE	CB-CG-CD2	-7.55	115.52	120.80
26	U	137	TYR	CB-CG-CD2	-7.55	116.47	121.00
1	a	32	PHE	CB-CG-CD1	-7.54	115.52	120.80
8	1	184	MET	CG-SD-CE	-7.54	88.13	100.20
12	l	245	TYR	CB-CG-CD2	7.54	125.53	121.00
22	S	52	TYR	CG-CD1-CE1	-7.54	115.27	121.30
21	N	415	PHE	CB-CG-CD1	-7.54	115.53	120.80
23	P	329	PHE	CB-CG-CD1	7.53	126.07	120.80
29	I	340	ARG	NE-CZ-NH1	7.53	124.06	120.30
2	b	170	ALA	N-CA-CB	7.52	120.63	110.10
1	a	110	TYR	CD1-CG-CD2	7.52	126.17	117.90
6	f	24	TYR	CB-CG-CD2	-7.52	116.49	121.00
4	D	48	ARG	NE-CZ-NH1	7.52	124.06	120.30
12	5	245	TYR	CG-CD2-CE2	7.52	127.31	121.30
33	J	48	ARG	NE-CZ-NH2	-7.51	116.54	120.30
6	F	51	ARG	NE-CZ-NH1	7.51	124.06	120.30
27	O	375	ASP	CB-CG-OD2	-7.50	111.55	118.30
2	b	89	SER	N-CA-CB	7.50	121.75	110.50
10	j	199	TYR	CB-CG-CD1	7.50	125.50	121.00
13	6	221	ARG	NE-CZ-NH2	7.49	124.05	120.30
11	k	190	ARG	NE-CZ-NH2	-7.49	116.56	120.30
12	5	179	TYR	CB-CG-CD1	7.49	125.49	121.00
30	K	207	ARG	NE-CZ-NH2	-7.48	116.56	120.30
3	C	20	TYR	CG-CD2-CE2	-7.48	115.32	121.30
21	N	762	ARG	NE-CZ-NH1	7.48	124.04	120.30
33	J	35	ARG	NE-CZ-NH1	-7.47	116.56	120.30
21	N	584	ARG	NH1-CZ-NH2	-7.47	111.18	119.40
29	I	316	PHE	CB-CG-CD1	-7.47	115.57	120.80
4	D	4	TYR	CB-CG-CD2	-7.47	116.52	121.00
23	P	238	ALA	N-CA-CB	7.47	120.56	110.10
7	G	48	PHE	CB-CG-CD1	-7.46	115.58	120.80
5	e	83	ALA	CB-CA-C	-7.44	98.95	110.10
1	a	143	PHE	CB-CG-CD2	-7.43	115.60	120.80
20	Z	287	ARG	NE-CZ-NH1	7.43	124.02	120.30
16	V	304	ALA	N-CA-CB	7.42	120.49	110.10
4	d	56	ASP	CB-CG-OD2	-7.42	111.62	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	150	ARG	NE-CZ-NH1	7.41	124.01	120.30
13	6	168	TYR	CB-CG-CD2	-7.41	116.56	121.00
4	D	111	ARG	NE-CZ-NH1	-7.40	116.60	120.30
13	m	56	ASP	CB-CG-OD2	7.39	124.95	118.30
6	f	42	THR	O-C-N	-7.39	110.87	122.70
11	4	124	THR	CA-CB-CG2	-7.38	102.07	112.40
24	Q	51	ARG	NE-CZ-NH1	-7.38	116.61	120.30
3	c	67	TYR	CG-CD2-CE2	-7.38	115.40	121.30
31	L	312	MET	CA-CB-CG	-7.38	100.76	113.30
7	G	20	ARG	NE-CZ-NH1	7.38	123.99	120.30
22	S	332	PHE	CB-CG-CD2	-7.37	115.64	120.80
7	g	149	TYR	CB-CG-CD2	-7.36	116.58	121.00
20	Z	722	ASP	CB-CG-OD1	-7.36	111.68	118.30
29	I	282	ASP	CB-CG-OD1	-7.36	111.68	118.30
3	C	143	ARG	NE-CZ-NH2	-7.36	116.62	120.30
10	3	164	PHE	CB-CG-CD2	-7.36	115.65	120.80
20	Z	901	PHE	CB-CG-CD1	-7.35	115.65	120.80
29	I	183	ASP	N-CA-CB	7.35	123.84	110.60
20	Z	761	PHE	CB-CG-CD2	-7.35	115.65	120.80
31	L	157	ARG	NE-CZ-NH2	-7.35	116.62	120.30
6	f	205	SER	O-C-N	-7.35	110.94	122.70
1	A	120	ARG	NE-CZ-NH1	-7.34	116.63	120.30
28	H	357	ARG	NE-CZ-NH1	7.34	123.97	120.30
3	C	188	ASP	CB-CG-OD1	-7.34	111.69	118.30
24	Q	149	LYS	N-CA-CB	7.34	123.81	110.60
28	H	370	ARG	NE-CZ-NH1	-7.34	116.63	120.30
33	J	200	ARG	NE-CZ-NH1	7.34	123.97	120.30
13	m	225	TYR	CG-CD1-CE1	-7.33	115.43	121.30
1	A	110	TYR	CB-CG-CD2	-7.33	116.60	121.00
7	g	157	TYR	CB-CG-CD1	7.33	125.40	121.00
31	L	392	ARG	NE-CZ-NH1	7.33	123.96	120.30
12	l	272	PHE	CB-CG-CD2	-7.33	115.67	120.80
3	C	114	ARG	NE-CZ-NH2	-7.33	116.64	120.30
32	M	77	TYR	CB-CG-CD2	7.33	125.39	121.00
3	C	226	TYR	CZ-CE2-CD2	7.32	126.39	119.80
15	W	101	ARG	NE-CZ-NH2	-7.32	116.64	120.30
33	J	282	PHE	CB-CG-CD1	7.31	125.92	120.80
3	C	4	ARG	NE-CZ-NH1	-7.31	116.65	120.30
24	Q	40	ALA	N-CA-CB	7.31	120.33	110.10
2	b	224	TYR	CB-CG-CD2	-7.30	116.62	121.00
3	C	208	TYR	CB-CG-CD1	7.30	125.38	121.00
5	E	138	PHE	CB-CG-CD1	7.30	125.91	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	X	111	LEU	CB-CG-CD1	7.30	123.40	111.00
20	Z	826	ARG	NE-CZ-NH2	-7.29	116.66	120.30
21	N	729	SER	N-CA-CB	7.29	121.44	110.50
22	S	274	PHE	CB-CG-CD1	-7.29	115.70	120.80
14	n	211	VAL	CA-CB-CG2	-7.29	99.97	110.90
8	h	163	PHE	CB-CG-CD1	-7.29	115.70	120.80
5	E	15	PHE	C-N-CA	7.28	139.90	121.70
9	i	153	TYR	CB-CG-CD1	-7.28	116.63	121.00
4	d	148	TYR	CG-CD1-CE1	7.27	127.12	121.30
25	R	321	TYR	CG-CD1-CE1	-7.27	115.48	121.30
4	D	5	ASP	CB-CG-OD1	7.26	124.84	118.30
5	E	8	TYR	CG-CD1-CE1	-7.26	115.49	121.30
16	V	214	MET	CG-SD-CE	-7.26	88.59	100.20
1	a	104	PHE	CB-CG-CD1	-7.25	115.72	120.80
3	c	208	TYR	CG-CD2-CE2	-7.25	115.50	121.30
13	6	203	HIS	CA-CB-CG	-7.24	101.29	113.60
20	Z	303	ASP	CB-CG-OD1	7.24	124.81	118.30
1	A	244	ARG	NE-CZ-NH1	7.23	123.92	120.30
28	H	254	THR	CA-CB-CG2	-7.23	102.28	112.40
31	L	161	ARG	NE-CZ-NH1	7.22	123.91	120.30
23	P	359	ARG	NE-CZ-NH2	-7.22	116.69	120.30
32	M	118	VAL	CG1-CB-CG2	7.22	122.45	110.90
5	E	103	TYR	CB-CG-CD2	7.21	125.33	121.00
20	Z	236	PHE	CB-CG-CD2	-7.20	115.76	120.80
29	I	337	ALA	CB-CA-C	-7.20	99.29	110.10
33	J	144	ASP	CB-CG-OD2	7.20	124.78	118.30
6	f	44	ALA	N-CA-CB	7.20	120.18	110.10
3	C	24	TYR	CB-CG-CD1	7.19	125.32	121.00
21	N	809	ARG	CD-NE-CZ	7.19	133.67	123.60
8	1	14	ALA	CB-CA-C	-7.19	99.31	110.10
9	i	212	ASP	CB-CG-OD1	7.18	124.76	118.30
5	E	237	ALA	CB-CA-C	-7.18	99.33	110.10
16	V	228	TYR	CG-CD2-CE2	-7.18	115.56	121.30
12	l	282	PHE	CB-CG-CD2	7.17	125.82	120.80
16	V	78	VAL	CA-CB-CG2	-7.17	100.14	110.90
11	4	75	LEU	CB-CG-CD2	7.17	123.18	111.00
24	Q	231	ASP	CB-CG-OD1	7.17	124.75	118.30
3	C	6	TYR	CG-CD1-CE1	-7.16	115.58	121.30
4	D	166	ARG	NE-CZ-NH2	7.16	123.88	120.30
10	j	154	TYR	CG-CD2-CE2	-7.15	115.58	121.30
1	a	73	PHE	CB-CG-CD2	-7.15	115.80	120.80
8	1	75	TYR	CB-CG-CD1	7.14	125.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	365	PHE	CG-CD2-CE2	-7.14	112.95	120.80
27	O	252	PHE	CB-CG-CD1	7.14	125.80	120.80
32	M	431	SER	N-CA-CB	7.14	121.21	110.50
21	N	415	PHE	CB-CG-CD2	7.13	125.79	120.80
24	Q	232	TYR	CB-CG-CD2	7.13	125.28	121.00
31	L	70	TYR	CG-CD2-CE2	-7.13	115.59	121.30
5	e	41	ALA	N-CA-CB	7.13	120.08	110.10
11	4	84	VAL	CA-CB-CG2	-7.13	100.20	110.90
21	N	697	PHE	CB-CG-CD2	7.13	125.79	120.80
1	a	128	TYR	CB-CG-CD2	-7.13	116.72	121.00
27	O	32	PHE	CB-CG-CD2	-7.13	115.81	120.80
22	S	452	TYR	CB-CG-CD2	-7.12	116.73	121.00
9	i	232	TYR	CB-CG-CD2	-7.12	116.73	121.00
13	m	155	MET	CG-SD-CE	-7.12	88.81	100.20
14	7	109	TYR	CB-CG-CD1	-7.12	116.73	121.00
11	k	187	ASP	CB-CG-OD1	7.11	124.70	118.30
18	X	98	PHE	CB-CG-CD1	-7.11	115.82	120.80
20	Z	567	ALA	N-CA-CB	7.11	120.06	110.10
18	X	17	TYR	CB-CG-CD2	7.11	125.27	121.00
2	b	56	ALA	N-CA-CB	7.11	120.05	110.10
7	g	230	PHE	CB-CG-CD1	-7.10	115.83	120.80
4	D	220	ASP	CB-CG-OD2	-7.10	111.91	118.30
3	c	102	TYR	CB-CG-CD2	7.10	125.26	121.00
32	M	309	LEU	CB-CG-CD2	7.10	123.07	111.00
16	V	181	ASN	N-CA-CB	7.09	123.37	110.60
2	B	99	ARG	NE-CZ-NH2	7.08	123.84	120.30
30	K	400	TYR	CB-CG-CD1	-7.07	116.76	121.00
27	O	183	ASN	N-CA-CB	7.07	123.33	110.60
5	E	97	VAL	CA-CB-CG2	-7.07	100.30	110.90
12	5	255	VAL	CA-CB-CG2	-7.07	100.30	110.90
5	e	72	ARG	CG-CD-NE	-7.07	96.96	111.80
4	d	75	PHE	CB-CG-CD1	-7.07	115.86	120.80
7	G	115	ARG	NE-CZ-NH2	7.06	123.83	120.30
5	E	69	GLU	OE1-CD-OE2	7.06	131.78	123.30
25	R	335	ARG	NE-CZ-NH1	-7.06	116.77	120.30
31	L	77	ARG	NE-CZ-NH2	-7.06	116.77	120.30
20	Z	838	TYR	CZ-CE2-CD2	-7.05	113.45	119.80
25	R	365	ASP	CB-CG-OD2	-7.05	111.95	118.30
32	M	226	THR	CA-CB-CG2	-7.05	102.53	112.40
22	S	171	TYR	CG-CD1-CE1	-7.05	115.66	121.30
5	e	226	ASP	CB-CG-OD1	7.05	124.65	118.30
28	H	96	PRO	O-C-N	7.05	133.97	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	47	ARG	N-CA-CB	7.04	123.28	110.60
14	n	241	PHE	CB-CG-CD2	-7.04	115.87	120.80
5	E	9	ASP	CB-CG-OD1	-7.04	111.97	118.30
20	Z	747	ALA	CB-CA-C	-7.04	99.54	110.10
33	J	309	ARG	NE-CZ-NH2	-7.04	116.78	120.30
10	j	36	VAL	CA-CB-CG2	-7.04	100.35	110.90
10	3	193	ASP	CB-CG-OD1	7.04	124.63	118.30
20	Z	210	TYR	CB-CG-CD1	7.04	125.22	121.00
20	Z	838	TYR	CD1-CE1-CZ	7.04	126.13	119.80
7	g	44	ASP	CB-CG-OD1	7.03	124.63	118.30
2	B	82	TYR	CG-CD2-CE2	-7.03	115.68	121.30
3	C	13	PHE	CB-CG-CD2	-7.03	115.88	120.80
13	6	75	ARG	NE-CZ-NH2	7.02	123.81	120.30
21	N	345	ASP	CB-CG-OD1	7.02	124.61	118.30
20	Z	489	ALA	N-CA-CB	7.01	119.92	110.10
32	M	376	TRP	CB-CG-CD2	-7.01	117.48	126.60
9	i	98	TYR	CB-CG-CD1	7.01	125.20	121.00
8	1	198	TYR	CB-CG-CD2	-7.00	116.80	121.00
5	e	103	TYR	CG-CD1-CE1	-7.00	115.70	121.30
2	b	168	SER	N-CA-CB	7.00	121.00	110.50
32	M	87	ASP	CB-CG-OD1	6.99	124.59	118.30
1	a	35	THR	CA-CB-CG2	-6.99	102.61	112.40
4	d	90	ARG	NE-CZ-NH1	6.99	123.80	120.30
9	2	186	ASP	CB-CG-OD2	6.99	124.59	118.30
14	7	123	SER	CB-CA-C	-6.98	96.84	110.10
20	Z	155	ARG	NE-CZ-NH2	-6.98	116.81	120.30
11	k	93	ARG	NE-CZ-NH2	-6.98	116.81	120.30
17	T	249	MET	CG-SD-CE	-6.98	89.04	100.20
25	R	125	GLU	N-CA-CB	6.98	123.16	110.60
22	S	377	TYR	CB-CG-CD1	-6.97	116.82	121.00
16	V	269	ARG	NE-CZ-NH2	-6.97	116.82	120.30
8	1	197	PHE	CB-CG-CD1	-6.96	115.92	120.80
22	S	286	TYR	CB-CG-CD1	6.96	125.18	121.00
31	L	104	LEU	CB-CG-CD1	6.96	122.84	111.00
20	Z	464	ASP	CB-CG-OD2	-6.96	112.03	118.30
2	b	54	PRO	N-CA-CB	6.96	111.65	103.30
23	P	267	PHE	CB-CG-CD1	-6.96	115.93	120.80
25	R	179	PHE	CB-CG-CD2	-6.96	115.93	120.80
7	G	72	ARG	NE-CZ-NH1	-6.96	116.82	120.30
23	P	208	PHE	CB-CG-CD2	-6.95	115.93	120.80
7	g	157	TYR	CB-CG-CD2	-6.94	116.83	121.00
21	N	339	MET	CG-SD-CE	-6.94	89.09	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	358	ALA	N-CA-CB	6.94	119.82	110.10
12	l	130	TRP	CB-CG-CD1	6.94	136.02	127.00
22	S	456	ASP	CB-CG-OD2	-6.93	112.06	118.30
23	P	415	TRP	CD1-CG-CD2	6.93	111.84	106.30
8	h	142	PHE	CB-CG-CD1	-6.93	115.95	120.80
25	R	20	ARG	NE-CZ-NH2	-6.93	116.84	120.30
25	R	206	ARG	NE-CZ-NH1	6.92	123.76	120.30
5	e	80	GLY	N-CA-C	-6.92	95.81	113.10
15	W	20	ASP	N-CA-CB	6.92	123.05	110.60
28	H	181	TYR	CG-CD2-CE2	6.91	126.83	121.30
2	B	97	TYR	CB-CG-CD2	6.91	125.14	121.00
21	N	36	TRP	CB-CG-CD2	-6.90	117.63	126.60
28	H	303	ALA	N-CA-CB	6.90	119.76	110.10
21	N	543	ASP	CB-CG-OD1	6.90	124.51	118.30
8	h	142	PHE	CB-CG-CD2	6.89	125.63	120.80
8	h	174	TRP	CB-CG-CD2	-6.89	117.64	126.60
4	D	112	TYR	CB-CG-CD2	-6.89	116.87	121.00
28	H	221	LEU	CB-CG-CD2	6.89	122.71	111.00
3	c	242	THR	CA-CB-CG2	-6.88	102.76	112.40
5	e	26	TYR	CB-CG-CD1	6.88	125.13	121.00
12	5	234	ARG	NE-CZ-NH1	6.88	123.74	120.30
11	k	117	TYR	CB-CG-CD1	-6.87	116.88	121.00
29	I	306	MET	CG-SD-CE	-6.87	89.20	100.20
13	m	133	PHE	CB-CG-CD2	6.87	125.61	120.80
29	I	128	TYR	CG-CD1-CE1	-6.87	115.81	121.30
13	6	139	TYR	CD1-CE1-CZ	-6.87	113.62	119.80
33	J	216	ALA	N-CA-CB	6.86	119.71	110.10
2	b	235	PHE	CB-CG-CD2	6.86	125.60	120.80
9	2	153	TYR	CB-CG-CD2	6.86	125.11	121.00
13	m	56	ASP	CB-CG-OD1	-6.86	112.13	118.30
1	A	46	ARG	NE-CZ-NH1	6.86	123.73	120.30
21	N	504	TYR	CB-CG-CD2	6.85	125.11	121.00
7	g	212	PHE	CG-CD1-CE1	-6.85	113.27	120.80
16	V	84	ASP	CB-CG-OD2	6.85	124.46	118.30
13	6	225	TYR	CB-CG-CD1	-6.84	116.89	121.00
18	X	122	TYR	CB-CG-CD1	-6.83	116.90	121.00
25	R	345	TYR	CB-CG-CD2	-6.83	116.90	121.00
15	W	35	PHE	CB-CG-CD1	-6.83	116.02	120.80
3	c	13	PHE	CB-CG-CD1	-6.83	116.02	120.80
2	B	239	THR	CA-CB-CG2	-6.83	102.84	112.40
20	Z	210	TYR	CB-CG-CD2	-6.82	116.91	121.00
2	B	174	PHE	CB-CG-CD1	-6.82	116.03	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	83	TYR	CB-CG-CD1	-6.82	116.91	121.00
13	6	106	TYR	CB-CG-CD1	6.82	125.09	121.00
21	N	404	SER	N-CA-CB	6.82	120.73	110.50
16	V	251	TYR	CB-CG-CD1	-6.82	116.91	121.00
24	Q	238	TYR	CB-CA-C	-6.82	96.77	110.40
1	A	106	TYR	CB-CG-CD2	-6.81	116.91	121.00
11	4	93	ARG	NE-CZ-NH2	6.81	123.70	120.30
12	5	115	PHE	CB-CG-CD2	6.80	125.56	120.80
28	H	364	ALA	CB-CA-C	-6.80	99.91	110.10
30	K	330	ARG	NE-CZ-NH1	6.80	123.70	120.30
25	R	170	VAL	CA-CB-CG2	-6.79	100.71	110.90
11	k	12	SER	N-CA-CB	6.79	120.69	110.50
12	5	155	SER	N-CA-CB	6.79	120.69	110.50
14	n	194	ARG	NE-CZ-NH2	-6.79	116.91	120.30
21	N	299	TYR	CB-CG-CD2	6.79	125.07	121.00
33	J	8	SER	N-CA-CB	6.79	120.68	110.50
21	N	242	PHE	CB-CG-CD2	6.78	125.55	120.80
14	n	218	TYR	CB-CG-CD2	-6.78	116.93	121.00
16	V	228	TYR	CB-CG-CD2	-6.78	116.93	121.00
25	R	180	PHE	CB-CG-CD2	6.78	125.55	120.80
32	M	319	ASP	CB-CG-OD2	-6.78	112.20	118.30
26	U	24	ARG	NE-CZ-NH2	-6.77	116.92	120.30
3	C	105	ASP	CB-CG-OD1	-6.77	112.21	118.30
24	Q	400	TYR	CG-CD2-CE2	6.76	126.71	121.30
21	N	866	TYR	CB-CG-CD2	6.76	125.06	121.00
29	I	125	MET	CA-C-O	-6.76	105.91	120.10
21	N	123	PHE	CB-CG-CD1	6.75	125.53	120.80
21	N	117	TYR	CB-CG-CD1	6.75	125.05	121.00
6	F	164	ARG	NE-CZ-NH2	-6.75	116.93	120.30
25	R	382	ASP	CB-CG-OD2	6.75	124.37	118.30
27	O	48	PHE	CB-CG-CD2	6.75	125.52	120.80
4	d	232	TYR	CB-CG-CD2	-6.75	116.95	121.00
11	4	39	SER	N-CA-CB	6.74	120.61	110.50
21	N	302	PHE	CB-CG-CD1	6.74	125.52	120.80
28	H	76	LEU	N-CA-CB	6.74	123.89	110.40
13	m	193	ARG	NE-CZ-NH2	-6.74	116.93	120.30
4	D	174	PHE	CB-CG-CD1	-6.73	116.09	120.80
17	T	149	ASP	CB-CG-OD2	-6.73	112.24	118.30
29	I	346	ARG	NE-CZ-NH2	-6.73	116.93	120.30
30	K	116	MET	CG-SD-CE	-6.73	89.43	100.20
14	n	92	ASP	CB-CG-OD1	6.73	124.36	118.30
12	5	281	SER	N-CA-CB	6.73	120.59	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	128	ARG	NE-CZ-NH1	-6.73	116.94	120.30
23	P	395	ARG	NE-CZ-NH2	6.73	123.66	120.30
30	K	256	ASP	CB-CG-OD2	6.73	124.35	118.30
25	R	214	TYR	CB-CG-CD1	6.72	125.03	121.00
27	O	248	TYR	CB-CG-CD1	6.72	125.03	121.00
4	d	156	TYR	CG-CD1-CE1	6.71	126.67	121.30
3	c	60	ASP	CB-CG-OD1	-6.71	112.26	118.30
14	7	74	ARG	NE-CZ-NH1	6.71	123.65	120.30
32	M	44	PHE	CB-CG-CD2	6.70	125.49	120.80
14	n	134	TYR	CG-CD1-CE1	-6.70	115.94	121.30
10	3	100	PHE	CB-CG-CD2	-6.70	116.11	120.80
12	5	245	TYR	CB-CG-CD1	6.70	125.02	121.00
30	K	236	ARG	NE-CZ-NH1	-6.70	116.95	120.30
20	Z	838	TYR	CG-CD2-CE2	6.69	126.65	121.30
14	n	89	ASP	CB-CG-OD1	6.69	124.32	118.30
23	P	13	TYR	CB-CG-CD1	6.69	125.01	121.00
15	W	140	ASP	CB-CG-OD1	-6.68	112.28	118.30
30	K	333	ARG	NE-CZ-NH1	6.68	123.64	120.30
5	E	93	ARG	NE-CZ-NH2	-6.68	116.96	120.30
7	G	149	TYR	CB-CG-CD1	-6.68	116.99	121.00
21	N	656	ALA	CB-CA-C	-6.68	100.08	110.10
24	Q	190	ASN	N-CA-CB	6.68	122.62	110.60
29	I	64	ARG	NE-CZ-NH2	-6.67	116.96	120.30
8	1	38	ARG	NE-CZ-NH1	6.67	123.64	120.30
3	c	70	ASN	N-CA-CB	6.67	122.61	110.60
25	R	180	PHE	CB-CG-CD1	-6.67	116.13	120.80
28	H	448	ASP	CB-CG-OD1	-6.67	112.30	118.30
12	l	189	TYR	CB-CG-CD2	-6.67	117.00	121.00
26	U	27	THR	CA-CB-CG2	-6.67	103.06	112.40
14	n	254	PHE	CB-CG-CD2	-6.66	116.14	120.80
2	b	224	TYR	CG-CD2-CE2	-6.66	115.97	121.30
3	C	146	TYR	CB-CG-CD2	6.66	125.00	121.00
30	K	411	TYR	CB-CG-CD2	6.66	124.99	121.00
27	O	263	PHE	CB-CG-CD1	-6.65	116.14	120.80
21	N	394	ARG	CG-CD-NE	-6.65	97.84	111.80
4	D	5	ASP	CB-CG-OD2	-6.64	112.32	118.30
21	N	471	TYR	CG-CD2-CE2	-6.64	115.99	121.30
22	S	467	PHE	CB-CG-CD2	-6.64	116.15	120.80
2	B	178	ARG	NE-CZ-NH1	-6.64	116.98	120.30
7	G	138	PHE	CB-CG-CD1	6.64	125.45	120.80
20	Z	236	PHE	CB-CG-CD1	6.64	125.45	120.80
3	c	143	ARG	NE-CZ-NH1	6.64	123.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	k	171	ARG	NE-CZ-NH1	6.64	123.62	120.30
31	L	255	TYR	CG-CD1-CE1	-6.63	115.99	121.30
16	V	87	PHE	CB-CG-CD1	6.63	125.44	120.80
21	N	743	PHE	CB-CG-CD2	-6.63	116.16	120.80
33	J	71	TYR	CG-CD2-CE2	-6.63	116.00	121.30
10	3	203	ARG	NH1-CZ-NH2	6.62	126.69	119.40
12	5	230	TYR	CB-CG-CD2	-6.62	117.03	121.00
31	L	329	ARG	NE-CZ-NH1	-6.62	116.99	120.30
32	M	153	TYR	CB-CG-CD1	-6.62	117.03	121.00
2	B	84	VAL	CA-CB-CG1	-6.62	100.97	110.90
21	N	697	PHE	CB-CG-CD1	-6.61	116.17	120.80
33	J	329	ARG	NE-CZ-NH2	6.61	123.61	120.30
31	L	400	PHE	CB-CG-CD1	-6.61	116.17	120.80
3	c	129	ARG	NE-CZ-NH1	6.60	123.60	120.30
5	E	20	ARG	NE-CZ-NH1	-6.60	117.00	120.30
21	N	528	ARG	NE-CZ-NH2	-6.60	117.00	120.30
24	Q	265	MET	CG-SD-CE	-6.60	89.64	100.20
4	d	28	LYS	CB-CA-C	-6.60	97.21	110.40
31	L	306	MET	CG-SD-CE	-6.59	89.66	100.20
5	E	77	ALA	N-CA-CB	6.59	119.32	110.10
5	E	151	ASP	CB-CG-OD2	-6.59	112.37	118.30
11	4	135	TYR	CG-CD1-CE1	-6.59	116.03	121.30
33	J	147	TYR	CB-CG-CD2	-6.59	117.05	121.00
17	T	269	SER	N-CA-CB	6.58	120.38	110.50
14	n	149	VAL	CA-CB-CG2	-6.58	101.03	110.90
1	A	157	THR	CA-CB-CG2	-6.58	103.18	112.40
2	B	156	TYR	CD1-CE1-CZ	-6.58	113.88	119.80
1	a	24	ARG	CD-NE-CZ	-6.58	114.39	123.60
9	i	65	ARG	NE-CZ-NH1	-6.58	117.01	120.30
22	S	285	ASP	CB-CG-OD2	-6.58	112.38	118.30
15	W	139	VAL	CA-CB-CG2	6.58	120.77	110.90
1	a	24	ARG	NE-CZ-NH2	-6.57	117.01	120.30
12	l	81	PHE	CB-CG-CD1	-6.57	116.20	120.80
3	C	6	TYR	CB-CG-CD2	-6.57	117.06	121.00
32	M	233	ARG	NE-CZ-NH1	-6.57	117.01	120.30
32	M	433	TYR	CZ-CE2-CD2	-6.57	113.89	119.80
11	k	185	ASP	CB-CG-OD2	-6.57	112.39	118.30
25	R	99	TYR	CB-CG-CD1	-6.57	117.06	121.00
22	S	272	TYR	CB-CG-CD1	6.57	124.94	121.00
25	R	221	VAL	CA-CB-CG2	6.57	120.75	110.90
1	a	91	ARG	NE-CZ-NH2	-6.57	117.02	120.30
9	2	48	ARG	NE-CZ-NH1	6.57	123.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	139	TYR	CG-CD2-CE2	-6.56	116.05	121.30
7	G	158	TRP	CD1-NE1-CE2	6.56	114.91	109.00
15	W	144	PHE	CB-CG-CD1	6.56	125.39	120.80
20	Z	48	ASP	CB-CG-OD1	6.56	124.21	118.30
22	S	170	TYR	CB-CG-CD2	-6.56	117.06	121.00
21	N	124	TYR	CG-CD2-CE2	6.56	126.55	121.30
28	H	443	PHE	CB-CG-CD1	-6.55	116.21	120.80
24	Q	124	PHE	CB-CG-CD2	-6.55	116.21	120.80
9	2	152	TYR	CG-CD2-CE2	-6.55	116.06	121.30
7	g	181	ASP	CB-CG-OD1	-6.55	112.41	118.30
13	6	41	TYR	CB-CG-CD1	-6.55	117.07	121.00
14	n	144	TRP	CE3-CZ3-CH2	-6.55	114.00	121.20
24	Q	291	TYR	CZ-CE2-CD2	6.55	125.69	119.80
11	4	85	ARG	NE-CZ-NH1	6.54	123.57	120.30
20	Z	272	TYR	CB-CG-CD2	-6.54	117.07	121.00
25	R	238	PHE	CG-CD1-CE1	-6.54	113.60	120.80
33	J	112	ARG	NE-CZ-NH1	-6.54	117.03	120.30
21	N	23	TYR	CG-CD2-CE2	6.54	126.53	121.30
22	S	429	ASP	CB-CA-C	-6.54	97.32	110.40
27	O	86	LEU	CB-CG-CD1	-6.54	99.88	111.00
8	1	68	VAL	CG1-CB-CG2	6.54	121.36	110.90
12	l	129	PHE	CB-CG-CD1	6.54	125.38	120.80
16	V	22	ASP	N-CA-CB	6.54	122.36	110.60
21	N	552	ALA	CB-CA-C	-6.54	100.30	110.10
21	N	753	PHE	CB-CG-CD1	6.53	125.37	120.80
22	S	270	ALA	CB-CA-C	-6.53	100.30	110.10
32	M	313	ASP	CB-CG-OD1	-6.53	112.42	118.30
21	N	69	TYR	CG-CD1-CE1	6.53	126.52	121.30
13	m	221	ARG	NE-CZ-NH2	-6.52	117.04	120.30
25	R	371	PHE	CB-CG-CD2	-6.52	116.23	120.80
13	m	138	SER	N-CA-CB	6.52	120.28	110.50
13	6	60	MET	CG-SD-CE	-6.52	89.77	100.20
30	K	141	ARG	NE-CZ-NH2	6.52	123.56	120.30
6	f	203	ASP	CB-CG-OD2	6.52	124.16	118.30
21	N	57	ASP	CB-CG-OD2	-6.51	112.44	118.30
20	Z	6	ASP	CB-CG-OD2	6.51	124.16	118.30
21	N	890	PHE	CZ-CE2-CD2	-6.51	112.29	120.10
29	I	202	LEU	CB-CG-CD1	6.51	122.07	111.00
26	U	59	ASP	CB-CG-OD2	-6.51	112.44	118.30
6	F	123	TYR	CB-CG-CD2	6.51	124.91	121.00
29	I	408	ARG	NH1-CZ-NH2	-6.51	112.24	119.40
8	1	198	TYR	CG-CD1-CE1	-6.50	116.10	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	849	ARG	NE-CZ-NH2	-6.50	117.05	120.30
4	D	29	ARG	NE-CZ-NH1	-6.50	117.05	120.30
17	T	119	THR	CA-CB-CG2	-6.50	103.30	112.40
26	U	24	ARG	NE-CZ-NH1	6.50	123.55	120.30
8	h	195	LEU	N-CA-CB	6.49	123.38	110.40
31	L	117	TYR	CA-CB-CG	-6.49	101.07	113.40
30	K	347	ARG	NE-CZ-NH2	-6.49	117.06	120.30
33	J	63	ARG	NE-CZ-NH2	6.49	123.54	120.30
6	F	188	GLU	OE1-CD-OE2	6.49	131.08	123.30
9	2	174	ASP	N-CA-CB	6.49	122.27	110.60
4	D	127	ARG	NE-CZ-NH2	-6.48	117.06	120.30
10	3	66	MET	CG-SD-CE	-6.48	89.83	100.20
20	Z	797	THR	CA-CB-CG2	-6.47	103.33	112.40
16	V	167	ASN	N-CA-CB	6.47	122.25	110.60
32	M	366	ARG	NE-CZ-NH2	6.47	123.54	120.30
5	E	123	PHE	CB-CG-CD1	-6.47	116.27	120.80
28	H	341	ASP	CB-CG-OD2	6.47	124.12	118.30
11	k	138	PHE	CB-CG-CD2	-6.47	116.27	120.80
12	l	130	TRP	CB-CG-CD2	-6.46	118.19	126.60
29	I	244	PHE	CB-CG-CD2	6.46	125.33	120.80
21	N	188	TYR	CG-CD2-CE2	-6.46	116.13	121.30
27	O	119	SER	N-CA-CB	6.46	120.19	110.50
28	H	389	PHE	CB-CG-CD2	-6.46	116.28	120.80
29	I	54	ARG	NE-CZ-NH2	-6.46	117.07	120.30
13	m	142	GLU	N-CA-CB	6.45	122.22	110.60
12	5	225	VAL	CA-CB-CG2	-6.45	101.22	110.90
22	S	76	PHE	CB-CG-CD2	-6.45	116.28	120.80
23	P	245	TYR	CZ-CE2-CD2	-6.45	114.00	119.80
11	k	32	ASP	CB-CG-OD1	-6.45	112.50	118.30
4	D	29	ARG	NE-CZ-NH2	-6.44	117.08	120.30
21	N	190	LEU	CB-CA-C	-6.44	97.96	110.20
5	e	8	TYR	CB-CG-CD2	-6.44	117.14	121.00
7	g	78	TYR	CB-CG-CD2	-6.44	117.14	121.00
20	Z	225	LEU	CB-CG-CD2	6.44	121.94	111.00
13	m	53	ASP	CB-CG-OD2	6.44	124.09	118.30
1	a	46	ARG	N-CA-CB	6.43	122.18	110.60
5	E	118	ASP	CB-CG-OD2	6.43	124.09	118.30
26	U	200	LEU	CB-CG-CD1	6.43	121.93	111.00
22	S	37	VAL	CA-CB-CG2	6.43	120.55	110.90
9	i	84	VAL	CA-CB-CG2	-6.43	101.25	110.90
14	n	220	ARG	NE-CZ-NH2	-6.43	117.08	120.30
21	N	269	LEU	CB-CG-CD1	6.43	121.93	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	133	SER	N-CA-C	-6.42	93.65	111.00
26	U	137	TYR	CB-CG-CD1	6.42	124.85	121.00
11	4	30	ASP	CB-CG-OD1	6.42	124.08	118.30
12	5	175	MET	CG-SD-CE	-6.42	89.92	100.20
12	l	282	PHE	CB-CG-CD1	-6.42	116.31	120.80
20	Z	446	GLU	OE1-CD-OE2	6.42	131.01	123.30
23	P	364	ARG	NE-CZ-NH2	6.42	123.51	120.30
23	P	13	TYR	CB-CG-CD2	-6.42	117.15	121.00
30	K	262	ARG	NE-CZ-NH1	6.42	123.51	120.30
14	n	116	ALA	N-CA-CB	-6.42	101.11	110.10
23	P	234	TYR	CG-CD1-CE1	-6.42	116.17	121.30
12	5	147	GLU	OE1-CD-OE2	6.42	131.00	123.30
30	K	46	ASP	CB-CG-OD2	-6.42	112.53	118.30
30	K	258	PHE	CB-CG-CD1	-6.42	116.31	120.80
7	g	160	TYR	CG-CD1-CE1	-6.41	116.17	121.30
4	D	105	THR	CA-CB-CG2	-6.41	103.42	112.40
24	Q	427	PHE	CB-CG-CD1	-6.41	116.31	120.80
28	H	139	ASP	CB-CG-OD1	-6.41	112.53	118.30
4	D	22	TYR	CB-CG-CD2	-6.41	117.16	121.00
4	D	161	ALA	N-CA-CB	6.41	119.07	110.10
25	R	252	TYR	CZ-CE2-CD2	6.41	125.57	119.80
25	R	95	ASP	CB-CG-OD2	-6.41	112.54	118.30
6	F	171	TYR	CZ-CE2-CD2	-6.40	114.04	119.80
13	6	81	LYS	N-CA-CB	6.40	122.12	110.60
10	j	104	PHE	CB-CG-CD2	-6.40	116.32	120.80
23	P	95	TYR	CB-CG-CD1	-6.40	117.16	121.00
30	K	400	TYR	CG-CD1-CE1	-6.39	116.18	121.30
7	g	206	ASP	CB-CG-OD1	-6.39	112.55	118.30
1	a	106	TYR	CB-CG-CD2	6.39	124.83	121.00
24	Q	203	THR	CA-CB-CG2	-6.39	103.46	112.40
20	Z	562	TRP	CB-CG-CD2	-6.39	118.30	126.60
20	Z	323	TYR	CB-CG-CD1	-6.38	117.17	121.00
20	Z	723	ASP	CB-CG-OD2	-6.38	112.56	118.30
6	F	123	TYR	CG-CD2-CE2	-6.38	116.20	121.30
15	W	113	PHE	CB-CG-CD1	6.38	125.27	120.80
23	P	310	ARG	NE-CZ-NH1	-6.38	117.11	120.30
22	S	76	PHE	CB-CG-CD1	6.38	125.26	120.80
6	F	104	ALA	CB-CA-C	6.37	119.66	110.10
10	j	103	TYR	CB-CG-CD2	-6.37	117.18	121.00
11	k	71	GLU	OE1-CD-OE2	6.37	130.95	123.30
33	J	85	LEU	CB-CG-CD2	-6.37	100.17	111.00
22	S	185	PHE	CB-CG-CD1	6.37	125.26	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	160	TYR	N-CA-CB	6.37	122.06	110.60
17	T	60	ARG	NE-CZ-NH1	-6.37	117.12	120.30
28	H	208	TYR	CD1-CE1-CZ	6.37	125.53	119.80
6	f	233	TYR	CB-CG-CD1	-6.36	117.18	121.00
8	h	146	TYR	CG-CD1-CE1	-6.36	116.21	121.30
30	K	88	ARG	NE-CZ-NH1	-6.36	117.12	120.30
29	I	291	ARG	N-CA-CB	6.36	122.04	110.60
1	a	73	PHE	CB-CG-CD1	6.35	125.25	120.80
12	l	262	TYR	CB-CG-CD1	-6.35	117.19	121.00
21	N	36	TRP	CB-CG-CD1	6.35	135.26	127.00
10	j	66	MET	CG-SD-CE	-6.35	90.04	100.20
8	1	153	GLU	N-CA-CB	6.35	122.03	110.60
30	K	275	ASP	CB-CG-OD2	6.35	124.02	118.30
14	n	170	TYR	CB-CG-CD1	-6.35	117.19	121.00
6	F	203	ASP	CB-CG-OD2	-6.35	112.58	118.30
7	G	86	ARG	NE-CZ-NH1	6.35	123.47	120.30
26	U	283	ARG	NE-CZ-NH1	-6.35	117.13	120.30
24	Q	124	PHE	CD1-CE1-CZ	6.35	127.72	120.10
27	O	139	LEU	CB-CG-CD2	6.35	121.79	111.00
7	g	234	ASP	CB-CG-OD2	-6.34	112.59	118.30
10	j	103	TYR	CB-CG-CD1	6.34	124.81	121.00
15	W	197	SER	N-CA-CB	6.34	120.01	110.50
7	g	84	ASP	CB-CG-OD1	6.34	124.01	118.30
5	E	51	GLU	N-CA-C	-6.34	93.88	111.00
21	N	299	TYR	CG-CD2-CE2	6.34	126.37	121.30
14	7	161	ARG	NE-CZ-NH1	-6.34	117.13	120.30
13	m	76	PHE	CB-CG-CD1	-6.33	116.37	120.80
7	G	48	PHE	CB-CG-CD2	6.33	125.23	120.80
23	P	41	VAL	CA-CB-CG2	-6.33	101.40	110.90
32	M	326	ALA	CB-CA-C	-6.33	100.60	110.10
28	H	343	PHE	CB-CG-CD2	6.33	125.23	120.80
5	e	142	LEU	CB-CG-CD1	6.33	121.76	111.00
6	F	177	ASP	CB-CG-OD2	-6.33	112.60	118.30
23	P	245	TYR	CB-CG-CD2	-6.33	117.20	121.00
32	M	320	ARG	NE-CZ-NH1	6.33	123.46	120.30
2	b	104	TYR	CB-CG-CD1	6.33	124.80	121.00
10	j	188	TYR	CB-CA-C	-6.33	97.75	110.40
4	d	166	ARG	NE-CZ-NH1	-6.32	117.14	120.30
20	Z	413	ASP	CB-CG-OD1	6.32	123.99	118.30
28	H	249	TYR	N-CA-CB	6.32	121.98	110.60
32	M	16	ASP	CB-CG-OD2	6.32	123.99	118.30
16	V	103	MET	CA-CB-CG	6.32	124.04	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	316	ASP	CB-CG-OD1	-6.32	112.61	118.30
32	M	45	ARG	NE-CZ-NH2	-6.32	117.14	120.30
33	J	257	ARG	NE-CZ-NH1	6.31	123.46	120.30
5	E	118	ASP	CB-CG-OD1	-6.31	112.62	118.30
11	4	195	PHE	CB-CG-CD1	6.31	125.22	120.80
24	Q	130	ARG	NE-CZ-NH1	6.31	123.45	120.30
10	j	188	TYR	CG-CD2-CE2	-6.30	116.26	121.30
3	C	11	THR	N-CA-CB	6.30	122.27	110.30
12	l	185	PRO	N-CD-CG	6.30	112.65	103.20
12	l	129	PHE	CB-CG-CD2	-6.30	116.39	120.80
1	a	30	TYR	CG-CD2-CE2	6.30	126.34	121.30
12	l	192	SER	N-CA-CB	-6.29	101.06	110.50
20	Z	408	TYR	CG-CD2-CE2	-6.29	116.27	121.30
19	Y	71	ASP	CB-CG-OD2	6.29	123.96	118.30
8	h	120	TYR	CB-CG-CD1	6.29	124.77	121.00
3	C	6	TYR	CG-CD2-CE2	-6.28	116.27	121.30
6	F	24	TYR	CB-CG-CD1	6.28	124.77	121.00
24	Q	185	TYR	CB-CG-CD2	-6.28	117.23	121.00
13	m	73	VAL	CA-CB-CG2	-6.28	101.48	110.90
9	2	119	TYR	CB-CG-CD1	6.28	124.77	121.00
30	K	171	TYR	CB-CG-CD1	6.28	124.77	121.00
3	C	6	TYR	CD1-CG-CD2	6.28	124.81	117.90
28	H	82	TRP	CA-CB-CG	6.28	125.63	113.70
25	R	357	PHE	CB-CG-CD1	-6.28	116.41	120.80
13	6	155	MET	CG-SD-CE	-6.27	90.17	100.20
15	W	83	GLY	C-N-CA	6.27	137.37	121.70
2	b	5	TYR	CZ-CE2-CD2	6.27	125.44	119.80
4	d	61	PRO	N-CA-CB	6.27	110.82	103.30
19	Y	7	ALA	CB-CA-C	-6.27	100.70	110.10
11	k	67	TYR	CB-CG-CD2	-6.26	117.24	121.00
33	J	122	LEU	CB-CA-C	-6.25	98.31	110.20
3	C	6	TYR	CB-CG-CD1	-6.25	117.25	121.00
7	g	93	ARG	CD-NE-CZ	-6.25	114.85	123.60
11	4	29	LYS	N-CA-CB	6.25	121.85	110.60
15	W	8	LEU	CB-CG-CD1	6.25	121.62	111.00
21	N	800	ALA	N-CA-CB	6.25	118.84	110.10
1	a	13	ASP	CB-CG-OD2	-6.24	112.68	118.30
25	R	204	TRP	CH2-CZ2-CE2	6.24	123.64	117.40
29	I	291	ARG	NE-CZ-NH1	-6.24	117.18	120.30
7	g	218	TRP	CA-CB-CG	6.24	125.55	113.70
24	Q	174	LEU	CB-CG-CD2	6.23	121.59	111.00
2	B	239	THR	N-CA-CB	6.23	122.14	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	26	TYR	CZ-CE2-CD2	6.23	125.41	119.80
33	J	57	PHE	CB-CG-CD2	-6.23	116.44	120.80
21	N	915	ALA	N-CA-CB	6.23	118.82	110.10
10	3	51	LEU	O-C-N	-6.22	112.62	123.20
31	L	304	THR	CA-CB-CG2	-6.22	103.69	112.40
12	l	253	TYR	CG-CD1-CE1	-6.22	116.33	121.30
3	C	54	SER	N-CA-CB	6.22	119.82	110.50
8	1	58	ALA	N-CA-CB	6.22	118.80	110.10
21	N	682	PHE	CB-CG-CD2	-6.22	116.45	120.80
14	7	254	PHE	CB-CG-CD2	-6.21	116.45	120.80
3	C	196	THR	CA-CB-CG2	-6.21	103.70	112.40
14	n	49	TYR	CG-CD2-CE2	-6.21	116.33	121.30
16	V	251	TYR	CB-CG-CD2	6.21	124.73	121.00
22	S	461	PHE	CB-CG-CD2	6.21	125.15	120.80
11	4	154	THR	CA-CB-CG2	-6.21	103.71	112.40
33	J	257	ARG	NE-CZ-NH2	-6.21	117.20	120.30
27	O	49	PHE	CB-CG-CD1	6.21	125.14	120.80
1	A	111	ASP	CB-CG-OD2	-6.20	112.72	118.30
20	Z	902	TYR	CB-CG-CD2	-6.20	117.28	121.00
29	I	316	PHE	CB-CG-CD2	6.20	125.14	120.80
33	J	144	ASP	CB-CG-OD1	-6.20	112.72	118.30
16	V	129	PHE	CB-CG-CD1	-6.20	116.46	120.80
16	V	197	TYR	CZ-CE2-CD2	-6.20	114.22	119.80
22	S	81	LEU	O-C-N	-6.20	112.78	122.70
14	7	257	ASP	CB-CG-OD1	-6.20	112.72	118.30
14	n	126	PHE	CB-CG-CD1	-6.19	116.46	120.80
8	h	102	LEU	N-CA-CB	6.19	122.78	110.40
13	6	15	ASP	CB-CG-OD1	6.19	123.87	118.30
16	V	235	GLU	OE1-CD-OE2	6.19	130.72	123.30
30	K	363	ALA	N-CA-CB	6.19	118.76	110.10
19	Y	83	ARG	NE-CZ-NH2	-6.18	117.21	120.30
2	B	12	PHE	CB-CG-CD1	6.18	125.13	120.80
10	3	131	ASP	CB-CG-OD2	6.18	123.86	118.30
13	6	225	TYR	CB-CG-CD2	6.18	124.71	121.00
6	f	203	ASP	CB-CG-OD1	-6.18	112.74	118.30
20	Z	951	GLN	N-CA-CB	6.18	121.72	110.60
4	D	220	ASP	CB-CG-OD1	6.17	123.86	118.30
10	3	203	ARG	NE-CZ-NH1	-6.17	117.21	120.30
24	Q	398	TYR	CD1-CG-CD2	6.17	124.69	117.90
28	H	99	VAL	CA-CB-CG2	-6.17	101.64	110.90
1	A	163	TYR	CB-CG-CD2	-6.17	117.30	121.00
6	f	24	TYR	CB-CG-CD1	6.17	124.70	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2	215	TYR	CB-CG-CD2	6.17	124.70	121.00
8	h	111	TYR	CB-CG-CD1	6.16	124.70	121.00
12	5	103	SER	N-CA-CB	6.16	119.74	110.50
5	E	234	GLU	O-C-N	-6.16	112.85	122.70
12	5	119	THR	N-CA-CB	6.15	121.99	110.30
17	T	226	TRP	N-CA-CB	6.15	121.67	110.60
1	A	244	ARG	NE-CZ-NH2	-6.15	117.23	120.30
8	1	155	MET	CG-SD-CE	-6.15	90.36	100.20
24	Q	271	MET	CG-SD-CE	-6.15	90.36	100.20
8	h	41	ASP	N-CA-C	-6.14	94.42	111.00
20	Z	194	GLU	N-CA-CB	6.14	121.66	110.60
14	7	193	ASP	CB-CG-OD2	-6.14	112.77	118.30
17	T	187	ASP	CB-CG-OD1	6.14	123.83	118.30
3	C	32	ALA	C-N-CA	6.14	135.19	122.30
12	5	245	TYR	CZ-CE2-CD2	-6.14	114.28	119.80
23	P	328	ALA	N-CA-CB	6.14	118.69	110.10
29	I	128	TYR	CG-CD2-CE2	-6.14	116.39	121.30
31	L	87	LEU	CB-CG-CD1	6.14	121.43	111.00
13	6	86	ASP	CA-CB-CG	-6.13	99.91	113.40
28	H	177	ASP	N-CA-CB	6.13	121.64	110.60
31	L	342	ARG	NE-CZ-NH1	6.13	123.37	120.30
1	A	218	PHE	CB-CG-CD2	6.13	125.09	120.80
20	Z	720	LYS	O-C-N	-6.13	112.89	122.70
21	N	139	ARG	NE-CZ-NH2	-6.13	117.24	120.30
3	C	216	ILE	O-C-N	-6.13	112.90	122.70
28	H	55	ASP	CB-CG-OD2	-6.12	112.79	118.30
13	m	65	PHE	CB-CG-CD1	6.12	125.09	120.80
21	N	157	ALA	N-CA-CB	6.12	118.67	110.10
24	Q	27	TYR	CB-CG-CD1	6.12	124.67	121.00
21	N	205	SER	N-CA-CB	6.12	119.67	110.50
25	R	422	ARG	NE-CZ-NH1	-6.12	117.24	120.30
9	i	151	GLY	N-CA-C	-6.11	97.82	113.10
30	K	155	ASP	CB-CG-OD1	-6.11	112.80	118.30
4	d	6	ARG	NE-CZ-NH2	-6.11	117.24	120.30
1	A	162	TYR	CZ-CE2-CD2	6.11	125.30	119.80
21	N	736	PHE	CB-CG-CD1	6.11	125.07	120.80
29	I	116	ASP	N-CA-CB	6.11	121.59	110.60
20	Z	410	THR	CA-CB-CG2	-6.10	103.86	112.40
31	L	132	ARG	N-CA-C	-6.10	94.52	111.00
4	D	136	ALA	N-CA-CB	6.10	118.64	110.10
14	7	41	GLY	N-CA-C	-6.10	97.84	113.10
2	B	130	PHE	CB-CG-CD2	-6.10	116.53	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	256	TYR	CG-CD1-CE1	-6.10	116.42	121.30
3	c	226	TYR	CB-CG-CD1	6.10	124.66	121.00
6	F	57	SER	N-CA-CB	6.10	119.65	110.50
15	W	26	PHE	CB-CG-CD1	-6.10	116.53	120.80
10	j	28	ARG	NE-CZ-NH1	6.09	123.35	120.30
12	l	219	TYR	CG-CD1-CE1	-6.09	116.42	121.30
13	m	41	TYR	CG-CD2-CE2	6.09	126.18	121.30
10	3	81	ALA	O-C-N	-6.09	112.95	122.70
13	6	102	GLN	N-CA-CB	6.09	121.57	110.60
6	f	39	ARG	NE-CZ-NH1	6.09	123.35	120.30
16	V	262	THR	N-CA-CB	6.09	121.88	110.30
25	R	209	ARG	NH1-CZ-NH2	6.09	126.10	119.40
19	Y	72	ASP	CB-CG-OD2	-6.09	112.82	118.30
25	R	154	LEU	CB-CG-CD2	6.08	121.34	111.00
14	7	220	ARG	NE-CZ-NH1	6.08	123.34	120.30
28	H	400	ARG	NH1-CZ-NH2	-6.08	112.71	119.40
33	J	329	ARG	CD-NE-CZ	-6.08	115.09	123.60
11	4	132	ALA	N-CA-CB	6.08	118.61	110.10
16	V	85	ASP	CB-CG-OD2	-6.08	112.83	118.30
20	Z	798	ARG	NE-CZ-NH2	-6.08	117.26	120.30
32	M	37	LEU	CB-CG-CD2	6.08	121.33	111.00
9	i	153	TYR	CB-CG-CD2	6.08	124.65	121.00
25	R	148	ASP	CB-CG-OD1	6.08	123.77	118.30
4	D	42	VAL	CA-CB-CG2	6.08	120.01	110.90
9	2	144	ALA	CB-CA-C	-6.07	100.99	110.10
32	M	93	ASP	CB-CG-OD1	-6.07	112.83	118.30
1	a	90	ALA	O-C-N	-6.07	112.99	122.70
5	E	231	TYR	CB-CG-CD1	6.07	124.64	121.00
22	S	258	GLU	N-CA-CB	6.07	121.52	110.60
28	H	297	MET	CG-SD-CE	-6.07	90.49	100.20
20	Z	242	PHE	CB-CG-CD2	-6.07	116.55	120.80
7	g	137	ILE	N-CA-C	-6.06	94.63	111.00
21	N	355	TRP	NE1-CE2-CZ2	6.06	137.07	130.40
23	P	47	ARG	NE-CZ-NH2	-6.06	117.27	120.30
28	H	135	ASP	CB-CG-OD2	6.06	123.76	118.30
23	P	111	ASP	CB-CG-OD2	-6.06	112.85	118.30
28	H	118	ASP	CB-CG-OD2	6.06	123.75	118.30
21	N	881	TYR	CG-CD2-CE2	-6.05	116.46	121.30
33	J	83	LYS	N-CA-CB	6.05	121.50	110.60
3	C	208	TYR	CG-CD1-CE1	6.05	126.14	121.30
29	I	125	MET	N-CA-CB	6.05	121.49	110.60
6	F	82	ARG	NE-CZ-NH2	-6.05	117.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	409	TYR	CG-CD2-CE2	6.05	126.14	121.30
24	Q	372	GLN	N-CA-CB	6.05	121.48	110.60
1	A	155	TYR	CG-CD2-CE2	-6.04	116.47	121.30
21	N	271	GLU	OE1-CD-OE2	6.04	130.55	123.30
27	O	375	ASP	CB-CG-OD1	6.04	123.73	118.30
8	1	146	TYR	CG-CD2-CE2	-6.03	116.47	121.30
20	Z	635	ALA	N-CA-CB	6.03	118.55	110.10
22	S	259	TYR	CB-CG-CD2	6.03	124.62	121.00
6	f	94	TYR	CD1-CE1-CZ	-6.03	114.38	119.80
14	n	197	ASP	CB-CG-OD2	-6.03	112.88	118.30
14	7	49	TYR	CB-CG-CD2	-6.03	117.38	121.00
22	S	188	TYR	CD1-CE1-CZ	-6.02	114.38	119.80
2	b	90	ARG	CD-NE-CZ	6.02	132.03	123.60
16	V	84	ASP	CB-CG-OD1	-6.02	112.88	118.30
21	N	651	PHE	CB-CG-CD1	-6.02	116.58	120.80
28	H	167	ASP	CA-CB-CG	-6.02	100.15	113.40
12	5	275	VAL	CA-CB-CG1	6.02	119.93	110.90
2	B	97	TYR	CZ-CE2-CD2	-6.02	114.38	119.80
25	R	301	TYR	CD1-CE1-CZ	6.02	125.22	119.80
28	H	463	TYR	CB-CG-CD2	6.02	124.61	121.00
7	g	71	ASP	CB-CG-OD2	6.01	123.71	118.30
21	N	784	TYR	CB-CG-CD1	-6.01	117.39	121.00
4	d	14	ASP	CB-CG-OD2	-6.01	112.89	118.30
5	e	15	PHE	O-C-N	-6.01	113.09	122.70
5	e	153	TYR	CZ-CE2-CD2	-6.01	114.39	119.80
8	1	28	ARG	N-CA-CB	6.01	121.41	110.60
31	L	191	ARG	NE-CZ-NH1	-6.01	117.30	120.30
4	D	190	GLU	OE1-CD-OE2	6.00	130.50	123.30
20	Z	970	TYR	CB-CG-CD1	-6.00	117.40	121.00
25	R	223	ASN	N-CA-C	-6.00	94.80	111.00
31	L	379	ALA	CB-CA-C	-6.00	101.10	110.10
21	N	389	TYR	CG-CD1-CE1	-6.00	116.50	121.30
21	N	881	TYR	CD1-CE1-CZ	6.00	125.20	119.80
2	B	99	ARG	CD-NE-CZ	-5.99	115.21	123.60
9	2	126	TYR	CB-CG-CD1	-5.99	117.40	121.00
9	2	135	THR	O-C-N	-5.99	113.01	123.20
1	A	106	TYR	CB-CG-CD1	5.99	124.59	121.00
17	T	132	HIS	C-N-CA	5.99	136.68	121.70
29	I	115	ASP	N-CA-CB	5.99	121.39	110.60
15	W	77	HIS	N-CA-CB	5.99	121.38	110.60
20	Z	231	ASP	CB-CG-OD1	5.99	123.69	118.30
6	F	153	VAL	CG1-CB-CG2	-5.99	101.32	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	129	ARG	N-CA-CB	5.99	121.38	110.60
20	Z	879	ALA	N-CA-CB	5.99	118.48	110.10
29	I	111	GLU	N-CA-CB	5.98	121.37	110.60
2	B	161	ALA	N-CA-CB	5.98	118.47	110.10
3	C	114	ARG	NE-CZ-NH1	-5.98	117.31	120.30
18	X	30	GLN	N-CA-CB	5.98	121.36	110.60
28	H	180	LYS	N-CA-C	-5.98	94.85	111.00
30	K	246	TYR	CD1-CE1-CZ	5.98	125.18	119.80
27	O	267	ASP	CB-CG-OD1	-5.98	112.92	118.30
25	R	115	GLU	OE1-CD-OE2	5.98	130.47	123.30
5	E	167	TYR	CB-CG-CD2	5.97	124.58	121.00
27	O	293	LEU	CB-CG-CD2	5.97	121.16	111.00
14	n	261	TYR	CG-CD1-CE1	-5.97	116.52	121.30
27	O	81	TYR	CB-CG-CD2	5.97	124.58	121.00
3	c	182	ASP	CB-CG-OD2	-5.97	112.93	118.30
5	e	118	ASP	CB-CG-OD1	5.97	123.67	118.30
21	N	570	ARG	NE-CZ-NH1	5.96	123.28	120.30
11	k	21	VAL	CB-CA-C	-5.96	100.08	111.40
13	m	106	TYR	CZ-CE2-CD2	-5.96	114.44	119.80
12	5	212	TYR	CD1-CE1-CZ	5.96	125.16	119.80
13	6	216	THR	CA-CB-CG2	-5.96	104.06	112.40
1	a	104	PHE	CB-CG-CD2	5.95	124.97	120.80
14	n	216	VAL	CA-CB-CG1	5.95	119.83	110.90
31	L	70	TYR	CZ-CE2-CD2	5.95	125.16	119.80
32	M	214	ALA	CB-CA-C	5.95	119.03	110.10
17	T	109	TYR	CG-CD1-CE1	-5.95	116.54	121.30
28	H	45	TYR	CG-CD1-CE1	-5.95	116.54	121.30
15	W	137	VAL	CB-CA-C	-5.95	100.10	111.40
29	I	254	GLN	CG-CD-OE1	-5.95	109.70	121.60
6	F	233	TYR	CZ-CE2-CD2	5.95	125.15	119.80
27	O	71	ASP	N-CA-CB	5.95	121.30	110.60
13	6	52	PHE	CB-CG-CD2	5.94	124.96	120.80
6	F	13	PHE	C-N-CA	5.94	136.56	121.70
11	k	187	ASP	CB-CG-OD2	-5.94	112.95	118.30
3	C	146	TYR	CB-CG-CD1	-5.94	117.44	121.00
3	C	162	ALA	N-CA-CB	5.94	118.42	110.10
21	N	753	PHE	CB-CG-CD2	-5.94	116.64	120.80
21	N	53	ASP	CB-CG-OD1	5.94	123.64	118.30
28	H	466	TYR	CG-CD1-CE1	5.94	126.05	121.30
12	l	165	TYR	CG-CD1-CE1	-5.93	116.55	121.30
14	7	92	ASP	CB-CG-OD1	-5.93	112.96	118.30
2	B	4	ARG	NE-CZ-NH1	5.93	123.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	188	TYR	CG-CD1-CE1	5.93	126.05	121.30
3	c	180	TYR	CG-CD1-CE1	5.93	126.04	121.30
14	n	137	ARG	NE-CZ-NH2	5.93	123.26	120.30
20	Z	789	GLN	N-CA-CB	5.93	121.27	110.60
28	H	463	TYR	CZ-CE2-CD2	-5.93	114.46	119.80
9	2	217	ARG	NE-CZ-NH1	5.93	123.26	120.30
25	R	183	ASP	CB-CG-OD1	-5.93	112.97	118.30
21	N	748	PHE	CB-CG-CD1	-5.93	116.65	120.80
20	Z	747	ALA	N-CA-CB	5.92	118.39	110.10
25	R	279	LEU	CB-CG-CD1	5.92	121.07	111.00
25	R	318	PRO	N-CA-CB	5.92	110.41	103.30
10	j	84	PRO	N-CA-CB	5.92	110.41	103.30
6	F	19	LEU	CB-CG-CD1	5.92	121.07	111.00
13	6	222	LYS	N-CA-C	-5.92	95.02	111.00
2	b	2	THR	CA-CB-CG2	-5.92	104.11	112.40
14	n	254	PHE	CB-CG-CD1	5.92	124.94	120.80
22	S	339	GLN	CG-CD-OE1	5.92	133.44	121.60
10	3	136	PHE	CB-CG-CD1	5.92	124.94	120.80
5	e	86	ARG	NE-CZ-NH2	-5.91	117.34	120.30
3	C	143	ARG	NE-CZ-NH1	5.91	123.26	120.30
5	e	20	ARG	NH1-CZ-NH2	5.91	125.90	119.40
6	F	92	CYS	N-CA-CB	5.91	121.23	110.60
25	R	167	LYS	CB-CA-C	-5.91	98.59	110.40
29	I	340	ARG	NH1-CZ-NH2	-5.91	112.91	119.40
4	D	46	CYS	N-CA-CB	5.90	121.23	110.60
13	6	141	ARG	NE-CZ-NH1	5.90	123.25	120.30
17	T	249	MET	CA-CB-CG	5.90	123.33	113.30
9	2	104	ARG	NE-CZ-NH2	-5.90	117.35	120.30
17	T	229	VAL	CA-CB-CG1	-5.90	102.05	110.90
25	R	38	VAL	CA-CB-CG1	-5.90	102.05	110.90
2	b	7	PHE	CB-CG-CD1	5.90	124.93	120.80
17	T	90	PHE	CG-CD2-CE2	5.90	127.29	120.80
24	Q	153	ASP	CB-CG-OD2	-5.90	112.99	118.30
27	O	64	ASN	N-CA-CB	5.90	121.22	110.60
5	E	181	ALA	O-C-N	-5.90	113.27	122.70
20	Z	408	TYR	CB-CG-CD1	-5.89	117.46	121.00
5	e	153	TYR	CB-CG-CD2	-5.89	117.47	121.00
21	N	438	ASP	CB-CA-C	-5.89	98.62	110.40
25	R	259	PHE	CB-CG-CD1	-5.89	116.68	120.80
24	Q	179	LEU	CB-CG-CD1	5.89	121.01	111.00
21	N	895	LYS	CD-CE-NZ	-5.89	98.16	111.70
26	U	52	PHE	CB-CG-CD1	-5.89	116.68	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	U	116	ASN	N-CA-C	-5.89	95.11	111.00
31	L	168	TYR	CG-CD2-CE2	-5.89	116.59	121.30
3	c	102	TYR	CB-CG-CD1	-5.88	117.47	121.00
8	h	174	TRP	CB-CG-CD1	5.88	134.65	127.00
24	Q	99	THR	CA-CB-CG2	-5.88	104.16	112.40
28	H	222	ARG	NE-CZ-NH2	-5.88	117.36	120.30
10	3	74	TYR	CD1-CE1-CZ	-5.88	114.51	119.80
33	J	174	PHE	CB-CG-CD1	-5.88	116.68	120.80
3	C	114	ARG	NH1-CZ-NH2	5.88	125.87	119.40
20	Z	486	SER	CB-CA-C	-5.88	98.93	110.10
10	j	199	TYR	CZ-CE2-CD2	-5.88	114.51	119.80
21	N	201	LYS	N-CA-CB	5.88	121.18	110.60
22	S	97	THR	CA-CB-CG2	-5.88	104.17	112.40
32	M	281	ASP	CB-CG-OD1	5.88	123.59	118.30
11	k	182	LYS	CB-CA-C	-5.88	98.65	110.40
2	b	93	ALA	N-CA-CB	5.88	118.33	110.10
4	d	39	LYS	CB-CA-C	-5.87	98.65	110.40
14	n	223	ARG	NE-CZ-NH1	5.87	123.24	120.30
13	6	97	ALA	N-CA-CB	5.87	118.32	110.10
21	N	711	ARG	NE-CZ-NH2	-5.87	117.36	120.30
5	E	151	ASP	CB-CG-OD1	5.87	123.58	118.30
5	E	191	LEU	N-CA-CB	5.87	122.14	110.40
25	R	204	TRP	CE2-CD2-CG	-5.87	102.60	107.30
13	6	68	ASP	CB-CG-OD1	5.87	123.58	118.30
10	3	20	CYS	O-C-N	5.87	132.09	122.70
8	1	200	ASP	CB-CG-OD1	-5.87	113.02	118.30
13	6	173	ASN	N-CA-CB	5.87	121.16	110.60
18	X	116	ALA	N-CA-C	-5.87	95.16	111.00
30	K	344	ARG	N-CA-CB	5.87	121.16	110.60
10	j	136	PHE	CB-CG-CD1	5.86	124.90	120.80
4	D	139	ASP	CB-CG-OD1	-5.86	113.03	118.30
20	Z	734	ASP	CB-CG-OD1	5.86	123.57	118.30
28	H	190	ARG	NE-CZ-NH1	5.86	123.23	120.30
5	e	158	ALA	CB-CA-C	5.85	118.88	110.10
21	N	789	GLU	OE1-CD-OE2	-5.85	116.28	123.30
4	D	156	TYR	CB-CG-CD1	-5.85	117.49	121.00
8	h	148	ASP	CB-CG-OD2	-5.85	113.03	118.30
2	b	3	ASP	CB-CG-OD2	-5.85	113.04	118.30
14	7	200	LYS	CB-CA-C	-5.85	98.70	110.40
22	S	137	PHE	CG-CD1-CE1	5.85	127.23	120.80
12	l	144	ARG	NE-CZ-NH1	5.84	123.22	120.30
13	m	21	LEU	CB-CG-CD1	5.84	120.93	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	144	TYR	CD1-CE1-CZ	5.84	125.06	119.80
2	B	220	ASP	CB-CG-OD2	5.84	123.56	118.30
30	K	322	ASP	N-CA-CB	5.84	121.11	110.60
10	3	104	PHE	N-CA-C	-5.84	95.24	111.00
33	J	97	ASP	CB-CG-OD1	-5.84	113.05	118.30
12	l	252	LEU	CB-CG-CD1	-5.83	101.08	111.00
3	c	113	ARG	NH1-CZ-NH2	-5.83	112.98	119.40
11	4	98	TYR	N-CA-C	-5.83	95.25	111.00
11	4	36	ARG	N-CA-CB	5.83	121.09	110.60
24	Q	339	TYR	CB-CG-CD2	-5.83	117.50	121.00
20	Z	410	THR	N-CA-CB	5.83	121.37	110.30
4	d	18	PHE	CB-CG-CD2	-5.83	116.72	120.80
7	g	160	TYR	CB-CG-CD1	-5.83	117.50	121.00
28	H	253	GLY	O-C-N	-5.83	113.38	122.70
29	I	334	LEU	CB-CA-C	-5.83	99.13	110.20
31	L	216	LYS	N-CA-C	-5.83	95.27	111.00
9	i	75	ALA	CB-CA-C	-5.82	101.36	110.10
3	C	8	SER	O-C-N	5.82	132.02	122.70
6	f	222	PHE	CG-CD2-CE2	-5.82	114.40	120.80
14	7	162	TYR	CB-CG-CD2	5.82	124.49	121.00
24	Q	123	GLU	OE1-CD-OE2	-5.82	116.31	123.30
20	Z	394	TYR	CG-CD2-CE2	-5.82	116.65	121.30
22	S	464	ARG	NE-CZ-NH2	5.82	123.21	120.30
25	R	307	TYR	CB-CG-CD1	5.82	124.49	121.00
15	W	20	ASP	CB-CA-C	-5.81	98.77	110.40
13	m	106	TYR	CD1-CE1-CZ	-5.81	114.57	119.80
13	6	106	TYR	CB-CG-CD2	-5.81	117.51	121.00
15	W	77	HIS	CB-CA-C	-5.81	98.77	110.40
21	N	642	ASP	CA-C-N	5.81	133.37	117.10
29	I	128	TYR	CD1-CE1-CZ	5.81	125.03	119.80
31	L	299	ARG	NE-CZ-NH2	-5.81	117.39	120.30
12	5	282	PHE	CB-CG-CD1	-5.81	116.73	120.80
12	l	94	ARG	NE-CZ-NH1	-5.81	117.40	120.30
11	4	151	ASP	CB-CG-OD1	-5.81	113.07	118.30
28	H	454	TYR	CB-CG-CD1	5.81	124.48	121.00
13	6	62	ALA	N-CA-CB	5.81	118.23	110.10
9	2	88	ILE	CB-CA-C	-5.80	99.99	111.60
21	N	419	THR	CA-CB-OG1	5.80	121.19	109.00
23	P	379	TYR	CD1-CE1-CZ	5.80	125.03	119.80
24	Q	8	LEU	CB-CG-CD1	5.80	120.86	111.00
30	K	418	ASP	CB-CG-OD2	5.80	123.52	118.30
11	4	2	ASP	CB-CG-OD1	-5.80	113.08	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	159	PHE	CG-CD1-CE1	-5.80	114.42	120.80
20	Z	439	TYR	CB-CG-CD2	-5.80	117.52	121.00
21	N	228	VAL	CG1-CB-CG2	5.80	120.18	110.90
23	P	223	LEU	N-CA-CB	5.80	122.00	110.40
25	R	204	TRP	CD2-CE2-CZ2	-5.80	115.34	122.30
13	6	139	TYR	CB-CG-CD2	5.79	124.48	121.00
20	Z	879	ALA	CB-CA-C	-5.79	101.41	110.10
31	L	269	TYR	CB-CG-CD2	5.79	124.48	121.00
11	k	139	TYR	CB-CG-CD2	-5.79	117.53	121.00
17	T	202	LEU	O-C-N	-5.79	113.44	122.70
32	M	166	ARG	NE-CZ-NH2	-5.79	117.41	120.30
14	7	49	TYR	N-CA-CB	5.79	121.02	110.60
2	B	212	ALA	N-CA-CB	5.79	118.20	110.10
11	4	170	LYS	O-C-N	-5.79	113.44	122.70
21	N	539	MET	CG-SD-CE	-5.79	90.94	100.20
25	R	239	THR	N-CA-C	-5.79	95.38	111.00
22	S	111	ARG	NE-CZ-NH2	-5.78	117.41	120.30
7	g	127	ASN	CB-CA-C	-5.78	98.84	110.40
20	Z	272	TYR	CB-CG-CD1	5.78	124.47	121.00
32	M	349	PHE	CB-CG-CD2	-5.78	116.75	120.80
4	d	141	ARG	NH1-CZ-NH2	-5.78	113.04	119.40
4	D	49	ARG	NH1-CZ-NH2	-5.78	113.05	119.40
12	5	106	VAL	CA-CB-CG2	-5.78	102.23	110.90
27	O	228	TYR	CB-CG-CD2	-5.78	117.53	121.00
21	N	675	VAL	CG1-CB-CG2	-5.78	101.66	110.90
23	P	225	VAL	CA-CB-CG2	-5.78	102.24	110.90
7	G	160	TYR	CB-CG-CD2	-5.77	117.54	121.00
20	Z	928	ARG	NH1-CZ-NH2	-5.77	113.05	119.40
23	P	232	ARG	NE-CZ-NH2	-5.77	117.42	120.30
3	c	50	ARG	NE-CZ-NH1	5.77	123.18	120.30
12	l	170	LEU	N-CA-CB	5.77	121.94	110.40
25	R	30	ALA	CB-CA-C	-5.77	101.45	110.10
27	O	369	ARG	NH1-CZ-NH2	5.77	125.74	119.40
28	H	185	LEU	CB-CG-CD1	5.77	120.81	111.00
11	k	172	MET	CG-SD-CE	5.77	109.43	100.20
11	4	161	LEU	CB-CG-CD1	5.77	120.80	111.00
2	b	89	SER	CB-CA-C	-5.76	99.15	110.10
10	j	199	TYR	CD1-CE1-CZ	-5.76	114.61	119.80
3	C	53	THR	CA-CB-CG2	-5.76	104.33	112.40
23	P	436	GLU	OE1-CD-OE2	5.76	130.22	123.30
1	A	122	ALA	CB-CA-C	-5.76	101.46	110.10
32	M	326	ALA	N-CA-CB	5.76	118.17	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	237	LYS	N-CA-CB	5.76	120.97	110.60
3	c	7	ASP	CB-CG-OD2	-5.76	113.12	118.30
17	T	128	TYR	CB-CG-CD2	-5.76	117.55	121.00
20	Z	511	PRO	N-CA-CB	5.76	110.21	103.30
20	Z	138	ARG	NH1-CZ-NH2	-5.75	113.07	119.40
32	M	247	ALA	N-CA-CB	5.75	118.15	110.10
32	M	187	ASP	CB-CG-OD1	5.75	123.48	118.30
4	D	23	ALA	CB-CA-C	-5.75	101.48	110.10
9	i	46	ASP	CB-CG-OD2	-5.75	113.13	118.30
25	R	232	VAL	CG1-CB-CG2	-5.75	101.70	110.90
33	J	206	THR	C-N-CA	5.75	136.07	121.70
9	i	101	ARG	NE-CZ-NH2	5.74	123.17	120.30
9	i	119	TYR	CZ-CE2-CD2	5.74	124.97	119.80
22	S	171	TYR	CB-CG-CD2	-5.74	117.55	121.00
22	S	399	TYR	CB-CA-C	-5.74	98.91	110.40
7	g	184	PRO	N-CD-CG	5.74	111.81	103.20
13	m	13	TYR	N-CA-CB	5.74	120.93	110.60
11	k	195	PHE	CD1-CE1-CZ	5.74	126.98	120.10
3	C	141	ASP	N-CA-CB	5.74	120.93	110.60
21	N	471	TYR	CD1-CE1-CZ	-5.74	114.64	119.80
17	T	233	VAL	CG1-CB-CG2	5.74	120.08	110.90
16	V	142	ASP	CB-CG-OD1	-5.73	113.14	118.30
3	c	180	TYR	CD1-CG-CD2	-5.73	111.60	117.90
33	J	212	ARG	NE-CZ-NH1	5.73	123.16	120.30
32	M	170	MET	CG-SD-CE	-5.73	91.04	100.20
33	J	134	VAL	CA-CB-CG2	-5.73	102.31	110.90
12	5	221	TRP	CG-CD2-CE3	-5.72	128.75	133.90
20	Z	215	ASN	O-C-N	5.72	132.93	123.20
20	Z	952	SER	N-CA-CB	5.72	119.09	110.50
27	O	309	SER	N-CA-CB	5.72	119.09	110.50
9	2	220	LEU	N-CA-CB	5.72	121.84	110.40
30	K	58	TYR	CB-CG-CD2	-5.72	117.57	121.00
3	c	24	TYR	CB-CG-CD1	5.72	124.43	121.00
10	3	15	MET	CG-SD-CE	5.72	109.35	100.20
15	W	173	THR	CA-CB-CG2	-5.72	104.39	112.40
13	m	151	ALA	CB-CA-C	-5.72	101.53	110.10
5	E	22	PHE	CB-CG-CD1	-5.72	116.80	120.80
13	6	113	TYR	CB-CG-CD2	-5.72	117.57	121.00
16	V	197	TYR	CB-CG-CD2	-5.71	117.57	121.00
21	N	581	ASP	CA-CB-CG	-5.71	100.83	113.40
28	H	457	PHE	CB-CG-CD2	-5.71	116.80	120.80
10	j	188	TYR	CD1-CE1-CZ	-5.71	114.66	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	893	PHE	CG-CD2-CE2	5.71	127.08	120.80
27	O	172	TYR	CG-CD2-CE2	5.71	125.87	121.30
3	c	237	ASP	CB-CG-OD2	-5.71	113.16	118.30
1	A	30	TYR	CB-CG-CD2	5.71	124.42	121.00
19	Y	32	ASP	CB-CG-OD2	-5.71	113.16	118.30
20	Z	562	TRP	CG-CD2-CE3	-5.71	128.76	133.90
29	I	142	GLU	N-CA-C	-5.71	95.59	111.00
32	M	254	MET	CG-SD-CE	-5.71	91.07	100.20
9	i	148	THR	CA-CB-CG2	-5.70	104.41	112.40
24	Q	43	GLY	CA-C-O	5.70	130.87	120.60
12	l	230	TYR	CG-CD2-CE2	-5.70	116.74	121.30
1	A	155	TYR	CG-CD1-CE1	5.70	125.86	121.30
13	6	149	ALA	N-CA-CB	5.70	118.08	110.10
28	H	464	MET	CG-SD-CE	-5.70	91.08	100.20
2	b	82	TYR	CB-CG-CD2	5.70	124.42	121.00
3	c	148	LEU	CB-CA-C	-5.70	99.38	110.20
1	A	219	SER	N-CA-CB	5.70	119.04	110.50
11	4	25	ILE	CA-CB-CG1	5.70	121.82	111.00
24	Q	86	MET	CB-CA-C	-5.70	99.01	110.40
26	U	9	THR	CA-CB-CG2	-5.70	104.43	112.40
22	S	330	LEU	CB-CG-CD2	5.69	120.68	111.00
29	I	271	ALA	N-CA-CB	5.69	118.07	110.10
7	G	230	PHE	CB-CG-CD2	5.69	124.78	120.80
9	i	212	ASP	CB-CG-OD2	-5.69	113.18	118.30
17	T	258	ASN	CA-CB-CG	-5.69	100.89	113.40
10	j	107	PRO	C-N-CA	5.68	135.91	121.70
31	L	180	PHE	CB-CG-CD2	-5.68	116.82	120.80
1	A	162	TYR	CB-CG-CD1	-5.68	117.59	121.00
20	Z	837	TYR	CB-CG-CD1	5.68	124.41	121.00
31	L	203	ASN	N-CA-CB	5.68	120.82	110.60
9	2	118	LYS	N-CA-CB	5.68	120.82	110.60
12	5	148	ARG	CB-CA-C	-5.68	99.04	110.40
21	N	183	VAL	CA-CB-CG1	5.68	119.42	110.90
13	m	21	LEU	N-CA-C	-5.68	95.67	111.00
1	a	173	PRO	N-CA-CB	5.67	110.11	103.30
14	7	163	VAL	O-C-N	-5.67	113.62	122.70
14	n	155	ASN	CB-CA-C	-5.67	99.05	110.40
21	N	526	TYR	CG-CD2-CE2	-5.67	116.76	121.30
22	S	118	PHE	N-CA-CB	5.67	120.81	110.60
6	f	219	ASP	CB-CG-OD1	-5.67	113.20	118.30
21	N	203	ARG	NE-CZ-NH2	5.67	123.14	120.30
27	O	70	TYR	CD1-CE1-CZ	5.67	124.90	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	402	ALA	N-CA-CB	5.67	118.04	110.10
1	a	147	ASP	C-N-CA	5.67	135.87	121.70
3	C	24	TYR	CG-CD2-CE2	-5.67	116.77	121.30
12	5	262	TYR	CB-CG-CD1	5.67	124.40	121.00
22	S	456	ASP	CB-CG-OD1	5.67	123.40	118.30
21	N	446	ALA	N-CA-CB	5.67	118.03	110.10
21	N	873	ARG	NE-CZ-NH1	-5.66	117.47	120.30
25	R	252	TYR	CG-CD2-CE2	-5.66	116.77	121.30
4	d	120	TYR	CG-CD2-CE2	-5.66	116.77	121.30
21	N	621	THR	N-CA-CB	5.66	121.06	110.30
26	U	72	TYR	CB-CG-CD1	5.66	124.40	121.00
29	I	246	ARG	NE-CZ-NH2	5.66	123.13	120.30
10	j	196	VAL	CA-CB-CG1	-5.66	102.41	110.90
4	D	138	PHE	CB-CG-CD1	-5.66	116.84	120.80
4	D	180	ASP	CB-CG-OD1	-5.66	113.20	118.30
13	6	204	ILE	O-C-N	-5.66	113.64	122.70
14	n	144	TRP	CB-CG-CD1	5.66	134.36	127.00
21	N	23	TYR	CB-CG-CD2	5.66	124.39	121.00
22	S	425	ARG	NE-CZ-NH2	5.66	123.13	120.30
10	3	124	PHE	CG-CD2-CE2	-5.66	114.58	120.80
16	V	214	MET	CA-CB-CG	5.66	122.91	113.30
4	d	195	THR	CA-CB-CG2	-5.65	104.48	112.40
20	Z	263	ALA	CB-CA-C	-5.65	101.62	110.10
13	6	102	GLN	CB-CA-C	-5.65	99.10	110.40
13	6	141	ARG	CG-CD-NE	-5.65	99.94	111.80
25	R	417	TYR	CB-CG-CD2	-5.65	117.61	121.00
28	H	56	LEU	CB-CG-CD2	5.65	120.61	111.00
6	f	6	TYR	CG-CD2-CE2	5.65	125.82	121.30
20	Z	534	PHE	CB-CG-CD1	-5.65	116.85	120.80
24	Q	64	LEU	CB-CG-CD2	5.65	120.60	111.00
29	I	219	VAL	N-CA-C	-5.65	95.75	111.00
9	2	215	TYR	CG-CD1-CE1	-5.65	116.78	121.30
3	C	198	SER	N-CA-CB	5.64	118.97	110.50
30	K	180	GLN	N-CA-CB	5.64	120.76	110.60
2	B	74	VAL	CA-CB-CG2	-5.64	102.44	110.90
6	F	225	TYR	CG-CD2-CE2	-5.64	116.78	121.30
10	3	69	TYR	CB-CG-CD1	5.64	124.39	121.00
22	S	114	TYR	CZ-CE2-CD2	5.64	124.88	119.80
11	k	182	LYS	N-CA-CB	5.64	120.75	110.60
20	Z	865	ASP	CB-CG-OD1	-5.64	113.22	118.30
18	X	45	PHE	CB-CG-CD1	-5.64	116.86	120.80
4	d	205	THR	CA-CB-CG2	-5.63	104.51	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	212	ASP	CB-CG-OD2	5.63	123.37	118.30
10	3	141	THR	CA-CB-CG2	-5.63	104.51	112.40
12	5	131	GLU	N-CA-CB	5.63	120.74	110.60
10	3	133	ALA	N-CA-CB	5.63	117.98	110.10
15	W	60	ARG	NE-CZ-NH2	-5.63	117.48	120.30
2	B	231	LYS	N-CA-CB	5.63	120.73	110.60
31	L	361	PHE	CB-CG-CD2	5.63	124.74	120.80
6	f	164	ARG	NE-CZ-NH2	-5.63	117.49	120.30
21	N	365	PHE	CB-CG-CD2	-5.63	116.86	120.80
8	h	146	TYR	CB-CG-CD2	-5.62	117.62	121.00
2	b	14	PRO	N-CA-CB	5.62	110.05	103.30
12	5	268	VAL	CA-CB-CG1	-5.62	102.46	110.90
19	Y	80	GLU	N-CA-CB	-5.62	100.48	110.60
9	i	202	VAL	CG1-CB-CG2	5.62	119.89	110.90
9	2	56	ALA	N-CA-CB	5.62	117.97	110.10
9	2	126	TYR	CZ-CE2-CD2	5.62	124.86	119.80
23	P	374	SER	N-CA-CB	5.62	118.93	110.50
7	G	191	GLU	CA-CB-CG	5.62	125.76	113.40
28	H	175	GLY	N-CA-C	-5.62	99.05	113.10
29	I	383	THR	C-N-CA	5.62	135.75	121.70
12	5	227	ASP	CB-CG-OD2	-5.62	113.24	118.30
8	1	152	ARG	NE-CZ-NH2	-5.62	117.49	120.30
29	I	373	GLU	O-C-N	-5.62	113.71	122.70
6	f	54	ASP	CB-CG-OD1	5.62	123.35	118.30
13	6	104	LEU	CB-CA-C	-5.62	99.53	110.20
25	R	164	THR	CA-CB-CG2	-5.62	104.54	112.40
25	R	73	ASN	N-CA-C	-5.61	95.84	111.00
25	R	272	ASP	CB-CG-OD2	-5.61	113.25	118.30
7	g	15	PHE	CB-CA-C	-5.61	99.18	110.40
30	K	46	ASP	CB-CG-OD1	5.61	123.35	118.30
33	J	42	ARG	NE-CZ-NH1	-5.61	117.50	120.30
1	A	199	TRP	CE3-CZ3-CH2	-5.61	115.03	121.20
21	N	222	TYR	CB-CG-CD1	5.61	124.36	121.00
32	M	303	ARG	NE-CZ-NH2	-5.61	117.50	120.30
11	4	122	LEU	C-N-CA	5.61	134.07	122.30
29	I	128	TYR	CB-CG-CD2	-5.61	117.64	121.00
24	Q	390	LEU	O-C-N	-5.60	113.73	122.70
2	B	68	THR	CA-CB-CG2	-5.60	104.56	112.40
4	d	129	PHE	CB-CG-CD2	5.60	124.72	120.80
21	N	857	TYR	CB-CG-CD1	-5.60	117.64	121.00
22	S	206	GLN	N-CA-CB	5.60	120.68	110.60
23	P	304	THR	CA-CB-CG2	-5.60	104.56	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	424	ASP	CB-CG-OD2	-5.60	113.26	118.30
7	g	189	ALA	N-CA-CB	5.60	117.94	110.10
20	Z	237	VAL	CA-CB-CG1	-5.60	102.51	110.90
4	d	112	TYR	CB-CG-CD2	-5.59	117.64	121.00
21	N	212	ASP	CB-CG-OD2	-5.59	113.26	118.30
25	R	86	ASP	CB-CG-OD1	5.59	123.33	118.30
9	2	186	ASP	CB-CG-OD1	-5.59	113.27	118.30
14	n	221	ASP	CB-CG-OD2	-5.59	113.27	118.30
12	5	173	GLY	N-CA-C	-5.59	99.12	113.10
25	R	171	MET	CG-SD-CE	-5.59	91.25	100.20
1	a	44	ALA	N-CA-CB	5.59	117.92	110.10
29	I	171	MET	CA-CB-CG	5.59	122.80	113.30
14	n	162	TYR	CB-CG-CD1	5.59	124.35	121.00
8	1	133	TYR	N-CA-CB	5.59	120.66	110.60
17	T	90	PHE	CZ-CE2-CD2	-5.59	113.40	120.10
32	M	393	ALA	N-CA-CB	5.59	117.92	110.10
2	b	23	TYR	CG-CD2-CE2	-5.58	116.83	121.30
17	T	168	SER	N-CA-CB	5.58	118.88	110.50
25	R	272	ASP	CB-CG-OD1	5.58	123.33	118.30
11	k	67	TYR	CB-CG-CD1	5.58	124.35	121.00
20	Z	724	GLU	OE1-CD-OE2	5.58	130.00	123.30
21	N	208	ARG	O-C-N	-5.58	113.77	122.70
25	R	70	TYR	CG-CD2-CE2	-5.58	116.83	121.30
3	c	180	TYR	CB-CG-CD2	-5.58	117.65	121.00
6	F	123	TYR	N-CA-CB	5.58	120.64	110.60
23	P	235	LEU	CB-CG-CD1	5.58	120.48	111.00
10	j	31	SER	N-CA-CB	5.58	118.86	110.50
10	j	178	ASP	CB-CG-OD2	-5.58	113.28	118.30
20	Z	269	TYR	CG-CD2-CE2	-5.58	116.84	121.30
3	C	225	VAL	CA-CB-CG1	-5.58	102.54	110.90
14	7	132	VAL	CG1-CB-CG2	-5.57	101.98	110.90
29	I	82	LEU	CB-CG-CD2	5.57	120.48	111.00
14	7	165	LEU	CB-CG-CD2	5.57	120.47	111.00
12	l	219	TYR	CZ-CE2-CD2	-5.57	114.79	119.80
20	Z	849	ARG	NE-CZ-NH1	5.57	123.08	120.30
12	l	181	ARG	NE-CZ-NH1	5.57	123.08	120.30
18	X	11	ARG	NH1-CZ-NH2	5.57	125.52	119.40
21	N	250	ASP	CB-CG-OD1	-5.57	113.29	118.30
29	I	275	ALA	N-CA-CB	5.57	117.89	110.10
23	P	325	ASP	CB-CG-OD2	-5.56	113.29	118.30
8	1	141	THR	N-CA-CB	5.56	120.87	110.30
21	N	231	ASN	N-CA-CB	5.56	120.61	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	30	TYR	CB-CG-CD2	-5.56	117.66	121.00
5	e	156	PHE	CZ-CE2-CD2	-5.56	113.43	120.10
17	T	78	PHE	N-CA-CB	5.56	120.61	110.60
17	T	245	TYR	CB-CG-CD2	-5.56	117.66	121.00
9	i	152	TYR	CB-CG-CD1	5.56	124.33	121.00
28	H	226	GLU	OE1-CD-OE2	5.56	129.97	123.30
7	g	216	ILE	N-CA-C	-5.55	96.00	111.00
13	m	164	PHE	N-CA-CB	5.55	120.60	110.60
2	B	120	GLU	OE1-CD-OE2	5.55	129.97	123.30
10	3	183	TRP	N-CA-CB	5.55	120.60	110.60
20	Z	489	ALA	CB-CA-C	-5.55	101.77	110.10
11	4	130	TYR	CZ-CE2-CD2	5.55	124.80	119.80
29	I	295	ASN	N-CA-CB	5.55	120.59	110.60
12	l	284	ASN	N-CA-CB	5.55	120.59	110.60
29	I	291	ARG	N-CA-C	-5.55	96.01	111.00
22	S	147	TRP	CE3-CZ3-CH2	-5.55	115.09	121.20
27	O	172	TYR	CZ-CE2-CD2	-5.55	114.81	119.80
20	Z	376	SER	N-CA-CB	5.55	118.82	110.50
6	f	216	VAL	CG1-CB-CG2	5.55	119.78	110.90
2	B	133	SER	CB-CA-C	-5.55	99.56	110.10
4	D	112	TYR	CG-CD2-CE2	5.55	125.74	121.30
10	3	190	ILE	N-CA-C	-5.55	96.03	111.00
15	W	142	ILE	CA-CB-CG2	5.55	121.99	110.90
28	H	225	VAL	CG1-CB-CG2	-5.54	102.03	110.90
3	c	209	ASP	CB-CG-OD1	5.54	123.29	118.30
2	b	82	TYR	CG-CD1-CE1	-5.54	116.87	121.30
18	X	10	PHE	CB-CG-CD2	-5.54	116.92	120.80
7	G	220	SER	N-CA-CB	5.54	118.81	110.50
22	S	367	TYR	CB-CG-CD1	5.54	124.32	121.00
8	h	136	ALA	N-CA-C	-5.54	96.05	111.00
21	N	378	ASN	CB-CG-OD1	-5.53	110.53	121.60
22	S	367	TYR	CB-CG-CD2	-5.53	117.68	121.00
31	L	270	ALA	N-CA-CB	5.53	117.85	110.10
14	7	138	SER	N-CA-CB	5.53	118.80	110.50
10	j	199	TYR	CG-CD2-CE2	5.53	125.72	121.30
5	E	144	ILE	CG1-CB-CG2	5.53	123.57	111.40
12	5	260	TRP	CZ3-CH2-CZ2	-5.53	114.97	121.60
25	R	408	ASP	CB-CG-OD2	5.53	123.27	118.30
23	P	136	ARG	NE-CZ-NH2	5.53	123.06	120.30
3	c	67	TYR	CG-CD1-CE1	-5.52	116.88	121.30
4	d	29	ARG	NE-CZ-NH1	5.52	123.06	120.30
21	N	60	MET	CG-SD-CE	-5.52	91.36	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	215	PRO	N-CD-CG	5.52	111.48	103.20
13	6	97	ALA	CB-CA-C	-5.52	101.82	110.10
7	g	53	LEU	CB-CG-CD2	5.52	120.38	111.00
5	E	16	SER	N-CA-CB	5.52	118.78	110.50
13	6	97	ALA	O-C-N	-5.52	113.87	122.70
1	a	96	ARG	NE-CZ-NH2	-5.52	117.54	120.30
4	d	148	TYR	CB-CG-CD2	5.52	124.31	121.00
28	H	443	PHE	CB-CG-CD2	5.52	124.66	120.80
13	m	82	TRP	CB-CG-CD1	5.52	134.17	127.00
32	M	293	SER	CB-CA-C	-5.52	99.62	110.10
4	D	225	SER	N-CA-CB	5.51	118.77	110.50
24	Q	326	MET	C-N-CA	5.51	133.88	122.30
3	C	4	ARG	N-CA-CB	5.51	120.52	110.60
20	Z	272	TYR	CD1-CE1-CZ	5.51	124.76	119.80
21	N	436	ASP	CB-CG-OD2	5.51	123.26	118.30
33	J	348	GLU	OE1-CD-OE2	-5.51	116.69	123.30
24	Q	100	LEU	CB-CG-CD1	5.51	120.36	111.00
28	H	271	PHE	N-CA-C	-5.51	96.13	111.00
2	B	75	TYR	CB-CG-CD1	-5.51	117.70	121.00
26	U	51	SER	N-CA-CB	5.51	118.76	110.50
17	T	267	ALA	CB-CA-C	-5.50	101.84	110.10
13	m	56	ASP	N-CA-CB	5.50	120.51	110.60
3	C	63	THR	N-CA-CB	5.50	120.76	110.30
9	2	88	ILE	CA-CB-CG1	5.50	121.46	111.00
7	G	243	ALA	N-CA-CB	5.50	117.80	110.10
24	Q	398	TYR	CG-CD2-CE2	-5.50	116.90	121.30
27	O	157	LEU	CB-CG-CD2	5.50	120.35	111.00
27	O	353	VAL	CA-CB-CG1	-5.50	102.65	110.90
1	a	166	TYR	CG-CD2-CE2	-5.50	116.90	121.30
2	b	148	TYR	CB-CG-CD1	-5.50	117.70	121.00
29	I	147	VAL	CA-CB-CG2	-5.50	102.65	110.90
29	I	310	LEU	CB-CG-CD2	5.50	120.34	111.00
33	J	223	ILE	N-CA-C	-5.50	96.16	111.00
33	J	228	ARG	NE-CZ-NH2	-5.50	117.55	120.30
1	a	123	ASN	N-CA-CB	5.50	120.49	110.60
23	P	221	TYR	CB-CA-C	-5.50	99.41	110.40
21	N	873	ARG	NE-CZ-NH2	5.49	123.05	120.30
9	2	55	VAL	CA-CB-CG2	-5.49	102.66	110.90
24	Q	20	TYR	CB-CG-CD2	5.49	124.29	121.00
31	L	281	ASP	CB-CA-C	-5.49	99.42	110.40
3	c	183	ASP	CB-CG-OD1	-5.49	113.36	118.30
1	A	166	TYR	CG-CD1-CE1	-5.49	116.91	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	Z	593	HIS	N-CA-C	-5.49	96.18	111.00
10	3	162	ASP	CB-CG-OD2	-5.49	113.36	118.30
11	4	135	TYR	CB-CG-CD2	5.49	124.29	121.00
2	B	99	ARG	NH1-CZ-NH2	-5.48	113.37	119.40
4	d	132	SER	N-CA-C	-5.48	96.20	111.00
6	F	202	ARG	NH1-CZ-NH2	-5.48	113.37	119.40
24	Q	68	MET	CG-SD-CE	5.48	108.97	100.20
13	m	168	TYR	CG-CD2-CE2	-5.48	116.92	121.30
20	Z	340	LEU	CB-CG-CD1	5.48	120.31	111.00
21	N	89	PHE	CB-CG-CD2	-5.48	116.97	120.80
5	e	123	PHE	CB-CG-CD1	5.48	124.64	120.80
3	c	208	TYR	CB-CG-CD2	-5.48	117.71	121.00
20	Z	482	ASP	CB-CG-OD2	5.48	123.23	118.30
10	j	198	ARG	NE-CZ-NH1	5.47	123.04	120.30
11	k	21	VAL	CA-CB-CG1	5.47	119.11	110.90
12	l	210	PHE	CB-CG-CD1	5.47	124.63	120.80
31	L	127	TYR	CB-CG-CD2	5.47	124.28	121.00
4	D	29	ARG	NH1-CZ-NH2	5.47	125.42	119.40
14	7	257	ASP	CB-CG-OD2	5.47	123.22	118.30
23	P	223	LEU	CB-CA-C	-5.47	99.80	110.20
5	e	198	LEU	CB-CG-CD2	5.47	120.30	111.00
10	j	3	ASP	CB-CG-OD2	5.47	123.22	118.30
24	Q	88	PHE	CB-CG-CD2	-5.47	116.97	120.80
31	L	237	ALA	CB-CA-C	-5.47	101.89	110.10
3	c	67	TYR	CD1-CG-CD2	5.47	123.92	117.90
1	A	229	THR	CA-CB-CG2	-5.47	104.74	112.40
14	7	124	TYR	CB-CG-CD1	5.47	124.28	121.00
22	S	186	TYR	CB-CG-CD2	-5.47	117.72	121.00
30	K	262	ARG	NE-CZ-NH2	-5.47	117.56	120.30
1	a	229	THR	CA-CB-CG2	-5.47	104.74	112.40
28	H	203	LYS	N-CA-CB	5.47	120.44	110.60
1	a	87	ILE	CA-C-N	5.47	132.40	117.10
12	5	130	TRP	CB-CA-C	-5.47	99.47	110.40
23	P	124	VAL	CB-CA-C	-5.47	101.01	111.40
23	P	209	LYS	N-CA-CB	5.47	120.44	110.60
11	k	73	TYR	CB-CG-CD1	-5.46	117.72	121.00
14	7	140	MET	N-CA-CB	5.46	120.44	110.60
21	N	802	ALA	N-CA-CB	5.46	117.75	110.10
14	7	49	TYR	CB-CG-CD1	5.46	124.28	121.00
2	b	181	ASP	CB-CG-OD2	-5.46	113.39	118.30
14	n	196	SER	CB-CA-C	5.46	120.47	110.10
31	L	69	ARG	NE-CZ-NH1	5.46	123.03	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	74	ARG	NE-CZ-NH2	-5.46	117.57	120.30
14	7	137	ARG	NE-CZ-NH2	5.46	123.03	120.30
23	P	37	ASP	N-CA-CB	5.46	120.42	110.60
6	f	116	ALA	N-CA-CB	5.46	117.74	110.10
3	C	66	LEU	N-CA-CB	5.46	121.31	110.40
2	B	53	SER	N-CA-C	-5.45	96.28	111.00
11	4	148	TYR	CB-CG-CD2	5.45	124.27	121.00
32	M	414	ASP	N-CA-CB	5.45	120.42	110.60
5	e	147	HIS	CB-CA-C	-5.45	99.50	110.40
9	i	215	TYR	CD1-CG-CD2	5.45	123.90	117.90
21	N	675	VAL	CA-CB-CG2	-5.45	102.72	110.90
27	O	171	PHE	CB-CG-CD1	5.45	124.61	120.80
21	N	45	ASP	CB-CG-OD1	-5.45	113.40	118.30
7	g	203	ALA	CB-CA-C	-5.45	101.93	110.10
30	K	121	ARG	NE-CZ-NH2	-5.45	117.58	120.30
32	M	330	VAL	CG1-CB-CG2	5.44	119.61	110.90
3	C	226	TYR	CG-CD2-CE2	-5.44	116.95	121.30
27	O	29	PHE	CB-CA-C	-5.44	99.52	110.40
13	m	120	ALA	N-CA-CB	5.44	117.72	110.10
17	T	100	ASP	CB-CG-OD2	-5.44	113.41	118.30
13	m	51	VAL	CA-CB-CG1	-5.44	102.74	110.90
29	I	326	MET	N-CA-CB	5.44	120.39	110.60
20	Z	98	ASP	CB-CG-OD2	-5.43	113.41	118.30
23	P	359	ARG	NE-CZ-NH1	5.43	123.02	120.30
28	H	235	PHE	CB-CG-CD1	-5.43	117.00	120.80
5	e	34	GLY	N-CA-C	-5.43	99.52	113.10
7	g	36	THR	CA-CB-CG2	-5.43	104.80	112.40
29	I	128	TYR	CZ-CE2-CD2	5.43	124.69	119.80
12	l	117	LEU	CB-CA-C	-5.43	99.88	110.20
10	3	103	TYR	CB-CG-CD2	-5.43	117.74	121.00
17	T	109	TYR	CB-CG-CD1	-5.43	117.74	121.00
27	O	178	TYR	CG-CD1-CE1	-5.43	116.96	121.30
9	2	45	ALA	O-C-N	5.43	131.38	122.70
16	V	111	HIS	N-CA-C	-5.43	96.34	111.00
1	a	13	ASP	CB-CG-OD1	5.43	123.18	118.30
3	c	137	TYR	CD1-CE1-CZ	-5.43	114.92	119.80
14	n	144	TRP	CB-CG-CD2	-5.43	119.55	126.60
12	5	253	TYR	CB-CG-CD2	-5.43	117.75	121.00
14	7	83	VAL	CA-CB-CG1	5.43	119.04	110.90
29	I	195	LYS	CA-CB-CG	-5.43	101.46	113.40
29	I	268	PHE	CB-CG-CD2	5.42	124.60	120.80
8	1	29	THR	N-CA-CB	5.42	120.60	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	423	LEU	CB-CG-CD1	5.42	120.22	111.00
31	L	62	ARG	NE-CZ-NH2	-5.42	117.59	120.30
32	M	203	ARG	NE-CZ-NH2	-5.42	117.59	120.30
3	c	94	HIS	N-CA-CB	5.42	120.36	110.60
3	C	58	GLU	N-CA-CB	5.42	120.36	110.60
21	N	653	ARG	NE-CZ-NH2	-5.42	117.59	120.30
25	R	204	TRP	NE1-CE2-CZ2	5.42	136.36	130.40
6	F	20	PHE	CD1-CG-CD2	5.42	125.34	118.30
9	i	132	VAL	CA-CB-CG1	-5.42	102.77	110.90
10	3	120	PHE	CZ-CE2-CD2	-5.42	113.60	120.10
21	N	406	TYR	CB-CG-CD2	-5.42	117.75	121.00
29	I	111	GLU	OE1-CD-OE2	5.42	129.80	123.30
10	3	185	ALA	CB-CA-C	-5.42	101.98	110.10
31	L	434	TYR	CD1-CE1-CZ	-5.42	114.93	119.80
32	M	128	PHE	CB-CG-CD2	5.42	124.59	120.80
3	c	221	ASN	N-CA-CB	5.41	120.34	110.60
8	1	105	GLY	N-CA-C	-5.41	99.56	113.10
21	N	871	MET	CG-SD-CE	-5.41	91.54	100.20
8	h	89	SER	CB-CA-C	-5.41	99.82	110.10
26	U	85	ALA	N-CA-CB	-5.41	102.52	110.10
27	O	206	THR	C-N-CA	5.41	135.23	121.70
6	f	94	TYR	CB-CG-CD1	5.41	124.25	121.00
13	m	61	SER	CB-CA-C	-5.41	99.82	110.10
2	B	81	ASP	CB-CG-OD2	-5.41	113.43	118.30
21	N	591	LEU	C-N-CA	5.41	133.66	122.30
5	E	80	GLY	N-CA-C	-5.41	99.58	113.10
28	H	249	TYR	CB-CG-CD2	-5.41	117.75	121.00
31	L	357	ARG	NH1-CZ-NH2	5.41	125.35	119.40
13	m	52	PHE	CB-CG-CD1	-5.41	117.02	120.80
13	m	192	VAL	CG1-CB-CG2	-5.41	102.25	110.90
13	6	19	THR	OG1-CB-CG2	-5.41	97.56	110.00
23	P	192	ASP	N-CA-CB	5.41	120.33	110.60
28	H	227	LEU	CB-CG-CD2	5.40	120.19	111.00
2	b	207	ASP	O-C-N	-5.40	114.06	122.70
3	c	112	VAL	CA-CB-CG2	-5.40	102.80	110.90
1	A	155	TYR	CD1-CE1-CZ	-5.40	114.94	119.80
8	1	163	PHE	CB-CG-CD1	5.40	124.58	120.80
14	7	206	ALA	N-CA-CB	5.40	117.66	110.10
6	F	221	PRO	N-CA-CB	5.40	109.78	103.30
21	N	921	ARG	NE-CZ-NH1	-5.40	117.60	120.30
1	a	133	TYR	O-C-N	5.40	131.34	122.70
9	i	180	ALA	N-CA-CB	5.40	117.66	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	7	100	LEU	CB-CG-CD1	5.39	120.17	111.00
26	U	217	LYS	C-N-CA	5.39	135.18	121.70
1	A	26	TYR	CA-CB-CG	-5.39	103.15	113.40
14	7	254	PHE	CB-CG-CD1	5.39	124.57	120.80
19	Y	14	ILE	N-CA-C	-5.39	96.44	111.00
29	I	395	MET	CG-SD-CE	-5.39	91.58	100.20
27	O	148	ASP	N-CA-CB	5.39	120.30	110.60
29	I	129	TYR	CB-CG-CD2	-5.39	117.77	121.00
32	M	355	ASP	CB-CG-OD2	-5.39	113.45	118.30
31	L	127	TYR	CG-CD2-CE2	5.38	125.61	121.30
33	J	390	MET	CA-CB-CG	-5.38	104.15	113.30
11	4	29	LYS	CB-CA-C	-5.38	99.63	110.40
28	H	142	ASP	CB-CG-OD1	-5.38	113.45	118.30
11	k	17	SER	N-CA-CB	5.38	118.57	110.50
32	M	232	ALA	N-CA-CB	-5.38	102.57	110.10
20	Z	85	VAL	CA-C-N	5.38	132.16	117.10
23	P	362	LEU	CB-CG-CD1	5.38	120.15	111.00
25	R	173	THR	CA-CB-CG2	-5.38	104.87	112.40
11	k	70	ARG	NE-CZ-NH1	5.38	122.99	120.30
13	6	76	PHE	CB-CG-CD1	5.38	124.56	120.80
13	6	182	TYR	CG-CD1-CE1	5.38	125.60	121.30
3	c	80	LEU	CB-CG-CD2	5.38	120.14	111.00
6	f	18	ARG	CD-NE-CZ	-5.38	116.07	123.60
13	m	180	LEU	N-CA-CB	5.38	121.15	110.40
5	E	179	ALA	CB-CA-C	-5.38	102.03	110.10
31	L	295	THR	CA-CB-CG2	-5.38	104.87	112.40
8	1	202	TYR	CD1-CE1-CZ	-5.38	114.96	119.80
9	2	68	PRO	N-CD-CG	5.38	111.26	103.20
4	d	239	GLU	CB-CG-CD	-5.37	99.69	114.20
29	I	437	LEU	CB-CG-CD2	5.37	120.13	111.00
24	Q	254	SER	CB-CA-C	-5.37	99.90	110.10
13	m	196	PHE	CB-CG-CD1	5.37	124.56	120.80
24	Q	386	PHE	CB-CG-CD1	5.37	124.56	120.80
23	P	225	VAL	CA-CB-CG1	5.37	118.95	110.90
24	Q	428	GLU	O-C-N	-5.37	114.11	122.70
9	i	33	VAL	CA-CB-CG2	5.37	118.95	110.90
13	m	133	PHE	CB-CG-CD1	-5.37	117.05	120.80
27	O	270	ILE	O-C-N	-5.37	114.11	122.70
7	G	49	ALA	N-CA-CB	5.36	117.61	110.10
20	Z	921	GLU	N-CA-C	-5.36	96.52	111.00
23	P	402	PHE	CB-CG-CD1	-5.36	117.05	120.80
6	f	18	ARG	NE-CZ-NH1	-5.36	117.62	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	W	186	ALA	N-CA-CB	5.36	117.60	110.10
20	Z	149	TRP	CB-CG-CD1	5.36	133.97	127.00
3	C	5	ARG	NE-CZ-NH1	5.36	122.98	120.30
7	G	127	ASN	N-CA-CB	5.36	120.25	110.60
19	Y	48	THR	CA-CB-CG2	-5.36	104.90	112.40
21	N	50	TYR	CB-CG-CD1	-5.36	117.79	121.00
26	U	240	GLY	C-N-CA	5.36	135.09	121.70
30	K	391	GLY	O-C-N	-5.36	114.13	122.70
32	M	44	PHE	CB-CG-CD1	-5.36	117.05	120.80
20	Z	935	THR	CA-CB-CG2	-5.36	104.90	112.40
20	Z	885	ALA	C-N-CA	5.35	135.08	121.70
30	K	175	GLY	N-CA-C	-5.35	99.72	113.10
13	m	162	VAL	CA-CB-CG2	-5.35	102.87	110.90
6	f	186	PRO	N-CD-CG	5.35	111.22	103.20
14	n	174	THR	CA-CB-CG2	-5.35	104.91	112.40
8	h	151	PHE	CG-CD2-CE2	5.35	126.68	120.80
8	h	135	ILE	N-CA-CB	5.35	123.10	110.80
11	4	17	SER	CA-CB-OG	5.35	125.64	111.20
5	e	122	ARG	NE-CZ-NH1	5.34	122.97	120.30
7	G	71	ASP	CB-CA-C	5.34	121.09	110.40
9	2	203	ASP	N-CA-CB	5.34	120.22	110.60
30	K	399	ARG	NH1-CZ-NH2	-5.34	113.52	119.40
7	g	129	VAL	C-N-CA	5.34	135.05	121.70
2	B	235	PHE	CB-CG-CD2	-5.34	117.06	120.80
10	j	100	PHE	CB-CA-C	-5.34	99.72	110.40
10	j	119	PRO	N-CD-CG	5.34	111.21	103.20
7	G	15	PHE	CD1-CE1-CZ	-5.34	113.69	120.10
21	N	389	TYR	CB-CG-CD1	-5.34	117.80	121.00
27	O	230	PHE	CB-CG-CD2	-5.34	117.06	120.80
7	g	115	ARG	NE-CZ-NH1	-5.34	117.63	120.30
6	F	99	PHE	CB-CG-CD1	-5.34	117.06	120.80
20	Z	298	PHE	CB-CG-CD2	-5.34	117.06	120.80
5	e	13	SER	N-CA-C	-5.34	96.59	111.00
5	e	53	ARG	NE-CZ-NH2	-5.34	117.63	120.30
9	i	119	TYR	CG-CD2-CE2	-5.34	117.03	121.30
12	5	126	ASP	CB-CG-OD2	5.34	123.10	118.30
4	D	126	VAL	CA-CB-CG2	5.33	118.90	110.90
5	e	8	TYR	CB-CG-CD1	5.33	124.20	121.00
8	h	79	TYR	CB-CG-CD1	-5.33	117.80	121.00
13	m	221	ARG	NE-CZ-NH1	5.33	122.97	120.30
3	C	50	ARG	NE-CZ-NH2	-5.33	117.63	120.30
22	S	467	PHE	CB-CG-CD1	5.33	124.53	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	119	ARG	CA-CB-CG	5.33	125.13	113.40
3	C	200	THR	CA-CB-CG2	-5.33	104.94	112.40
3	C	208	TYR	CD1-CG-CD2	-5.33	112.04	117.90
18	X	130	ASN	CB-CA-C	-5.33	99.74	110.40
4	d	8	LEU	CB-CG-CD1	5.33	120.06	111.00
1	A	120	ARG	NE-CZ-NH2	5.33	122.96	120.30
27	O	312	ASP	CB-CG-OD2	-5.33	113.50	118.30
2	B	62	SER	O-C-N	5.33	131.22	122.70
7	G	86	ARG	NE-CZ-NH2	-5.32	117.64	120.30
20	Z	261	ASP	CB-CG-OD1	-5.32	113.51	118.30
8	h	75	TYR	CZ-CE2-CD2	5.32	124.59	119.80
13	6	39	THR	N-CA-C	-5.32	96.64	111.00
14	7	116	ALA	N-CA-CB	5.32	117.55	110.10
3	C	154	SER	N-CA-CB	5.32	118.48	110.50
29	I	345	ASP	CB-CG-OD2	-5.32	113.51	118.30
17	T	224	ARG	NE-CZ-NH1	-5.32	117.64	120.30
11	4	194	ASP	CB-CG-OD1	-5.31	113.52	118.30
28	H	222	ARG	NE-CZ-NH1	5.31	122.96	120.30
33	J	116	ARG	CG-CD-NE	-5.31	100.65	111.80
22	S	272	TYR	CB-CG-CD2	-5.31	117.81	121.00
3	c	123	THR	CA-CB-CG2	-5.31	104.97	112.40
33	J	225	GLU	OE1-CD-OE2	-5.31	116.93	123.30
7	g	72	ARG	NE-CZ-NH2	-5.31	117.65	120.30
8	h	175	ASP	CB-CG-OD2	-5.30	113.53	118.30
6	F	35	THR	N-CA-C	-5.30	96.68	111.00
15	W	140	ASP	N-CA-CB	5.30	120.15	110.60
21	N	217	MET	CG-SD-CE	-5.30	91.71	100.20
29	I	77	SER	CA-C-O	-5.30	108.96	120.10
25	R	203	ASP	CB-CG-OD2	-5.30	113.53	118.30
28	H	129	SER	N-CA-CB	5.30	118.45	110.50
13	6	203	HIS	C-N-CA	5.30	134.95	121.70
16	V	197	TYR	CG-CD2-CE2	5.30	125.54	121.30
22	S	390	THR	N-CA-CB	5.30	120.37	110.30
27	O	195	TYR	CB-CG-CD1	-5.30	117.82	121.00
6	f	8	GLY	N-CA-C	-5.30	99.86	113.10
13	m	75	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	B	92	VAL	CA-CB-CG1	5.30	118.85	110.90
7	G	103	TYR	CB-CG-CD1	-5.30	117.82	121.00
12	5	144	ARG	NE-CZ-NH1	-5.30	117.65	120.30
14	7	143	LEU	CB-CG-CD1	5.30	120.00	111.00
28	H	317	ALA	N-CA-CB	5.30	117.52	110.10
33	J	331	HIS	CA-CB-CG	-5.30	104.60	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	32	ASP	CB-CG-OD1	5.29	123.07	118.30
30	K	237	VAL	CA-CB-CG2	5.29	118.84	110.90
1	a	24	ARG	NE-CZ-NH1	5.29	122.95	120.30
11	4	141	PHE	CB-CG-CD1	5.29	124.50	120.80
11	4	176	PHE	CB-CG-CD1	-5.29	117.09	120.80
12	l	249	SER	N-CA-CB	5.29	118.44	110.50
6	F	212	SER	N-CA-C	-5.29	96.72	111.00
20	Z	406	TRP	CZ3-CH2-CZ2	-5.29	115.25	121.60
33	J	134	VAL	CG1-CB-CG2	5.29	119.37	110.90
27	O	337	LEU	CB-CA-C	-5.29	100.15	110.20
6	f	81	ALA	N-CA-CB	5.29	117.50	110.10
10	j	144	ASP	CB-CG-OD2	-5.29	113.54	118.30
3	C	226	TYR	CG-CD1-CE1	-5.29	117.07	121.30
21	N	157	ALA	CB-CA-C	-5.29	102.17	110.10
23	P	69	ARG	NE-CZ-NH1	5.29	122.94	120.30
27	O	47	LYS	CA-CB-CG	5.29	125.03	113.40
30	K	198	TYR	CD1-CE1-CZ	-5.29	115.04	119.80
32	M	409	SER	N-CA-CB	5.29	118.43	110.50
7	G	169	ARG	NE-CZ-NH2	-5.29	117.66	120.30
22	S	442	PHE	CB-CG-CD2	-5.29	117.10	120.80
9	i	234	PHE	CD1-CE1-CZ	-5.29	113.76	120.10
29	I	354	ASP	CB-CG-OD1	-5.28	113.55	118.30
15	W	25	ARG	CD-NE-CZ	-5.28	116.21	123.60
17	T	199	PHE	CZ-CE2-CD2	5.28	126.44	120.10
25	R	266	LEU	C-N-CA	5.28	134.90	121.70
10	j	27	LEU	CB-CG-CD1	-5.28	102.03	111.00
25	R	357	PHE	CG-CD1-CE1	-5.28	115.00	120.80
33	J	357	ASP	CB-CG-OD2	5.28	123.05	118.30
20	Z	302	SER	CB-CA-C	-5.28	100.08	110.10
25	R	251	THR	N-CA-CB	5.28	120.32	110.30
9	i	61	ALA	CB-CA-C	-5.27	102.19	110.10
21	N	724	THR	CA-CB-CG2	-5.27	105.02	112.40
24	Q	12	ARG	NE-CZ-NH2	5.27	122.94	120.30
14	7	109	TYR	CB-CG-CD2	5.27	124.16	121.00
33	J	271	THR	CA-CB-CG2	-5.27	105.02	112.40
2	B	207	ASP	CB-CG-OD2	5.27	123.04	118.30
11	4	98	TYR	CB-CG-CD1	5.27	124.16	121.00
12	5	148	ARG	NE-CZ-NH1	-5.27	117.67	120.30
30	K	58	TYR	CB-CG-CD1	5.27	124.16	121.00
30	K	141	ARG	N-CA-CB	5.27	120.08	110.60
24	Q	1	MET	CG-SD-CE	-5.27	91.77	100.20
4	d	129	PHE	CB-CG-CD1	-5.26	117.11	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	43	ASP	CB-CG-OD1	-5.26	113.56	118.30
24	Q	12	ARG	CA-CB-CG	5.26	124.98	113.40
24	Q	319	LYS	N-CA-CB	5.26	120.08	110.60
30	K	376	ASP	CB-CG-OD1	5.26	123.04	118.30
21	N	598	ASP	N-CA-C	-5.26	96.79	111.00
23	P	257	TRP	N-CA-CB	5.26	120.07	110.60
31	L	137	ARG	NE-CZ-NH1	5.26	122.93	120.30
32	M	345	ARG	NE-CZ-NH1	-5.26	117.67	120.30
22	S	139	HIS	O-C-N	5.26	131.11	122.70
30	K	39	ALA	N-CA-CB	5.26	117.46	110.10
18	X	99	PHE	CB-CG-CD1	-5.25	117.12	120.80
28	H	181	TYR	CB-CG-CD2	5.25	124.15	121.00
4	D	173	GLU	N-CA-CB	5.25	120.06	110.60
22	S	393	ARG	NE-CZ-NH1	-5.25	117.67	120.30
23	P	432	LEU	CB-CG-CD2	-5.25	102.07	111.00
24	Q	354	PHE	CB-CG-CD2	-5.25	117.12	120.80
31	L	375	ASP	CB-CG-OD1	5.25	123.03	118.30
20	Z	137	TYR	CB-CG-CD2	-5.25	117.85	121.00
21	N	173	LYS	O-C-N	5.25	131.10	122.70
26	U	132	LEU	CB-CG-CD2	5.25	119.93	111.00
22	S	69	LEU	N-CA-CB	5.25	120.90	110.40
23	P	95	TYR	CG-CD1-CE1	-5.25	117.10	121.30
28	H	377	PHE	CG-CD2-CE2	-5.25	115.03	120.80
1	A	104	PHE	CG-CD1-CE1	5.25	126.57	120.80
4	D	232	TYR	CZ-CE2-CD2	5.25	124.52	119.80
7	G	138	PHE	CG-CD1-CE1	5.25	126.57	120.80
20	Z	738	TYR	CB-CG-CD2	5.25	124.15	121.00
22	S	248	ASP	CB-CG-OD2	-5.25	113.58	118.30
10	3	135	ASP	CB-CG-OD1	5.24	123.02	118.30
23	P	41	VAL	CB-CA-C	-5.24	101.44	111.40
11	k	8	ARG	CB-CA-C	-5.24	99.92	110.40
20	Z	757	SER	N-CA-CB	5.24	118.36	110.50
10	3	104	PHE	CB-CG-CD2	5.24	124.47	120.80
12	5	272	PHE	CB-CG-CD1	-5.24	117.13	120.80
28	H	205	ASP	CB-CG-OD2	-5.24	113.58	118.30
1	a	89	ASP	O-C-N	-5.24	114.32	122.70
9	2	178	GLU	CB-CA-C	-5.24	99.93	110.40
20	Z	104	ASP	CB-CG-OD1	-5.24	113.59	118.30
26	U	29	GLU	CB-CA-C	-5.24	99.92	110.40
25	R	150	ALA	CB-CA-C	-5.24	102.25	110.10
13	m	208	ASP	N-CA-CB	5.23	120.02	110.60
3	C	46	LEU	N-CA-CB	5.23	120.87	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	158	GLU	OE1-CD-OE2	5.23	129.58	123.30
10	3	67	PHE	N-CA-CB	5.23	120.02	110.60
2	B	177	LYS	CB-CA-C	-5.23	99.94	110.40
25	R	339	ALA	CB-CA-C	-5.23	102.25	110.10
6	f	36	VAL	CG1-CB-CG2	-5.23	102.53	110.90
10	3	69	TYR	CZ-CE2-CD2	-5.23	115.09	119.80
13	6	61	SER	N-CA-C	-5.23	96.88	111.00
33	J	50	ALA	CB-CA-C	-5.23	102.25	110.10
20	Z	145	ASP	O-C-N	5.23	131.07	122.70
31	L	307	GLU	N-CA-CB	5.23	120.01	110.60
2	b	93	ALA	CB-CA-C	-5.23	102.26	110.10
8	h	127	SER	N-CA-C	-5.23	96.89	111.00
17	T	235	PHE	CD1-CE1-CZ	5.23	126.37	120.10
28	H	284	VAL	C-N-CA	5.23	133.28	122.30
30	K	311	ASN	CB-CA-C	-5.22	99.95	110.40
32	M	266	ALA	N-CA-CB	5.22	117.42	110.10
2	b	239	THR	CA-CB-CG2	-5.22	105.09	112.40
5	e	165	TYR	CD1-CE1-CZ	-5.22	115.10	119.80
6	f	199	GLN	CB-CA-C	5.22	120.85	110.40
2	B	156	TYR	CG-CD1-CE1	5.22	125.48	121.30
2	B	220	ASP	CB-CG-OD1	-5.22	113.60	118.30
13	6	220	VAL	CG1-CB-CG2	-5.22	102.54	110.90
16	V	244	MET	CA-CB-CG	5.22	122.18	113.30
20	Z	491	LEU	N-CA-CB	5.22	120.84	110.40
21	N	865	PRO	O-C-N	5.22	131.06	122.70
24	Q	314	PHE	CG-CD1-CE1	-5.22	115.06	120.80
27	O	166	ARG	NE-CZ-NH2	5.22	122.91	120.30
21	N	55	PHE	CB-CG-CD1	5.22	124.45	120.80
3	c	9	ARG	N-CA-CB	5.22	120.00	110.60
1	A	110	TYR	N-CA-CB	5.22	120.00	110.60
12	5	120	MET	CG-SD-CE	-5.22	91.85	100.20
4	d	56	ASP	CB-CG-OD1	5.22	123.00	118.30
8	h	54	ARG	NE-CZ-NH1	-5.22	117.69	120.30
6	f	225	TYR	CZ-CE2-CD2	-5.22	115.11	119.80
28	H	261	ARG	NH1-CZ-NH2	5.22	125.14	119.40
5	e	176	SER	N-CA-CB	5.21	118.32	110.50
8	1	107	ILE	N-CA-C	-5.21	96.92	111.00
20	Z	328	ASP	CB-CG-OD2	5.21	122.99	118.30
28	H	69	VAL	C-N-CA	5.21	134.74	121.70
17	T	187	ASP	CB-CG-OD2	-5.21	113.61	118.30
33	J	236	MET	CA-CB-CG	5.21	122.16	113.30
4	d	83	ARG	NH1-CZ-NH2	-5.21	113.67	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	87	TYR	CD1-CE1-CZ	5.21	124.49	119.80
19	Y	46	GLY	N-CA-C	-5.21	100.07	113.10
20	Z	24	THR	CA-C-O	-5.21	109.16	120.10
2	b	3	ASP	CB-CG-OD1	5.21	122.99	118.30
2	b	145	PHE	N-CA-CB	5.21	119.98	110.60
7	g	20	ARG	CG-CD-NE	-5.21	100.86	111.80
12	l	260	TRP	CG-CD2-CE3	-5.21	129.21	133.90
3	C	144	TYR	CD1-CE1-CZ	-5.21	115.11	119.80
5	E	72	ARG	NE-CZ-NH2	-5.21	117.69	120.30
12	5	266	HIS	N-CA-C	-5.21	96.94	111.00
32	M	412	HIS	O-C-N	5.21	131.03	122.70
20	Z	61	SER	N-CA-CB	5.21	118.31	110.50
20	Z	456	GLY	O-C-N	5.21	131.03	122.70
22	S	346	TYR	CB-CG-CD1	5.21	124.12	121.00
24	Q	124	PHE	CG-CD1-CE1	-5.21	115.07	120.80
25	R	328	PHE	CB-CG-CD1	-5.21	117.16	120.80
26	U	294	ASN	N-CA-CB	5.21	119.97	110.60
29	I	320	GLY	CA-C-O	5.21	129.97	120.60
6	f	89	ARG	NH1-CZ-NH2	5.20	125.12	119.40
12	l	210	PHE	CB-CG-CD2	-5.20	117.16	120.80
2	B	142	PHE	CB-CA-C	-5.20	99.99	110.40
9	2	232	TYR	CG-CD2-CE2	-5.20	117.14	121.30
33	J	382	PHE	CB-CG-CD1	5.20	124.44	120.80
5	e	111	SER	N-CA-CB	5.20	118.30	110.50
21	N	685	VAL	CA-CB-CG2	-5.20	103.10	110.90
25	R	408	ASP	CB-CG-OD1	-5.20	113.62	118.30
32	M	89	ASN	N-CA-CB	5.20	119.96	110.60
10	j	52	GLY	N-CA-C	-5.20	100.10	113.10
17	T	15	PHE	CB-CG-CD2	5.20	124.44	120.80
8	h	34	TYR	CB-CG-CD2	-5.20	117.88	121.00
10	j	60	VAL	CA-CB-CG2	-5.20	103.10	110.90
4	D	163	THR	CA-CB-CG2	-5.20	105.12	112.40
31	L	70	TYR	CB-CG-CD1	-5.20	117.88	121.00
1	A	199	TRP	CG-CD1-NE1	5.20	115.30	110.10
3	C	137	TYR	CD1-CE1-CZ	-5.20	115.12	119.80
11	4	143	LEU	CB-CA-C	-5.20	100.33	110.20
21	N	436	ASP	CB-CG-OD1	-5.20	113.62	118.30
33	J	143	PRO	N-CD-CG	5.20	110.99	103.20
15	W	121	SER	CB-CA-C	-5.19	100.23	110.10
17	T	77	SER	N-CA-CB	5.19	118.29	110.50
26	U	113	TYR	CB-CG-CD1	-5.19	117.88	121.00
10	j	50	PHE	CB-CG-CD2	-5.19	117.17	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	157	TYR	N-CA-CB	5.19	119.95	110.60
29	I	252	LEU	O-C-N	-5.19	114.39	122.70
6	F	183	ASP	CB-CG-OD1	-5.19	113.63	118.30
15	W	86	HIS	N-CA-CB	5.19	119.94	110.60
19	Y	54	VAL	CA-CB-CG1	-5.19	103.11	110.90
3	C	230	PHE	CB-CG-CD1	-5.19	117.17	120.80
21	N	717	LEU	O-C-N	5.19	131.00	122.70
2	B	178	ARG	NE-CZ-NH2	5.19	122.89	120.30
15	W	114	VAL	CA-CB-CG2	-5.19	103.12	110.90
21	N	250	ASP	CB-CG-OD2	5.19	122.97	118.30
26	U	290	ASP	CB-CG-OD2	-5.19	113.63	118.30
1	a	81	MET	CG-SD-CE	5.19	108.50	100.20
4	d	148	TYR	CB-CA-C	-5.19	100.03	110.40
1	A	228	ALA	N-CA-CB	5.19	117.36	110.10
12	5	125	ALA	N-CA-CB	5.19	117.36	110.10
12	l	121	ALA	N-CA-CB	5.18	117.36	110.10
17	T	82	PHE	CZ-CE2-CD2	-5.18	113.88	120.10
21	N	677	ASP	CB-CG-OD1	-5.18	113.63	118.30
29	I	125	MET	CA-C-N	5.18	131.62	117.10
11	k	26	SER	N-CA-CB	5.18	118.28	110.50
5	E	26	TYR	CB-CG-CD2	5.18	124.11	121.00
11	4	98	TYR	N-CA-CB	5.18	119.93	110.60
29	I	122	SER	CA-C-O	-5.18	109.22	120.10
20	Z	138	ARG	NE-CZ-NH1	5.18	122.89	120.30
7	g	150	MET	CG-SD-CE	-5.18	91.92	100.20
4	D	18	PHE	CB-CG-CD2	5.18	124.42	120.80
20	Z	303	ASP	CB-CG-OD2	-5.18	113.64	118.30
4	d	121	THR	N-CA-CB	5.18	120.14	110.30
2	B	135	LEU	N-CA-C	-5.18	97.02	111.00
15	W	168	THR	N-CA-C	-5.18	97.02	111.00
22	S	285	ASP	N-CA-C	-5.18	97.02	111.00
3	C	50	ARG	NE-CZ-NH1	5.17	122.89	120.30
23	P	326	ASP	N-CA-CB	5.17	119.91	110.60
27	O	294	MET	CG-SD-CE	-5.17	91.92	100.20
31	L	269	TYR	CB-CG-CD1	-5.17	117.90	121.00
33	J	53	ASP	N-CA-CB	5.17	119.91	110.60
23	P	213	TYR	CB-CG-CD2	5.17	124.10	121.00
32	M	432	PHE	CB-CG-CD1	-5.17	117.18	120.80
1	a	46	ARG	CB-CA-C	-5.17	100.06	110.40
2	B	105	PRO	N-CD-CG	5.17	110.95	103.20
20	Z	732	ILE	C-N-CA	5.17	134.61	121.70
4	d	116	VAL	CG1-CB-CG2	-5.16	102.64	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	48	ALA	N-CA-CB	5.16	117.33	110.10
27	O	67	SER	N-CA-CB	5.16	118.24	110.50
28	H	59	ILE	O-C-N	-5.16	114.44	122.70
32	M	309	LEU	CB-CA-C	-5.16	100.39	110.20
7	G	140	GLY	N-CA-C	-5.16	100.19	113.10
4	d	141	ARG	N-CA-CB	5.16	119.89	110.60
30	K	170	THR	CA-CB-CG2	-5.16	105.17	112.40
12	l	94	ARG	CD-NE-CZ	-5.16	116.38	123.60
6	f	13	PHE	C-N-CA	5.16	134.59	121.70
27	O	231	GLY	C-N-CA	5.16	134.59	121.70
17	T	54	ASP	CB-CG-OD2	-5.16	113.66	118.30
18	X	91	PHE	CZ-CE2-CD2	5.15	126.28	120.10
30	K	213	GLY	N-CA-C	-5.15	100.22	113.10
2	B	66	LEU	N-CA-C	-5.15	97.10	111.00
11	4	36	ARG	NH1-CZ-NH2	5.15	125.06	119.40
14	7	214	MET	CG-SD-CE	-5.15	91.96	100.20
25	R	20	ARG	NH1-CZ-NH2	5.15	125.07	119.40
25	R	335	ARG	NH1-CZ-NH2	5.15	125.06	119.40
24	Q	50	ARG	NE-CZ-NH1	5.15	122.87	120.30
12	l	91	VAL	CA-CB-CG2	5.15	118.62	110.90
13	m	68	ASP	CB-CG-OD1	5.15	122.93	118.30
16	V	239	ALA	N-CA-CB	5.15	117.31	110.10
23	P	303	PHE	CB-CG-CD2	-5.15	117.20	120.80
27	O	76	LEU	CB-CG-CD1	5.15	119.75	111.00
28	H	447	VAL	O-C-N	-5.15	114.46	122.70
33	J	275	LEU	CB-CG-CD2	5.15	119.75	111.00
5	e	136	ARG	N-CA-CB	5.15	119.86	110.60
15	W	119	SER	N-CA-CB	5.15	118.22	110.50
4	D	82	SER	O-C-N	5.14	130.93	122.70
11	4	18	SER	CB-CA-C	-5.14	100.32	110.10
14	7	60	LEU	CB-CG-CD1	5.14	119.75	111.00
21	N	50	TYR	CG-CD2-CE2	-5.14	117.19	121.30
14	n	84	VAL	CB-CA-C	-5.14	101.63	111.40
28	H	463	TYR	CG-CD2-CE2	5.14	125.42	121.30
7	g	76	CYS	N-CA-C	-5.14	97.12	111.00
3	c	7	ASP	CB-CG-OD1	5.14	122.92	118.30
12	l	257	GLU	OE1-CD-OE2	5.14	129.47	123.30
11	4	177	LYS	N-CA-C	5.14	124.88	111.00
20	Z	206	ASP	CA-CB-CG	-5.14	102.09	113.40
31	L	371	THR	CA-CB-CG2	-5.14	105.20	112.40
8	1	44	THR	CA-CB-CG2	5.14	119.59	112.40
12	5	93	SER	CB-CA-C	-5.14	100.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	73	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
18	X	96	ARG	NH1-CZ-NH2	-5.14	113.75	119.40
6	F	99	PHE	CB-CA-C	-5.13	100.13	110.40
12	5	248	GLY	N-CA-C	-5.13	100.27	113.10
4	d	35	GLY	N-CA-C	-5.13	100.27	113.10
2	B	181	ASP	CB-CG-OD1	5.13	122.92	118.30
4	D	54	LEU	N-CA-CB	5.13	120.66	110.40
20	Z	42	ASP	CB-CG-OD1	-5.13	113.68	118.30
28	H	448	ASP	CB-CG-OD2	5.13	122.92	118.30
29	I	424	MET	CG-SD-CE	-5.13	91.99	100.20
1	A	110	TYR	CA-CB-CG	5.13	123.15	113.40
5	E	165	TYR	CG-CD2-CE2	5.13	125.40	121.30
30	K	148	ASP	CB-CG-OD1	-5.13	113.68	118.30
1	A	103	GLU	OE1-CD-OE2	5.13	129.45	123.30
8	1	183	ARG	NE-CZ-NH1	5.13	122.86	120.30
14	7	124	TYR	CB-CG-CD2	-5.13	117.92	121.00
20	Z	556	ILE	CA-CB-CG1	5.13	120.74	111.00
25	R	43	ARG	O-C-N	-5.13	114.49	122.70
32	M	266	ALA	CA-C-O	5.13	130.87	120.10
1	a	162	TYR	CB-CG-CD2	5.13	124.08	121.00
11	k	52	ASP	CB-CG-OD1	5.13	122.91	118.30
3	C	214	ALA	N-CA-CB	5.13	117.28	110.10
24	Q	306	TYR	CB-CG-CD1	5.13	124.08	121.00
28	H	463	TYR	CB-CG-CD1	-5.13	117.92	121.00
33	J	150	VAL	C-N-CA	5.13	133.06	122.30
21	N	629	CYS	CA-CB-SG	5.12	123.22	114.00
4	d	144	GLU	CA-CB-CG	5.12	124.67	113.40
5	E	215	ASN	CA-CB-CG	-5.12	102.13	113.40
26	U	113	TYR	CD1-CE1-CZ	5.12	124.41	119.80
22	S	479	MET	CG-SD-CE	-5.12	92.01	100.20
29	I	433	GLU	CB-CA-C	-5.12	100.17	110.40
24	Q	399	VAL	N-CA-C	-5.12	97.19	111.00
25	R	336	LYS	CB-CA-C	-5.12	100.17	110.40
28	H	466	TYR	CA-CB-CG	-5.12	103.68	113.40
5	e	49	GLY	N-CA-C	-5.11	100.32	113.10
5	e	222	ILE	N-CA-C	-5.11	97.20	111.00
14	n	205	VAL	CA-CB-CG2	-5.11	103.23	110.90
6	F	51	ARG	NE-CZ-NH2	-5.11	117.75	120.30
10	3	28	ARG	CD-NE-CZ	-5.11	116.45	123.60
10	3	181	SER	N-CA-CB	5.11	118.17	110.50
6	f	172	LEU	CB-CG-CD2	-5.11	102.31	111.00
8	h	111	TYR	CD1-CG-CD2	-5.11	112.28	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	77	THR	N-CA-C	-5.11	97.21	111.00
1	A	146	VAL	CG1-CB-CG2	5.11	119.07	110.90
17	T	91	SER	C-N-CA	5.11	134.47	121.70
22	S	323	LEU	CB-CG-CD2	-5.11	102.32	111.00
23	P	257	TRP	CE3-CZ3-CH2	-5.11	115.58	121.20
30	K	225	ALA	CB-CA-C	-5.11	102.44	110.10
2	B	224	TYR	N-CA-CB	5.11	119.79	110.60
12	5	94	ARG	NE-CZ-NH2	-5.11	117.75	120.30
21	N	368	THR	N-CA-CB	5.11	120.00	110.30
21	N	891	VAL	CA-CB-CG2	-5.11	103.24	110.90
12	l	106	VAL	CA-CB-CG2	-5.10	103.25	110.90
27	O	172	TYR	CG-CD1-CE1	-5.10	117.22	121.30
12	l	146	LYS	N-CA-CB	5.10	119.78	110.60
6	F	114	ASP	N-CA-CB	5.10	119.78	110.60
23	P	245	TYR	CD1-CE1-CZ	-5.10	115.21	119.80
24	Q	258	ALA	N-CA-CB	5.10	117.24	110.10
11	k	36	ARG	NE-CZ-NH1	5.10	122.85	120.30
7	G	144	ASN	CA-CB-CG	-5.10	102.18	113.40
16	V	89	ALA	N-CA-CB	5.10	117.24	110.10
10	j	11	ILE	N-CA-CB	5.10	122.52	110.80
13	m	54	CYS	CA-CB-SG	-5.10	104.82	114.00
5	E	84	ASP	CB-CG-OD1	-5.10	113.71	118.30
20	Z	358	TYR	CB-CG-CD1	5.10	124.06	121.00
22	S	95	PHE	CB-CG-CD2	-5.10	117.23	120.80
28	H	208	TYR	CG-CD1-CE1	-5.10	117.22	121.30
12	l	230	TYR	CB-CG-CD2	-5.10	117.94	121.00
24	Q	229	ASP	CB-CG-OD2	5.10	122.89	118.30
6	f	137	TYR	CA-CB-CG	-5.09	103.72	113.40
2	B	151	ASP	CB-CG-OD2	-5.09	113.71	118.30
4	D	14	ASP	CB-CG-OD2	-5.09	113.72	118.30
7	G	199	ILE	CA-CB-CG1	5.09	120.68	111.00
12	5	219	TYR	CB-CG-CD2	-5.09	117.94	121.00
21	N	328	PHE	CG-CD2-CE2	5.09	126.40	120.80
20	Z	483	THR	CA-CB-OG1	5.09	119.69	109.00
33	J	251	ASP	N-CA-CB	5.09	119.76	110.60
9	i	126	TYR	CB-CG-CD1	-5.09	117.95	121.00
13	m	153	LEU	CB-CA-C	-5.09	100.53	110.20
21	N	230	VAL	O-C-N	-5.09	114.56	122.70
30	K	346	ARG	NH1-CZ-NH2	5.09	125.00	119.40
31	L	376	PHE	CB-CG-CD2	-5.09	117.24	120.80
12	5	109	VAL	CA-CB-CG1	-5.09	103.27	110.90
15	W	188	SER	N-CA-CB	5.09	118.13	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	432	VAL	CA-CB-CG1	5.09	118.53	110.90
24	Q	398	TYR	CB-CG-CD2	5.08	124.05	121.00
25	R	263	ARG	NE-CZ-NH1	5.08	122.84	120.30
28	H	280	VAL	CG1-CB-CG2	-5.08	102.77	110.90
9	i	98	TYR	CB-CG-CD2	-5.08	117.95	121.00
13	6	70	ASP	CB-CG-OD1	5.08	122.87	118.30
6	F	205	SER	N-CA-CB	5.08	118.12	110.50
13	m	41	TYR	CD1-CG-CD2	-5.08	112.31	117.90
14	n	163	VAL	CB-CA-C	5.08	121.05	111.40
4	D	189	GLU	N-CA-CB	5.08	119.74	110.60
13	6	152	SER	N-CA-CB	5.08	118.12	110.50
20	Z	584	VAL	CA-CB-CG1	-5.08	103.28	110.90
21	N	471	TYR	CZ-CE2-CD2	5.08	124.37	119.80
26	U	58	GLU	CA-CB-CG	5.08	124.57	113.40
3	C	183	ASP	CB-CG-OD2	5.08	122.87	118.30
9	2	108	ALA	CB-CA-C	-5.08	102.48	110.10
9	2	217	ARG	NE-CZ-NH2	-5.08	117.76	120.30
7	g	119	TYR	CB-CG-CD2	-5.07	117.96	121.00
27	O	216	ASP	CB-CG-OD2	5.07	122.87	118.30
12	l	202	PHE	CG-CD2-CE2	-5.07	115.22	120.80
7	G	245	LYS	O-C-N	-5.07	114.58	122.70
8	h	61	THR	CA-CB-CG2	-5.07	105.30	112.40
11	k	135	TYR	CB-CG-CD2	-5.07	117.96	121.00
30	K	81	ARG	NE-CZ-NH2	-5.07	117.77	120.30
23	P	3	ARG	NE-CZ-NH1	5.07	122.83	120.30
24	Q	173	SER	N-CA-CB	5.07	118.10	110.50
31	L	236	ALA	CB-CA-C	-5.07	102.50	110.10
15	W	151	THR	N-CA-C	-5.07	97.32	111.00
20	Z	765	MET	CG-SD-CE	-5.07	92.09	100.20
16	V	275	ASP	CB-CG-OD2	-5.07	113.74	118.30
30	K	99	PHE	CG-CD1-CE1	5.07	126.37	120.80
32	M	108	LEU	CB-CG-CD1	5.07	119.61	111.00
32	M	190	ILE	CA-CB-CG1	5.07	120.62	111.00
21	N	41	ASN	CB-CA-C	-5.06	100.27	110.40
22	S	274	PHE	CB-CG-CD2	5.06	124.34	120.80
24	Q	34	ASP	CB-CG-OD1	5.06	122.86	118.30
9	i	118	LYS	CD-CE-NZ	-5.06	100.06	111.70
12	l	279	GLU	O-C-N	-5.06	114.59	123.20
7	g	119	TYR	CG-CD1-CE1	-5.06	117.25	121.30
11	k	120	ASP	CB-CG-OD1	5.06	122.85	118.30
20	Z	520	ILE	CG1-CB-CG2	5.06	122.53	111.40
3	c	98	TYR	CB-CG-CD2	5.06	124.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	82	ARG	O-C-N	-5.06	114.61	122.70
14	7	132	VAL	CA-CB-CG1	5.06	118.49	110.90
20	Z	798	ARG	NE-CZ-NH1	5.06	122.83	120.30
2	B	170	ALA	O-C-N	-5.06	114.61	122.70
25	R	94	PHE	CB-CG-CD2	5.06	124.34	120.80
27	O	251	LEU	CB-CG-CD2	-5.06	102.40	111.00
27	O	352	TRP	CG-CD2-CE3	-5.06	129.35	133.90
10	3	13	VAL	CG1-CB-CG2	5.05	118.99	110.90
22	S	60	LEU	CB-CG-CD2	-5.05	102.41	111.00
9	2	71	TRP	CG-CD2-CE3	-5.05	129.35	133.90
11	k	128	LEU	N-CA-C	-5.05	97.36	111.00
3	C	149	TYR	CG-CD2-CE2	-5.05	117.26	121.30
32	M	233	ARG	NE-CZ-NH2	5.05	122.83	120.30
33	J	357	ASP	CB-CG-OD1	-5.05	113.76	118.30
12	l	188	TYR	CB-CG-CD2	5.05	124.03	121.00
3	C	151	SER	N-CA-CB	5.05	118.07	110.50
24	Q	314	PHE	CD1-CE1-CZ	5.05	126.16	120.10
23	P	12	ASP	CB-CG-OD1	5.04	122.84	118.30
2	b	147	LEU	CB-CG-CD1	5.04	119.58	111.00
2	b	207	ASP	CB-CG-OD2	-5.04	113.76	118.30
3	c	4	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
14	n	255	ALA	N-CA-CB	-5.04	103.04	110.10
2	B	179	TRP	CE2-CD2-CE3	5.04	124.75	118.70
24	Q	290	THR	CA-CB-CG2	-5.04	105.34	112.40
26	U	32	ARG	NE-CZ-NH2	-5.04	117.78	120.30
11	k	109	LYS	O-C-N	-5.04	114.63	122.70
12	l	195	THR	N-CA-CB	5.04	119.88	110.30
20	Z	326	VAL	CA-CB-CG2	-5.04	103.34	110.90
22	S	54	TRP	NE1-CE2-CD2	5.04	112.34	107.30
22	S	275	TYR	CB-CG-CD2	-5.04	117.98	121.00
29	I	435	LEU	C-N-CA	5.04	134.30	121.70
32	M	386	PHE	CB-CG-CD2	-5.04	117.27	120.80
17	T	249	MET	N-CA-C	-5.04	97.39	111.00
5	e	21	LEU	CB-CA-C	5.04	119.78	110.20
8	1	113	ASP	CB-CA-C	-5.04	100.32	110.40
23	P	273	TYR	CB-CG-CD2	5.04	124.02	121.00
29	I	137	ASP	CB-CG-OD1	-5.04	113.77	118.30
29	I	376	ASN	N-CA-C	-5.04	97.40	111.00
23	P	417	HIS	N-CA-CB	5.03	119.66	110.60
28	H	426	ALA	CB-CA-C	-5.03	102.55	110.10
16	V	49	VAL	CA-CB-CG1	-5.03	103.35	110.90
3	c	83	ASP	CB-CG-OD1	-5.03	113.77	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Y	83	ARG	N-CA-CB	5.03	119.65	110.60
21	N	21	LYS	CB-CA-C	-5.03	100.34	110.40
25	R	210	TYR	CB-CG-CD2	-5.03	117.98	121.00
5	E	249	ALA	N-CA-CB	5.03	117.14	110.10
11	4	192	VAL	CA-CB-CG2	5.03	118.44	110.90
20	Z	233	LEU	O-C-N	-5.03	111.55	121.10
3	c	237	ASP	CB-CG-OD1	5.03	122.82	118.30
3	C	7	ASP	CB-CG-OD1	5.03	122.82	118.30
12	5	115	PHE	CB-CG-CD1	-5.03	117.28	120.80
23	P	82	LEU	N-CA-CB	5.03	120.45	110.40
26	U	82	LYS	CA-C-N	5.03	128.26	117.20
33	J	154	THR	O-C-N	5.03	130.74	122.70
20	Z	426	TYR	CB-CG-CD1	-5.02	117.98	121.00
33	J	324	ARG	NH1-CZ-NH2	-5.02	113.87	119.40
3	C	26	LEU	CB-CG-CD2	-5.02	102.46	111.00
3	c	149	TYR	CB-CG-CD1	-5.02	117.99	121.00
25	R	140	TYR	CB-CG-CD2	-5.02	117.99	121.00
3	c	149	TYR	CB-CG-CD2	5.02	124.01	121.00
8	1	100	ASP	CB-CG-OD2	-5.02	113.78	118.30
28	H	167	ASP	CB-CG-OD1	-5.02	113.78	118.30
31	L	304	THR	N-CA-CB	5.02	119.83	110.30
33	J	82	LYS	N-CA-CB	5.02	119.63	110.60
29	I	337	ALA	N-CA-CB	5.02	117.12	110.10
31	L	342	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
32	M	207	PHE	CB-CG-CD1	-5.02	117.29	120.80
6	f	74	LEU	CB-CG-CD1	-5.01	102.47	111.00
18	X	62	ASP	CB-CA-C	5.01	120.43	110.40
19	Y	65	ASP	CB-CG-OD1	-5.01	113.79	118.30
20	Z	259	PRO	N-CD-CG	5.01	110.72	103.20
21	N	79	VAL	CA-CB-CG2	-5.01	103.38	110.90
24	Q	286	TYR	CD1-CG-CD2	-5.01	112.38	117.90
32	M	290	ARG	CB-CA-C	-5.01	100.37	110.40
11	4	139	TYR	CB-CG-CD2	-5.01	117.99	121.00
5	e	15	PHE	CB-CG-CD2	5.01	124.31	120.80
7	G	44	ASP	CB-CG-OD1	-5.01	113.79	118.30
21	N	591	LEU	CB-CA-C	-5.01	100.68	110.20
24	Q	298	ALA	N-CA-CB	5.01	117.12	110.10
27	O	31	LYS	CB-CA-C	-5.01	100.38	110.40
27	O	51	ASP	CB-CG-OD1	-5.01	113.79	118.30
9	i	236	ARG	NE-CZ-NH2	-5.01	117.80	120.30
2	B	103	GLU	OE1-CD-OE2	5.01	129.31	123.30
16	V	146	SER	N-CA-CB	5.01	118.01	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	306	TYR	CG-CD1-CE1	-5.01	117.29	121.30
12	5	262	TYR	CB-CA-C	5.01	120.42	110.40
5	e	71	ASP	CB-CG-OD2	5.01	122.81	118.30
14	n	194	ARG	NE-CZ-NH1	5.01	122.80	120.30
8	1	186	VAL	CA-CB-CG2	-5.01	103.39	110.90
14	7	169	THR	N-CA-CB	5.01	119.81	110.30
20	Z	831	LEU	CB-CG-CD2	5.01	119.51	111.00
23	P	396	PRO	C-N-CA	5.01	134.22	121.70
31	L	119	VAL	CA-CB-CG2	-5.01	103.39	110.90
25	R	308	LEU	CA-CB-CG	5.00	126.81	115.30
16	V	171	ARG	N-CA-CB	5.00	119.61	110.60
29	I	163	ASP	CB-CG-OD2	-5.00	113.80	118.30
33	J	221	LYS	CA-CB-CG	5.00	124.41	113.40
7	G	130	ARG	CD-NE-CZ	-5.00	116.60	123.60

There are no chirality outliers.

All (347) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	133	TYR	Sidechain
8	1	144	TYR	Sidechain
8	1	146	TYR	Sidechain
8	1	152	ARG	Sidechain
8	1	198	TYR	Sidechain
8	1	34	TYR	Sidechain
8	1	70	TYR	Sidechain
8	1	79	TYR	Sidechain
9	2	119	TYR	Sidechain
9	2	152	TYR	Sidechain
9	2	153	TYR	Sidechain
9	2	217	ARG	Sidechain
9	2	65	ARG	Sidechain
10	3	164	PHE	Sidechain
10	3	177	ARG	Sidechain
10	3	203	ARG	Sidechain
10	3	74	TYR	Sidechain
10	3	87	PHE	Sidechain
10	3	96	TYR	Sidechain
10	3	98	ARG	Sidechain
11	4	149	ARG	Sidechain
11	4	190	ARG	Sidechain
11	4	23	ARG	Sidechain

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Mol	Chain	Res	Type	Group
11	4	36	ARG	Sidechain
11	4	46	PHE	Sidechain
11	4	59	TYR	Sidechain
11	4	67	TYR	Sidechain
12	5	139	ARG	Sidechain
12	5	179	TYR	Sidechain
12	5	242	ARG	Sidechain
12	5	83	PHE	Sidechain
13	6	10	PHE	Sidechain
13	6	114	TYR	Sidechain
13	6	13	TYR	Sidechain
13	6	168	TYR	Sidechain
13	6	182	TYR	Sidechain
13	6	229	ARG	Peptide
13	6	36	ARG	Sidechain
13	6	41	TYR	Sidechain
13	6	83	TYR	Sidechain
14	7	109	TYR	Sidechain
14	7	134	TYR	Sidechain
14	7	136	ARG	Sidechain
14	7	162	TYR	Sidechain
14	7	170	TYR	Sidechain
14	7	49	TYR	Sidechain
14	7	63	TYR	Sidechain
14	7	74	ARG	Sidechain
14	7	95	HIS	Sidechain
1	A	106	TYR	Sidechain
1	A	110	TYR	Sidechain
1	A	128	TYR	Sidechain
1	A	131	ARG	Sidechain
1	A	135	ARG	Sidechain
1	A	233	PHE	Sidechain
1	A	24	ARG	Sidechain
2	B	128	ARG	Sidechain
2	B	156	TYR	Sidechain
2	B	246	ARG	Sidechain
2	B	97	TYR	Sidechain
3	C	114	ARG	Sidechain
3	C	137	TYR	Sidechain
3	C	146	TYR	Sidechain
3	C	149	TYR	Sidechain
3	C	18	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	C	208	TYR	Sidechain
3	C	217	ARG	Sidechain
3	C	226	TYR	Sidechain
3	C	230	PHE	Sidechain
3	C	50	ARG	Sidechain
4	D	120	TYR	Sidechain
4	D	141	ARG	Sidechain
4	D	16	HIS	Peptide
4	D	18	PHE	Sidechain
4	D	232	TYR	Sidechain
4	D	4	TYR	Sidechain
4	D	49	ARG	Sidechain
4	D	58	ARG	Sidechain
4	D	90	ARG	Sidechain
4	D	97	ARG	Sidechain
5	E	136	ARG	Sidechain
5	E	165	TYR	Sidechain
5	E	20	ARG	Sidechain
5	E	228	PHE	Sidechain
5	E	231	TYR	Sidechain
5	E	26	TYR	Sidechain
5	E	8	TYR	Sidechain
6	F	101	ARG	Sidechain
6	F	107	ARG	Sidechain
6	F	123	TYR	Sidechain
6	F	126	ARG	Sidechain
6	F	147	PHE	Sidechain
6	F	157	TYR	Sidechain
6	F	164	ARG	Sidechain
6	F	18	ARG	Peptide,Mainchain
6	F	202	ARG	Sidechain
6	F	21	GLN	Sidechain
6	F	233	TYR	Sidechain
6	F	24	TYR	Sidechain
6	F	94	TYR	Sidechain
7	G	13	SER	Peptide
7	G	157	TYR	Sidechain
7	G	20	ARG	Sidechain
7	G	21	ASN	Peptide
7	G	242	PHE	Sidechain
7	G	91	ARG	Sidechain
7	G	93	ARG	Sidechain

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Mol	Chain	Res	Type	Group
28	H	145	TYR	Sidechain
28	H	173	ARG	Sidechain
28	H	178	ARG	Sidechain
28	H	190	ARG	Sidechain
28	H	234	ARG	Sidechain
28	H	261	ARG	Sidechain
28	H	266	ARG	Sidechain
28	H	283	TYR	Sidechain
28	H	307	PHE	Sidechain
28	H	342	GLY	Peptide
28	H	357	ARG	Sidechain
28	H	420	ARG	Sidechain
28	H	462	ARG	Sidechain
28	H	69	VAL	Peptide
29	I	100	ARG	Sidechain
29	I	129	TYR	Sidechain
29	I	181	TYR	Sidechain
29	I	256	TYR	Sidechain
29	I	292	TYR	Sidechain
29	I	304	ARG	Sidechain
29	I	436	TYR	Sidechain
29	I	54	ARG	Sidechain
33	J	120	TYR	Sidechain
33	J	147	TYR	Sidechain
33	J	88	VAL	Peptide
33	J	94	TYR	Sidechain
30	K	118	TYR	Sidechain
30	K	128	ARG	Sidechain
30	K	141	ARG	Sidechain
30	K	236	ARG	Peptide,Mainchain,Sidechain
30	K	246	TYR	Sidechain
30	K	330	ARG	Sidechain
30	K	340	PHE	Sidechain
30	K	350	ARG	Sidechain
30	K	400	TYR	Sidechain
30	K	411	TYR	Sidechain
30	K	426	PHE	Sidechain
30	K	67	TYR	Sidechain
30	K	73	ARG	Sidechain
31	L	126	ARG	Sidechain
31	L	127	TYR	Sidechain
31	L	137	ARG	Sidechain

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Mol	Chain	Res	Type	Group
31	L	180	PHE	Sidechain
31	L	221	TYR	Sidechain
31	L	255	TYR	Sidechain
31	L	329	ARG	Sidechain
32	M	153	TYR	Sidechain
32	M	180	TYR	Sidechain
32	M	342	ARG	Sidechain
32	M	345	ARG	Sidechain
32	M	357	ARG	Sidechain
21	N	161	TYR	Sidechain
21	N	222	TYR	Sidechain
21	N	23	TYR	Sidechain
21	N	282	TYR	Sidechain
21	N	338	PHE	Sidechain
21	N	389	TYR	Sidechain
21	N	394	ARG	Sidechain
21	N	463	TYR	Sidechain
21	N	50	TYR	Sidechain
21	N	515	ARG	Sidechain
21	N	580	ASN	Peptide
21	N	736	PHE	Sidechain
21	N	809	ARG	Sidechain
21	N	881	TYR	Sidechain
21	N	894	ARG	Sidechain
21	N	906	ARG	Sidechain
27	O	135	ARG	Sidechain
27	O	172	TYR	Sidechain
27	O	178	TYR	Sidechain
27	O	190	TYR	Sidechain
27	O	228	TYR	Sidechain
27	O	306	ARG	Sidechain
27	O	32	PHE	Sidechain
27	O	330	ARG	Sidechain
27	O	70	TYR	Sidechain
23	P	103	TYR	Sidechain
23	P	13	TYR	Sidechain
23	P	234	TYR	Sidechain
23	P	240	TYR	Sidechain
23	P	273	TYR	Sidechain
23	P	3	ARG	Sidechain
23	P	318	TYR	Sidechain
23	P	359	ARG	Sidechain

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Mol	Chain	Res	Type	Group
24	Q	135	HIS	Sidechain
24	Q	151	TYR	Sidechain
24	Q	161	LEU	Peptide
24	Q	189	ARG	Sidechain
24	Q	20	TYR	Sidechain
24	Q	209	TYR	Sidechain
24	Q	246	TYR	Sidechain
24	Q	286	TYR	Sidechain
24	Q	291	TYR	Sidechain
24	Q	354	PHE	Peptide,Sidechain
24	Q	65	TYR	Sidechain
25	R	123	ASP	Peptide
25	R	181	TYR	Sidechain
25	R	209	ARG	Sidechain
25	R	24	TYR	Sidechain
25	R	252	TYR	Sidechain
25	R	304	TYR	Sidechain
25	R	357	PHE	Sidechain
25	R	417	TYR	Sidechain
25	R	70	TYR	Peptide
25	R	99	TYR	Sidechain
22	S	118	PHE	Sidechain
22	S	186	TYR	Sidechain
22	S	197	SER	Peptide
22	S	211	ARG	Sidechain
22	S	241	PHE	Sidechain
22	S	25	TYR	Sidechain
22	S	273	PHE	Sidechain
22	S	275	TYR	Sidechain
22	S	334	HIS	Sidechain
22	S	346	TYR	Sidechain
22	S	425	ARG	Sidechain
22	S	64	ARG	Sidechain
22	S	82	TYR	Sidechain
17	T	109	TYR	Sidechain
17	T	144	TYR	Sidechain
17	T	20	TYR	Sidechain
17	T	210	PHE	Sidechain
17	T	220	PHE	Sidechain
17	T	245	TYR	Sidechain
17	T	266	TYR	Sidechain
17	T	81	TYR	Sidechain

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Mol	Chain	Res	Type	Group
26	U	113	TYR	Sidechain
26	U	176	ARG	Sidechain
26	U	179	ARG	Sidechain
26	U	277	TYR	Sidechain
26	U	288	PHE	Sidechain
26	U	67	PHE	Sidechain
16	V	171	ARG	Sidechain
16	V	228	TYR	Sidechain
15	W	101	ARG	Sidechain
15	W	15	TYR	Sidechain
15	W	164	PRO	Peptide
15	W	41	ARG	Sidechain
18	X	11	ARG	Sidechain
18	X	51	ARG	Sidechain
18	X	97	TYR	Sidechain
20	Z	126	TYR	Sidechain
20	Z	202	ARG	Sidechain
20	Z	210	TYR	Sidechain
20	Z	269	TYR	Sidechain
20	Z	341	TYR	Sidechain
20	Z	358	TYR	Sidechain
20	Z	408	TYR	Sidechain
20	Z	426	TYR	Sidechain
20	Z	477	TYR	Sidechain
20	Z	574	TYR	Sidechain
20	Z	623	ARG	Sidechain
20	Z	64	TYR	Sidechain
20	Z	738	TYR	Sidechain
20	Z	766	HIS	Sidechain
20	Z	838	TYR	Sidechain
1	a	108	TYR	Sidechain
1	a	133	TYR	Sidechain
1	a	14	ARG	Sidechain
1	a	143	PHE	Sidechain
1	a	162	TYR	Sidechain
1	a	26	TYR	Sidechain
1	a	46	ARG	Sidechain
1	a	77	ARG	Sidechain
2	b	104	TYR	Sidechain
2	b	128	ARG	Sidechain
2	b	75	TYR	Sidechain
3	c	102	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	c	129	ARG	Sidechain
3	c	144	TYR	Sidechain
3	c	146	TYR	Sidechain
3	c	149	TYR	Sidechain
3	c	210	ARG	Sidechain
3	c	226	TYR	Sidechain
3	c	230	PHE	Sidechain
4	d	112	TYR	Sidechain
4	d	120	TYR	Sidechain
4	d	148	TYR	Sidechain
4	d	181	ARG	Sidechain
4	d	197	ARG	Sidechain
4	d	22	TYR	Sidechain
4	d	48	ARG	Sidechain
4	d	75	PHE	Sidechain
4	d	83	ARG	Sidechain
4	d	90	ARG	Sidechain
5	e	102	TYR	Sidechain
6	f	123	TYR	Sidechain
6	f	147	PHE	Sidechain
6	f	171	TYR	Sidechain
6	f	18	ARG	Peptide,Sidechain
6	f	20	PHE	Sidechain
6	f	51	ARG	Sidechain
7	g	103	TYR	Sidechain
7	g	13	SER	Peptide
7	g	130	ARG	Sidechain
7	g	21	ASN	Peptide,Mainchain
7	g	72	ARG	Sidechain
7	g	8	TYR	Sidechain
7	g	93	ARG	Sidechain
8	h	144	TYR	Sidechain
8	h	163	PHE	Sidechain
8	h	183	ARG	Sidechain
8	h	202	TYR	Sidechain
8	h	34	TYR	Sidechain
8	h	79	TYR	Sidechain
9	i	215	TYR	Sidechain
9	i	219	TYR	Sidechain
10	j	124	PHE	Sidechain
10	j	177	ARG	Sidechain
10	j	199	TYR	Sidechain

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Mol	Chain	Res	Type	Group
10	j	28	ARG	Sidechain
10	j	80	ARG	Sidechain
11	k	117	TYR	Sidechain
11	k	23	ARG	Sidechain
11	k	59	TYR	Sidechain
11	k	70	ARG	Sidechain
11	k	98	TYR	Sidechain
12	l	163	TYR	Sidechain
12	l	189	TYR	Sidechain
12	l	196	ARG	Sidechain
12	l	219	TYR	Sidechain
12	l	245	TYR	Sidechain
12	l	81	PHE	Sidechain
13	m	157	PHE	Sidechain
13	m	221	ARG	Sidechain
13	m	41	TYR	Sidechain
13	m	52	PHE	Sidechain
13	m	85	PHE	Sidechain
13	m	87	HIS	Peptide
14	n	161	ARG	Sidechain
14	n	220	ARG	Sidechain
14	n	49	TYR	Sidechain
14	n	63	TYR	Sidechain
14	n	68	ARG	Sidechain

5.2 Too-close contacts

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

5.3 Torsion angles

5.3.1 Protein backbone

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

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

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/241 (99%)	221 (92%)	16 (7%)	2 (1%)	19	58
1	a	239/241 (99%)	224 (94%)	11 (5%)	4 (2%)	9	42
2	B	247/249 (99%)	226 (92%)	18 (7%)	3 (1%)	13	48
2	b	247/249 (99%)	228 (92%)	13 (5%)	6 (2%)	6	35
3	C	242/244 (99%)	232 (96%)	10 (4%)	0	100	100
3	c	242/244 (99%)	228 (94%)	12 (5%)	2 (1%)	19	58
4	D	235/251 (94%)	217 (92%)	13 (6%)	5 (2%)	7	38
4	d	249/251 (99%)	232 (93%)	16 (6%)	1 (0%)	34	71
5	E	242/244 (99%)	224 (93%)	15 (6%)	3 (1%)	13	48
5	e	242/244 (99%)	224 (93%)	16 (7%)	2 (1%)	19	58
6	F	229/231 (99%)	212 (93%)	15 (7%)	2 (1%)	17	54
6	f	229/231 (99%)	217 (95%)	9 (4%)	3 (1%)	12	47
7	G	243/245 (99%)	230 (95%)	11 (4%)	2 (1%)	19	58
7	g	243/245 (99%)	230 (95%)	11 (4%)	2 (1%)	19	58
8	1	194/196 (99%)	185 (95%)	6 (3%)	3 (2%)	10	44
8	h	194/196 (99%)	176 (91%)	14 (7%)	4 (2%)	7	38
9	2	224/226 (99%)	210 (94%)	13 (6%)	1 (0%)	34	71
9	i	224/226 (99%)	208 (93%)	14 (6%)	2 (1%)	17	54
10	3	202/204 (99%)	181 (90%)	20 (10%)	1 (0%)	29	67
10	j	202/204 (99%)	184 (91%)	14 (7%)	4 (2%)	7	39
11	4	193/195 (99%)	178 (92%)	12 (6%)	3 (2%)	9	43
11	k	193/195 (99%)	177 (92%)	14 (7%)	2 (1%)	15	52
12	5	210/212 (99%)	196 (93%)	14 (7%)	0	100	100
12	l	210/212 (99%)	196 (93%)	9 (4%)	5 (2%)	6	35
13	6	220/222 (99%)	200 (91%)	17 (8%)	3 (1%)	11	45
13	m	220/222 (99%)	203 (92%)	15 (7%)	2 (1%)	17	54
14	7	227/232 (98%)	197 (87%)	23 (10%)	7 (3%)	4	31
14	n	230/232 (99%)	206 (90%)	18 (8%)	6 (3%)	5	34
15	W	195/197 (99%)	181 (93%)	6 (3%)	8 (4%)	3	25
16	V	287/289 (99%)	265 (92%)	16 (6%)	6 (2%)	7	38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
17	T	264/266 (99%)	238 (90%)	23 (9%)	3 (1%)	14 50
18	X	125/127 (98%)	105 (84%)	15 (12%)	5 (4%)	3 25
19	Y	87/89 (98%)	73 (84%)	11 (13%)	3 (3%)	3 29
20	Z	902/970 (93%)	813 (90%)	71 (8%)	18 (2%)	7 39
21	N	920/922 (100%)	861 (94%)	43 (5%)	16 (2%)	9 42
22	S	473/475 (100%)	438 (93%)	24 (5%)	11 (2%)	6 36
23	P	438/440 (100%)	410 (94%)	18 (4%)	10 (2%)	6 36
24	Q	432/434 (100%)	393 (91%)	28 (6%)	11 (2%)	5 34
25	R	403/405 (100%)	377 (94%)	18 (4%)	8 (2%)	7 39
26	U	302/304 (99%)	290 (96%)	9 (3%)	3 (1%)	15 52
27	O	386/388 (100%)	371 (96%)	14 (4%)	1 (0%)	41 75
28	H	424/426 (100%)	380 (90%)	32 (8%)	12 (3%)	5 32
29	I	383/385 (100%)	362 (94%)	15 (4%)	6 (2%)	9 43
30	K	392/394 (100%)	363 (93%)	25 (6%)	4 (1%)	15 52
31	L	386/388 (100%)	365 (95%)	18 (5%)	3 (1%)	19 58
32	M	419/421 (100%)	379 (90%)	32 (8%)	8 (2%)	8 39
33	J	403/405 (100%)	362 (90%)	29 (7%)	12 (3%)	4 31
All	All	13932/14109 (99%)	12868 (92%)	836 (6%)	228 (2%)	13 43

All (228) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	a	196	GLU
5	e	16	SER
11	k	4	ILE
1	A	196	GLU
7	G	9	ASP
8	1	153	GLU
10	3	183	TRP
11	4	151	ASP
15	W	57	ALA
15	W	84	LYS
15	W	149	GLN
16	V	196	TYR
16	V	274	GLN
18	X	116	ALA

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Mol	Chain	Res	Type
20	Z	85	VAL
20	Z	462	VAL
20	Z	802	ASP
20	Z	926	ASN
21	N	832	HIS
21	N	915	ALA
24	Q	40	ALA
24	Q	46	VAL
24	Q	110	SER
25	R	76	GLN
25	R	125	GLU
25	R	280	ILE
25	R	395	ASN
28	H	70	LYS
28	H	76	LEU
28	H	194	SER
29	I	87	LYS
29	I	115	ASP
29	I	125	MET
30	K	237	VAL
31	L	174	GLU
32	M	97	SER
32	M	112	ALA
33	J	118	ASP
33	J	353	CYS
1	a	13	ASP
2	b	219	PRO
10	j	7	ILE
4	D	50	SER
4	D	218	ASP
5	E	9	ASP
6	F	14	SER
7	G	22	PHE
8	1	126	GLY
11	4	11	ASP
14	7	140	MET
14	7	199	PRO
15	W	190	ILE
17	T	131	LYS
20	Z	309	GLN
20	Z	825	ALA
21	N	87	ASP

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Mol	Chain	Res	Type
21	N	718	GLU
21	N	739	PHE
21	N	859	ASN
21	N	861	TYR
21	N	894	ARG
22	S	102	SER
22	S	198	SER
22	S	258	GLU
23	P	47	ARG
23	P	86	HIS
23	P	130	ILE
23	P	327	LEU
25	R	223	ASN
28	H	152	ILE
29	I	86	GLU
29	I	159	VAL
31	L	288	GLY
33	J	110	SER
33	J	151	GLY
33	J	230	VAL
2	b	97	TYR
3	c	167	ALA
6	f	14	SER
7	g	207	ASN
8	h	27	SER
9	i	146	GLY
12	l	286	ILE
13	m	208	ASP
14	n	35	GLN
14	n	80	ASP
4	D	5	ASP
4	D	15	GLY
5	E	16	SER
6	F	222	PHE
13	6	27	ASP
15	W	165	GLN
15	W	179	ARG
15	W	191	ILE
17	T	140	SER
18	X	38	ASN
18	X	94	ASN
18	X	107	GLY

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Mol	Chain	Res	Type
19	Y	13	LYS
20	Z	57	LYS
20	Z	578	GLY
20	Z	727	GLU
20	Z	885	ALA
20	Z	939	ALA
20	Z	940	GLY
20	Z	947	GLY
21	N	858	LYS
22	S	257	LEU
22	S	263	ASP
23	P	6	PRO
23	P	328	ALA
24	Q	44	ALA
24	Q	70	ALA
24	Q	252	HIS
25	R	82	ASP
27	O	119	SER
28	H	188	PRO
28	H	412	PRO
29	I	429	GLU
30	K	164	ASN
30	K	321	ALA
31	L	110	LYS
33	J	90	PRO
33	J	285	SER
1	a	76	SER
4	d	141	ARG
6	f	205	SER
6	f	221	PRO
7	g	22	PHE
8	h	138	SER
10	j	8	ASN
10	j	157	ASN
12	l	147	GLU
14	n	110	ASP
14	n	249	ASN
2	B	232	GLY
5	E	53	ARG
9	2	174	ASP
16	V	61	TYR
16	V	185	ILE

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Mol	Chain	Res	Type
17	T	132	HIS
19	Y	45	ASN
20	Z	397	ASP
21	N	31	VAL
21	N	490	LEU
21	N	882	ILE
22	S	152	LEU
22	S	225	HIS
23	P	331	GLY
24	Q	71	LYS
24	Q	75	ARG
25	R	238	PHE
26	U	133	PRO
28	H	190	ARG
28	H	203	LYS
28	H	215	LYS
28	H	315	GLY
28	H	324	GLY
30	K	103	ILE
32	M	318	ASP
32	M	339	ARG
2	b	4	ARG
2	b	124	SER
3	c	42	ASP
5	e	53	ARG
8	h	39	VAL
8	h	49	LYS
12	l	114	PRO
12	l	115	PHE
14	n	117	GLU
1	A	60	PRO
8	1	123	PRO
13	6	48	GLU
14	7	43	SER
14	7	80	ASP
14	7	110	ASP
14	7	116	ALA
14	7	244	ASN
16	V	262	THR
18	X	95	GLU
20	Z	5	SER
20	Z	82	MET

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Mol	Chain	Res	Type
20	Z	233	LEU
21	N	785	PRO
21	N	853	ASP
22	S	96	ILE
22	S	118	PHE
22	S	126	LYS
23	P	7	ILE
23	P	397	ALA
25	R	245	SER
26	U	150	THR
26	U	180	ASP
28	H	314	VAL
32	M	106	VAL
32	M	290	ARG
33	J	228	ARG
33	J	281	GLY
2	b	17	LYS
2	b	220	ASP
10	j	156	PRO
14	n	119	ALA
2	B	106	PRO
4	D	102	ASP
13	6	137	GLY
16	V	22	ASP
19	Y	70	ASP
20	Z	25	PRO
21	N	791	ALA
23	P	5	ALA
24	Q	49	LYS
24	Q	128	GLU
32	M	143	ASN
32	M	292	ASP
33	J	280	ASP
33	J	284	THR
12	l	173	GLY
21	N	914	VAL
9	i	222	PRO
11	k	178	GLY
22	S	451	ILE
33	J	190	PRO
13	m	49	PRO
2	B	32	VAL

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Mol	Chain	Res	Type
15	W	178	PRO
1	a	16	ILE
11	4	150	PRO
24	Q	66	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	206/206 (100%)	199 (97%)	7 (3%)	37	61
1	a	206/206 (100%)	199 (97%)	7 (3%)	37	61
2	B	208/208 (100%)	202 (97%)	6 (3%)	42	64
2	b	208/208 (100%)	201 (97%)	7 (3%)	37	61
3	C	203/203 (100%)	198 (98%)	5 (2%)	47	68
3	c	203/203 (100%)	203 (100%)	0	100	100
4	D	210/224 (94%)	203 (97%)	7 (3%)	38	62
4	d	224/224 (100%)	221 (99%)	3 (1%)	69	81
5	E	200/200 (100%)	191 (96%)	9 (4%)	27	54
5	e	200/200 (100%)	193 (96%)	7 (4%)	36	61
6	F	190/190 (100%)	180 (95%)	10 (5%)	22	51
6	f	190/190 (100%)	186 (98%)	4 (2%)	53	72
7	G	202/202 (100%)	200 (99%)	2 (1%)	76	85
7	g	202/202 (100%)	197 (98%)	5 (2%)	47	68
8	1	162/162 (100%)	159 (98%)	3 (2%)	57	75
8	h	162/162 (100%)	155 (96%)	7 (4%)	29	56
9	2	185/185 (100%)	183 (99%)	2 (1%)	73	84
9	i	185/185 (100%)	179 (97%)	6 (3%)	39	62
10	3	172/172 (100%)	168 (98%)	4 (2%)	50	70
10	j	172/172 (100%)	168 (98%)	4 (2%)	50	70

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
11	4	173/173 (100%)	170 (98%)	3 (2%)	60	78
11	k	173/173 (100%)	167 (96%)	6 (4%)	36	61
12	5	169/169 (100%)	164 (97%)	5 (3%)	41	64
12	l	169/169 (100%)	164 (97%)	5 (3%)	41	64
13	6	185/185 (100%)	182 (98%)	3 (2%)	62	78
13	m	185/185 (100%)	179 (97%)	6 (3%)	39	62
14	7	195/198 (98%)	191 (98%)	4 (2%)	53	72
14	n	198/198 (100%)	191 (96%)	7 (4%)	36	61
15	W	171/171 (100%)	170 (99%)	1 (1%)	86	92
16	V	253/253 (100%)	246 (97%)	7 (3%)	43	65
17	T	249/249 (100%)	241 (97%)	8 (3%)	39	62
18	X	116/116 (100%)	109 (94%)	7 (6%)	19	47
19	Y	81/81 (100%)	78 (96%)	3 (4%)	34	59
20	Z	773/828 (93%)	744 (96%)	29 (4%)	33	59
21	N	776/776 (100%)	757 (98%)	19 (2%)	49	69
22	S	447/447 (100%)	439 (98%)	8 (2%)	59	77
23	P	412/412 (100%)	403 (98%)	9 (2%)	52	71
24	Q	391/391 (100%)	380 (97%)	11 (3%)	43	65
25	R	356/356 (100%)	350 (98%)	6 (2%)	60	78
26	U	277/277 (100%)	273 (99%)	4 (1%)	67	80
27	O	363/363 (100%)	350 (96%)	13 (4%)	35	60
28	H	361/361 (100%)	350 (97%)	11 (3%)	41	64
29	I	342/342 (100%)	334 (98%)	8 (2%)	50	70
30	K	346/346 (100%)	335 (97%)	11 (3%)	39	62
31	L	332/332 (100%)	320 (96%)	12 (4%)	35	60
32	M	364/364 (100%)	352 (97%)	12 (3%)	38	62
33	J	352/352 (100%)	344 (98%)	8 (2%)	50	70
All	All	12099/12171 (99%)	11768 (97%)	331 (3%)	48	66

All (331) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	13	ASP

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Mol	Chain	Res	Type
1	a	86	PRO
1	a	139	VAL
1	a	171	THR
1	a	175	GLN
1	a	181	ASN
1	a	219	SER
2	b	53	SER
2	b	118	MET
2	b	124	SER
2	b	128	ARG
2	b	132	VAL
2	b	217	GLU
2	b	233	PRO
4	d	11	PHE
4	d	118	GLN
4	d	178	ASN
5	e	22	PHE
5	e	78	MET
5	e	82	THR
5	e	121	LEU
5	e	136	ARG
5	e	214	GLU
5	e	222	ILE
6	f	54	ASP
6	f	72	LEU
6	f	74	LEU
6	f	189	LEU
7	g	11	SER
7	g	46	VAL
7	g	134	VAL
7	g	185	GLU
7	g	218	TRP
8	h	48	ASP
8	h	84	THR
8	h	85	GLU
8	h	135	ILE
8	h	144	TYR
8	h	156	SER
8	h	173	LYS
9	i	60	CYS
9	i	143	HIS
9	i	148	THR

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Mol	Chain	Res	Type
9	i	201	ASN
9	i	209	ILE
9	i	243	LYS
10	j	46	TYR
10	j	48	HIS
10	j	66	MET
10	j	172	LEU
11	k	31	SER
11	k	32	ASP
11	k	75	LEU
11	k	78	GLN
11	k	169	GLU
11	k	180	ILE
12	l	79	LEU
12	l	83	PHE
12	l	109	VAL
12	l	181	ARG
12	l	258	ASP
13	m	11	ASN
13	m	30	VAL
13	m	114	TYR
13	m	115	VAL
13	m	135	PRO
13	m	136	VAL
14	n	36	GLN
14	n	113	LEU
14	n	115	ASP
14	n	152	VAL
14	n	165	LEU
14	n	182	HIS
14	n	195	GLU
1	A	16	ILE
1	A	17	THR
1	A	110	TYR
1	A	131	ARG
1	A	139	VAL
1	A	175	GLN
1	A	239	GLU
2	B	35	LEU
2	B	41	ASN
2	B	118	MET
2	B	128	ARG

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Mol	Chain	Res	Type
2	B	162	THR
2	B	179	TRP
3	C	63	THR
3	C	80	LEU
3	C	89	ASN
3	C	120	GLN
3	C	154	SER
4	D	11	PHE
4	D	62	SER
4	D	81	ASP
4	D	118	GLN
4	D	142	ASP
4	D	152	PRO
4	D	194	LEU
5	E	14	THR
5	E	20	ARG
5	E	22	PHE
5	E	68	VAL
5	E	76	CYS
5	E	112	LEU
5	E	136	ARG
5	E	164	PHE
5	E	214	GLU
6	F	5	ASN
6	F	15	PRO
6	F	57	SER
6	F	69	HIS
6	F	74	LEU
6	F	80	ASP
6	F	117	GLN
6	F	161	ILE
6	F	179	PHE
6	F	209	ASP
7	G	185	GLU
7	G	218	TRP
8	1	48	ASP
8	1	135	ILE
8	1	155	MET
9	2	167	LEU
9	2	241	VAL
10	3	82	ILE
10	3	147	PHE

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Mol	Chain	Res	Type
10	3	150	CYS
10	3	192	LYS
11	4	78	GLN
11	4	124	THR
11	4	141	PHE
12	5	79	LEU
12	5	128	GLN
12	5	139	ARG
12	5	181	ARG
12	5	268	VAL
13	6	39	THR
13	6	115	VAL
13	6	123	ASP
14	7	39	VAL
14	7	95	HIS
14	7	102	ASP
14	7	186	PRO
15	W	2	VAL
16	V	24	LYS
16	V	58	VAL
16	V	80	VAL
16	V	188	LEU
16	V	196	TYR
16	V	199	LEU
16	V	259	LYS
17	T	19	ASP
17	T	85	LEU
17	T	138	ASP
17	T	140	SER
17	T	171	ILE
17	T	197	TYR
17	T	248	GLU
17	T	254	ASP
18	X	14	VAL
18	X	18	ASN
18	X	38	ASN
18	X	63	PRO
18	X	65	SER
18	X	80	SER
18	X	87	PHE
19	Y	21	ASN
19	Y	57	THR

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Mol	Chain	Res	Type
19	Y	74	THR
20	Z	63	LEU
20	Z	120	SER
20	Z	154	ILE
20	Z	175	ASP
20	Z	195	PHE
20	Z	210	TYR
20	Z	213	LYS
20	Z	284	LEU
20	Z	293	MET
20	Z	317	GLN
20	Z	323	TYR
20	Z	411	LYS
20	Z	534	PHE
20	Z	546	ILE
20	Z	548	ASP
20	Z	566	LEU
20	Z	583	ASP
20	Z	609	THR
20	Z	613	ASP
20	Z	722	ASP
20	Z	728	LYS
20	Z	741	LEU
20	Z	756	MET
20	Z	815	MET
20	Z	817	LEU
20	Z	850	LEU
20	Z	859	LYS
20	Z	874	ASN
20	Z	945	ILE
21	N	38	GLU
21	N	263	SER
21	N	318	LYS
21	N	381	GLU
21	N	417	ARG
21	N	418	ASP
21	N	436	ASP
21	N	492	THR
21	N	508	THR
21	N	530	GLU
21	N	546	LEU
21	N	773	MET

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Mol	Chain	Res	Type
21	N	824	ASN
21	N	829	LYS
21	N	862	SER
21	N	866	TYR
21	N	869	ASP
21	N	919	THR
21	N	922	GLN
22	S	82	TYR
22	S	93	LEU
22	S	253	PHE
22	S	339	GLN
22	S	378	GLN
22	S	392	ILE
22	S	404	LEU
22	S	475	TYR
23	P	6	PRO
23	P	129	LYS
23	P	163	LEU
23	P	203	ILE
23	P	208	PHE
23	P	214	GLU
23	P	308	LEU
23	P	309	MET
23	P	326	ASP
24	Q	50	ARG
24	Q	79	PRO
24	Q	118	CYS
24	Q	153	ASP
24	Q	157	LEU
24	Q	166	LYS
24	Q	198	LEU
24	Q	222	SER
24	Q	226	HIS
24	Q	306	TYR
24	Q	313	ASP
25	R	22	PRO
25	R	33	LEU
25	R	98	LEU
25	R	184	GLN
25	R	199	GLU
25	R	380	VAL
26	U	28	LYS

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Mol	Chain	Res	Type
26	U	229	LEU
26	U	246	GLU
26	U	257	ILE
27	O	9	THR
27	O	58	ARG
27	O	98	TYR
27	O	110	ASP
27	O	126	ILE
27	O	130	ASP
27	O	152	ASP
27	O	166	ARG
27	O	185	PHE
27	O	237	PRO
27	O	258	LEU
27	O	307	MET
27	O	343	GLN
28	H	161	GLU
28	H	163	VAL
28	H	174	VAL
28	H	195	VAL
28	H	203	LYS
28	H	208	TYR
28	H	240	ILE
28	H	268	ASP
28	H	367	ARG
28	H	389	PHE
28	H	459	SER
29	I	54	ARG
29	I	159	VAL
29	I	219	VAL
29	I	254	GLN
29	I	257	LEU
29	I	341	PRO
29	I	368	LYS
29	I	415	ASP
30	K	128	ARG
30	K	153	ASP
30	K	237	VAL
30	K	264	ASN
30	K	272	ASP
30	K	286	THR
30	K	335	ASP

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Mol	Chain	Res	Type
30	K	370	SER
30	K	376	ASP
30	K	404	GLN
30	K	425	ASP
31	L	93	ASN
31	L	126	ARG
31	L	132	ARG
31	L	141	LYS
31	L	144	VAL
31	L	206	ILE
31	L	216	LYS
31	L	235	VAL
31	L	334	ASP
31	L	361	PHE
31	L	415	LEU
31	L	421	LYS
32	M	18	LEU
32	M	76	PRO
32	M	85	VAL
32	M	129	LEU
32	M	146	VAL
32	M	162	GLU
32	M	172	VAL
32	M	182	ASP
32	M	254	MET
32	M	296	SER
32	M	344	ASP
32	M	415	PHE
33	J	121	MET
33	J	218	LEU
33	J	279	LEU
33	J	282	PHE
33	J	353	CYS
33	J	370	LEU
33	J	391	ASN
33	J	403	LEU

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (122) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	15	HIS
1	a	56	GLN

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Mol	Chain	Res	Type
1	a	92	ASN
1	a	130	GLN
2	b	241	GLN
2	b	244	ASN
3	c	94	HIS
3	c	124	GLN
4	d	94	GLN
4	d	178	ASN
5	e	157	HIS
5	e	233	ASN
6	f	117	GLN
7	g	183	HIS
8	h	71	HIS
9	i	95	HIS
10	j	173	ASN
11	k	65	GLN
11	k	133	HIS
12	l	241	HIS
13	m	11	ASN
13	m	16	ASN
14	n	95	HIS
1	A	15	HIS
1	A	92	ASN
1	A	184	ASN
2	B	94	HIS
2	B	139	HIS
2	B	190	HIS
5	E	73	HIS
5	E	168	ASN
5	E	216	ASN
6	F	31	GLN
6	F	117	GLN
6	F	121	GLN
6	F	185	ASN
7	G	204	HIS
9	2	59	ASN
9	2	143	HIS
10	3	45	HIS
11	4	99	GLN
11	4	166	GLN
12	5	141	HIS
14	7	35	GLN

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Mol	Chain	Res	Type
15	W	38	GLN
15	W	80	GLN
15	W	100	HIS
16	V	88	GLN
16	V	102	GLN
17	T	135	ASN
18	X	102	GLN
20	Z	129	ASN
20	Z	156	HIS
20	Z	243	GLN
20	Z	307	HIS
20	Z	378	GLN
20	Z	391	ASN
20	Z	405	ASN
20	Z	434	GLN
20	Z	463	HIS
20	Z	593	HIS
20	Z	760	HIS
20	Z	769	ASN
20	Z	823	ASN
20	Z	833	GLN
20	Z	842	GLN
20	Z	868	ASN
20	Z	905	ASN
20	Z	917	ASN
20	Z	926	ASN
21	N	17	GLN
21	N	375	HIS
21	N	613	HIS
21	N	738	GLN
21	N	824	ASN
22	S	139	HIS
22	S	159	ASN
22	S	244	ASN
22	S	378	GLN
23	P	98	GLN
23	P	230	HIS
23	P	401	ASN
23	P	410	GLN
24	Q	63	GLN
24	Q	186	HIS
24	Q	252	HIS

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Mol	Chain	Res	Type
24	Q	280	ASN
24	Q	334	HIS
24	Q	346	ASN
24	Q	405	GLN
25	R	42	GLN
25	R	374	ASN
26	U	62	ASN
26	U	116	ASN
26	U	192	ASN
26	U	260	ASN
26	U	270	ASN
27	O	75	GLN
27	O	175	ASN
28	H	339	GLN
29	I	151	HIS
29	I	204	HIS
29	I	254	GLN
29	I	295	ASN
29	I	311	ASN
30	K	83	GLN
30	K	98	GLN
30	K	285	GLN
30	K	302	GLN
30	K	311	ASN
30	K	375	ASN
31	L	169	ASN
31	L	393	ASN
31	L	409	HIS
32	M	55	ASN
32	M	96	ASN
32	M	189	GLN
32	M	250	GLN
32	M	390	GLN
33	J	123	HIS
33	J	336	ASN
33	J	394	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
34	ATP	M	501	35	26,33,33	1.18	3 (11%)	31,52,52	2.29	9 (29%)
34	ATP	K	501	35	26,33,33	1.30	4 (15%)	31,52,52	1.77	5 (16%)
34	ATP	I	501	-	26,33,33	1.17	2 (7%)	31,52,52	1.89	5 (16%)
36	ADP	J	501	-	24,29,29	1.65	6 (25%)	29,45,45	2.18	6 (20%)
34	ATP	L	501	-	26,33,33	1.09	1 (3%)	31,52,52	1.87	7 (22%)
34	ATP	H	501	35	26,33,33	1.51	5 (19%)	31,52,52	1.75	6 (19%)

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
34	ATP	M	501	35	-	3/18/38/38	0/3/3/3
34	ATP	K	501	35	-	5/18/38/38	0/3/3/3
34	ATP	I	501	-	-	6/18/38/38	0/3/3/3
36	ADP	J	501	-	-	5/12/32/32	0/3/3/3
34	ATP	L	501	-	-	2/18/38/38	0/3/3/3
34	ATP	H	501	35	-	9/18/38/38	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	J	501	ADP	O4'-C1'	5.10	1.48	1.41
34	H	501	ATP	C4-N3	-3.70	1.30	1.35
34	K	501	ATP	O4'-C1'	3.00	1.45	1.41
34	H	501	ATP	C8-N7	-2.93	1.29	1.34
34	H	501	ATP	C2-N3	2.91	1.36	1.32
34	K	501	ATP	C2-N3	2.85	1.36	1.32
34	K	501	ATP	C4-N3	2.65	1.39	1.35
34	M	501	ATP	O2'-C2'	-2.51	1.37	1.43
34	L	501	ATP	C8-N7	-2.51	1.30	1.34
36	J	501	ADP	C8-N7	-2.35	1.30	1.34
36	J	501	ADP	C2-N1	-2.34	1.29	1.33
34	I	501	ATP	C4-N3	-2.32	1.32	1.35
36	J	501	ADP	C2'-C1'	2.27	1.57	1.53
36	J	501	ADP	C2-N3	2.25	1.35	1.32
34	I	501	ATP	C2-N3	2.24	1.35	1.32
34	M	501	ATP	C3'-C4'	2.23	1.58	1.53
34	M	501	ATP	PA-O2A	-2.22	1.44	1.55
34	H	501	ATP	PG-O2G	-2.22	1.46	1.54
36	J	501	ADP	PA-O2A	-2.11	1.45	1.55
34	K	501	ATP	C8-N7	-2.02	1.31	1.34
34	H	501	ATP	O4'-C4'	2.01	1.49	1.45

All (38) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	J	501	ADP	PA-O3A-PB	9.56	165.62	132.83
34	M	501	ATP	PB-O3B-PG	7.72	159.31	132.83
34	H	501	ATP	PA-O3A-PB	6.09	153.74	132.83
34	K	501	ATP	PA-O3A-PB	5.92	153.13	132.83
34	I	501	ATP	PA-O3A-PB	5.84	152.87	132.83
34	L	501	ATP	PB-O3B-PG	5.71	152.44	132.83
34	M	501	ATP	PA-O3A-PB	4.93	149.74	132.83
34	M	501	ATP	C4-C5-N7	-4.51	104.70	109.40
34	L	501	ATP	PA-O3A-PB	4.48	148.20	132.83
34	K	501	ATP	PB-O3B-PG	3.98	146.48	132.83
34	L	501	ATP	N6-C6-N1	3.93	126.74	118.57
34	I	501	ATP	N6-C6-N1	3.58	126.01	118.57
34	I	501	ATP	PB-O3B-PG	3.50	144.84	132.83
34	I	501	ATP	C5-C6-N1	-3.34	112.78	120.35
34	M	501	ATP	C5-C6-N1	-3.22	113.05	120.35
36	J	501	ADP	N6-C6-N1	3.03	124.86	118.57
34	H	501	ATP	N6-C6-N1	2.86	124.50	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	K	501	ATP	N3-C2-N1	2.77	133.01	128.68
34	I	501	ATP	C3'-C2'-C1'	2.71	105.06	100.98
36	J	501	ADP	C5-C6-N1	-2.70	114.23	120.35
34	L	501	ATP	C5-C6-N1	-2.63	114.40	120.35
34	H	501	ATP	C2'-C3'-C4'	-2.60	97.59	102.64
34	K	501	ATP	N6-C6-N1	2.59	123.95	118.57
34	H	501	ATP	C3'-C2'-C1'	2.58	104.86	100.98
34	M	501	ATP	O3G-PG-O2G	2.53	117.31	107.64
34	M	501	ATP	O2B-PB-O1B	2.42	124.19	112.24
34	H	501	ATP	PB-O3B-PG	2.35	140.89	132.83
34	M	501	ATP	C3'-C2'-C1'	2.35	104.51	100.98
34	L	501	ATP	N3-C2-N1	2.32	132.30	128.68
34	M	501	ATP	N6-C6-N1	2.31	123.38	118.57
36	J	501	ADP	C2'-C3'-C4'	2.27	107.05	102.64
36	J	501	ADP	O3B-PB-O3A	2.14	111.80	104.64
34	M	501	ATP	C5-C6-N6	2.12	123.57	120.35
34	L	501	ATP	O3'-C3'-C2'	2.10	118.62	111.82
34	H	501	ATP	O3G-PG-O2G	2.09	115.64	107.64
34	L	501	ATP	O3G-PG-O2G	2.09	115.62	107.64
36	J	501	ADP	O3A-PB-O1B	-2.06	99.75	111.19
34	K	501	ATP	C5'-C4'-C3'	2.01	122.71	115.18

There are no chirality outliers.

All (30) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	H	501	ATP	C5'-O5'-PA-O1A
34	H	501	ATP	C5'-O5'-PA-O3A
34	I	501	ATP	C5'-O5'-PA-O3A
34	K	501	ATP	C5'-O5'-PA-O2A
34	L	501	ATP	C5'-O5'-PA-O3A
36	J	501	ADP	PA-O3A-PB-O3B
36	J	501	ADP	C5'-O5'-PA-O1A
36	J	501	ADP	C5'-O5'-PA-O2A
34	I	501	ATP	PA-O3A-PB-O1B
34	H	501	ATP	C4'-C5'-O5'-PA
34	H	501	ATP	PB-O3B-PG-O2G
34	K	501	ATP	C5'-O5'-PA-O3A
34	I	501	ATP	C5'-O5'-PA-O1A
34	K	501	ATP	C5'-O5'-PA-O1A
34	L	501	ATP	C5'-O5'-PA-O2A
34	M	501	ATP	C5'-O5'-PA-O2A

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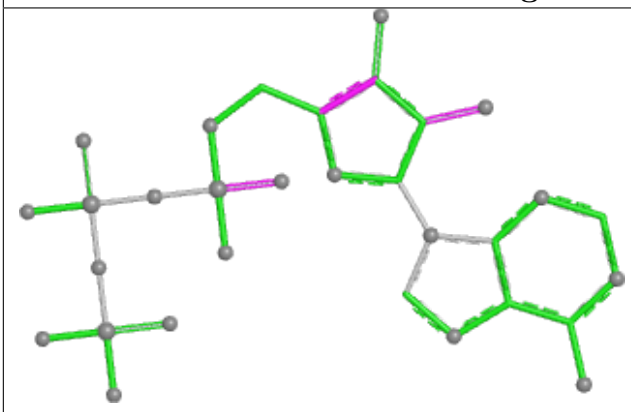
Mol	Chain	Res	Type	Atoms
34	I	501	ATP	PG-O3B-PB-O2B
34	I	501	ATP	PA-O3A-PB-O2B
34	K	501	ATP	PA-O3A-PB-O1B
34	K	501	ATP	PA-O3A-PB-O2B
34	I	501	ATP	C4'-C5'-O5'-PA
34	M	501	ATP	C4'-C5'-O5'-PA
34	H	501	ATP	PB-O3A-PA-O2A
34	H	501	ATP	PB-O3B-PG-O3G
36	J	501	ADP	PA-O3A-PB-O2B
34	M	501	ATP	C5'-O5'-PA-O3A
36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

There are no ring outliers.

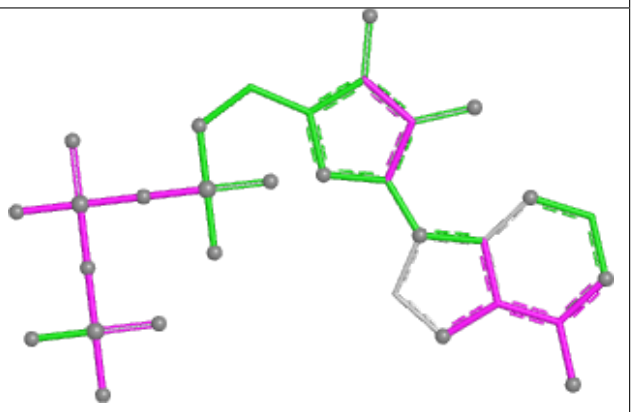
No monomer is involved in short contacts.

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

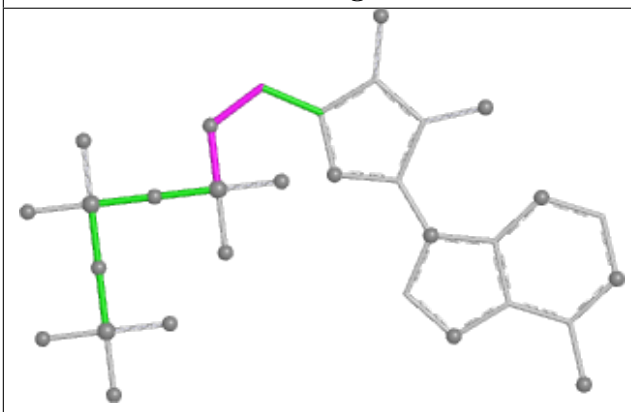
Ligand ATP M 501



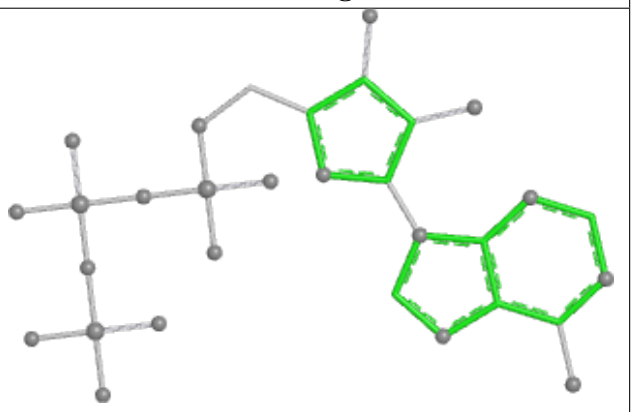
Bond lengths



Bond angles

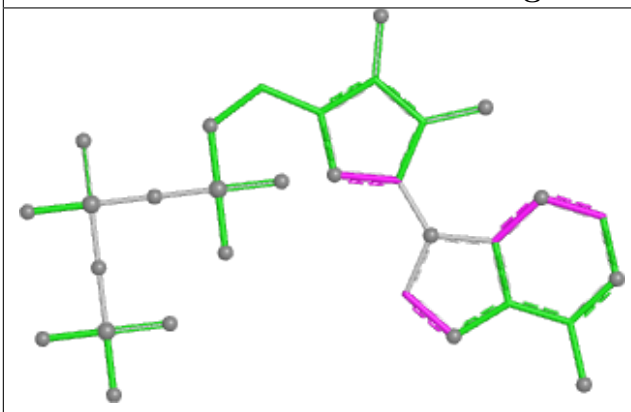


Torsions



Rings

Ligand ATP K 501



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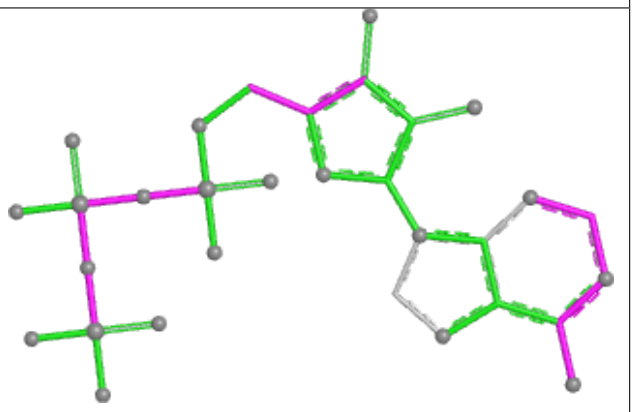
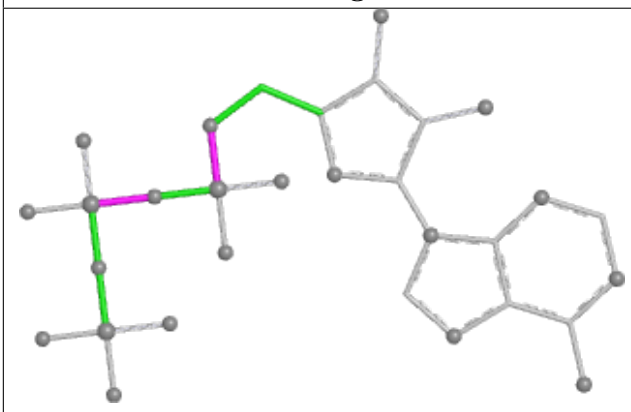
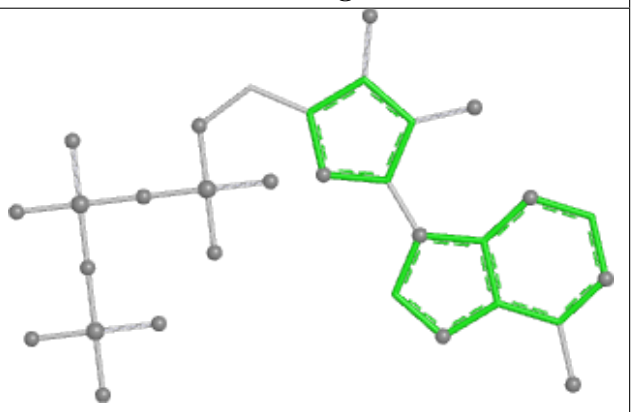


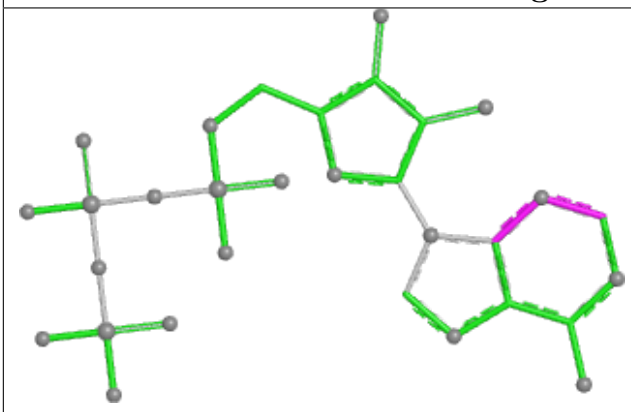
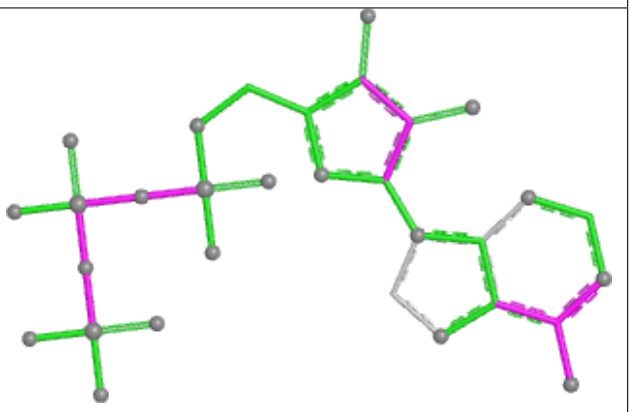
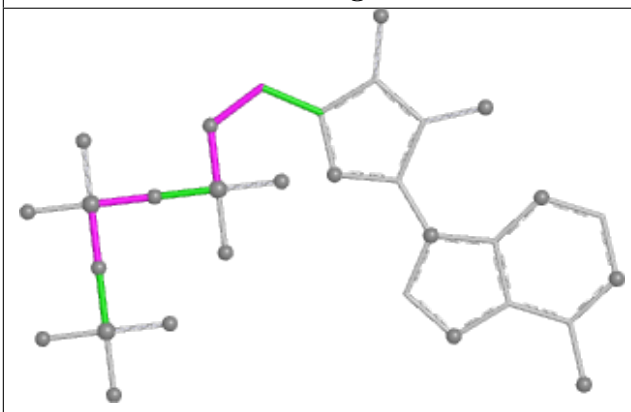
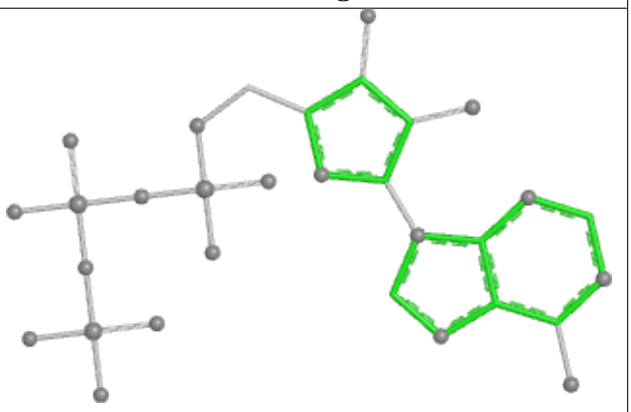
Bond angles

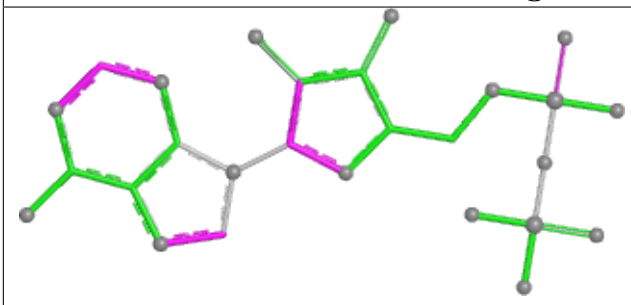
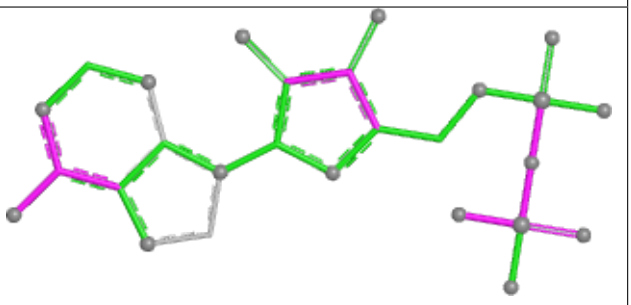
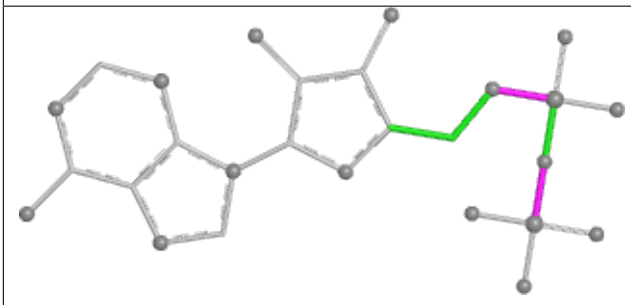
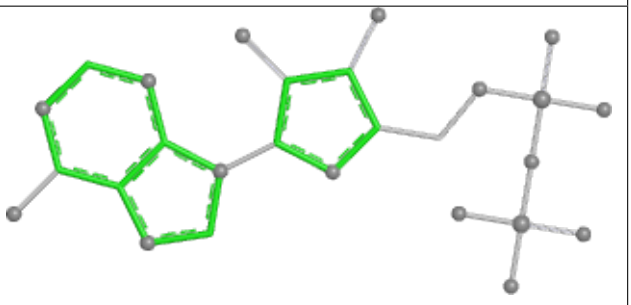


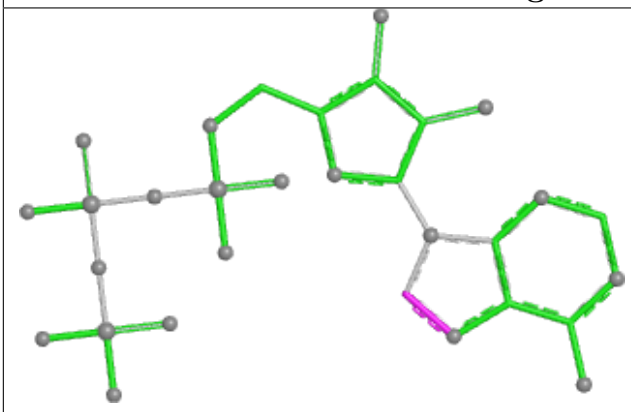
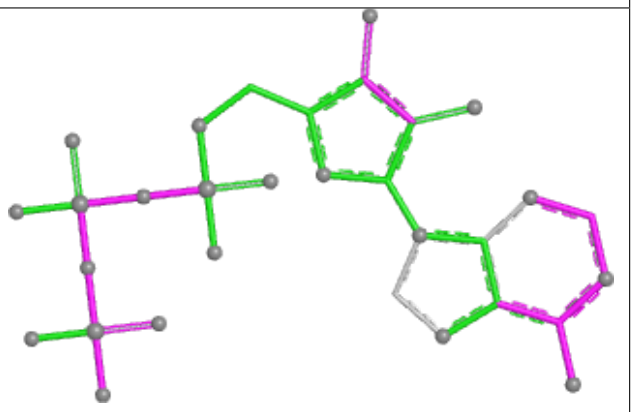
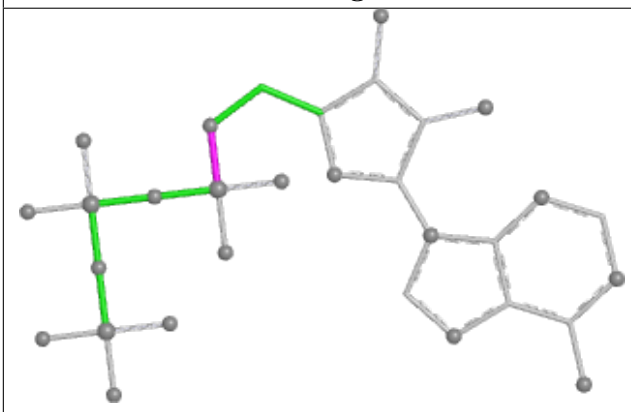
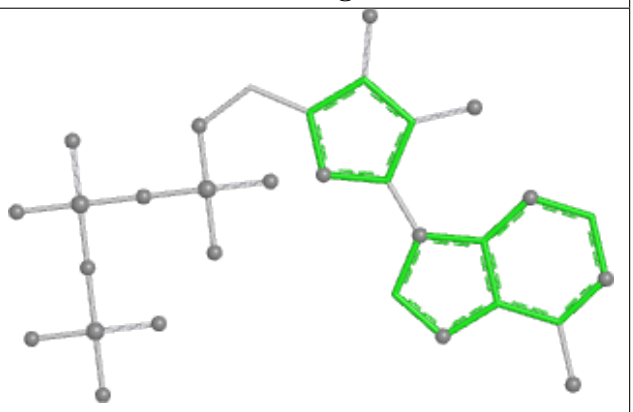
Torsions

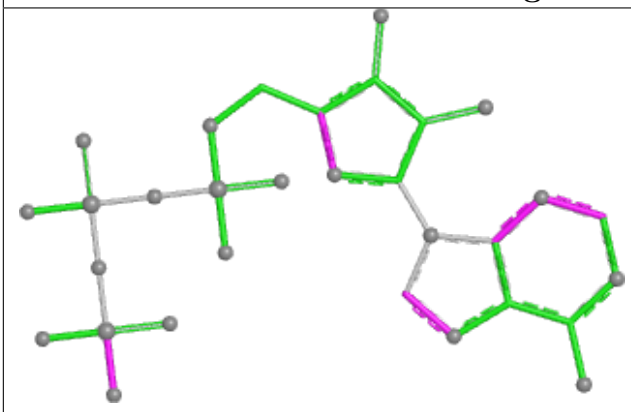
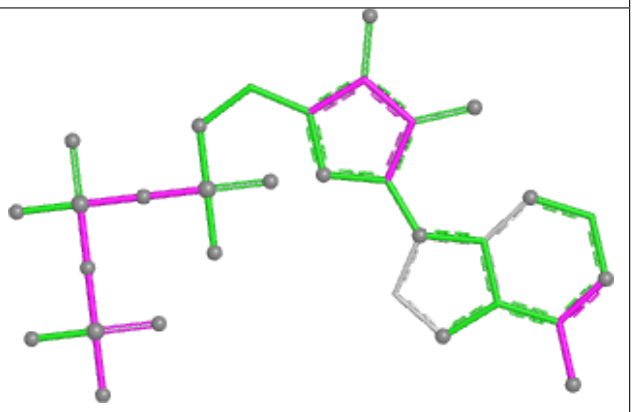
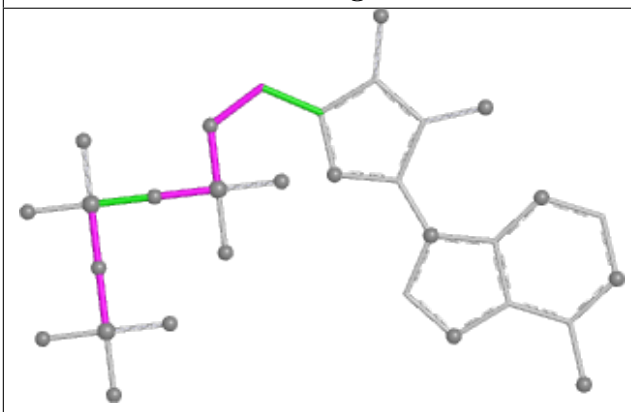
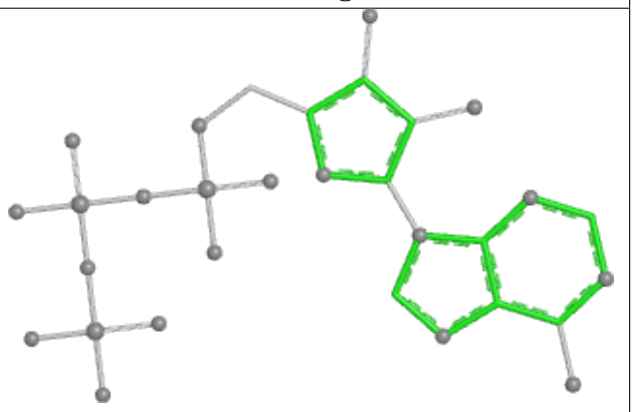


Rings

Ligand ATP I 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ADP J 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP L 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP H 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

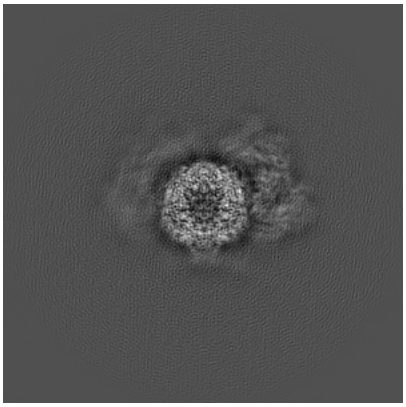
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3534. These allow visual inspection of the internal detail of the map and identification of artifacts.

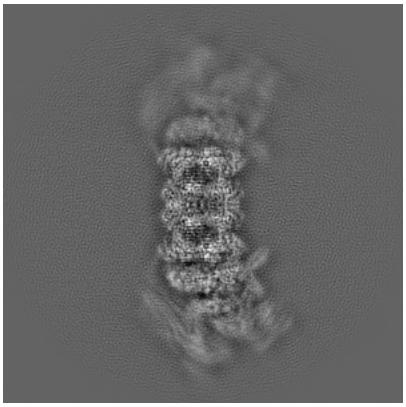
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

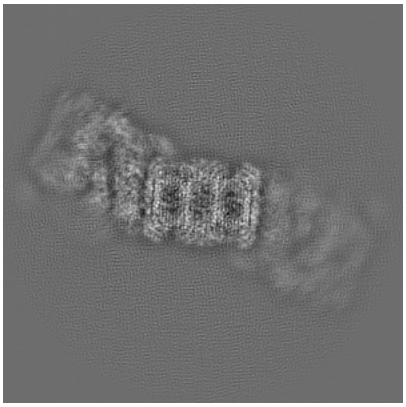
6.1.1 Primary map



X



Y

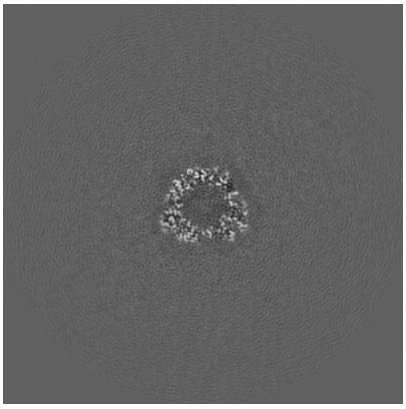


Z

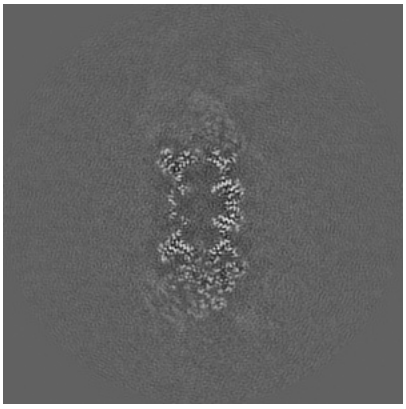
The images above show the map projected in three orthogonal directions.

6.2 Central slices

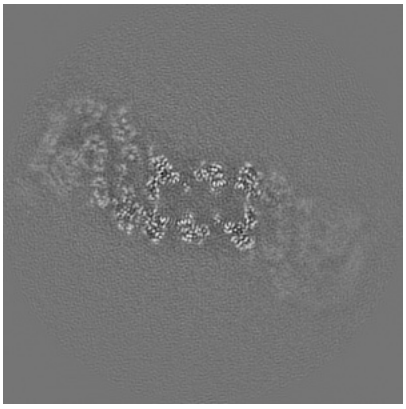
6.2.1 Primary map



X Index: 192



Y Index: 192

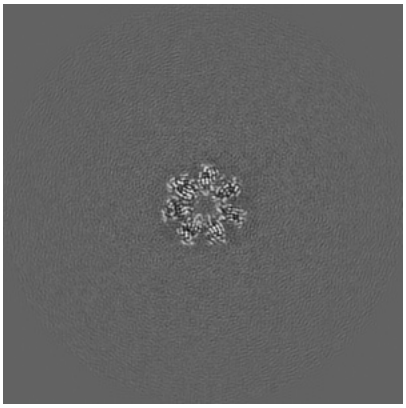


Z Index: 192

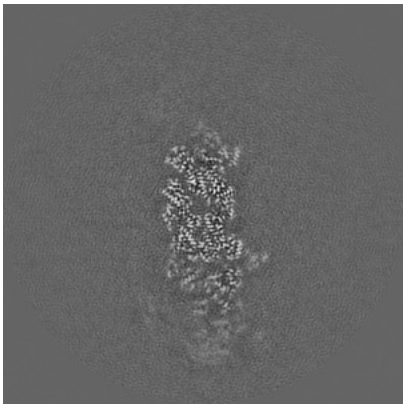
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

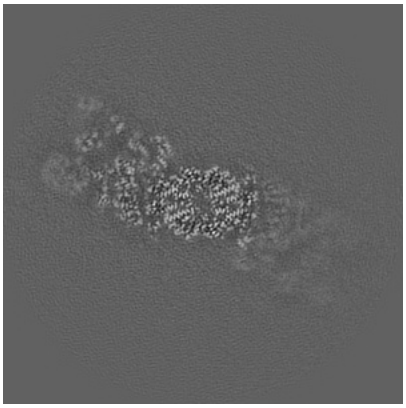
6.3.1 Primary map



X Index: 177



Y Index: 212



Z Index: 208

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

6.4 Orthogonal surface views (i)

6.4.1 Primary map

X

Y

Z

The images above show the 3D surface view of the map at the recommended contour level 0.02. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

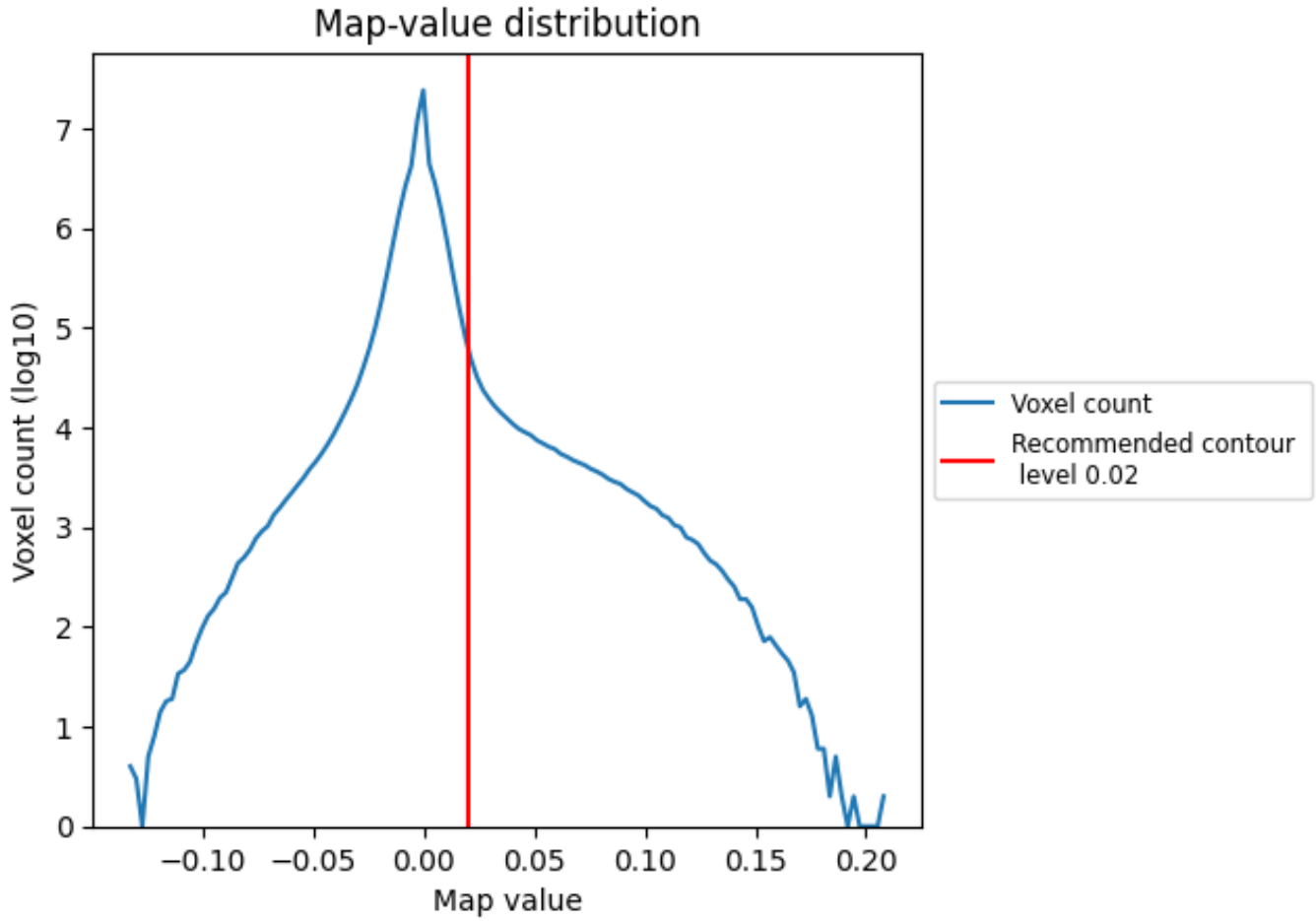
6.5 Mask visualisation (i)

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

7 Map analysis

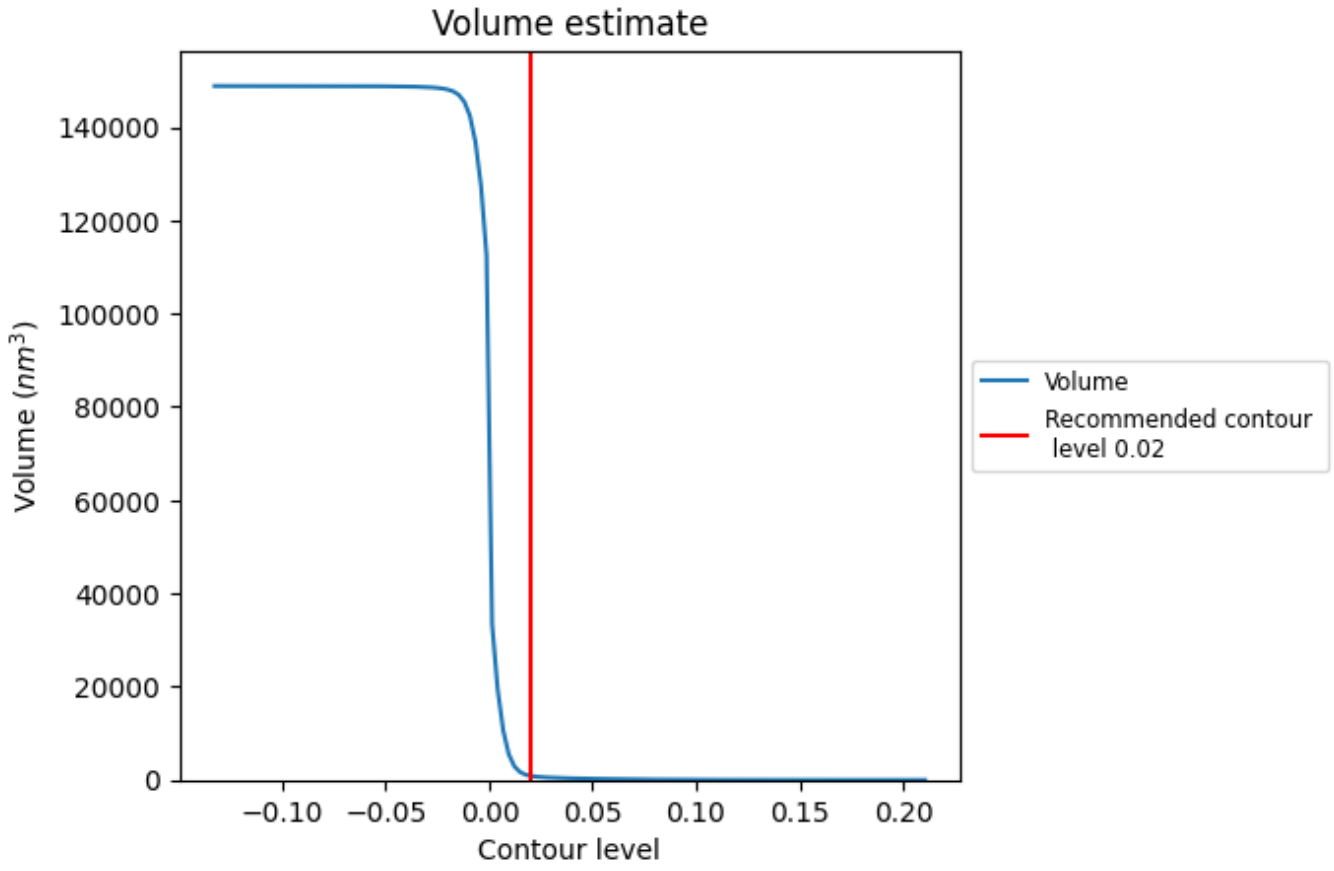
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

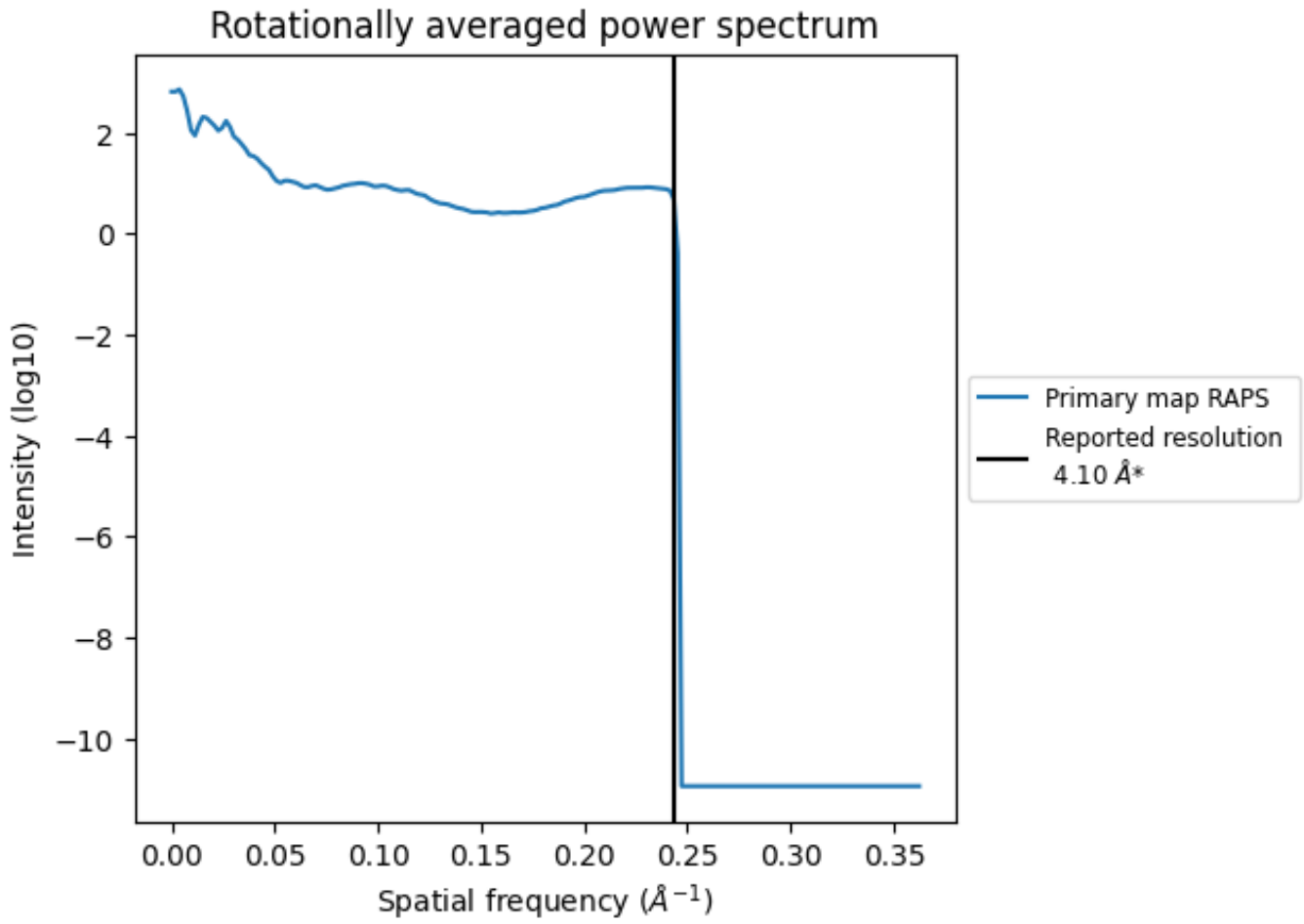
7.2 Volume estimate



The volume at the recommended contour level is 881 nm^3; this corresponds to an approximate mass of 796 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 0.244 Å^{-1}

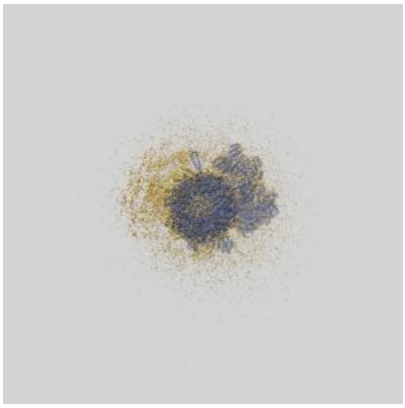
8 Fourier-Shell correlation

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

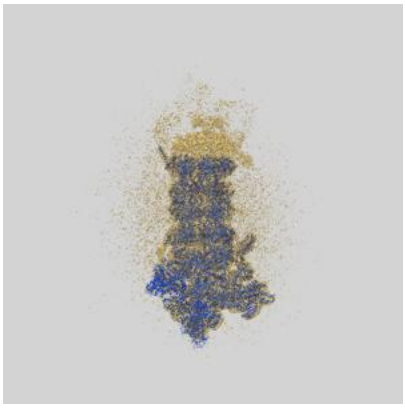
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3534 and PDB model 6FVT. Per-residue inclusion information can be found in section 3 on page 13.

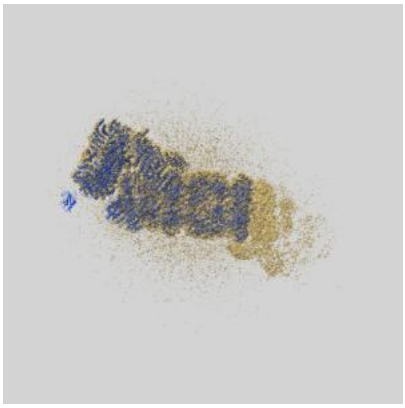
9.1 Map-model overlay



X



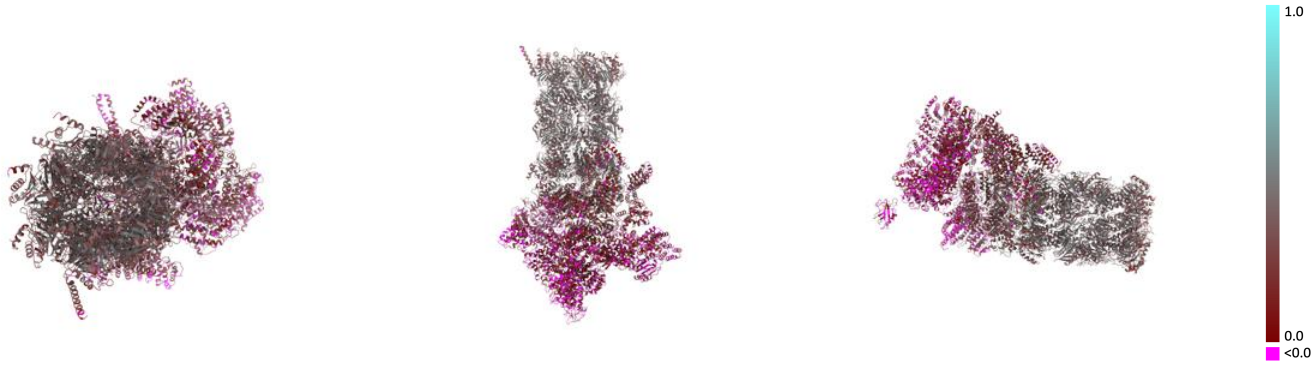
Y



Z

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

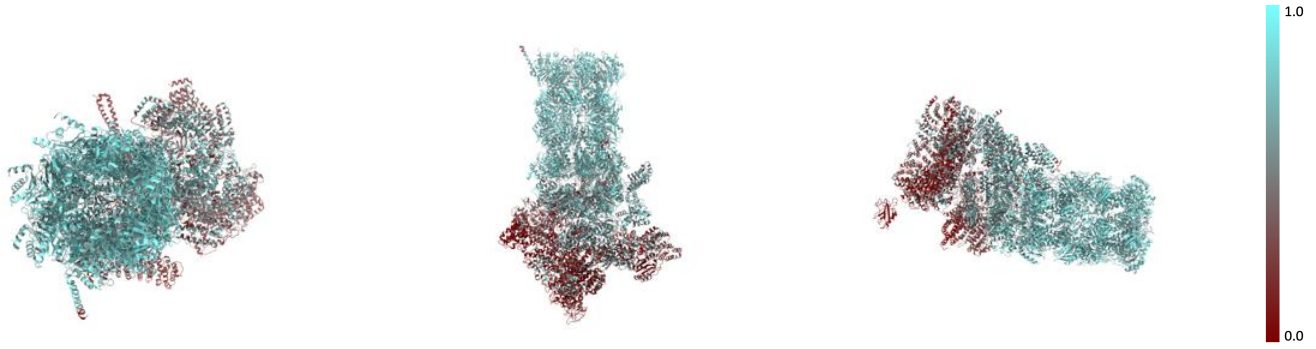
9.2 Q-score mapped to coordinate model



X Y Z

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

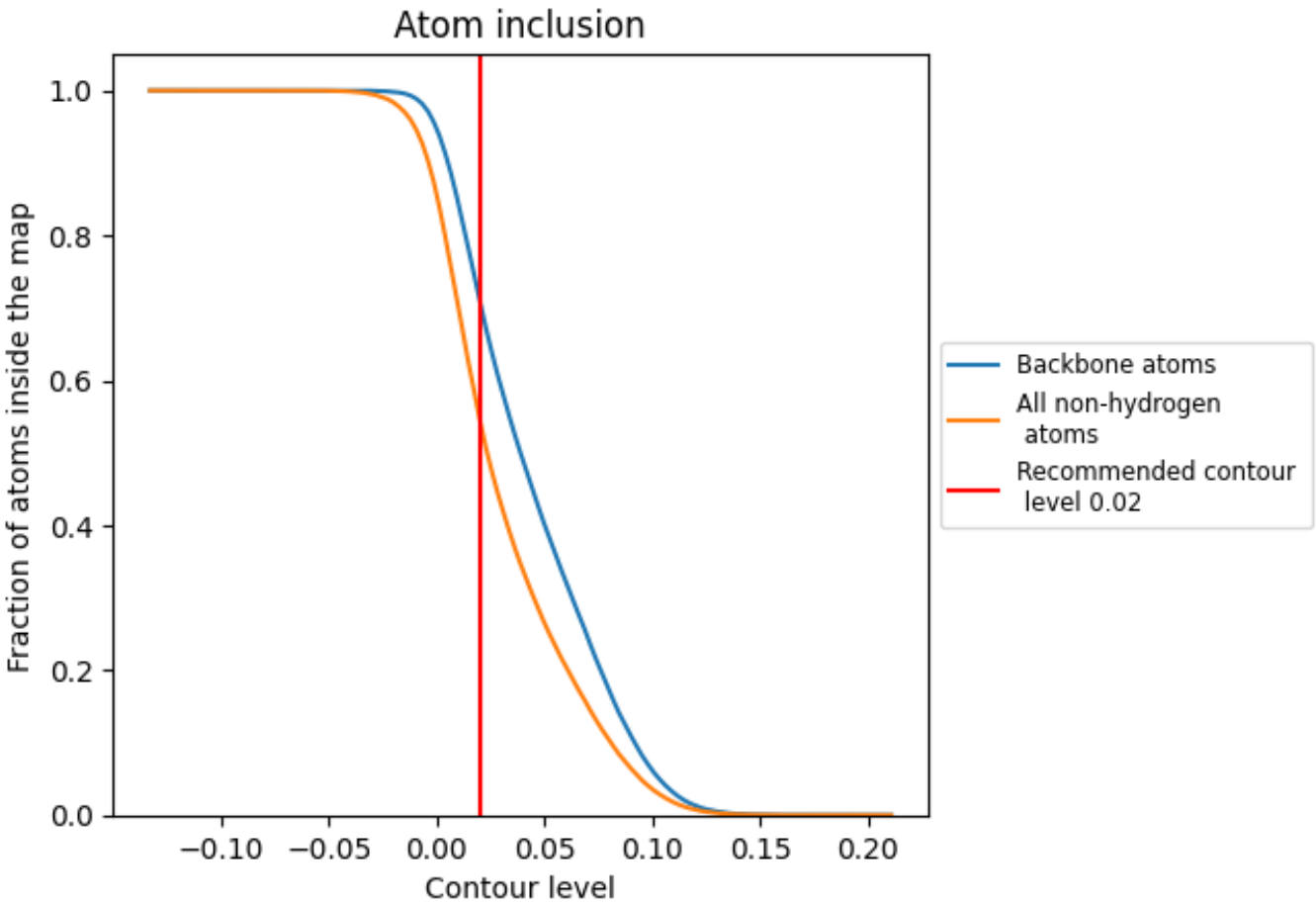
9.3 Atom inclusion mapped to coordinate model



X Y Z

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

9.4 Atom inclusion (i)



At the recommended contour level, 71% of all backbone atoms, 55% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.02) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.5462	0.2540
1	0.7743	0.3920
2	0.7546	0.3840
3	0.7596	0.4000
4	0.7554	0.3830
5	0.7794	0.3970
6	0.7689	0.3870
7	0.7867	0.3900
A	0.7431	0.3520
B	0.7373	0.3720
C	0.7307	0.3670
D	0.7474	0.3640
E	0.7104	0.3500
F	0.7476	0.3750
G	0.7472	0.3640
H	0.5616	0.2690
I	0.5744	0.2590
J	0.5072	0.2250
K	0.5738	0.2430
L	0.5749	0.2510
M	0.5366	0.2540
N	0.1714	0.0720
O	0.3339	0.1040
P	0.5782	0.1840
Q	0.5923	0.1990
R	0.4792	0.1640
S	0.3182	0.1160
T	0.2536	0.1190
U	0.3471	0.1260
V	0.3971	0.1480
W	0.1256	0.0520
X	0.0039	0.0270
Y	0.2033	0.0560
Z	0.1114	0.0900
a	0.7318	0.3490

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Chain	Atom inclusion	Q-score
b	0.7176	0.3470
c	0.7124	0.3430
d	0.7191	0.3460
e	0.7157	0.3480
f	0.7418	0.3560
g	0.7328	0.3540
h	0.7810	0.3900
i	0.7499	0.3790
j	0.7468	0.3840
k	0.7652	0.3960
l	0.7974	0.4080
m	0.7718	0.3870
n	0.7830	0.3850