Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 08:48 am GMT

PDB ID	:	5LN3
EMDB ID	:	EMD-4089
Title	:	The human 26S Proteasome at 6.8 Ang.
Authors	:	Schweitzer, A.; Beck, F.; Sakata, E.; Unverdorben, P.
Deposited on	:	2016-08-03
Resolution	:	6.80 Å(reported)

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

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

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

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

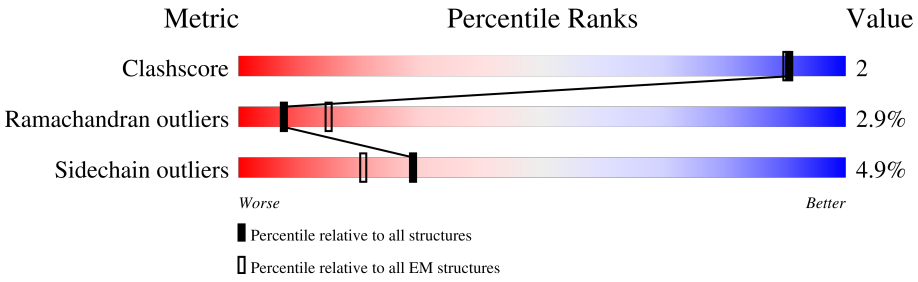
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.80 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
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	Z	908	79% 63% 21% • 13%
2	1	239	27% 68% 18% • 10%
3	2	277	15% 58% 17% • 20%
4	3	205	32% 70% 20% 8% •
5	4	201	20% 62% 30% • •
6	5	263	19% 54% 16% • 26%
7	6	241	25% 60% 23% 5% • 12%
8	7	264	27% 57% 20% 6% 17%

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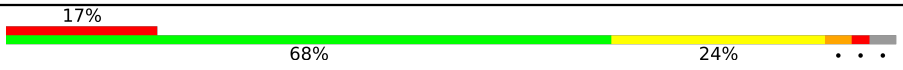
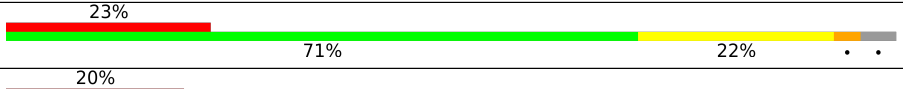
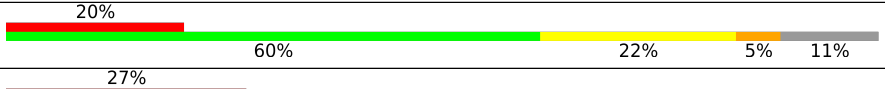
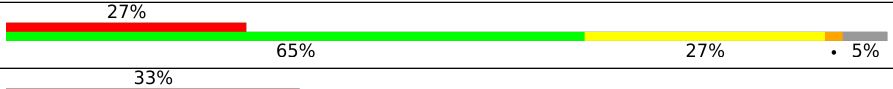
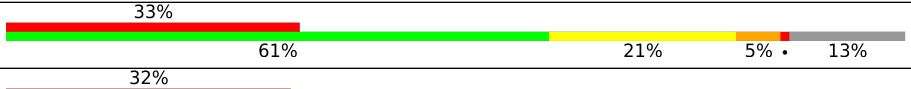
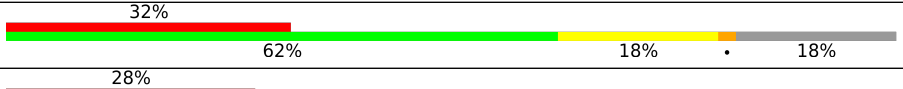
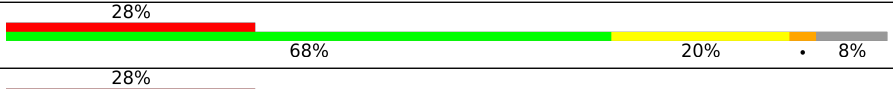
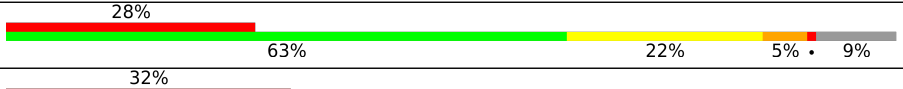
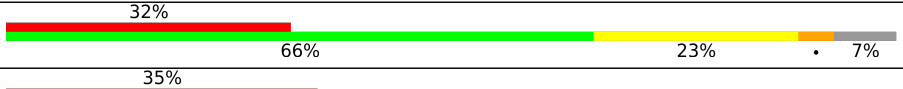
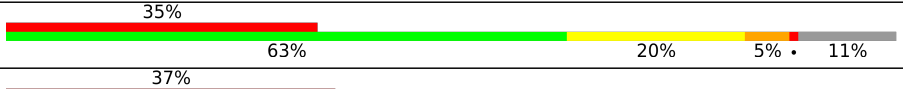
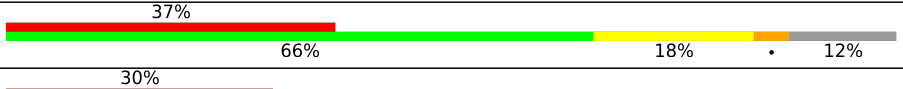
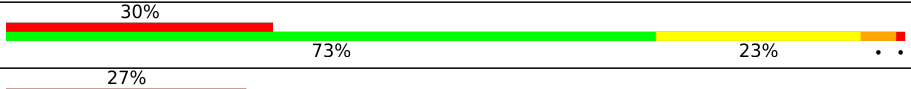
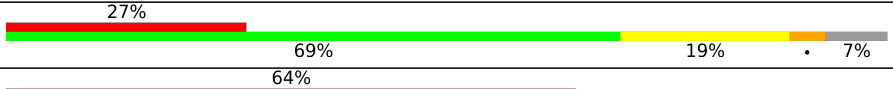
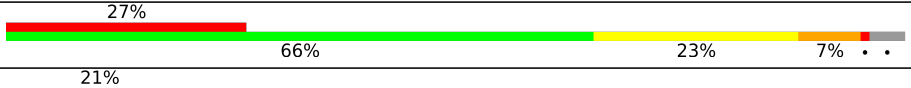
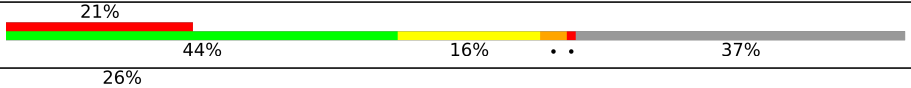
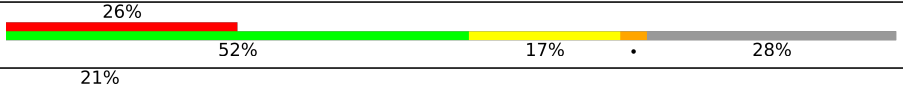
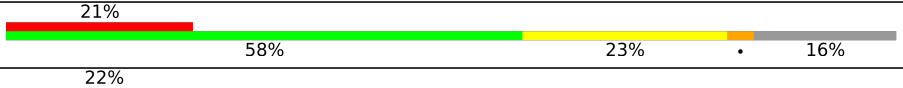
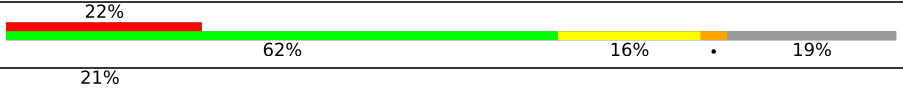
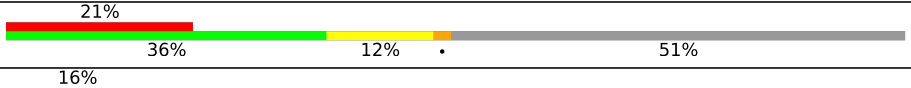
Mol	Chain	Length	Quality of chain
9	A	246	
10	B	234	
11	C	261	
12	D	248	
13	E	241	
14	F	263	
15	G	255	
16	H	433	
17	I	440	
18	J	406	
19	K	418	
20	L	389	
21	M	439	
22	N	953	
23	O	376	
24	P	456	
25	Q	422	
26	R	389	
27	S	534	
28	T	350	
29	U	324	
30	V	310	
31	W	377	
32	Y	70	

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 78323 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 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	Z	794	6146	3893	1043	1166	44	0	0

- Molecule 2 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	1	214	1607	1006	274	315	12	0	0

- Molecule 3 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	2	222	1676	1055	285	324	12	0	0

- Molecule 4 is a protein called Proteasome subunit beta type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	3	205	1599	1018	266	295	20	0	0

- Molecule 5 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	4	194	1554	994	265	286	9	0	0

- Molecule 6 is a protein called Proteasome subunit beta type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	5	195	1509	951	265	284	9	0	0

- Molecule 7 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	6	213	Total	C	N	O	S	0	0
			1654	1047	284	313	10		

- Molecule 8 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	7	218	Total	C	N	O	S	0	0
			1705	1076	293	324	12		

- Molecule 9 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	A	239	Total	C	N	O	S	0	0
			1874	1190	312	359	13		

- Molecule 10 is a protein called Proteasome subunit alpha type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	B	234	Total	C	N	O	S	0	0
			1826	1166	309	344	7		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	C	261	Total	C	N	O	S	0	0
			2069	1304	356	398	11		

- Molecule 12 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	D	248	Total	C	N	O	S	0	0
			1961	1229	349	377	6		

- Molecule 13 is a protein called Proteasome subunit alpha type-5.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	E	232	Total	C	N	O	S	0	0
			1770	1112	293	354	11		

- Molecule 14 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	F	233	Total	C	N	O	S	0	0
			1837	1153	331	341	12		

- Molecule 15 is a protein called Proteasome subunit alpha type-3.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	G	242	Total	C	N	O	S	0	0
			1894	1200	323	360	11		

- Molecule 16 is a protein called 26S protease regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	H	378	Total	C	N	O	S	0	0
			2962	1865	522	558	17		

- Molecule 17 is a protein called 26S protease regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	I	362	Total	C	N	O	S	0	0
			2840	1782	483	562	13		

- Molecule 18 is a protein called 26S protease regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	J	373	Total	C	N	O	S	0	0
			2929	1839	525	548	17		

- Molecule 19 is a protein called 26S protease regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	K	379	Total	C	N	O	S	0	0
			3032	1919	523	577	13		

- Molecule 20 is a protein called 26S protease regulatory subunit 10B.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	L	361	Total	C	N	O	S	0	0
			2862	1797	512	537	16		

- Molecule 21 is a protein called 26S protease regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	M	389	Total	C	N	O	S	0	0
			3046	1914	526	589	17		

- Molecule 22 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	N	836	Total	C	N	O	S	0	0
			6508	4130	1106	1229	43		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 13.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	O	376	Total	C	N	O	S	0	0
			3020	1926	514	564	16		

- Molecule 24 is a protein called 26S proteasome non-ATPase regulatory subunit 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	P	422	Total	C	N	O	S	0	0
			3447	2185	589	651	22		

- Molecule 25 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	Q	422	Total	C	N	O	S	0	0
			3335	2116	567	639	13		

- Molecule 26 is a protein called 26S proteasome non-ATPase regulatory subunit 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	R	374	Total	C	N	O	S	0	0
			3084	1967	527	573	17		

- Molecule 27 is a protein called 26S proteasome non-ATPase regulatory subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	S	338	Total	C	N	O	S	0	0
			2757	1761	489	497	10		

- Molecule 28 is a protein called 26S proteasome non-ATPase regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	T	253	Total	C	N	O	S	0	0
			2056	1332	337	378	9		

- Molecule 29 is a protein called 26S proteasome non-ATPase regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	U	272	Total	C	N	O	S	0	0
			2183	1401	373	403	6		

- Molecule 30 is a protein called 26S proteasome non-ATPase regulatory subunit 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	V	252	Total	C	N	O	S	0	0
			1986	1261	342	366	17		

- Molecule 31 is a protein called 26S proteasome non-ATPase regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	W	185	Total	C	N	O	S	0	0
			1420	885	255	272	8		

- Molecule 32 is a protein called 26S proteasome complex subunit DSS1.

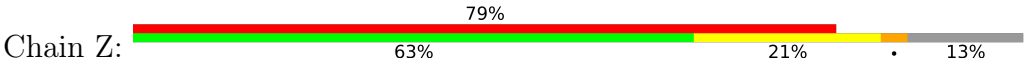
Mol	Chain	Residues	Atoms					AltConf	Trace
32	Y	21	Total	C	N	O	S	0	0
			175	106	30	38	1		

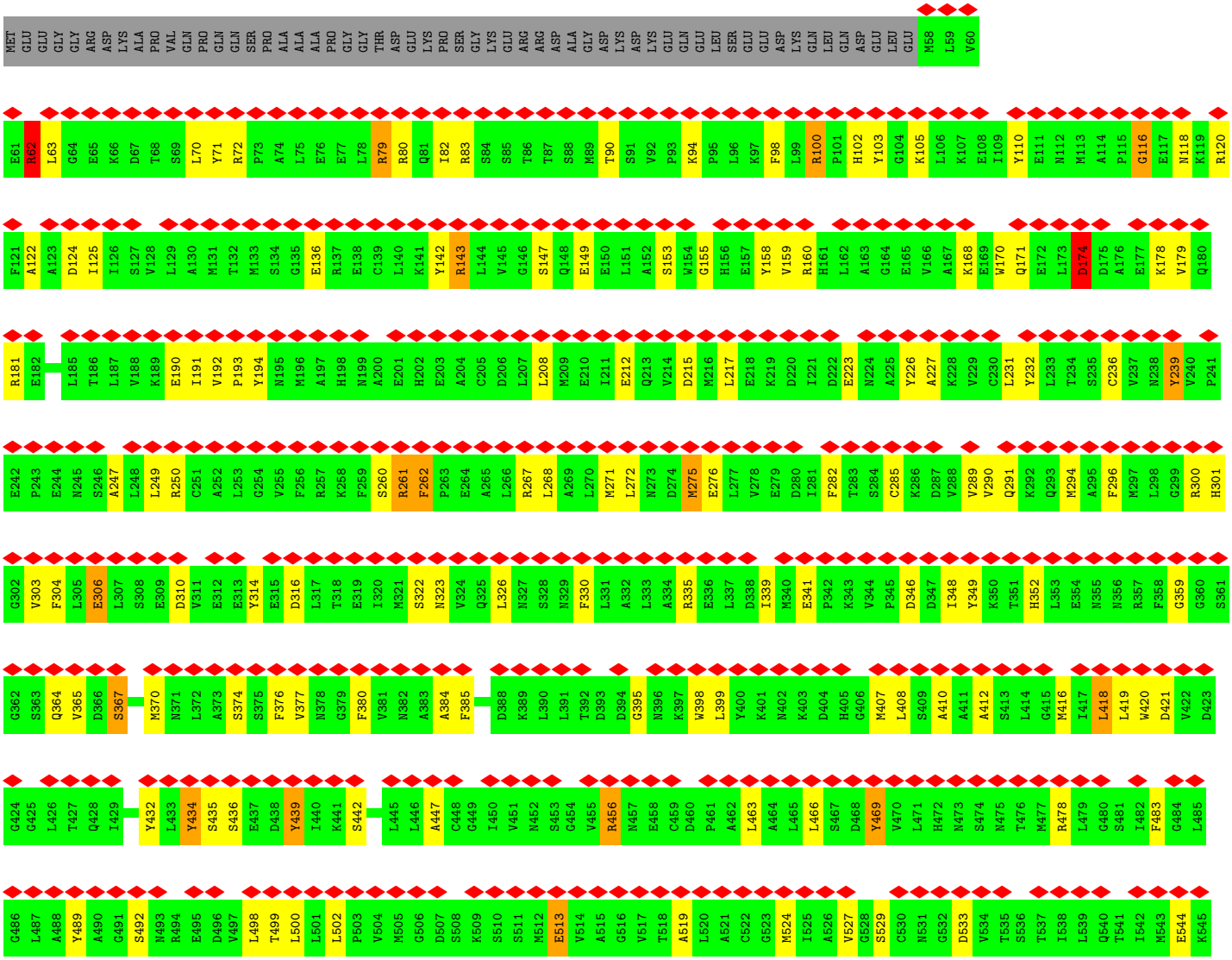
3 Residue-property plots (i)

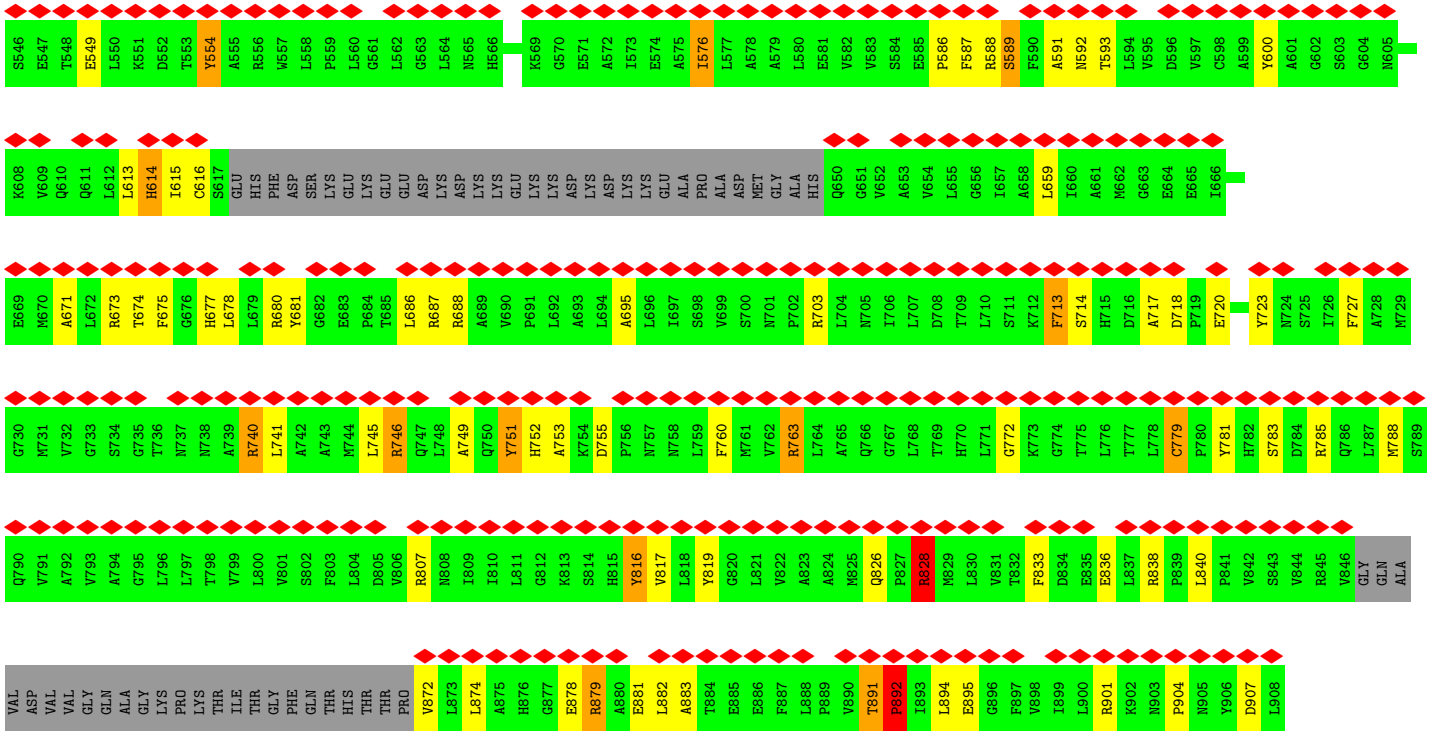
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: 26S proteasome non-ATPase regulatory subunit 2

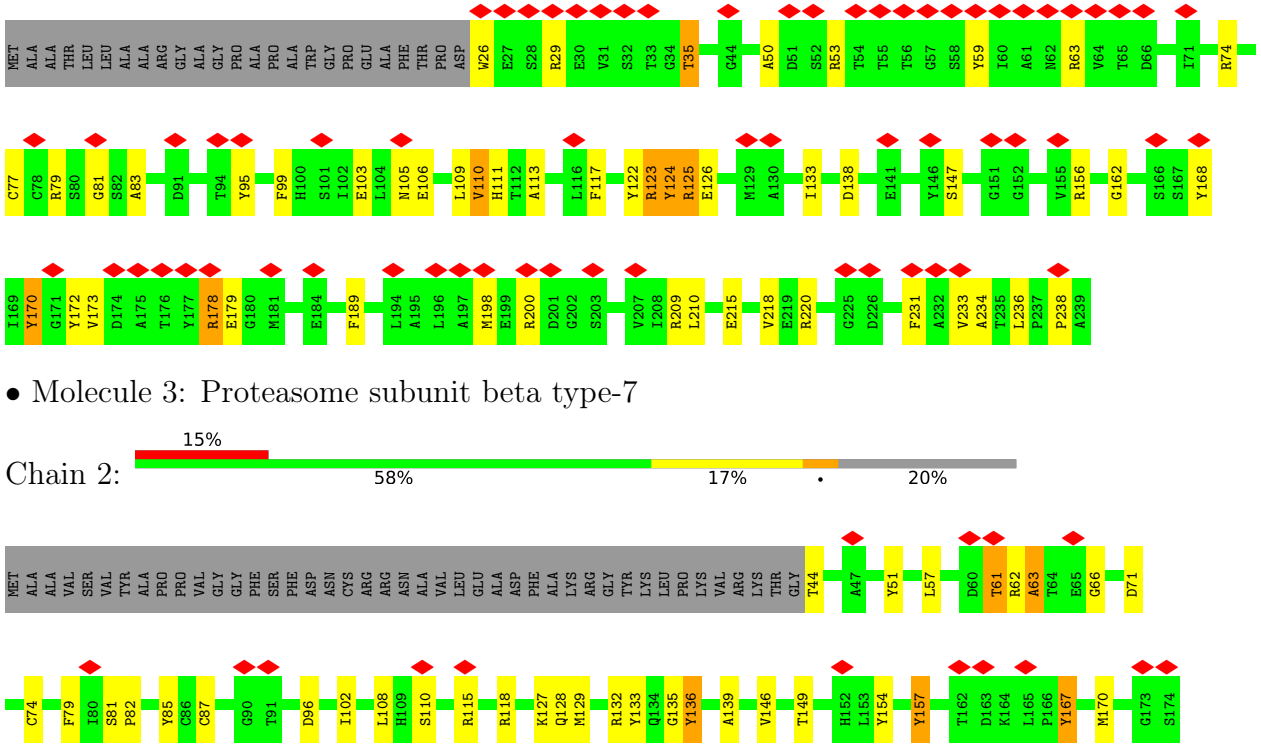
Chain Z:



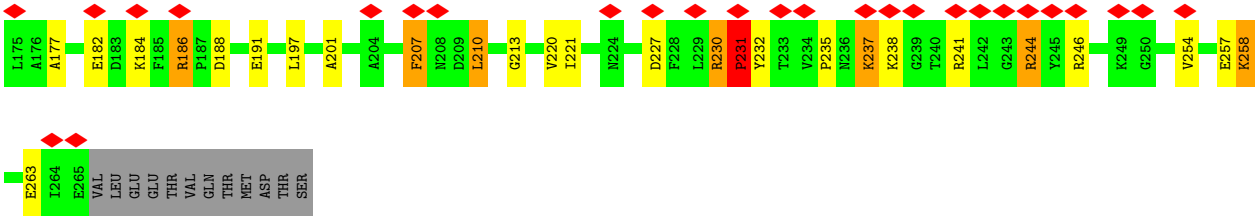




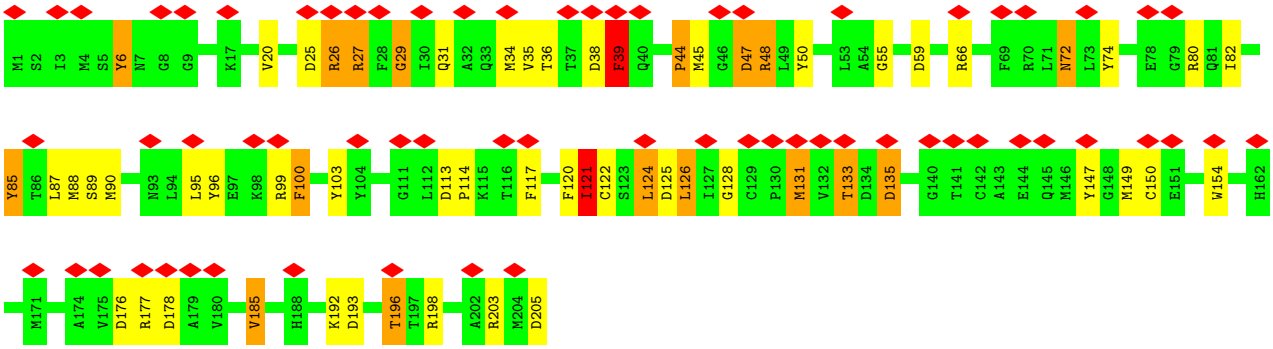
• Molecule 2: Proteasome subunit beta type-6



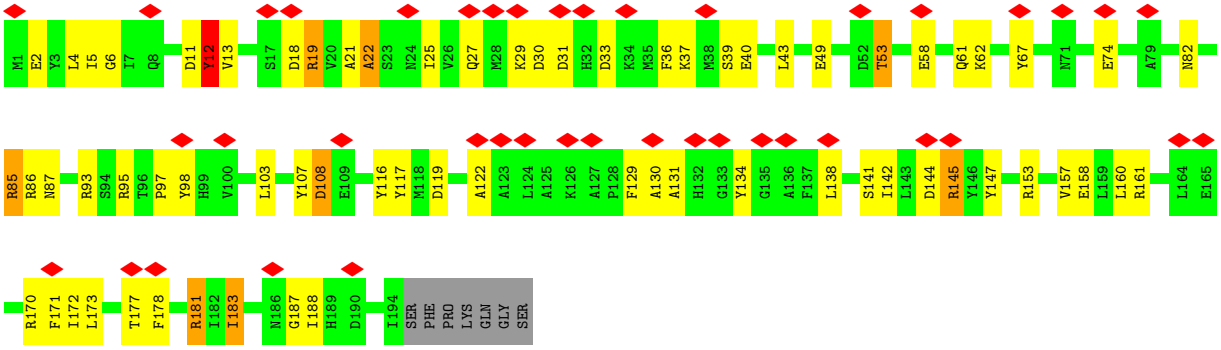
• Molecule 3: Proteasome subunit beta type-7



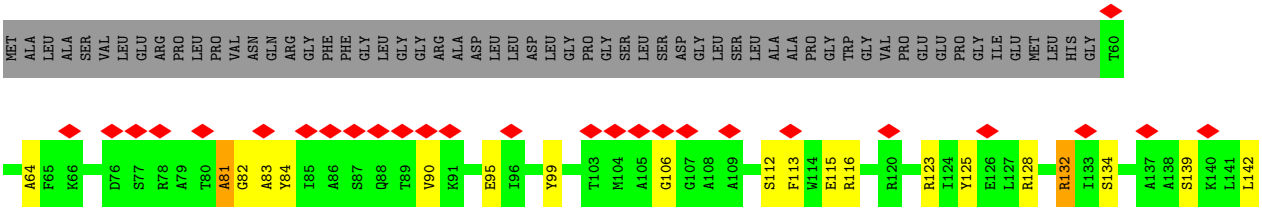
• Molecule 4: Proteasome subunit beta type-3

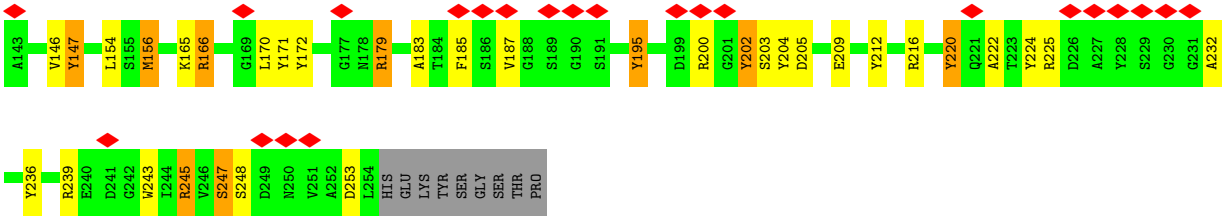


• Molecule 5: Proteasome subunit beta type-2



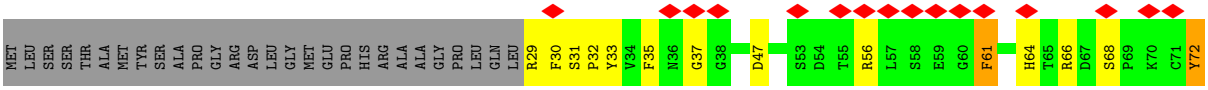
• Molecule 6: Proteasome subunit beta type-5

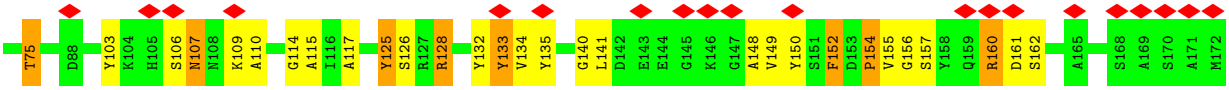


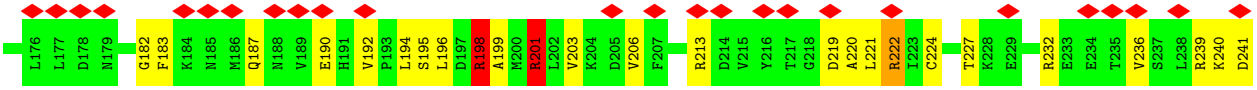


• Molecule 7: Proteasome subunit beta type-1

Chain 6:

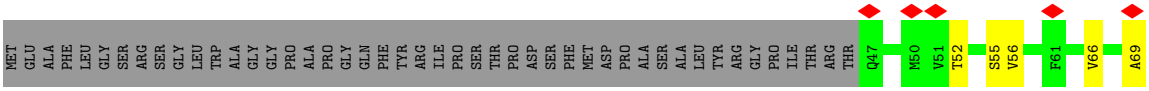


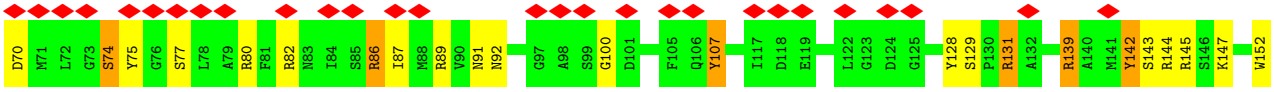


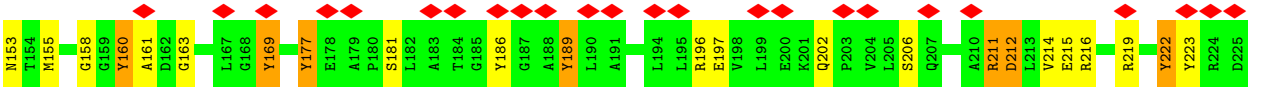


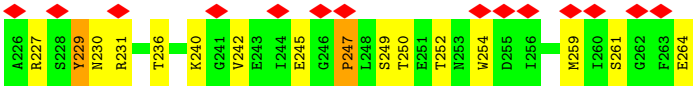
• Molecule 8: Proteasome subunit beta type-4

Chain 7:



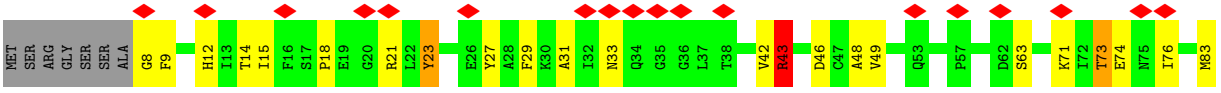


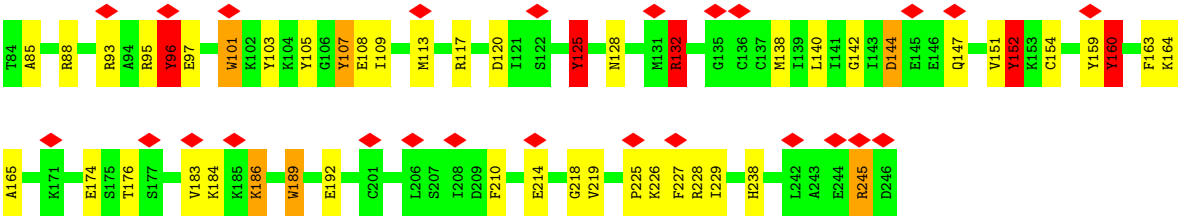




• Molecule 9: Proteasome subunit alpha type-6

Chain A:

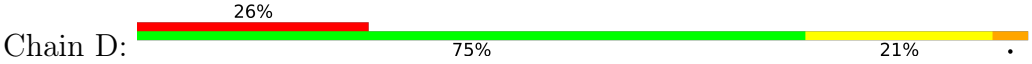


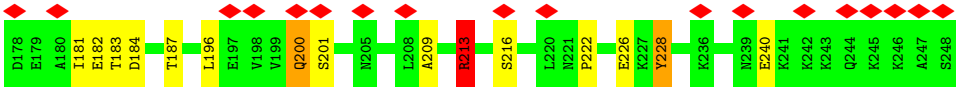


• Molecule 10: Proteasome subunit alpha type-2

• Molecule 11: Proteasome subunit alpha type-4

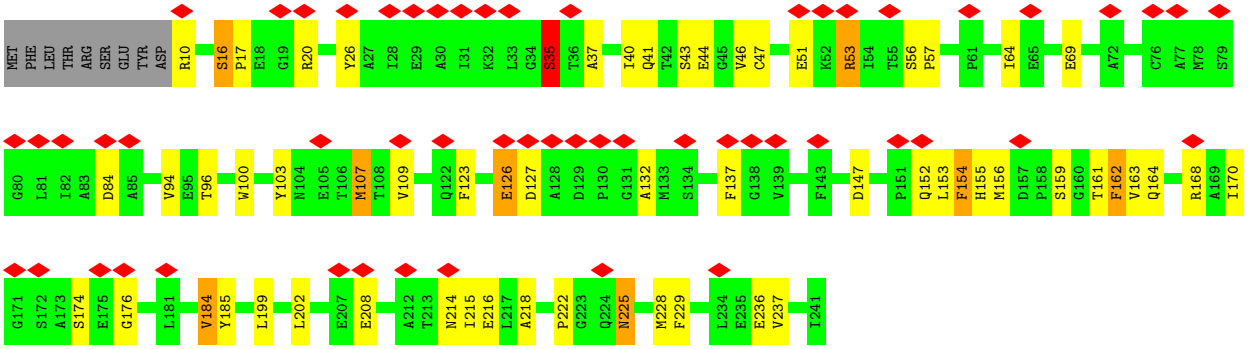
• Molecule 12: Proteasome subunit alpha type-7





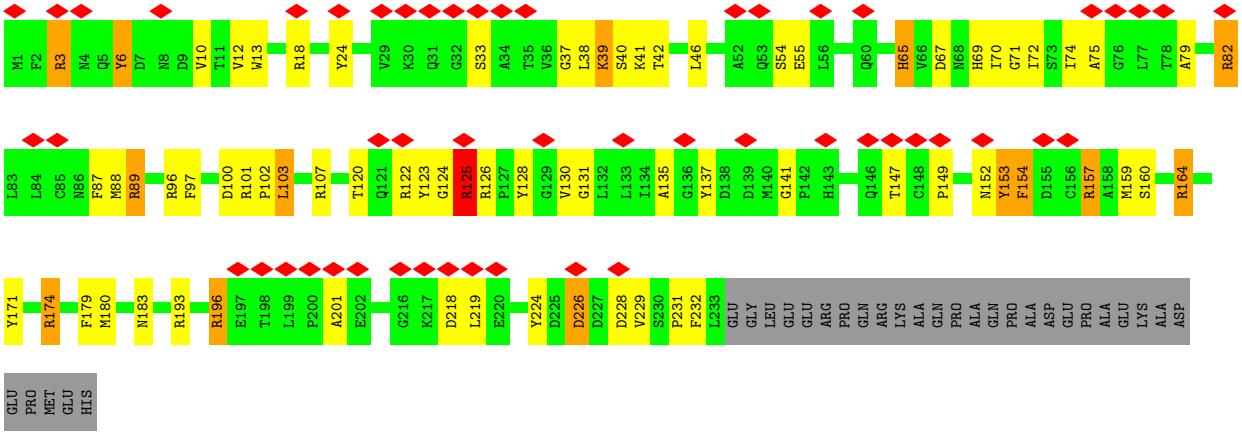
• Molecule 13: Proteasome subunit alpha type-5

Chain E:



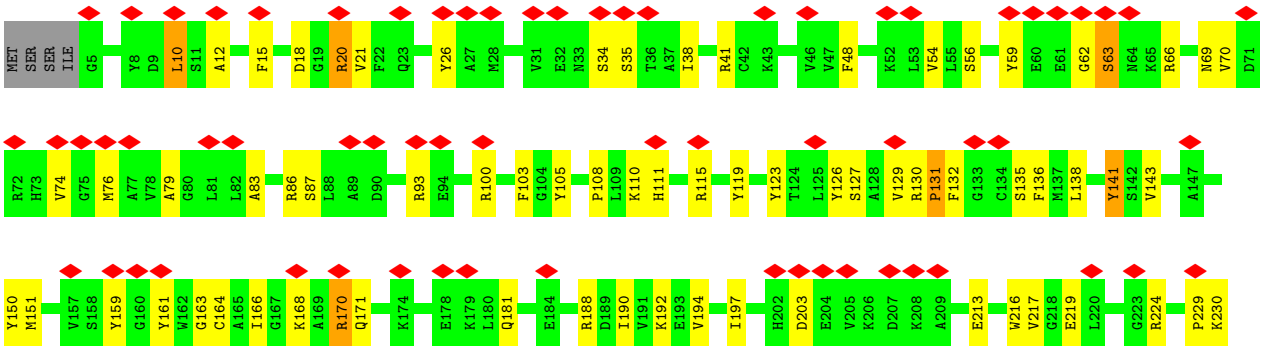
• Molecule 14: Proteasome subunit alpha type-1

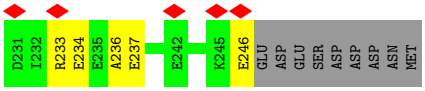
Chain F:



• Molecule 15: Proteasome subunit alpha type-3

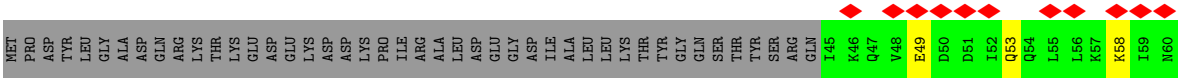
Chain G:

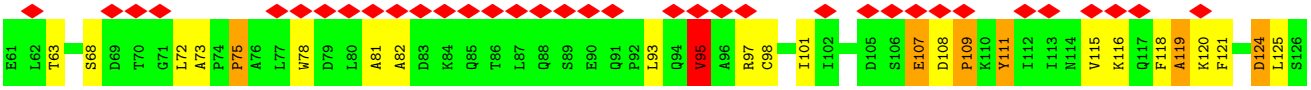


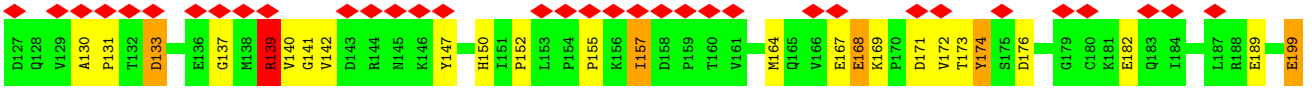


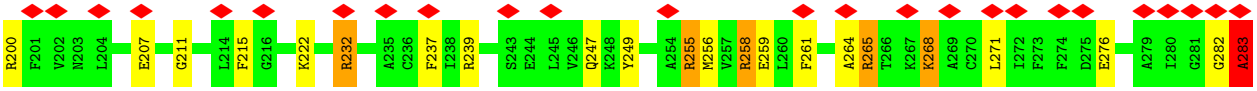
• Molecule 16: 26S protease regulatory subunit 7

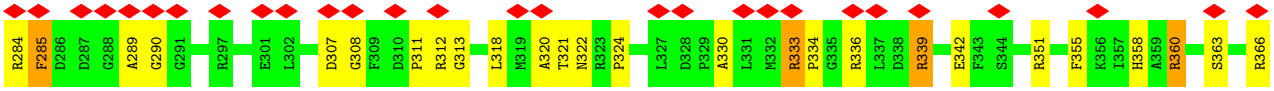
Chain H:

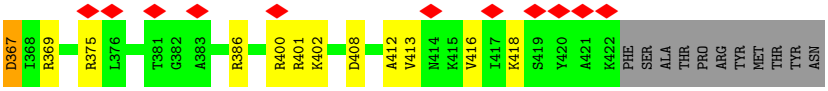






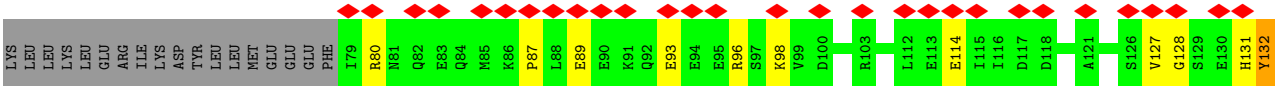


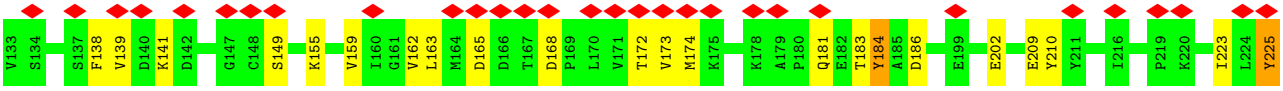


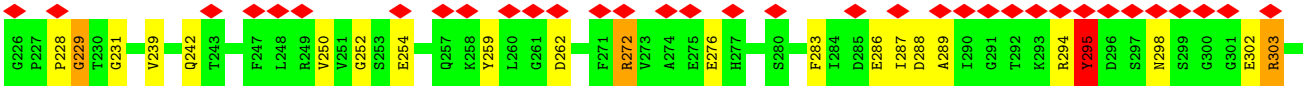


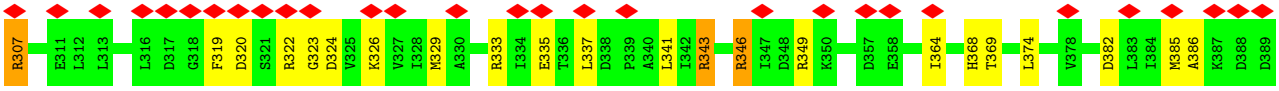
• Molecule 17: 26S protease regulatory subunit 4

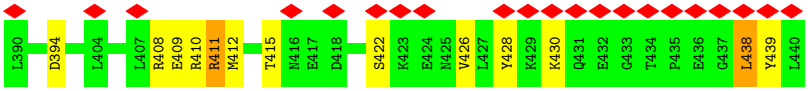
Chain I:





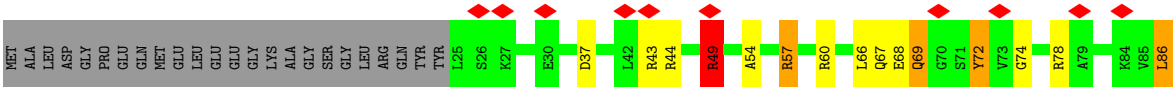


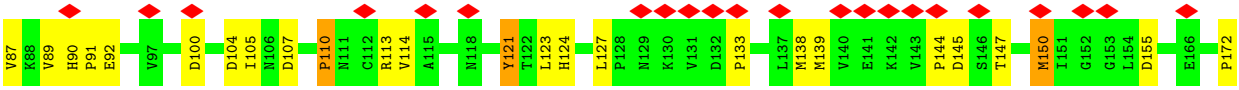


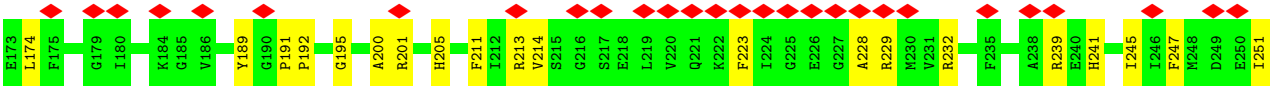


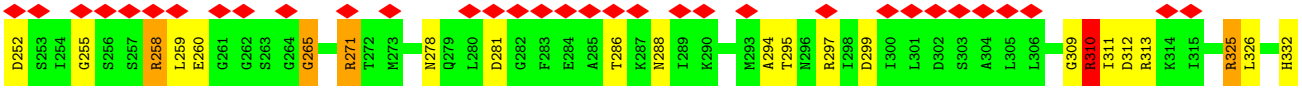
• Molecule 18: 26S protease regulatory subunit 8

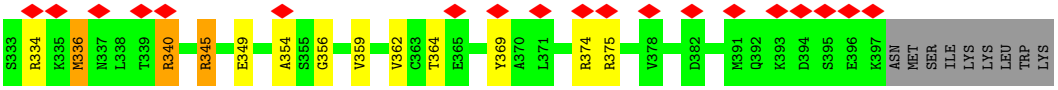
Chain J:





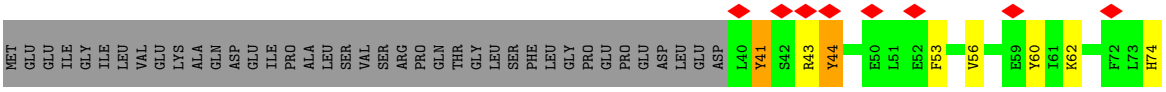


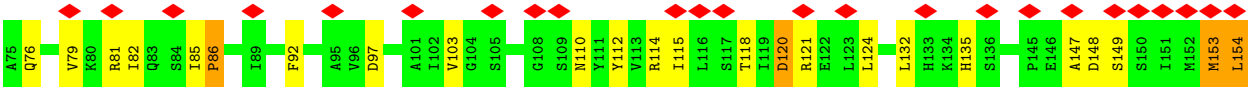


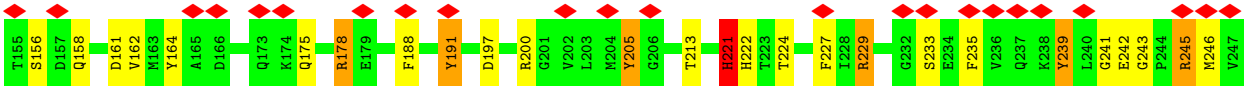


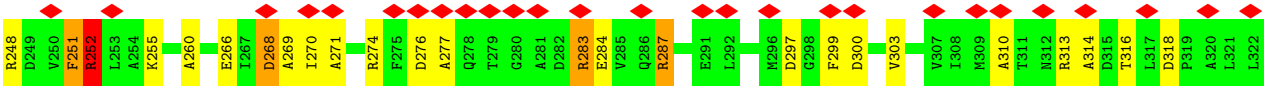
• Molecule 19: 26S protease regulatory subunit 6B

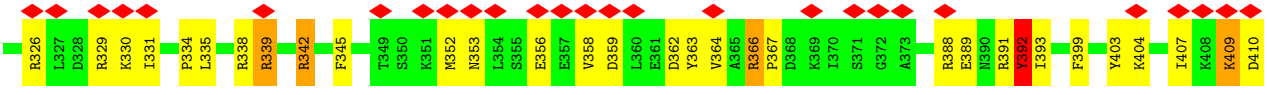
Chain K:

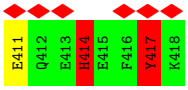






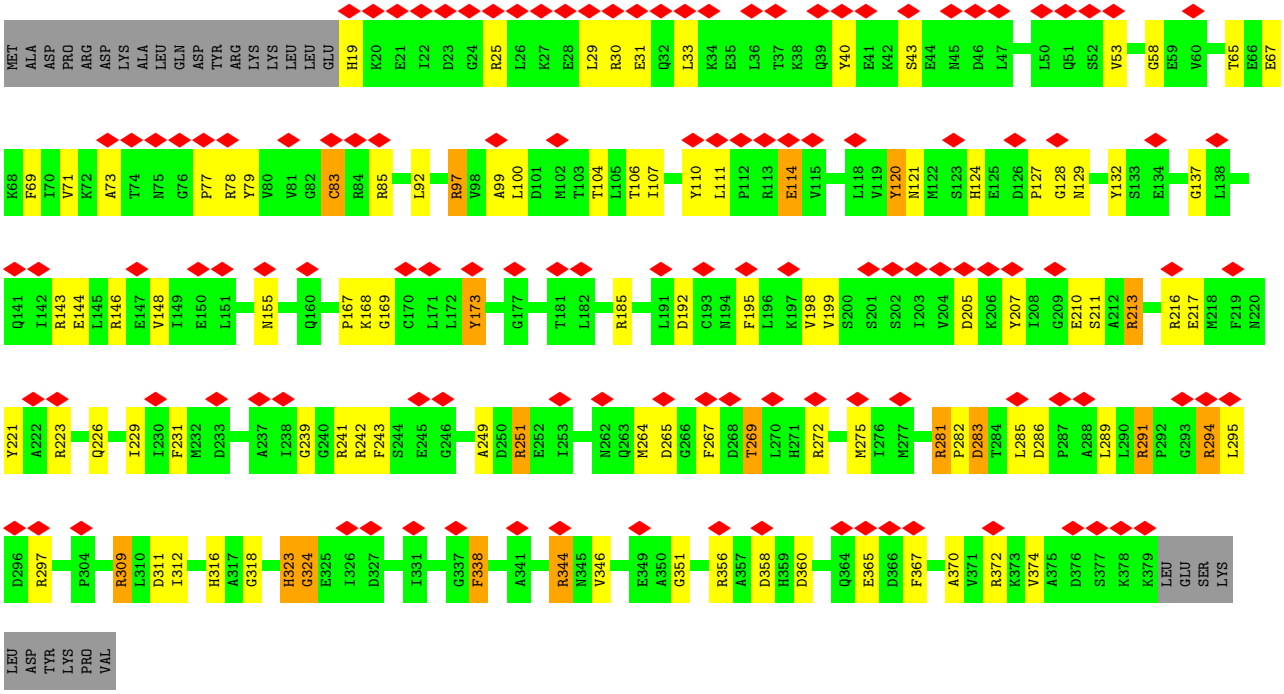






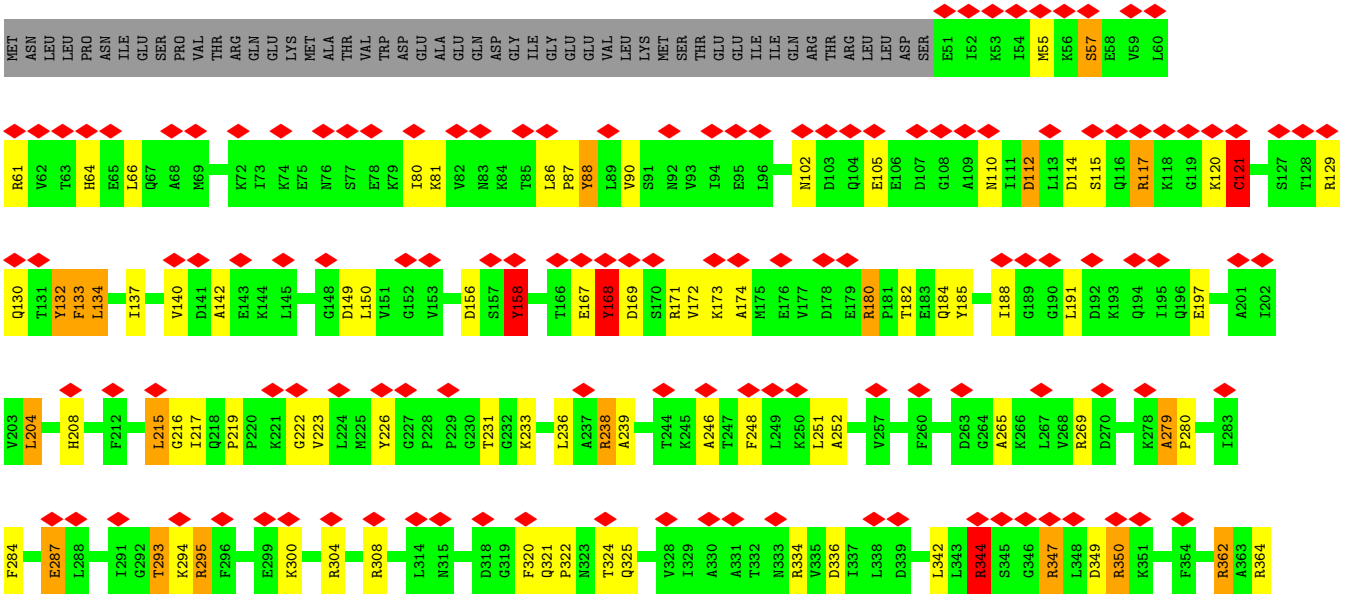
• Molecule 20: 26S protease regulatory subunit 10B

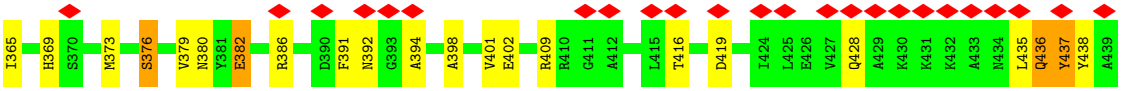
Chain L:



• Molecule 21: 26S protease regulatory subunit 6A

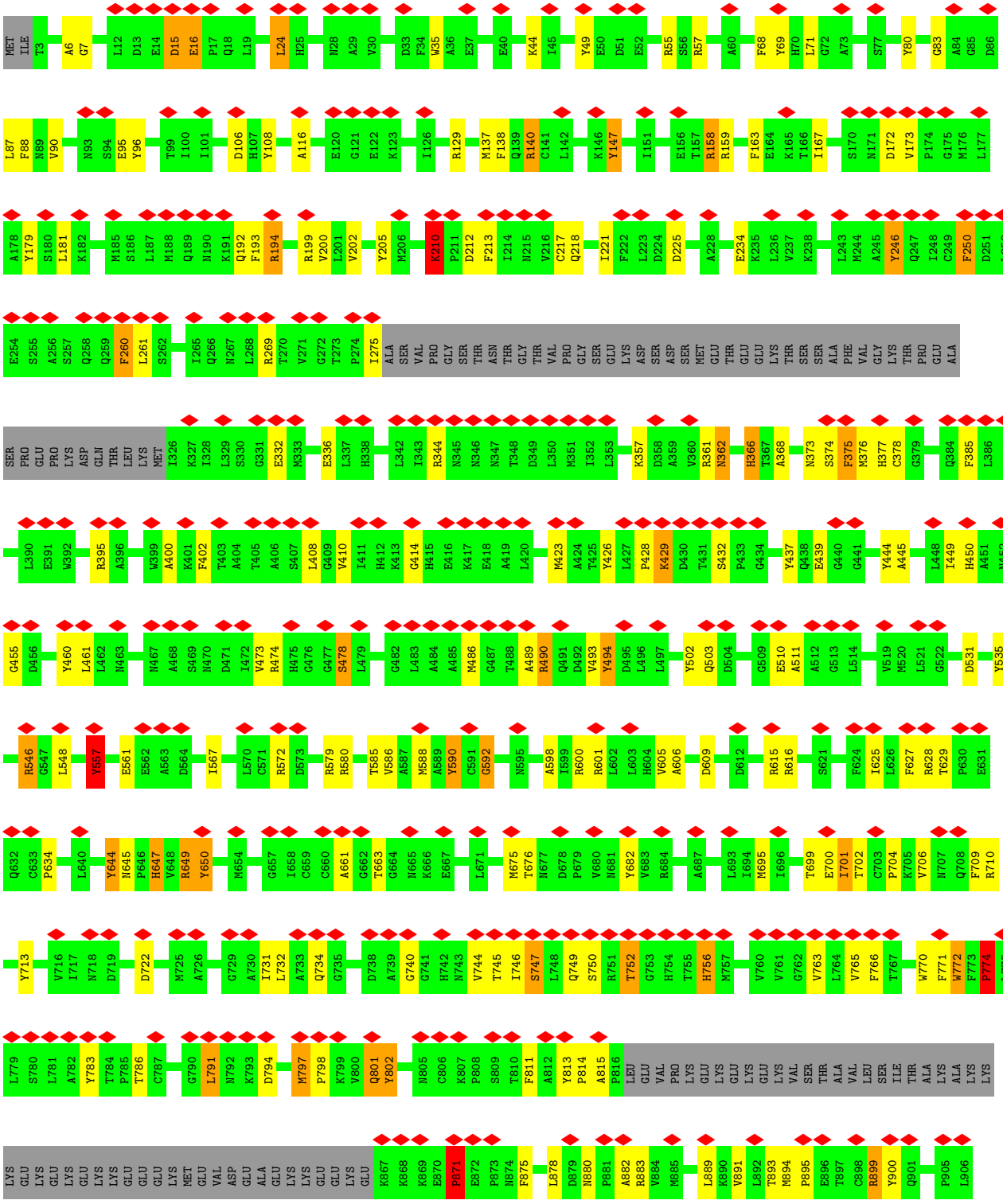
Chain M:

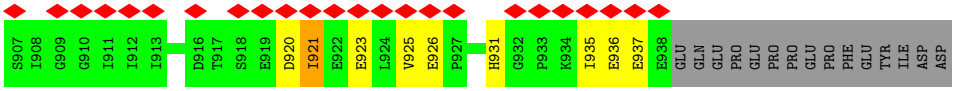




• Molecule 22: 26S proteasome non-ATPase regulatory subunit 1

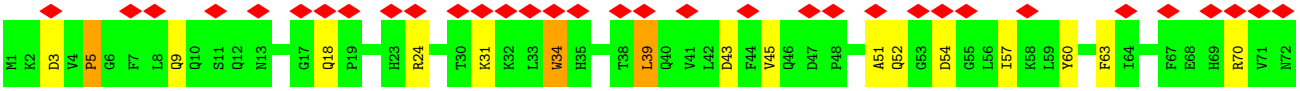
Chain N:

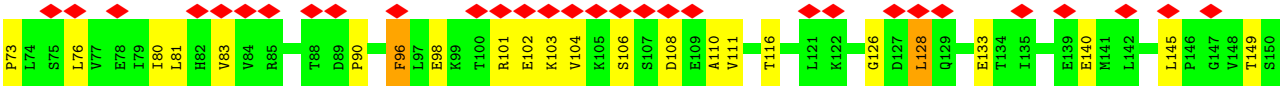


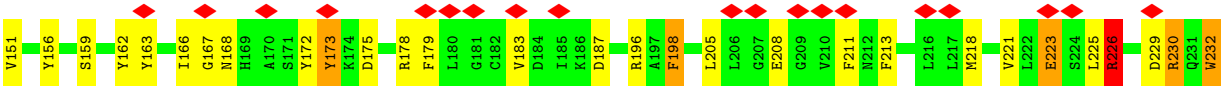


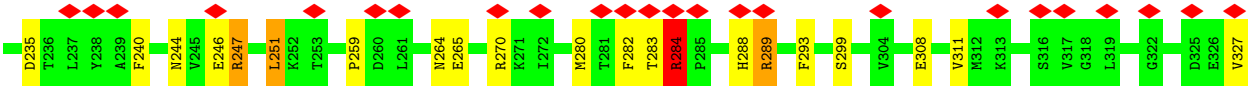
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 13

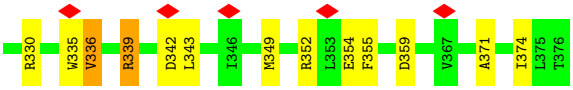
Chain O:





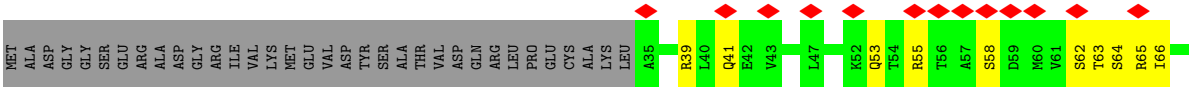


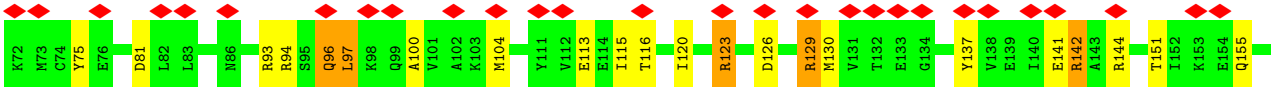


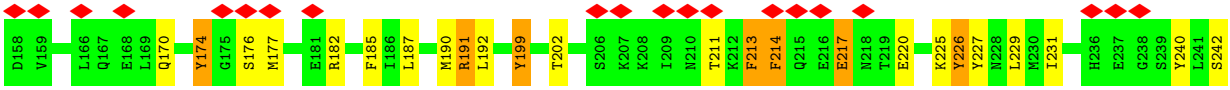


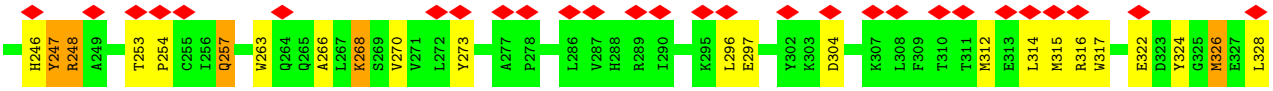
• Molecule 24: 26S proteasome non-ATPase regulatory subunit 12

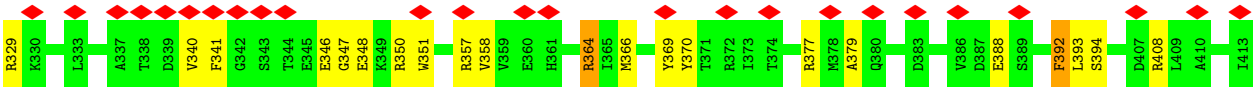
Chain P:

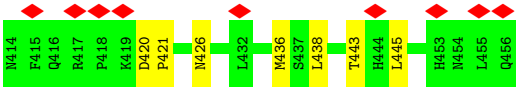






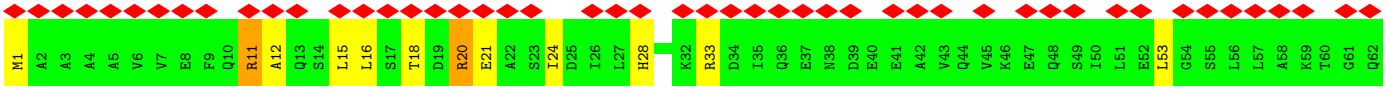


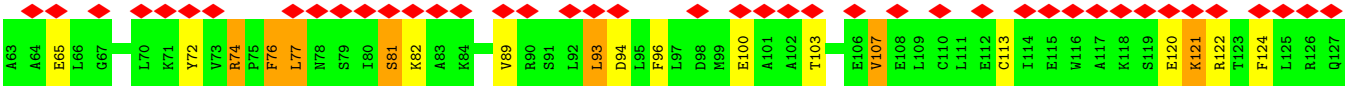


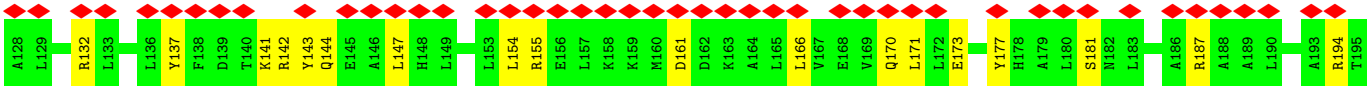


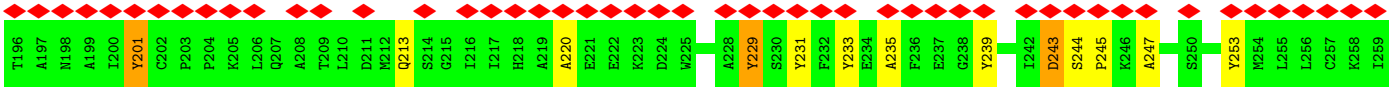
• Molecule 25: 26S proteasome non-ATPase regulatory subunit 11

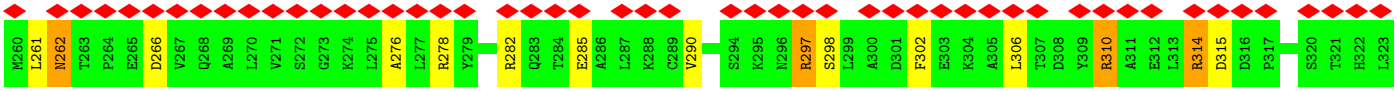
Chain Q:

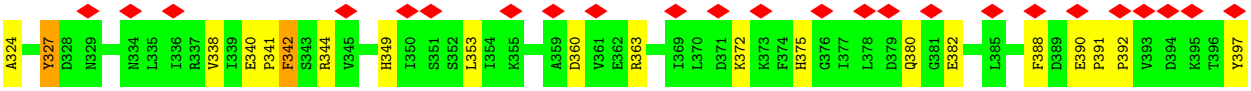


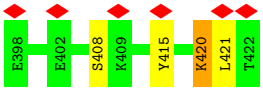






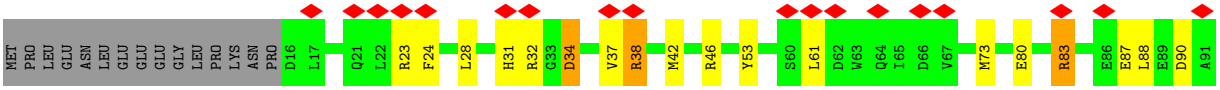


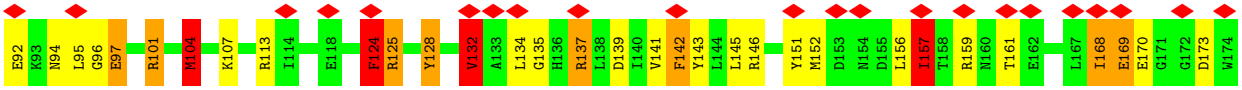


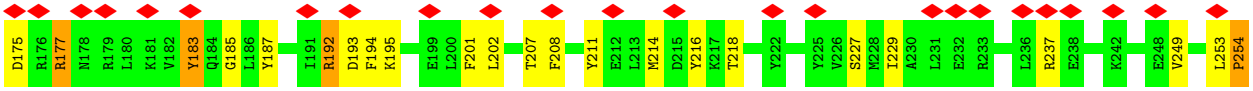


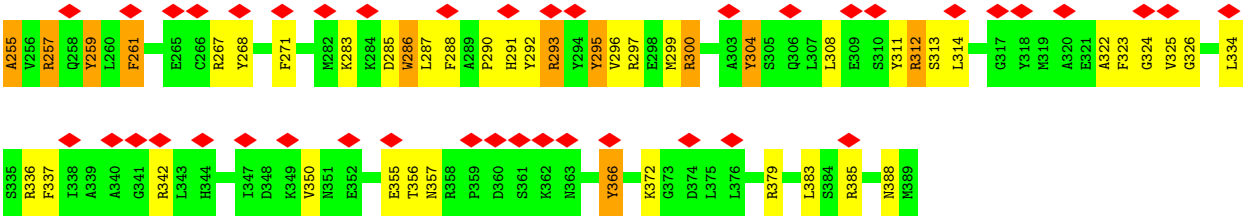
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 6

Chain R:



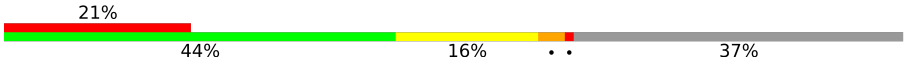


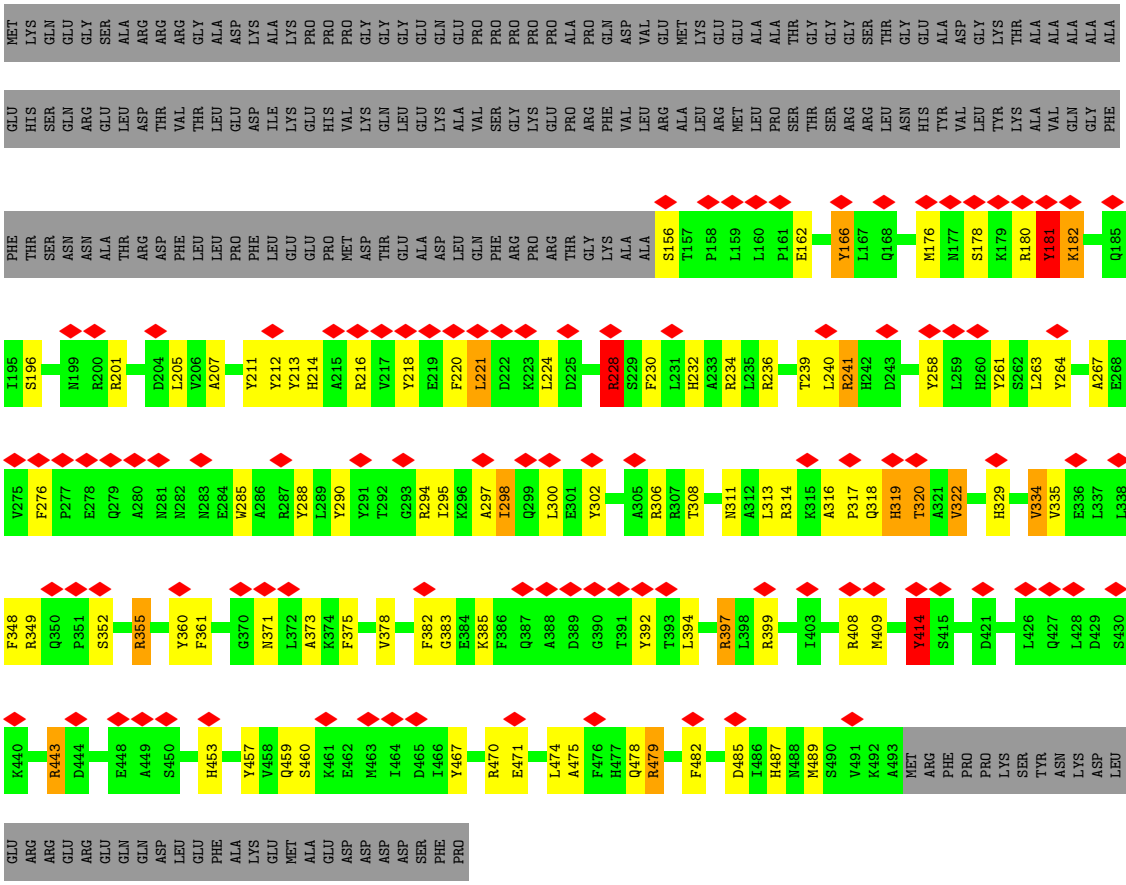




• Molecule 27: 26S proteasome non-ATPase regulatory subunit 3

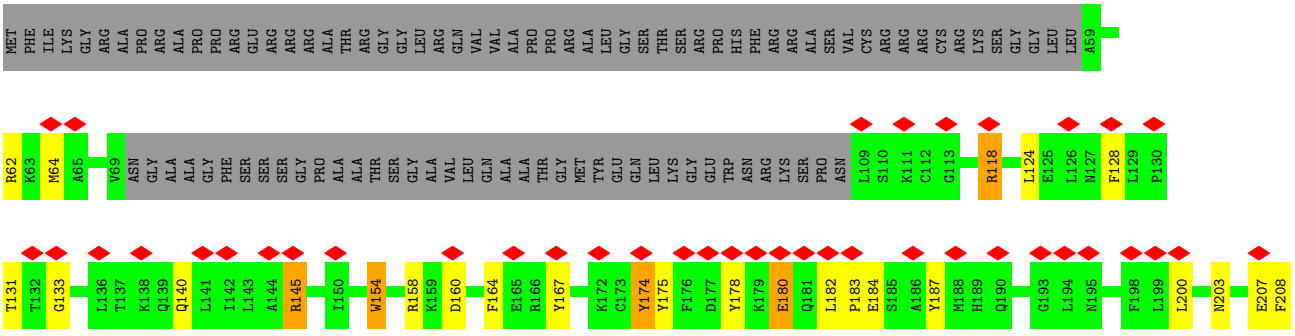
Chain S:

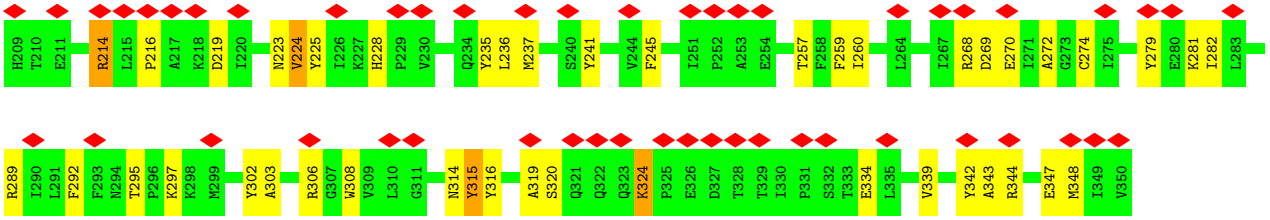




• Molecule 28: 26S proteasome non-ATPase regulatory subunit 8

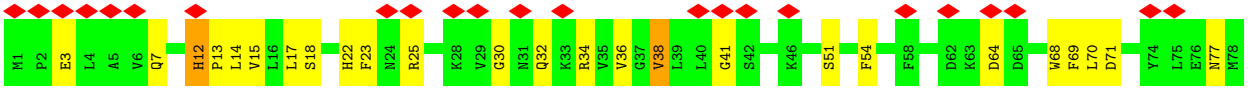
Chain T:

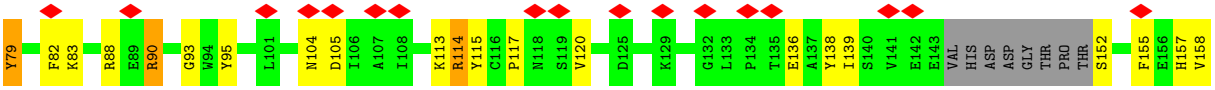


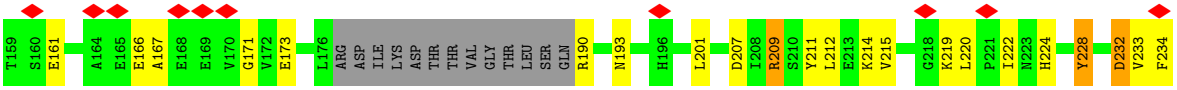


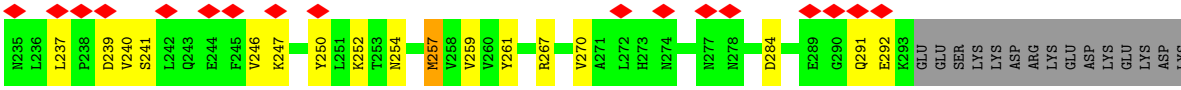
• Molecule 29: 26S proteasome non-ATPase regulatory subunit 7

Chain U:



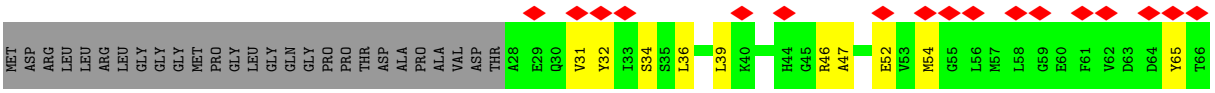


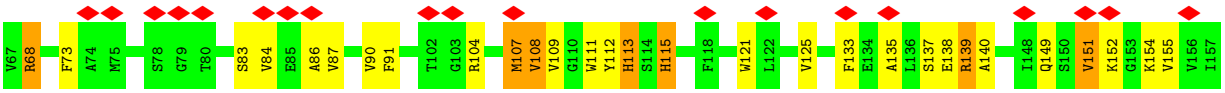


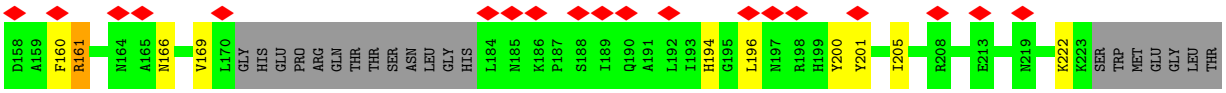


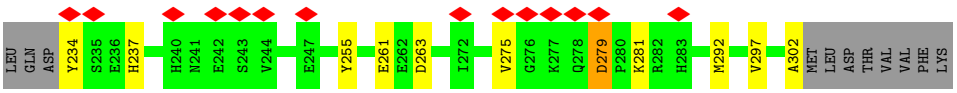
• Molecule 30: 26S proteasome non-ATPase regulatory subunit 14

Chain V:



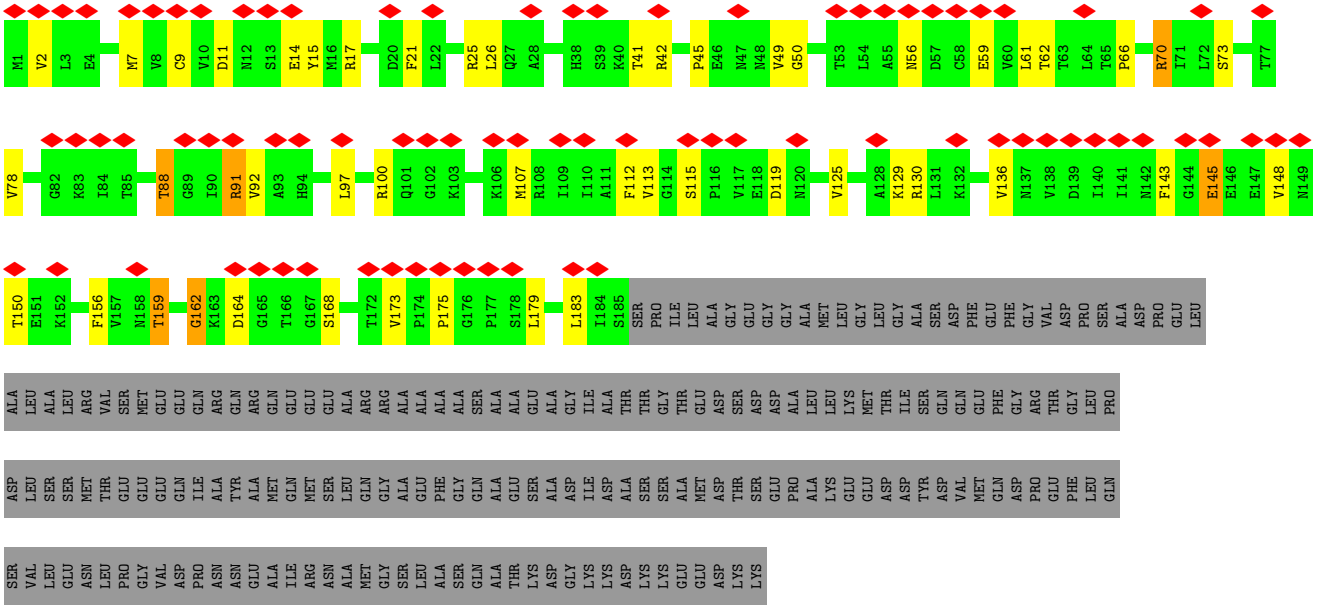




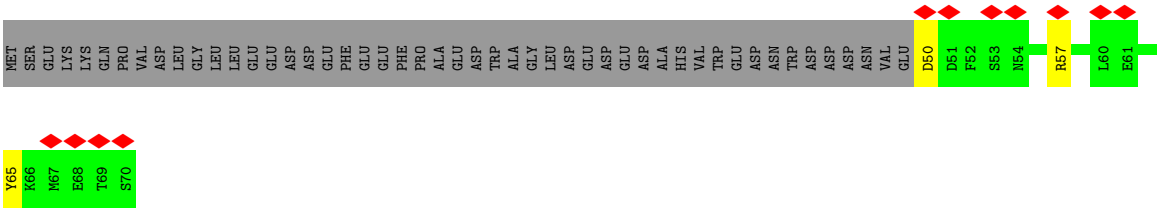


• Molecule 31: 26S proteasome non-ATPase regulatory subunit 4

Chain W:



• Molecule 32: 26S proteasome complex subunit DSS1



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	252000	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)	800	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	Not provided	
Image detector	FEI FALCON II (4k x 4k)	Depositor
Maximum map value	0.549	Depositor
Minimum map value	-0.463	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.012	Depositor
Recommended contour level	0.088	Depositor
Map size (Å)	604.80005, 604.80005, 604.80005	wwPDB
Map dimensions	280, 280, 280	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.16, 2.16, 2.16	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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	Z	1.76	67/6249 (1.1%)	1.95	133/8457 (1.6%)
2	1	1.75	14/1637 (0.9%)	2.09	42/2218 (1.9%)
3	2	1.79	25/1703 (1.5%)	2.03	49/2305 (2.1%)
4	3	1.73	15/1628 (0.9%)	2.01	47/2194 (2.1%)
5	4	1.82	15/1585 (0.9%)	2.03	51/2144 (2.4%)
6	5	1.81	17/1538 (1.1%)	2.05	44/2078 (2.1%)
7	6	1.80	24/1684 (1.4%)	2.04	42/2268 (1.9%)
8	7	1.77	25/1739 (1.4%)	2.03	56/2351 (2.4%)
9	A	1.76	24/1908 (1.3%)	1.95	45/2578 (1.7%)
10	B	1.78	17/1865 (0.9%)	2.06	61/2524 (2.4%)
11	C	1.74	14/2099 (0.7%)	1.97	50/2818 (1.8%)
12	D	1.78	24/1987 (1.2%)	2.01	51/2673 (1.9%)
13	E	1.70	14/1797 (0.8%)	1.91	40/2426 (1.6%)
14	F	1.79	24/1872 (1.3%)	2.06	60/2529 (2.4%)
15	G	1.79	18/1929 (0.9%)	2.03	51/2597 (2.0%)
16	H	1.73	32/3009 (1.1%)	1.87	51/4061 (1.3%)
17	I	1.70	24/2881 (0.8%)	1.89	54/3887 (1.4%)
18	J	1.74	24/2966 (0.8%)	1.94	67/3989 (1.7%)
19	K	1.75	32/3082 (1.0%)	1.99	91/4157 (2.2%)
20	L	1.74	27/2906 (0.9%)	1.96	74/3913 (1.9%)
21	M	1.72	27/3087 (0.9%)	1.95	77/4160 (1.9%)
22	N	1.73	66/6626 (1.0%)	1.92	154/8970 (1.7%)
23	O	1.72	29/3078 (0.9%)	1.93	57/4165 (1.4%)
24	P	1.71	32/3493 (0.9%)	1.96	75/4696 (1.6%)
25	Q	1.71	25/3381 (0.7%)	1.91	74/4558 (1.6%)
26	R	1.79	34/3140 (1.1%)	2.06	86/4228 (2.0%)
27	S	1.79	30/2808 (1.1%)	2.02	78/3791 (2.1%)
28	T	1.72	20/2097 (1.0%)	1.90	50/2830 (1.8%)
29	U	1.71	17/2223 (0.8%)	1.93	59/3006 (2.0%)
30	V	1.65	10/2020 (0.5%)	1.85	40/2724 (1.5%)
31	W	1.70	11/1439 (0.8%)	1.89	28/1947 (1.4%)
32	Y	1.81	2/177 (1.1%)	1.79	2/233 (0.9%)
All	All	1.74	779/79633 (1.0%)	1.96	1939/107475 (1.8%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	Z	0	19
2	1	0	3
3	2	0	5
4	3	0	3
5	4	0	7
6	5	0	6
7	6	0	9
8	7	0	9
9	A	0	10
10	B	0	3
11	C	0	9
12	D	0	5
14	F	0	8
15	G	0	4
16	H	1	12
17	I	0	5
18	J	0	10
19	K	0	19
20	L	0	11
21	M	0	12
22	N	1	16
23	O	0	8
24	P	0	13
25	Q	0	12
26	R	0	18
27	S	0	11
28	T	0	8
29	U	0	7
30	V	0	3
31	W	0	3
32	Y	0	1
All	All	2	269

All (779) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	174	SER	CA-CB	9.23	1.66	1.52
7	6	222	ARG	NE-CZ	9.11	1.44	1.33
22	N	7	GLY	CA-C	-9.01	1.37	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	114	ARG	NE-CZ	8.96	1.44	1.33
15	G	130	ARG	NE-CZ	8.86	1.44	1.33
6	5	195	TYR	CE1-CZ	8.57	1.49	1.38
28	T	279	TYR	CE2-CZ	8.54	1.49	1.38
3	2	191	GLU	CG-CD	8.49	1.64	1.51
25	Q	392	PRO	N-CD	-8.38	1.36	1.47
26	R	304	TYR	CE2-CZ	8.36	1.49	1.38
16	H	68	SER	CA-CB	8.28	1.65	1.52
3	2	132	ARG	CZ-NH2	8.10	1.43	1.33
12	D	226	GLU	CG-CD	8.06	1.64	1.51
17	I	303	ARG	NE-CZ	8.01	1.43	1.33
7	6	31	SER	CA-CB	7.96	1.64	1.52
27	S	479	ARG	CZ-NH2	7.92	1.43	1.33
26	R	183	TYR	CB-CG	-7.86	1.39	1.51
26	R	192	ARG	NE-CZ	7.86	1.43	1.33
14	F	3	ARG	NE-CZ	7.84	1.43	1.33
3	2	110	SER	CA-CB	7.83	1.64	1.52
19	K	389	GLU	CG-CD	7.74	1.63	1.51
29	U	88	ARG	CZ-NH2	7.69	1.43	1.33
9	A	21	ARG	NE-CZ	7.69	1.43	1.33
10	B	91	ARG	CZ-NH2	7.68	1.43	1.33
25	Q	33	ARG	NE-CZ	7.60	1.43	1.33
8	7	189	TYR	CE2-CZ	7.58	1.48	1.38
1	Z	589	SER	CA-CB	7.53	1.64	1.52
27	S	408	ARG	NE-CZ	7.50	1.42	1.33
15	G	48	PHE	CG-CD1	7.49	1.50	1.38
17	I	294	ARG	CZ-NH1	7.48	1.42	1.33
4	3	177	ARG	CZ-NH2	7.43	1.42	1.33
22	N	205	TYR	CG-CD2	7.42	1.48	1.39
19	K	326	ARG	NE-CZ	7.40	1.42	1.33
1	Z	335	ARG	NE-CZ	7.39	1.42	1.33
19	K	329	ARG	CZ-NH2	7.38	1.42	1.33
31	W	130	ARG	NE-CZ	7.34	1.42	1.33
21	M	61	ARG	CZ-NH2	7.34	1.42	1.33
1	Z	687	ARG	CZ-NH2	7.33	1.42	1.33
24	P	247	TYR	CG-CD2	-7.32	1.29	1.39
20	L	43	SER	CA-CB	7.24	1.63	1.52
25	Q	278	ARG	NE-CZ	7.24	1.42	1.33
13	E	185	TYR	CG-CD2	7.22	1.48	1.39
14	F	18	ARG	CZ-NH2	7.22	1.42	1.33
12	D	213	ARG	CZ-NH1	7.20	1.42	1.33
30	V	160	PHE	CE2-CZ	7.20	1.51	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	23	ARG	CD-NE	7.18	1.58	1.46
22	N	616	ARG	CZ-NH2	7.18	1.42	1.33
26	R	38	ARG	CZ-NH1	7.16	1.42	1.33
3	2	186	ARG	CZ-NH2	7.16	1.42	1.33
24	P	144	ARG	CZ-NH2	7.16	1.42	1.33
27	S	272	SER	CA-CB	7.16	1.63	1.52
23	O	339	ARG	CD-NE	7.14	1.58	1.46
24	P	247	TYR	CE2-CZ	7.13	1.47	1.38
1	Z	819	TYR	CG-CD1	7.12	1.48	1.39
31	W	42	ARG	NE-CZ	7.09	1.42	1.33
16	H	199	GLU	CD-OE1	7.06	1.33	1.25
10	B	131	GLY	N-CA	-7.04	1.35	1.46
1	Z	232	TYR	CG-CD2	7.03	1.48	1.39
1	Z	720	GLU	CG-CD	7.03	1.62	1.51
16	H	174	TYR	CG-CD2	7.02	1.48	1.39
9	A	152	TYR	CE1-CZ	6.98	1.47	1.38
18	J	74	GLY	CA-C	-6.97	1.40	1.51
12	D	21	TYR	CE2-CZ	6.97	1.47	1.38
21	M	129	ARG	NE-CZ	6.96	1.42	1.33
3	2	232	TYR	CE2-CZ	6.96	1.47	1.38
1	Z	763	ARG	CD-NE	6.93	1.58	1.46
10	B	121	TYR	CB-CG	6.93	1.62	1.51
10	B	217	GLY	N-CA	-6.91	1.35	1.46
24	P	142	ARG	CZ-NH1	6.90	1.42	1.33
16	H	97	ARG	NE-CZ	6.89	1.42	1.33
8	7	142	TYR	CE2-CZ	6.88	1.47	1.38
25	Q	20	ARG	CZ-NH1	6.81	1.42	1.33
11	C	5	TYR	CE1-CZ	6.80	1.47	1.38
4	3	26	ARG	NE-CZ	6.80	1.41	1.33
4	3	89	SER	CA-CB	6.80	1.63	1.52
21	M	364	ARG	CD-NE	6.80	1.58	1.46
21	M	402	GLU	CG-CD	-6.78	1.41	1.51
28	T	154	TRP	CG-CD2	6.78	1.55	1.43
18	J	229	ARG	CZ-NH2	6.75	1.41	1.33
8	7	222	TYR	CZ-OH	6.74	1.49	1.37
8	7	222	TYR	CE2-CZ	6.74	1.47	1.38
1	Z	116	GLY	CA-C	-6.74	1.41	1.51
12	D	182	GLU	CG-CD	6.74	1.62	1.51
29	U	90	ARG	CD-NE	6.72	1.57	1.46
5	4	187	GLY	CA-C	-6.70	1.41	1.51
26	R	101	ARG	CD-NE	6.70	1.57	1.46
9	A	117	ARG	CZ-NH2	6.70	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	239	ARG	CZ-NH2	6.69	1.41	1.33
26	R	326	GLY	CA-C	-6.69	1.41	1.51
5	4	58	GLU	CD-OE1	6.68	1.32	1.25
19	K	362	ASP	CB-CG	6.67	1.65	1.51
20	L	297	ARG	CD-NE	6.67	1.57	1.46
9	A	8	GLY	CA-C	-6.66	1.41	1.51
19	K	287	ARG	CZ-NH1	6.66	1.41	1.33
28	T	145	ARG	CZ-NH1	6.65	1.41	1.33
1	Z	680	ARG	CD-NE	6.63	1.57	1.46
12	D	109	ARG	NE-CZ	6.63	1.41	1.33
14	F	71	GLY	CA-C	-6.61	1.41	1.51
22	N	147	TYR	CG-CD2	6.60	1.47	1.39
2	1	74	ARG	CZ-NH2	6.60	1.41	1.33
21	M	61	ARG	CD-NE	6.60	1.57	1.46
1	Z	194	TYR	CG-CD2	6.60	1.47	1.39
12	D	142	PRO	N-CA	-6.60	1.36	1.47
16	H	167	GLU	CD-OE1	6.59	1.32	1.25
22	N	494	TYR	CZ-OH	6.59	1.49	1.37
6	5	116	ARG	CZ-NH2	6.58	1.41	1.33
19	K	245	ARG	CZ-NH2	6.57	1.41	1.33
9	A	210	PHE	CG-CD2	6.55	1.48	1.38
6	5	216	ARG	CZ-NH2	6.53	1.41	1.33
20	L	291	ARG	CZ-NH1	6.52	1.41	1.33
17	I	184	TYR	CE1-CZ	6.51	1.47	1.38
7	6	33	TYR	CZ-OH	6.51	1.49	1.37
26	R	342	ARG	NE-CZ	6.50	1.41	1.33
8	7	215	GLU	CD-OE2	-6.49	1.18	1.25
22	N	490	ARG	NE-CZ	6.47	1.41	1.33
7	6	222	ARG	CD-NE	6.46	1.57	1.46
16	H	401	ARG	CZ-NH2	6.46	1.41	1.33
15	G	119	TYR	CE1-CZ	6.46	1.47	1.38
16	H	155	PRO	N-CD	-6.46	1.38	1.47
2	1	123	ARG	CZ-NH2	6.45	1.41	1.33
8	7	197	GLU	CG-CD	6.44	1.61	1.51
16	H	139	ARG	NE-CZ	6.43	1.41	1.33
26	R	312	ARG	CZ-NH2	6.42	1.41	1.33
18	J	239	ARG	CD-NE	6.41	1.57	1.46
20	L	231	PHE	CG-CD2	6.41	1.48	1.38
17	I	283	PHE	CG-CD2	6.40	1.48	1.38
1	Z	79	ARG	NE-CZ	6.40	1.41	1.33
11	C	226	ARG	CD-NE	6.39	1.57	1.46
21	M	438	TYR	CE2-CZ	6.39	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
16	H	255	ARG	CZ-NH1	6.37	1.41	1.33
7	6	162	SER	CA-CB	6.35	1.62	1.52
28	T	167	TYR	CG-CD2	6.35	1.47	1.39
10	B	6	TYR	CE1-CZ	6.35	1.46	1.38
28	T	214	ARG	CD-NE	6.34	1.57	1.46
2	1	231	PHE	CE2-CZ	6.34	1.49	1.37
21	M	344	ARG	NE-CZ	6.33	1.41	1.33
11	C	128	ARG	NE-CZ	6.33	1.41	1.33
1	Z	143	ARG	NE-CZ	6.32	1.41	1.33
1	Z	751	TYR	CG-CD2	6.31	1.47	1.39
8	7	142	TYR	CG-CD2	6.29	1.47	1.39
1	Z	170	TRP	NE1-CE2	6.29	1.45	1.37
20	L	281	ARG	CZ-NH2	6.29	1.41	1.33
1	Z	456	ARG	CD-NE	6.28	1.57	1.46
20	L	114	GLU	CD-OE1	6.28	1.32	1.25
29	U	171	GLY	CA-C	-6.28	1.41	1.51
14	F	101	ARG	CZ-NH2	6.27	1.41	1.33
17	I	184	TYR	CD2-CE2	6.27	1.48	1.39
19	K	114	ARG	CZ-NH1	6.26	1.41	1.33
1	Z	398	TRP	CE3-CZ3	6.26	1.49	1.38
18	J	345	ARG	CD-NE	6.26	1.57	1.46
30	V	46	ARG	NE-CZ	6.26	1.41	1.33
25	Q	21	GLU	CD-OE1	6.25	1.32	1.25
26	R	267	ARG	NE-CZ	6.25	1.41	1.33
23	O	289	ARG	CZ-NH1	6.25	1.41	1.33
24	P	364	ARG	CD-NE	6.25	1.57	1.46
4	3	44	PRO	N-CD	-6.24	1.39	1.47
24	P	226	TYR	CG-CD1	6.23	1.47	1.39
16	H	259	GLU	CB-CG	6.23	1.64	1.52
22	N	83	GLY	CA-C	-6.23	1.41	1.51
22	N	57	ARG	NE-CZ	6.22	1.41	1.33
3	2	79	PHE	CG-CD2	6.22	1.48	1.38
26	R	137	ARG	NE-CZ	6.22	1.41	1.33
31	W	14	GLU	CB-CG	6.21	1.64	1.52
20	L	30	ARG	CD-NE	6.21	1.57	1.46
25	Q	100	GLU	CB-CG	6.21	1.64	1.52
17	I	272	ARG	NE-CZ	6.19	1.41	1.33
16	H	258	ARG	NE-CZ	6.19	1.41	1.33
24	P	53	GLN	CG-CD	6.18	1.65	1.51
22	N	194	ARG	CZ-NH2	6.18	1.41	1.33
19	K	112	TYR	CD2-CE2	6.18	1.48	1.39
10	B	83	TYR	CB-CG	-6.17	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	F	224	TYR	CG-CD2	6.17	1.47	1.39
27	S	241	ARG	CZ-NH2	6.17	1.41	1.33
3	2	44	THR	N-CA	6.16	1.58	1.46
21	M	171	ARG	NE-CZ	6.16	1.41	1.33
22	N	361	ARG	NE-CZ	6.15	1.41	1.33
11	C	91	ARG	NE-CZ	6.14	1.41	1.33
18	J	49	ARG	CD-NE	6.14	1.56	1.46
25	Q	327	TYR	CB-CG	-6.14	1.42	1.51
12	D	118	TYR	CG-CD1	6.14	1.47	1.39
24	P	39	ARG	CZ-NH1	6.14	1.41	1.33
26	R	257	ARG	CZ-NH1	6.14	1.41	1.33
10	B	5	GLY	CA-C	-6.12	1.42	1.51
17	I	202	GLU	CG-CD	6.12	1.61	1.51
26	R	259	TYR	CE2-CZ	6.12	1.46	1.38
19	K	41	TYR	CG-CD1	6.11	1.47	1.39
16	H	182	GLU	CD-OE1	6.10	1.32	1.25
28	T	184	GLU	CG-CD	-6.10	1.42	1.51
2	1	156	ARG	CZ-NH2	6.10	1.41	1.33
20	L	251	ARG	CD-NE	6.10	1.56	1.46
17	I	242	GLN	N-CA	-6.10	1.34	1.46
22	N	474	ARG	CZ-NH1	6.10	1.41	1.33
6	5	216	ARG	NE-CZ	6.09	1.41	1.33
1	Z	723	TYR	CE2-CZ	6.08	1.46	1.38
28	T	145	ARG	CD-NE	6.08	1.56	1.46
7	6	135	TYR	CZ-OH	6.08	1.48	1.37
10	B	143	ARG	CZ-NH1	6.07	1.41	1.33
27	S	213	TYR	CZ-OH	6.07	1.48	1.37
30	V	112	TYR	CG-CD1	6.06	1.47	1.39
6	5	128	ARG	CZ-NH1	6.05	1.41	1.33
1	Z	478	ARG	NE-CZ	6.05	1.41	1.33
22	N	158	ARG	NE-CZ	6.05	1.41	1.33
20	L	351	GLY	C-O	-6.05	1.14	1.23
18	J	325	ARG	CZ-NH1	6.04	1.41	1.33
30	V	34	SER	CB-OG	6.04	1.50	1.42
8	7	89	ARG	CD-NE	6.04	1.56	1.46
6	5	224	TYR	CZ-OH	6.03	1.48	1.37
25	Q	408	SER	CB-OG	-6.03	1.34	1.42
29	U	228	TYR	CZ-OH	6.02	1.48	1.37
24	P	357	ARG	CD-NE	6.02	1.56	1.46
12	D	125	ARG	NE-CZ	6.02	1.40	1.33
14	F	141	GLY	CA-C	-6.02	1.42	1.51
10	B	155	TYR	CE2-CZ	6.02	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	E	185	TYR	CE2-CZ	6.02	1.46	1.38
12	D	170	GLU	N-CA	-6.01	1.34	1.46
26	R	170	GLU	CB-CG	6.01	1.63	1.52
1	Z	554	TYR	CE2-CZ	6.01	1.46	1.38
17	I	346	ARG	CZ-NH1	6.01	1.40	1.33
19	K	53	PHE	CG-CD1	6.01	1.47	1.38
11	C	158	GLY	N-CA	-6.00	1.37	1.46
27	S	234	ARG	CZ-NH2	5.99	1.40	1.33
5	4	147	TYR	CB-CG	-5.99	1.42	1.51
9	A	163	PHE	CB-CG	5.98	1.61	1.51
23	O	289	ARG	CZ-NH2	5.98	1.40	1.33
8	7	158	GLY	CA-C	-5.98	1.42	1.51
1	Z	779	CYS	CB-SG	5.98	1.92	1.82
1	Z	322	SER	CA-CB	5.97	1.61	1.52
9	A	245	ARG	NE-CZ	5.97	1.40	1.33
16	H	139	ARG	CZ-NH2	5.97	1.40	1.33
26	R	257	ARG	CZ-NH2	5.96	1.40	1.33
6	5	84	TYR	CB-CG	5.96	1.60	1.51
27	S	471	GLU	CB-CG	5.96	1.63	1.52
27	S	355	ARG	NE-CZ	5.95	1.40	1.33
20	L	137	GLY	CA-C	-5.95	1.42	1.51
6	5	123	ARG	NE-CZ	5.94	1.40	1.33
30	V	73	PHE	CG-CD2	5.94	1.47	1.38
9	A	43	ARG	NE-CZ	5.94	1.40	1.33
1	Z	588	ARG	NE-CZ	5.94	1.40	1.33
22	N	159	ARG	NE-CZ	5.93	1.40	1.33
6	5	95	GLU	CD-OE2	5.93	1.32	1.25
1	Z	300	ARG	CZ-NH2	5.93	1.40	1.33
5	4	107	TYR	CD2-CE2	-5.93	1.30	1.39
15	G	130	ARG	CZ-NH2	5.93	1.40	1.33
23	O	34	TRP	NE1-CE2	5.92	1.45	1.37
14	F	82	ARG	NE-CZ	5.92	1.40	1.33
24	P	329	ARG	CD-NE	5.92	1.56	1.46
21	M	376	SER	CA-CB	5.91	1.61	1.52
8	7	144	ARG	CZ-NH2	5.91	1.40	1.33
9	A	132	ARG	CZ-NH1	5.91	1.40	1.33
3	2	167	TYR	CA-C	-5.90	1.37	1.52
23	O	172	TYR	CE1-CZ	5.90	1.46	1.38
24	P	214	PHE	CD2-CE2	5.90	1.51	1.39
1	Z	80	ARG	CD-NE	5.89	1.56	1.46
23	O	299	SER	CA-CB	5.89	1.61	1.52
1	Z	687	ARG	CZ-NH1	5.88	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	D	39	ASP	CB-CG	5.88	1.64	1.51
23	O	167	GLY	CA-C	-5.88	1.42	1.51
1	Z	588	ARG	CD-NE	5.88	1.56	1.46
3	2	82	PRO	N-CD	-5.87	1.39	1.47
18	J	60	ARG	NE-CZ	5.87	1.40	1.33
21	M	320	PHE	CG-CD2	5.87	1.47	1.38
30	V	111	TRP	CD2-CE2	5.87	1.48	1.41
20	L	239	GLY	CA-C	-5.87	1.42	1.51
15	G	87	SER	CA-CB	5.87	1.61	1.52
28	T	245	PHE	CG-CD1	5.86	1.47	1.38
1	Z	492	SER	CB-OG	-5.86	1.34	1.42
3	2	154	TYR	CG-CD1	5.86	1.46	1.39
10	B	229	TYR	CZ-OH	5.86	1.47	1.37
17	I	411	ARG	CZ-NH1	5.86	1.40	1.33
6	5	245	ARG	NE-CZ	5.86	1.40	1.33
7	6	198	ARG	CZ-NH1	5.86	1.40	1.33
2	1	178	ARG	CD-NE	5.86	1.56	1.46
7	6	72	TYR	CE2-CZ	5.86	1.46	1.38
1	Z	879	ARG	NE-CZ	5.85	1.40	1.33
19	K	314	ALA	CA-CB	5.85	1.64	1.52
30	V	255	TYR	CB-CG	-5.85	1.42	1.51
13	E	154	PHE	CG-CD2	5.85	1.47	1.38
26	R	297	ARG	CZ-NH1	5.85	1.40	1.33
18	J	201	ARG	CZ-NH2	5.84	1.40	1.33
21	M	322	PRO	N-CD	-5.84	1.39	1.47
22	N	344	ARG	CZ-NH1	5.84	1.40	1.33
22	N	429	LYS	CA-CB	5.83	1.66	1.53
5	4	19	ARG	NE-CZ	5.83	1.40	1.33
25	Q	415	TYR	CE1-CZ	5.83	1.46	1.38
11	C	108	GLU	CB-CG	5.82	1.63	1.52
1	Z	323	ASN	CB-CG	5.82	1.64	1.51
20	L	210	GLU	CD-OE2	5.82	1.32	1.25
1	Z	250	ARG	CZ-NH1	5.82	1.40	1.33
23	O	24	ARG	CD-NE	5.82	1.56	1.46
20	L	25	ARG	CD-NE	5.81	1.56	1.46
24	P	357	ARG	NE-CZ	5.81	1.40	1.33
18	J	205	HIS	CB-CG	-5.81	1.39	1.50
25	Q	72	TYR	CZ-OH	5.81	1.47	1.37
26	R	295	TYR	CE2-CZ	5.80	1.46	1.38
28	T	187	TYR	CE1-CZ	5.80	1.46	1.38
26	R	46	ARG	CZ-NH2	5.80	1.40	1.33
24	P	191	ARG	NE-CZ	5.79	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	97	GLU	CD-OE2	5.79	1.32	1.25
22	N	710	ARG	CZ-NH1	5.79	1.40	1.33
24	P	350	ARG	CZ-NH2	5.79	1.40	1.33
15	G	93	ARG	CD-NE	5.79	1.56	1.46
7	6	148	ALA	CA-C	-5.79	1.38	1.52
30	V	65	TYR	CZ-OH	5.78	1.47	1.37
1	Z	529	SER	CA-CB	5.78	1.61	1.52
3	2	213	GLY	CA-C	-5.78	1.42	1.51
4	3	85	TYR	CG-CD2	5.77	1.46	1.39
19	K	188	PHE	CB-CG	5.77	1.61	1.51
31	W	91	ARG	NE-CZ	5.77	1.40	1.33
22	N	275	ILE	C-O	5.77	1.34	1.23
12	D	240	GLU	CG-CD	5.76	1.60	1.51
23	O	45	VAL	CB-CG1	5.76	1.65	1.52
31	W	78	VAL	CB-CG2	5.76	1.65	1.52
4	3	55	GLY	CA-C	-5.76	1.42	1.51
7	6	187	GLN	C-N	5.76	1.47	1.34
27	S	156	SER	CA-CB	5.76	1.61	1.52
26	R	385	ARG	CZ-NH1	5.76	1.40	1.33
3	2	167	TYR	CZ-OH	5.75	1.47	1.37
18	J	57	ARG	CD-NE	5.75	1.56	1.46
9	A	63	SER	CA-CB	5.75	1.61	1.52
17	I	89	GLU	CD-OE2	5.75	1.31	1.25
22	N	137	MET	CA-CB	5.75	1.66	1.53
26	R	304	TYR	CB-CG	-5.75	1.43	1.51
1	Z	282	PHE	CG-CD1	5.74	1.47	1.38
7	6	114	GLY	N-CA	-5.74	1.37	1.46
27	S	383	GLY	CA-C	-5.74	1.42	1.51
1	Z	881	GLU	CG-CD	5.73	1.60	1.51
21	M	265	ALA	CA-CB	5.73	1.64	1.52
23	O	270	ARG	NE-CZ	5.73	1.40	1.33
25	Q	132	ARG	CZ-NH2	5.73	1.40	1.33
22	N	55	ARG	CZ-NH2	5.72	1.40	1.33
3	2	244	ARG	CZ-NH2	5.72	1.40	1.33
22	N	439	GLU	CD-OE2	5.72	1.31	1.25
23	O	140	GLU	CA-CB	5.72	1.66	1.53
19	K	339	ARG	CZ-NH2	5.72	1.40	1.33
15	G	135	SER	CA-CB	5.71	1.61	1.52
13	E	17	PRO	CA-C	-5.71	1.41	1.52
20	L	242	ARG	NE-CZ	5.71	1.40	1.33
16	H	239	ARG	CZ-NH2	5.71	1.40	1.33
25	Q	194	ARG	CD-NE	5.71	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	N	747	SER	CA-CB	5.70	1.61	1.52
1	Z	314	TYR	CZ-OH	5.69	1.47	1.37
27	S	467	TYR	CG-CD2	5.68	1.46	1.39
31	W	115	SER	CA-CB	5.68	1.61	1.52
12	D	36	ARG	NE-CZ	5.68	1.40	1.33
23	O	282	PHE	CA-CB	5.68	1.66	1.53
17	I	411	ARG	CD-NE	5.67	1.56	1.46
21	M	347	ARG	CZ-NH1	5.67	1.40	1.33
21	M	57	SER	CA-CB	5.67	1.61	1.52
19	K	251	PHE	CE2-CZ	5.67	1.48	1.37
29	U	209	ARG	CZ-NH1	5.66	1.40	1.33
1	Z	807	ARG	CZ-NH2	5.66	1.40	1.33
9	A	105	TYR	CZ-OH	5.66	1.47	1.37
4	3	26	ARG	CD-NE	5.66	1.56	1.46
14	F	6	TYR	CE1-CZ	5.66	1.46	1.38
13	E	20	ARG	NE-CZ	5.66	1.40	1.33
9	A	101	TRP	CB-CG	5.64	1.60	1.50
5	4	86	ARG	CZ-NH2	5.64	1.40	1.33
1	Z	335	ARG	CZ-NH1	5.64	1.40	1.33
1	Z	763	ARG	CZ-NH1	5.64	1.40	1.33
16	H	189	GLU	CD-OE1	5.64	1.31	1.25
31	W	113	VAL	CA-CB	-5.64	1.43	1.54
28	T	175	TYR	CE2-CZ	5.64	1.45	1.38
12	D	110	TYR	CB-CG	-5.64	1.43	1.51
12	D	106	TYR	CD1-CE1	5.63	1.47	1.39
26	R	83	ARG	CD-NE	5.62	1.56	1.46
7	6	56	ARG	NE-CZ	5.62	1.40	1.33
2	1	95	TYR	CG-CD1	5.62	1.46	1.39
22	N	246	TYR	CE2-CZ	5.62	1.45	1.38
32	Y	57	ARG	CZ-NH1	5.62	1.40	1.33
1	Z	492	SER	CA-CB	5.61	1.61	1.52
19	K	388	ARG	CD-NE	5.61	1.55	1.46
19	K	366	ARG	CD-NE	5.61	1.55	1.46
23	O	60	TYR	CB-CG	5.60	1.60	1.51
2	1	79	ARG	CZ-NH2	5.60	1.40	1.33
16	H	369	ARG	CZ-NH1	5.60	1.40	1.33
25	Q	363	ARG	CD-NE	5.60	1.55	1.46
2	1	168	TYR	CG-CD1	5.60	1.46	1.39
10	B	89	ARG	CD-NE	5.60	1.55	1.46
12	D	86	ARG	CZ-NH2	5.60	1.40	1.33
14	F	40	SER	CA-CB	5.60	1.61	1.52
8	7	80	ARG	NE-CZ	5.59	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	2	184	LYS	CD-CE	5.59	1.65	1.51
9	A	160	TYR	CE2-CZ	5.59	1.45	1.38
2	1	103	GLU	CB-CG	5.59	1.62	1.52
31	W	175	PRO	N-CD	5.59	1.55	1.47
1	Z	72	ARG	CZ-NH1	5.59	1.40	1.33
11	C	3	ARG	CZ-NH2	5.59	1.40	1.33
22	N	644	TYR	CZ-OH	5.59	1.47	1.37
26	R	324	GLY	CA-C	-5.59	1.43	1.51
8	7	86	ARG	NE-CZ	5.58	1.40	1.33
17	I	430	LYS	CA-CB	5.58	1.66	1.53
1	Z	816	TYR	CG-CD2	5.58	1.46	1.39
7	6	152	PHE	CE1-CZ	5.58	1.48	1.37
17	I	252	GLY	N-CA	-5.57	1.37	1.46
1	Z	783	SER	CA-CB	5.57	1.61	1.52
3	2	135	GLY	CA-C	-5.57	1.43	1.51
16	H	282	GLY	CA-C	-5.56	1.43	1.51
17	I	254	GLU	N-CA	-5.56	1.35	1.46
14	F	174	ARG	CD-NE	5.56	1.55	1.46
22	N	16	GLU	CB-CG	5.55	1.62	1.52
22	N	361	ARG	CD-NE	5.55	1.55	1.46
27	S	201	ARG	CZ-NH1	5.55	1.40	1.33
6	5	113	PHE	CB-CG	5.55	1.60	1.51
24	P	120	ILE	CA-CB	-5.55	1.42	1.54
8	7	245	GLU	CB-CG	5.55	1.62	1.52
17	I	168	ASP	CB-CG	5.55	1.63	1.51
21	M	438	TYR	CD1-CE1	5.54	1.47	1.39
12	D	110	TYR	CE2-CZ	5.54	1.45	1.38
22	N	937	GLU	CB-CG	5.54	1.62	1.52
9	A	74	GLU	CG-CD	5.54	1.60	1.51
27	S	205	LEU	N-CA	-5.54	1.35	1.46
22	N	494	TYR	CG-CD2	5.54	1.46	1.39
15	G	163	GLY	CA-C	-5.54	1.43	1.51
22	N	213	PHE	CG-CD2	5.53	1.47	1.38
9	A	144	ASP	CA-CB	5.53	1.66	1.53
11	C	66	TYR	CZ-OH	5.53	1.47	1.37
21	M	222	GLY	N-CA	-5.53	1.37	1.46
1	Z	262	PHE	CG-CD1	5.53	1.47	1.38
23	O	230	ARG	CZ-NH1	5.53	1.40	1.33
24	P	217	GLU	CG-CD	5.53	1.60	1.51
21	M	216	GLY	N-CA	-5.52	1.37	1.46
7	6	72	TYR	N-CA	-5.52	1.35	1.46
16	H	168	GLU	CD-OE2	5.52	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
18	J	356	GLY	CA-C	-5.52	1.43	1.51
14	F	102	PRO	N-CA	-5.52	1.37	1.47
25	Q	201	TYR	CZ-OH	5.52	1.47	1.37
12	D	81	ARG	NE-CZ	5.51	1.40	1.33
17	I	295	TYR	CG-CD1	5.51	1.46	1.39
24	P	248	ARG	CD-NE	5.51	1.55	1.46
21	M	117	ARG	CZ-NH2	5.51	1.40	1.33
22	N	710	ARG	CZ-NH2	5.51	1.40	1.33
6	5	248	SER	CB-OG	-5.51	1.35	1.42
22	N	899	ARG	CZ-NH2	5.51	1.40	1.33
5	4	181	ARG	NE-CZ	5.51	1.40	1.33
19	K	299	PHE	CG-CD1	5.51	1.47	1.38
26	R	128	TYR	CE1-CZ	5.51	1.45	1.38
8	7	82	ARG	CD-NE	5.50	1.55	1.46
1	Z	226	TYR	CZ-OH	5.50	1.47	1.37
3	2	220	VAL	CB-CG1	5.50	1.64	1.52
23	O	240	PHE	CG-CD1	5.50	1.47	1.38
20	L	143	ARG	NE-CZ	5.50	1.40	1.33
24	P	350	ARG	CZ-NH1	5.50	1.40	1.33
29	U	190	ARG	CZ-NH2	5.50	1.40	1.33
10	B	97	TYR	CZ-OH	5.49	1.47	1.37
23	O	145	LEU	C-N	-5.49	1.23	1.34
21	M	437	TYR	CE1-CZ	5.49	1.45	1.38
18	J	68	GLU	CD-OE2	5.49	1.31	1.25
22	N	426	TYR	CG-CD2	5.49	1.46	1.39
1	Z	346	ASP	N-CA	-5.48	1.35	1.46
21	M	304	ARG	CZ-NH2	5.48	1.40	1.33
24	P	141	GLU	CG-CD	5.48	1.60	1.51
11	C	226	ARG	CZ-NH1	5.48	1.40	1.33
14	F	122	ARG	NE-CZ	5.48	1.40	1.33
17	I	98	LYS	CA-CB	5.48	1.66	1.53
18	J	345	ARG	NE-CZ	5.47	1.40	1.33
4	3	66	ARG	CZ-NH1	5.47	1.40	1.33
1	Z	149	GLU	CD-OE1	5.47	1.31	1.25
6	5	172	TYR	CG-CD1	5.47	1.46	1.39
27	S	322	VAL	N-CA	-5.47	1.35	1.46
7	6	232	ARG	CZ-NH1	5.46	1.40	1.33
23	O	162	TYR	CE2-CZ	5.46	1.45	1.38
1	Z	349	TYR	CG-CD1	5.46	1.46	1.39
27	S	341	GLU	CG-CD	5.46	1.60	1.51
28	T	289	ARG	CZ-NH1	5.45	1.40	1.33
5	4	74	GLU	CB-CG	5.44	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	5	134	SER	CA-CB	5.44	1.61	1.52
23	O	196	ARG	NE-CZ	5.44	1.40	1.33
24	P	263	TRP	CZ2-CH2	5.44	1.47	1.37
21	M	167	GLU	CG-CD	5.44	1.60	1.51
12	D	145	TYR	CG-CD1	5.43	1.46	1.39
18	J	189	TYR	CE1-CZ	5.43	1.45	1.38
18	J	278	ASN	CB-CG	5.43	1.63	1.51
12	D	216	SER	N-CA	-5.43	1.35	1.46
16	H	313	GLY	N-CA	-5.43	1.38	1.46
20	L	372	ARG	CZ-NH1	5.43	1.40	1.33
26	R	293	ARG	CA-C	-5.43	1.38	1.52
17	I	93	GLU	CG-CD	5.43	1.60	1.51
22	N	900	TYR	CE2-CZ	5.42	1.45	1.38
1	Z	330	PHE	CG-CD1	5.42	1.46	1.38
7	6	232	ARG	NE-CZ	5.42	1.40	1.33
13	E	47	CYS	CA-C	-5.42	1.38	1.52
19	K	241	GLY	N-CA	-5.42	1.38	1.46
22	N	628	ARG	CZ-NH2	5.42	1.40	1.33
24	P	113	GLU	CD-OE2	-5.42	1.19	1.25
27	S	360	TYR	CG-CD1	5.42	1.46	1.39
15	G	119	TYR	CB-CG	-5.42	1.43	1.51
15	G	233	ARG	CD-NE	5.42	1.55	1.46
22	N	734	GLN	C-N	5.42	1.42	1.33
22	N	801	GLN	CG-CD	5.42	1.63	1.51
14	F	164	ARG	NE-CZ	5.42	1.40	1.33
14	F	157	ARG	NE-CZ	5.41	1.40	1.33
13	E	44	GLU	CG-CD	5.41	1.60	1.51
12	D	213	ARG	CD-NE	5.41	1.55	1.46
19	K	411	GLU	CD-OE2	5.41	1.31	1.25
1	Z	434	TYR	CE1-CZ	5.41	1.45	1.38
26	R	185	GLY	CA-C	-5.40	1.43	1.51
22	N	771	PHE	CD2-CE2	5.39	1.50	1.39
1	Z	143	ARG	CD-NE	5.39	1.55	1.46
5	4	145	ARG	NE-CZ	5.39	1.40	1.33
21	M	295	ARG	CZ-NH2	5.39	1.40	1.33
13	E	159	SER	C-N	5.39	1.42	1.33
16	H	49	GLU	CD-OE2	5.39	1.31	1.25
22	N	486	MET	C-N	5.39	1.42	1.33
10	B	65	VAL	CB-CG1	5.38	1.64	1.52
12	D	38	ARG	CD-NE	5.38	1.55	1.46
13	E	94	VAL	N-CA	-5.38	1.35	1.46
32	Y	57	ARG	CD-NE	5.38	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
15	G	126	TYR	CE2-CZ	5.38	1.45	1.38
28	T	207	GLU	CG-CD	5.38	1.60	1.51
22	N	783	TYR	CE1-CZ	5.38	1.45	1.38
22	N	199	ARG	CZ-NH1	5.38	1.40	1.33
28	T	306	ARG	NE-CZ	5.38	1.40	1.33
19	K	81	ARG	CD-NE	5.37	1.55	1.46
20	L	168	LYS	C-N	5.36	1.42	1.33
16	H	366	ARG	CZ-NH2	5.36	1.40	1.33
27	S	460	SER	CA-CB	5.36	1.60	1.52
23	O	265	GLU	CG-CD	5.36	1.59	1.51
16	H	265	ARG	CD-NE	5.35	1.55	1.46
14	F	196	ARG	CZ-NH1	5.35	1.40	1.33
25	Q	276	ALA	CA-CB	5.35	1.63	1.52
22	N	510	GLU	CB-CG	5.35	1.62	1.52
28	T	180	GLU	CB-CG	5.34	1.62	1.52
24	P	421	PRO	CA-C	-5.34	1.42	1.52
10	B	227	LYS	CD-CE	5.34	1.64	1.51
18	J	223	PHE	CG-CD1	5.34	1.46	1.38
15	G	219	GLU	CB-CG	5.34	1.62	1.52
24	P	348	GLU	N-CA	-5.34	1.35	1.46
11	C	91	ARG	CZ-NH2	5.34	1.40	1.33
19	K	268	ASP	CA-CB	5.34	1.65	1.53
22	N	766	PHE	CE2-CZ	5.34	1.47	1.37
19	K	242	GLU	CB-CG	5.33	1.62	1.52
16	H	174	TYR	CB-CG	-5.33	1.43	1.51
1	Z	772	GLY	CA-C	-5.33	1.43	1.51
27	S	294	ARG	NE-CZ	5.33	1.40	1.33
22	N	192	GLN	CA-C	-5.33	1.39	1.52
29	U	136	GLU	CB-CG	5.33	1.62	1.52
24	P	394	SER	CA-CB	5.33	1.60	1.52
16	H	200	ARG	NE-CZ	5.32	1.40	1.33
20	L	367	PHE	CB-CG	-5.32	1.42	1.51
23	O	172	TYR	CG-CD1	5.32	1.46	1.39
28	T	315	TYR	CE2-CZ	5.32	1.45	1.38
25	Q	235	ALA	CA-CB	5.32	1.63	1.52
14	F	96	ARG	CD-NE	5.32	1.55	1.46
20	L	294	ARG	CZ-NH1	5.31	1.40	1.33
3	2	66	GLY	CA-C	-5.31	1.43	1.51
5	4	67	TYR	CE2-CZ	-5.31	1.31	1.38
2	1	125	ARG	N-CA	-5.30	1.35	1.46
27	S	399	ARG	CZ-NH2	5.30	1.40	1.33
7	6	239	ARG	NE-CZ	5.30	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	A	214	GLU	CG-CD	5.30	1.59	1.51
20	L	67	GLU	CD-OE1	5.30	1.31	1.25
26	R	304	TYR	CG-CD1	5.30	1.46	1.39
1	Z	385	PHE	CE1-CZ	5.29	1.47	1.37
1	Z	261	ARG	CZ-NH2	5.29	1.40	1.33
3	2	254	VAL	CB-CG1	5.29	1.64	1.52
23	O	308	GLU	CD-OE2	5.29	1.31	1.25
25	Q	77	LEU	N-CA	-5.29	1.35	1.46
26	R	88	LEU	CA-CB	5.29	1.66	1.53
26	R	151	TYR	CD1-CE1	5.29	1.47	1.39
8	7	249	SER	CA-CB	5.29	1.60	1.52
12	D	228	TYR	CZ-OH	5.29	1.46	1.37
15	G	159	TYR	CB-CG	-5.29	1.43	1.51
22	N	35	TRP	CE2-CZ2	-5.29	1.30	1.39
31	W	15	TYR	CD2-CE2	5.29	1.47	1.39
19	K	342	ARG	CZ-NH1	5.29	1.40	1.33
29	U	36	VAL	CA-C	-5.29	1.39	1.52
3	2	157	TYR	CZ-OH	5.28	1.46	1.37
26	R	187	TYR	CG-CD2	5.28	1.46	1.39
25	Q	173	GLU	CD-OE1	-5.28	1.19	1.25
20	L	110	TYR	CB-CG	-5.28	1.43	1.51
8	7	231	ARG	CZ-NH2	5.27	1.40	1.33
26	R	237	ARG	CZ-NH1	5.27	1.40	1.33
9	A	107	TYR	CE1-CZ	5.27	1.45	1.38
22	N	616	ARG	NE-CZ	5.27	1.40	1.33
2	1	81	GLY	N-CA	-5.27	1.38	1.46
15	G	131	PRO	N-CA	-5.27	1.38	1.47
21	M	105	GLU	CB-CG	5.26	1.62	1.52
1	Z	432	TYR	CE1-CZ	5.26	1.45	1.38
22	N	455	GLY	N-CA	5.26	1.53	1.46
3	2	263	GLU	CD-OE2	5.26	1.31	1.25
23	O	70	ARG	CZ-NH1	5.26	1.39	1.33
14	F	70	ILE	C-N	5.26	1.42	1.33
11	C	17	ARG	CZ-NH1	5.26	1.39	1.33
22	N	374	SER	CB-OG	5.26	1.49	1.42
3	2	81	SER	N-CA	-5.25	1.35	1.46
18	J	265	GLY	N-CA	-5.25	1.38	1.46
1	Z	155	GLY	CA-C	-5.25	1.43	1.51
7	6	154	PRO	N-CD	-5.25	1.40	1.47
16	H	142	VAL	N-CA	-5.24	1.35	1.46
22	N	615	ARG	CD-NE	5.24	1.55	1.46
16	H	207	GLU	CG-CD	5.24	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	L	365	GLU	CG-CD	5.24	1.59	1.51
29	U	207	ASP	CA-CB	5.24	1.65	1.53
21	M	197	GLU	CD-OE2	5.24	1.31	1.25
25	Q	341	PRO	CA-C	-5.24	1.42	1.52
1	Z	892	PRO	N-CA	-5.24	1.38	1.47
5	4	170	ARG	NE-CZ	5.24	1.39	1.33
20	L	272	ARG	CZ-NH2	5.24	1.39	1.33
23	O	126	GLY	CA-C	-5.24	1.43	1.51
16	H	259	GLU	CD-OE2	5.23	1.31	1.25
16	H	258	ARG	CZ-NH1	5.23	1.39	1.33
22	N	740	GLY	CA-C	5.23	1.60	1.51
27	S	180	ARG	CZ-NH2	5.23	1.39	1.33
22	N	649	ARG	CD-NE	5.22	1.55	1.46
23	O	354	GLU	CD-OE2	5.22	1.31	1.25
1	Z	160	ARG	CZ-NH1	5.22	1.39	1.33
5	4	19	ARG	CZ-NH1	5.22	1.39	1.33
8	7	222	TYR	CG-CD1	5.22	1.46	1.39
9	A	103	TYR	CG-CD1	5.22	1.46	1.39
29	U	95	TYR	CE1-CZ	5.22	1.45	1.38
24	P	58	SER	CA-CB	5.21	1.60	1.52
3	2	257	GLU	CG-CD	5.21	1.59	1.51
17	I	411	ARG	CZ-NH2	5.21	1.39	1.33
27	S	334	VAL	CA-CB	-5.21	1.43	1.54
15	G	115	ARG	CZ-NH2	5.21	1.39	1.33
18	J	295	THR	N-CA	-5.21	1.35	1.46
8	7	129	SER	CA-CB	5.20	1.60	1.52
26	R	38	ARG	CZ-NH2	5.20	1.39	1.33
7	6	150	TYR	CE2-CZ	5.20	1.45	1.38
19	K	229	ARG	CD-NE	5.20	1.55	1.46
4	3	203	ARG	NE-CZ	5.20	1.39	1.33
12	D	169	ARG	CZ-NH1	5.20	1.39	1.33
13	E	152	GLN	CG-CD	5.20	1.63	1.51
16	H	211	GLY	CA-C	-5.20	1.43	1.51
22	N	937	GLU	CD-OE1	5.20	1.31	1.25
25	Q	65	GLU	CG-CD	-5.20	1.44	1.51
23	O	235	ASP	C-N	5.20	1.46	1.34
24	P	254	PRO	N-CD	-5.20	1.40	1.47
29	U	259	VAL	C-N	5.20	1.46	1.34
4	3	196	THR	CA-C	-5.19	1.39	1.52
22	N	138	PHE	CG-CD1	5.19	1.46	1.38
3	2	133	TYR	CE1-CZ	5.19	1.45	1.38
23	O	60	TYR	CE1-CZ	5.19	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	V	107	MET	CA-CB	5.19	1.65	1.53
1	Z	83	ARG	CZ-NH2	5.19	1.39	1.33
14	F	101	ARG	NE-CZ	5.19	1.39	1.33
19	K	283	ARG	CD-NE	5.19	1.55	1.46
24	P	129	ARG	CD-NE	5.19	1.55	1.46
22	N	108	TYR	CG-CD1	5.18	1.45	1.39
2	1	162	GLY	N-CA	-5.18	1.38	1.46
22	N	6	ALA	C-N	5.18	1.42	1.33
31	W	162	GLY	N-CA	-5.18	1.38	1.46
17	I	289	ALA	N-CA	-5.17	1.36	1.46
23	O	159	SER	CB-OG	5.17	1.49	1.42
14	F	89	ARG	NE-CZ	5.17	1.39	1.33
15	G	83	ALA	N-CA	-5.17	1.36	1.46
4	3	47	ASP	CA-CB	5.17	1.65	1.53
20	L	173	TYR	CG-CD1	5.17	1.45	1.39
22	N	80	TYR	CZ-OH	5.17	1.46	1.37
9	A	154	CYS	CB-SG	5.16	1.91	1.82
19	K	392	TYR	CG-CD2	5.16	1.45	1.39
22	N	68	PHE	CG-CD1	5.16	1.46	1.38
30	V	52	GLU	CB-CG	5.16	1.61	1.52
22	N	744	VAL	CA-CB	-5.16	1.44	1.54
22	N	763	VAL	CB-CG1	5.16	1.63	1.52
4	3	29	GLY	CA-C	-5.16	1.43	1.51
19	K	411	GLU	CG-CD	5.15	1.59	1.51
24	P	137	TYR	CZ-OH	5.15	1.46	1.37
24	P	144	ARG	NE-CZ	5.15	1.39	1.33
1	Z	746	ARG	NE-CZ	5.15	1.39	1.33
22	N	750	SER	CA-CB	5.15	1.60	1.52
25	Q	124	PHE	CB-CG	5.15	1.60	1.51
18	J	92	GLU	N-CA	-5.15	1.36	1.46
17	I	272	ARG	CZ-NH2	5.15	1.39	1.33
21	M	369	HIS	CB-CG	5.15	1.59	1.50
29	U	12	HIS	CG-CD2	-5.15	1.26	1.35
25	Q	298	SER	CA-CB	5.14	1.60	1.52
8	7	227	ARG	NE-CZ	5.14	1.39	1.33
14	F	101	ARG	CZ-NH1	5.14	1.39	1.33
22	N	899	ARG	CZ-NH1	5.14	1.39	1.33
25	Q	266	ASP	N-CA	-5.14	1.36	1.46
1	Z	586	PRO	CA-C	-5.13	1.42	1.52
9	A	132	ARG	NE-CZ	5.13	1.39	1.33
1	Z	395	GLY	CA-C	-5.12	1.43	1.51
14	F	107	ARG	NE-CZ	5.12	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	K	283	ARG	NE-CZ	5.12	1.39	1.33
31	W	145	GLU	CD-OE1	5.12	1.31	1.25
7	6	132	TYR	CA-CB	5.12	1.65	1.53
27	S	181	TYR	CZ-OH	5.12	1.46	1.37
19	K	266	GLU	CD-OE2	5.11	1.31	1.25
27	S	314	ARG	CZ-NH1	5.11	1.39	1.33
28	T	235	TYR	CE1-CZ	5.11	1.45	1.38
1	Z	673	ARG	CZ-NH1	5.11	1.39	1.33
4	3	177	ARG	CZ-NH1	5.11	1.39	1.33
5	4	11	ASP	CB-CG	5.11	1.62	1.51
7	6	125	TYR	CD1-CE1	5.11	1.47	1.39
28	T	320	SER	CB-OG	5.11	1.48	1.42
28	T	343	ALA	CA-CB	5.11	1.63	1.52
15	G	86	ARG	NE-CZ	5.11	1.39	1.33
18	J	362	VAL	CB-CG2	5.11	1.63	1.52
29	U	79	TYR	CG-CD2	5.11	1.45	1.39
8	7	206	SER	CB-OG	5.11	1.48	1.42
6	5	115	GLU	CG-CD	5.10	1.59	1.51
13	E	69	GLU	CD-OE1	5.10	1.31	1.25
25	Q	397	TYR	CE2-CZ	5.10	1.45	1.38
29	U	34	ARG	CZ-NH2	5.10	1.39	1.33
14	F	160	SER	CA-CB	5.10	1.60	1.52
19	K	103	VAL	N-CA	-5.10	1.36	1.46
1	Z	675	PHE	CG-CD1	5.10	1.46	1.38
9	A	142	GLY	CA-C	-5.09	1.43	1.51
14	F	54	SER	CA-CB	5.09	1.60	1.52
10	B	185	GLU	CD-OE2	5.09	1.31	1.25
29	U	93	GLY	CA-C	-5.09	1.43	1.51
10	B	60	ARG	CZ-NH2	5.09	1.39	1.33
17	I	322	ARG	NE-CZ	5.09	1.39	1.33
28	T	334	GLU	CB-CG	5.09	1.61	1.52
22	N	883	ARG	NE-CZ	5.08	1.39	1.33
1	Z	276	GLU	CB-CG	5.08	1.61	1.52
5	4	145	ARG	CZ-NH2	5.08	1.39	1.33
24	P	64	SER	CA-CB	5.08	1.60	1.52
16	H	363	SER	CA-CB	5.08	1.60	1.52
22	N	408	LEU	C-N	5.08	1.42	1.33
20	L	83	CYS	CB-SG	5.08	1.90	1.82
23	O	213	PHE	CE1-CZ	5.08	1.47	1.37
18	J	325	ARG	CD-NE	5.08	1.55	1.46
27	S	349	ARG	NE-CZ	5.08	1.39	1.33
3	2	85	TYR	CA-C	-5.07	1.39	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	S	298	ILE	CA-CB	-5.07	1.43	1.54
14	F	137	TYR	CZ-OH	5.07	1.46	1.37
13	E	51	GLU	CB-CG	5.07	1.61	1.52
4	3	128	GLY	N-CA	-5.07	1.38	1.46
9	A	108	GLU	CB-CG	5.07	1.61	1.52
24	P	322	GLU	CG-CD	5.07	1.59	1.51
8	7	143	SER	CB-OG	5.06	1.48	1.42
28	T	315	TYR	CZ-OH	5.06	1.46	1.37
27	S	347	GLN	CA-C	-5.06	1.39	1.52
1	Z	746	ARG	CD-NE	5.06	1.55	1.46
7	6	37	GLY	C-N	5.06	1.42	1.33
17	I	408	ARG	NE-CZ	5.05	1.39	1.33
22	N	615	ARG	CZ-NH2	5.05	1.39	1.33
8	7	74	SER	CA-CB	5.05	1.60	1.52
12	D	213	ARG	CZ-NH2	5.05	1.39	1.33
1	Z	439	TYR	CE2-CZ	5.05	1.45	1.38
22	N	194	ARG	NE-CZ	5.05	1.39	1.33
5	4	12	TYR	CE2-CZ	5.04	1.45	1.38
8	7	216	ARG	NE-CZ	5.04	1.39	1.33
16	H	285	PHE	CG-CD2	5.04	1.46	1.38
10	B	71	HIS	N-CA	-5.04	1.36	1.46
29	U	166	GLU	CB-CG	5.04	1.61	1.52
16	H	98	CYS	CB-SG	5.04	1.90	1.82
2	1	53	ARG	CD-NE	5.04	1.55	1.46
11	C	19	TYR	CG-CD2	5.04	1.45	1.39
7	6	190	GLU	CD-OE1	5.04	1.31	1.25
11	C	181	GLU	CD-OE2	5.04	1.31	1.25
8	7	86	ARG	CZ-NH2	5.03	1.39	1.33
18	J	229	ARG	NE-CZ	5.03	1.39	1.33
1	Z	190	GLU	CB-CG	5.03	1.61	1.52
4	3	100	PHE	CG-CD1	5.03	1.46	1.38
6	5	139	SER	CA-CB	5.03	1.60	1.52
20	L	217	GLU	CD-OE2	5.03	1.31	1.25
27	S	361	PHE	N-CA	-5.03	1.36	1.46
13	E	57	PRO	N-CA	-5.02	1.38	1.47
26	R	267	ARG	CZ-NH2	5.02	1.39	1.33
7	6	33	TYR	CE2-CZ	5.02	1.45	1.38
11	C	179	TYR	CG-CD1	5.02	1.45	1.39
26	R	135	GLY	C-N	5.02	1.45	1.34
25	Q	397	TYR	CE1-CZ	5.02	1.45	1.38
1	Z	740	ARG	NE-CZ	5.02	1.39	1.33
3	2	197	LEU	N-CA	-5.02	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	O	270	ARG	CZ-NH1	5.02	1.39	1.33
20	L	207	TYR	CE2-CZ	5.01	1.45	1.38
21	M	238	ARG	CD-NE	5.01	1.54	1.46
22	N	159	ARG	CZ-NH1	5.01	1.39	1.33
26	R	146	ARG	CZ-NH1	5.01	1.39	1.33
2	1	77	CYS	CB-SG	5.01	1.90	1.82
9	A	228	ARG	N-CA	-5.01	1.36	1.46
8	7	152	TRP	CZ2-CH2	5.01	1.46	1.37
18	J	113	ARG	CD-NE	5.01	1.54	1.46
24	P	248	ARG	CZ-NH1	5.01	1.39	1.33
27	S	261	TYR	CB-CG	-5.01	1.44	1.51
27	S	348	PHE	CE1-CZ	5.01	1.46	1.37
15	G	224	ARG	CZ-NH2	5.01	1.39	1.33
22	N	163	PHE	CG-CD2	5.01	1.46	1.38
22	N	336	GLU	CG-CD	5.01	1.59	1.51
27	S	382	PHE	CB-CG	5.01	1.59	1.51
19	K	121	ARG	CD-NE	5.00	1.54	1.46
21	M	398	ALA	N-CA	-5.00	1.36	1.46
29	U	13	PRO	N-CA	-5.00	1.38	1.47
18	J	201	ARG	NE-CZ	5.00	1.39	1.33

All (1939) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	R	304	TYR	CB-CG-CD1	-18.88	109.67	121.00
19	K	338	ARG	NE-CZ-NH1	18.82	129.71	120.30
4	3	27	ARG	NE-CZ-NH2	-17.84	111.38	120.30
26	R	142	PHE	CB-CG-CD1	17.53	133.07	120.80
27	S	399	ARG	NE-CZ-NH2	-17.01	111.80	120.30
10	B	6	TYR	CB-CG-CD2	-16.90	110.86	121.00
22	N	205	TYR	CB-CG-CD1	16.57	130.94	121.00
5	4	12	TYR	CB-CG-CD2	-16.48	111.11	121.00
27	S	276	PHE	CB-CG-CD2	-16.35	109.35	120.80
1	Z	469	TYR	CB-CG-CD2	-16.18	111.29	121.00
11	C	156	TYR	CB-CG-CD2	-16.01	111.39	121.00
21	M	180	ARG	NE-CZ-NH1	15.89	128.25	120.30
26	R	297	ARG	NE-CZ-NH2	15.81	128.21	120.30
19	K	326	ARG	NE-CZ-NH2	-15.60	112.50	120.30
29	U	228	TYR	CB-CG-CD2	15.45	130.27	121.00
27	S	399	ARG	NE-CZ-NH1	15.33	127.96	120.30
2	1	156	ARG	NE-CZ-NH2	-15.24	112.68	120.30
27	S	479	ARG	NE-CZ-NH1	15.03	127.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	126	TYR	CB-CG-CD1	-14.95	112.03	121.00
15	G	130	ARG	NE-CZ-NH2	-14.86	112.87	120.30
11	C	249	ARG	NE-CZ-NH1	14.75	127.68	120.30
17	I	132	TYR	CB-CG-CD1	14.41	129.65	121.00
14	F	18	ARG	NE-CZ-NH1	14.36	127.48	120.30
2	1	53	ARG	NE-CZ-NH2	-14.31	113.15	120.30
17	I	210	TYR	CB-CG-CD2	-14.30	112.42	121.00
26	R	304	TYR	CB-CG-CD2	14.09	129.46	121.00
21	M	334	ARG	NE-CZ-NH1	14.03	127.31	120.30
18	J	72	TYR	CB-CG-CD2	-14.00	112.60	121.00
27	S	276	PHE	CB-CG-CD1	13.55	130.29	120.80
13	E	162	PHE	CB-CG-CD1	-13.54	111.32	120.80
21	M	158	TYR	CB-CG-CD2	-13.53	112.88	121.00
1	Z	72	ARG	NE-CZ-NH1	13.51	127.05	120.30
26	R	192	ARG	NE-CZ-NH1	13.46	127.03	120.30
24	P	369	TYR	CB-CG-CD1	13.43	129.06	121.00
3	2	244	ARG	NE-CZ-NH1	13.35	126.98	120.30
26	R	46	ARG	NE-CZ-NH2	-13.34	113.63	120.30
22	N	650	TYR	CB-CG-CD1	13.31	128.98	121.00
15	G	233	ARG	NE-CZ-NH1	13.28	126.94	120.30
10	B	130	PHE	CB-CG-CD2	-13.25	111.53	120.80
11	C	128	ARG	NE-CZ-NH2	-13.24	113.68	120.30
17	I	132	TYR	CB-CG-CD2	-13.23	113.06	121.00
18	J	60	ARG	NE-CZ-NH2	13.21	126.91	120.30
15	G	170	ARG	NE-CZ-NH1	13.11	126.86	120.30
7	6	61	PHE	CB-CG-CD2	-13.03	111.68	120.80
20	L	309	ARG	NE-CZ-NH2	13.00	126.80	120.30
20	L	344	ARG	NE-CZ-NH1	12.95	126.78	120.30
4	3	103	TYR	CB-CG-CD1	-12.92	113.25	121.00
24	P	191	ARG	NE-CZ-NH2	-12.92	113.84	120.30
1	Z	901	ARG	NE-CZ-NH2	-12.90	113.85	120.30
1	Z	349	TYR	CB-CG-CD2	-12.85	113.29	121.00
7	6	160	ARG	NE-CZ-NH1	12.83	126.72	120.30
2	1	156	ARG	NE-CZ-NH1	12.79	126.70	120.30
18	J	60	ARG	NE-CZ-NH1	-12.78	113.91	120.30
23	O	198	PHE	CB-CG-CD2	-12.75	111.87	120.80
3	2	133	TYR	CB-CG-CD2	-12.72	113.37	121.00
25	Q	20	ARG	NE-CZ-NH2	12.68	126.64	120.30
9	A	125	TYR	CB-CG-CD2	-12.62	113.43	121.00
4	3	103	TYR	CB-CG-CD2	12.62	128.57	121.00
23	O	198	PHE	CB-CG-CD1	12.59	129.61	120.80
25	Q	74	ARG	NE-CZ-NH2	-12.56	114.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	7	227	ARG	NE-CZ-NH2	-12.54	114.03	120.30
22	N	811	PHE	CB-CG-CD2	12.53	129.57	120.80
15	G	141	TYR	CB-CG-CD1	-12.51	113.49	121.00
9	A	159	TYR	CB-CG-CD2	12.48	128.49	121.00
22	N	269	ARG	NE-CZ-NH2	-12.48	114.06	120.30
1	Z	71	TYR	CB-CG-CD2	-12.47	113.52	121.00
2	1	53	ARG	NE-CZ-NH1	12.39	126.50	120.30
24	P	369	TYR	CB-CG-CD2	-12.37	113.58	121.00
6	5	236	TYR	CB-CG-CD1	-12.36	113.58	121.00
12	D	3	TYR	CB-CG-CD2	-12.36	113.58	121.00
6	5	236	TYR	CB-CG-CD2	12.30	128.38	121.00
5	4	12	TYR	CB-CG-CD1	12.29	128.37	121.00
19	K	178	ARG	NE-CZ-NH2	-12.27	114.17	120.30
2	1	63	ARG	NE-CZ-NH2	-12.25	114.17	120.30
16	H	200	ARG	NE-CZ-NH1	12.25	126.43	120.30
27	S	408	ARG	NE-CZ-NH2	-12.24	114.18	120.30
23	O	156	TYR	CB-CG-CD1	12.22	128.33	121.00
26	R	295	TYR	CB-CG-CD1	-12.14	113.72	121.00
10	B	130	PHE	CB-CG-CD1	12.12	129.28	120.80
20	L	367	PHE	CB-CG-CD1	12.09	129.26	120.80
18	J	334	ARG	NE-CZ-NH1	12.08	126.34	120.30
10	B	6	TYR	CB-CG-CD1	12.07	128.24	121.00
7	6	61	PHE	CB-CG-CD1	11.99	129.19	120.80
22	N	253	TYR	CB-CG-CD1	11.97	128.19	121.00
4	3	120	PHE	CB-CG-CD1	-11.97	112.42	120.80
4	3	99	ARG	NE-CZ-NH1	11.97	126.28	120.30
26	R	101	ARG	NE-CZ-NH2	-11.96	114.32	120.30
9	A	27	TYR	CB-CG-CD2	-11.93	113.84	121.00
26	R	312	ARG	NE-CZ-NH1	11.93	126.26	120.30
6	5	202	TYR	CB-CG-CD2	-11.91	113.85	121.00
22	N	179	TYR	CB-CG-CD1	11.91	128.15	121.00
15	G	93	ARG	NE-CZ-NH1	11.85	126.22	120.30
25	Q	415	TYR	CB-CG-CD1	-11.83	113.90	121.00
24	P	185	PHE	CB-CG-CD2	-11.82	112.52	120.80
29	U	190	ARG	NE-CZ-NH1	11.78	126.19	120.30
14	F	193	ARG	NE-CZ-NH2	-11.73	114.44	120.30
8	7	189	TYR	CB-CG-CD2	-11.72	113.97	121.00
10	B	24	TYR	CB-CG-CD1	11.68	128.01	121.00
22	N	96	TYR	CB-CG-CD2	-11.67	114.00	121.00
19	K	391	ARG	NE-CZ-NH1	11.64	126.12	120.30
22	N	55	ARG	NE-CZ-NH1	11.60	126.10	120.30
14	F	157	ARG	NE-CZ-NH1	11.54	126.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	D	169	ARG	NE-CZ-NH1	11.54	126.07	120.30
14	F	123	TYR	CB-CG-CD1	-11.54	114.08	121.00
26	R	312	ARG	NE-CZ-NH2	-11.54	114.53	120.30
15	G	126	TYR	CB-CG-CD2	11.52	127.91	121.00
12	D	109	ARG	NE-CZ-NH1	11.51	126.06	120.30
16	H	284	ARG	NE-CZ-NH1	11.51	126.05	120.30
11	C	121	TYR	CB-CG-CD2	-11.47	114.11	121.00
21	M	158	TYR	CB-CG-CD1	11.46	127.88	121.00
7	6	201	ARG	NE-CZ-NH1	11.45	126.02	120.30
27	S	228	ARG	NE-CZ-NH1	-11.43	114.59	120.30
18	J	297	ARG	NE-CZ-NH1	11.40	126.00	120.30
22	N	108	TYR	CB-CG-CD2	-11.37	114.18	121.00
16	H	118	PHE	CB-CG-CD1	11.37	128.76	120.80
1	Z	469	TYR	CB-CG-CD1	11.33	127.80	121.00
22	N	269	ARG	NE-CZ-NH1	11.31	125.96	120.30
24	P	214	PHE	CB-CG-CD1	-11.30	112.89	120.80
1	Z	816	TYR	CB-CG-CD1	-11.28	114.23	121.00
26	R	337	PHE	CB-CG-CD1	11.27	128.69	120.80
26	R	142	PHE	CB-CG-CD2	-11.20	112.96	120.80
6	5	220	TYR	CB-CG-CD1	11.11	127.67	121.00
16	H	200	ARG	NE-CZ-NH2	-11.10	114.75	120.30
22	N	650	TYR	CB-CG-CD2	-11.10	114.34	121.00
22	N	395	ARG	NE-CZ-NH2	-11.08	114.76	120.30
18	J	369	TYR	CB-CG-CD1	-11.07	114.36	121.00
1	Z	103	TYR	CB-CG-CD1	-10.96	114.42	121.00
22	N	644	TYR	CB-CG-CD1	-10.95	114.43	121.00
27	S	181	TYR	CB-CG-CD1	-10.94	114.44	121.00
12	D	57	ARG	NE-CZ-NH1	-10.92	114.84	120.30
23	O	213	PHE	CB-CG-CD2	-10.90	113.17	120.80
1	Z	439	TYR	CB-CG-CD2	-10.90	114.46	121.00
20	L	243	PHE	CB-CG-CD1	10.87	128.41	120.80
28	T	268	ARG	NE-CZ-NH2	-10.87	114.86	120.30
3	2	244	ARG	NE-CZ-NH2	-10.85	114.88	120.30
25	Q	233	TYR	CB-CG-CD2	-10.82	114.51	121.00
20	L	146	ARG	NE-CZ-NH2	-10.78	114.91	120.30
17	I	411	ARG	NE-CZ-NH2	-10.70	114.95	120.30
4	3	100	PHE	CB-CG-CD2	10.65	128.25	120.80
28	T	178	TYR	CG-CD1-CE1	-10.60	112.82	121.30
1	Z	380	PHE	CB-CG-CD1	10.57	128.20	120.80
7	6	125	TYR	CB-CG-CD1	-10.56	114.66	121.00
8	7	169	TYR	CB-CG-CD2	10.56	127.34	121.00
10	B	89	ARG	NE-CZ-NH1	-10.48	115.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	713	TYR	CB-CG-CD2	-10.46	114.72	121.00
21	M	185	TYR	CB-CG-CD2	-10.46	114.72	121.00
22	N	199	ARG	NE-CZ-NH1	-10.46	115.07	120.30
18	J	271	ARG	NE-CZ-NH2	-10.45	115.07	120.30
20	L	344	ARG	NE-CZ-NH2	-10.44	115.08	120.30
10	B	83	TYR	CG-CD1-CE1	-10.44	112.95	121.30
24	P	304	ASP	CB-CG-OD2	-10.42	108.92	118.30
27	S	264	TYR	CB-CG-CD1	-10.41	114.75	121.00
25	Q	72	TYR	CB-CG-CD2	10.41	127.25	121.00
2	1	200	ARG	NE-CZ-NH1	10.41	125.50	120.30
25	Q	11	ARG	NE-CZ-NH2	-10.38	115.11	120.30
24	P	55	ARG	NE-CZ-NH1	10.37	125.48	120.30
1	Z	838	ARG	NE-CZ-NH1	10.37	125.48	120.30
13	E	162	PHE	CB-CG-CD2	10.34	128.04	120.80
25	Q	278	ARG	NE-CZ-NH2	-10.34	115.13	120.30
16	H	339	ARG	NE-CZ-NH1	10.34	125.47	120.30
16	H	258	ARG	NE-CZ-NH1	-10.33	115.13	120.30
21	M	248	PHE	CB-CG-CD2	-10.32	113.58	120.80
25	Q	229	TYR	CB-CG-CD2	-10.28	114.83	121.00
24	P	191	ARG	NE-CZ-NH1	10.26	125.43	120.30
20	L	69	PHE	CB-CG-CD2	-10.25	113.62	120.80
22	N	572	ARG	NE-CZ-NH2	-10.24	115.18	120.30
27	S	467	TYR	CB-CG-CD1	-10.24	114.86	121.00
2	1	122	TYR	CB-CG-CD2	10.20	127.12	121.00
22	N	55	ARG	NE-CZ-NH2	-10.21	115.20	120.30
9	A	27	TYR	CB-CG-CD1	10.20	127.12	121.00
14	F	18	ARG	NE-CZ-NH2	-10.20	115.20	120.30
16	H	386	ARG	NE-CZ-NH2	10.19	125.39	120.30
12	D	106	TYR	CB-CG-CD2	10.18	127.11	121.00
1	Z	100	ARG	NE-CZ-NH1	10.18	125.39	120.30
4	3	203	ARG	NE-CZ-NH2	-10.16	115.22	120.30
26	R	192	ARG	NE-CZ-NH2	-10.15	115.22	120.30
27	S	216	ARG	NE-CZ-NH2	-10.15	115.22	120.30
25	Q	310	ARG	NE-CZ-NH2	-10.14	115.23	120.30
25	Q	415	TYR	CB-CG-CD2	10.13	127.08	121.00
3	2	133	TYR	CG-CD2-CE2	-10.13	113.20	121.30
5	4	116	TYR	CG-CD1-CE1	-10.11	113.21	121.30
26	R	337	PHE	CB-CG-CD2	-10.11	113.72	120.80
3	2	51	TYR	CB-CG-CD1	10.11	127.07	121.00
23	O	352	ARG	NE-CZ-NH1	10.11	125.35	120.30
24	P	227	TYR	CB-CG-CD2	-10.10	114.94	121.00
5	4	134	TYR	CB-CG-CD2	10.09	127.06	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	226	TYR	CB-CG-CD1	10.07	127.04	121.00
23	O	63	PHE	CB-CG-CD1	-10.06	113.76	120.80
20	L	360	ASP	CB-CG-OD1	10.00	127.30	118.30
3	2	85	TYR	CB-CG-CD2	9.99	126.99	121.00
24	P	392	PHE	CB-CG-CD2	-9.98	113.81	120.80
11	C	96	ARG	NE-CZ-NH1	9.93	125.27	120.30
12	D	95	ARG	NE-CZ-NH1	9.93	125.27	120.30
21	M	129	ARG	NE-CZ-NH2	-9.86	115.37	120.30
25	Q	231	TYR	CB-CG-CD1	-9.86	115.09	121.00
5	4	134	TYR	CB-CG-CD1	-9.85	115.09	121.00
1	Z	407	MET	CG-SD-CE	-9.85	84.45	100.20
6	5	212	TYR	CB-CG-CD2	-9.83	115.10	121.00
10	B	220	ARG	NE-CZ-NH2	9.83	125.21	120.30
16	H	118	PHE	CB-CG-CD2	-9.81	113.93	120.80
25	Q	72	TYR	CB-CG-CD1	-9.81	115.11	121.00
28	T	208	PHE	CB-CG-CD1	-9.79	113.94	120.80
7	6	213	ARG	NE-CZ-NH2	9.78	125.19	120.30
12	D	171	PHE	CB-CG-CD2	-9.76	113.97	120.80
17	I	210	TYR	CB-CG-CD1	9.74	126.84	121.00
12	D	163	ARG	NE-CZ-NH2	-9.72	115.44	120.30
27	S	349	ARG	NE-CZ-NH2	-9.71	115.45	120.30
20	L	367	PHE	CB-CG-CD2	-9.70	114.01	120.80
1	Z	713	PHE	CB-CG-CD2	-9.70	114.01	120.80
23	O	156	TYR	CB-CG-CD2	-9.70	115.18	121.00
5	4	130	ALA	N-CA-CB	9.64	123.60	110.10
14	F	180	MET	CG-SD-CE	-9.64	84.78	100.20
2	1	29	ARG	NE-CZ-NH1	9.61	125.11	120.30
12	D	139	ASP	CB-CG-OD1	-9.57	109.69	118.30
23	O	240	PHE	CB-CG-CD1	9.56	127.49	120.80
28	T	178	TYR	CB-CG-CD1	-9.54	115.27	121.00
2	1	200	ARG	NE-CZ-NH2	-9.53	115.53	120.30
18	J	375	ARG	NE-CZ-NH2	-9.51	115.54	120.30
26	R	259	TYR	CB-CG-CD2	-9.49	115.31	121.00
29	U	90	ARG	NE-CZ-NH2	-9.49	115.56	120.30
31	W	21	PHE	CB-CG-CD1	9.48	127.44	120.80
8	7	75	TYR	CB-CG-CD2	-9.46	115.32	121.00
10	B	199	PHE	CB-CG-CD1	-9.46	114.18	120.80
8	7	222	TYR	CB-CG-CD2	9.44	126.66	121.00
22	N	811	PHE	CB-CG-CD1	-9.43	114.20	120.80
1	Z	819	TYR	CB-CG-CD2	9.42	126.65	121.00
22	N	875	PHE	CB-CG-CD2	-9.40	114.22	120.80
25	Q	194	ARG	NE-CZ-NH1	-9.39	115.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	J	44	ARG	NE-CZ-NH2	9.38	124.99	120.30
16	H	237	PHE	CB-CG-CD2	-9.36	114.25	120.80
25	Q	243	ASP	CB-CG-OD1	9.35	126.72	118.30
1	Z	416	MET	CG-SD-CE	-9.35	85.24	100.20
20	L	223	ARG	NE-CZ-NH2	-9.35	115.63	120.30
8	7	169	TYR	CB-CG-CD1	-9.33	115.41	121.00
3	2	79	PHE	CB-CG-CD2	-9.32	114.27	120.80
4	3	74	TYR	CB-CG-CD2	-9.32	115.41	121.00
18	J	43	ARG	NE-CZ-NH2	-9.32	115.64	120.30
12	D	3	TYR	CB-CG-CD1	9.31	126.59	121.00
16	H	258	ARG	NE-CZ-NH2	9.31	124.96	120.30
7	6	128	ARG	NE-CZ-NH2	-9.30	115.65	120.30
20	L	223	ARG	NE-CZ-NH1	9.29	124.95	120.30
10	B	145	TYR	CB-CG-CD1	9.29	126.58	121.00
31	W	112	PHE	CB-CG-CD1	-9.29	114.30	120.80
22	N	205	TYR	CB-CG-CD2	-9.27	115.44	121.00
8	7	155	MET	CG-SD-CE	-9.24	85.41	100.20
24	P	266	ALA	N-CA-CB	-9.21	97.21	110.10
14	F	193	ARG	NE-CZ-NH1	9.16	124.88	120.30
27	S	306	ARG	NE-CZ-NH1	9.15	124.87	120.30
25	Q	231	TYR	CG-CD2-CE2	-9.13	113.99	121.30
6	5	116	ARG	NE-CZ-NH2	-9.13	115.73	120.30
16	H	237	PHE	CB-CG-CD1	9.12	127.19	120.80
25	Q	81	SER	N-CA-CB	9.07	124.11	110.50
7	6	239	ARG	NE-CZ-NH2	-9.04	115.78	120.30
28	T	344	ARG	NE-CZ-NH2	9.04	124.82	120.30
16	H	366	ARG	NE-CZ-NH2	-9.02	115.79	120.30
2	1	168	TYR	CB-CG-CD2	-9.02	115.59	121.00
24	P	312	MET	CG-SD-CE	-9.00	85.81	100.20
27	S	181	TYR	CB-CG-CD2	8.98	126.39	121.00
12	D	88	ARG	NE-CZ-NH1	8.97	124.79	120.30
31	W	143	PHE	CB-CG-CD1	-8.97	114.52	120.80
19	K	313	ARG	NE-CZ-NH2	-8.94	115.83	120.30
18	J	43	ARG	NE-CZ-NH1	8.94	124.77	120.30
23	O	96	PHE	CB-CG-CD2	8.93	127.05	120.80
24	P	351	TRP	CB-CG-CD2	-8.93	115.00	126.60
1	Z	250	ARG	NE-CZ-NH2	-8.92	115.84	120.30
27	S	166	TYR	CB-CG-CD1	8.91	126.35	121.00
26	R	257	ARG	NE-CZ-NH1	8.88	124.74	120.30
1	Z	103	TYR	CB-CG-CD2	8.88	126.33	121.00
18	J	72	TYR	CG-CD2-CE2	-8.87	114.20	121.30
27	S	230	PHE	CB-CG-CD2	8.85	126.99	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	G	161	TYR	CB-CG-CD1	8.85	126.31	121.00
21	M	248	PHE	CB-CG-CD1	8.83	126.98	120.80
5	4	18	ASP	CB-CG-OD2	-8.82	110.36	118.30
21	M	295	ARG	NE-CZ-NH1	8.82	124.71	120.30
1	Z	703	ARG	NE-CZ-NH1	8.81	124.71	120.30
8	7	229	TYR	CB-CG-CD2	8.81	126.29	121.00
29	U	25	ARG	NE-CZ-NH1	-8.80	115.90	120.30
1	Z	434	TYR	CB-CG-CD2	-8.79	115.72	121.00
5	4	144	ASP	CB-CG-OD2	-8.79	110.39	118.30
2	1	29	ARG	NE-CZ-NH2	-8.79	115.91	120.30
19	K	60	TYR	CB-CG-CD1	8.79	126.27	121.00
1	Z	62	ARG	NE-CZ-NH1	-8.78	115.91	120.30
27	S	414	TYR	CB-CG-CD2	-8.78	115.73	121.00
8	7	186	TYR	CB-CG-CD1	-8.77	115.74	121.00
24	P	227	TYR	CB-CG-CD1	8.77	126.26	121.00
24	P	39	ARG	NE-CZ-NH1	8.76	124.68	120.30
20	L	294	ARG	NE-CZ-NH2	8.75	124.67	120.30
22	N	695	MET	CG-SD-CE	-8.74	86.22	100.20
18	J	247	PHE	CB-CG-CD1	8.73	126.91	120.80
26	R	311	TYR	CB-CG-CD1	-8.73	115.77	121.00
6	5	84	TYR	CB-CG-CD2	-8.72	115.77	121.00
19	K	338	ARG	NE-CZ-NH2	-8.72	115.94	120.30
18	J	258	ARG	NE-CZ-NH2	8.71	124.66	120.30
25	Q	96	PHE	CB-CG-CD1	-8.70	114.71	120.80
12	D	117	ARG	NE-CZ-NH1	-8.69	115.95	120.30
17	I	333	ARG	NE-CZ-NH2	-8.69	115.95	120.30
25	Q	20	ARG	NE-CZ-NH1	-8.69	115.95	120.30
15	G	130	ARG	NE-CZ-NH1	8.68	124.64	120.30
22	N	628	ARG	NE-CZ-NH2	-8.68	115.96	120.30
6	5	212	TYR	CB-CG-CD1	8.68	126.21	121.00
4	3	135	ASP	CB-CG-OD1	8.66	126.10	118.30
11	C	19	TYR	CB-CG-CD1	-8.66	115.80	121.00
30	V	68	ARG	NE-CZ-NH1	8.66	124.63	120.30
1	Z	673	ARG	NE-CZ-NH1	8.66	124.63	120.30
8	7	222	TYR	CB-CG-CD1	-8.66	115.81	121.00
24	P	226	TYR	CB-CG-CD2	-8.65	115.81	121.00
22	N	361	ARG	NE-CZ-NH2	8.64	124.62	120.30
25	Q	315	ASP	CB-CG-OD2	-8.62	110.54	118.30
18	J	369	TYR	CB-CG-CD2	8.58	126.14	121.00
8	7	216	ARG	NE-CZ-NH1	-8.57	116.02	120.30
22	N	813	TYR	CD1-CE1-CZ	8.55	127.50	119.80
5	4	178	PHE	CB-CG-CD2	8.54	126.77	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	T	167	TYR	CB-CG-CD2	-8.53	115.89	121.00
29	U	267	ARG	NE-CZ-NH1	8.52	124.56	120.30
26	R	300	ARG	NE-CZ-NH1	-8.52	116.04	120.30
23	O	240	PHE	CB-CG-CD2	-8.51	114.84	120.80
3	2	132	ARG	NE-CZ-NH1	-8.50	116.05	120.30
9	A	144	ASP	CB-CG-OD1	-8.48	110.66	118.30
19	K	121	ARG	NE-CZ-NH1	8.48	124.54	120.30
22	N	108	TYR	CB-CG-CD1	8.47	126.08	121.00
20	L	294	ARG	NE-CZ-NH1	-8.47	116.07	120.30
19	K	191	TYR	CB-CG-CD1	8.46	126.08	121.00
9	A	245	ARG	NE-CZ-NH2	8.44	124.52	120.30
24	P	351	TRP	CB-CG-CD1	8.44	137.97	127.00
23	O	116	THR	CA-CB-CG2	-8.44	100.59	112.40
3	2	133	TYR	CZ-CE2-CD2	8.42	127.38	119.80
1	Z	833	PHE	CB-CG-CD2	8.41	126.69	120.80
5	4	86	ARG	NE-CZ-NH1	8.40	124.50	120.30
11	C	3	ARG	NE-CZ-NH1	8.39	124.50	120.30
17	I	333	ARG	NE-CZ-NH1	8.37	124.48	120.30
19	K	60	TYR	CB-CG-CD2	-8.35	115.99	121.00
30	V	73	PHE	CB-CG-CD1	8.35	126.64	120.80
24	P	185	PHE	CB-CG-CD1	8.34	126.64	120.80
20	L	25	ARG	NE-CZ-NH1	8.34	124.47	120.30
25	Q	229	TYR	CB-CG-CD1	8.34	126.00	121.00
17	I	319	PHE	CB-CG-CD1	-8.33	114.97	120.80
23	O	232	TRP	CB-CG-CD2	-8.33	115.77	126.60
5	4	161	ARG	NE-CZ-NH1	8.32	124.46	120.30
17	I	294	ARG	NE-CZ-NH1	8.32	124.46	120.30
18	J	211	PHE	CB-CG-CD2	-8.32	114.97	120.80
2	1	123	ARG	NE-CZ-NH2	-8.32	116.14	120.30
1	Z	330	PHE	CB-CG-CD1	8.32	126.62	120.80
14	F	171	TYR	CB-CG-CD2	8.31	125.99	121.00
27	S	306	ARG	NE-CZ-NH2	-8.29	116.15	120.30
8	7	160	TYR	CB-CG-CD2	-8.29	116.03	121.00
26	R	292	TYR	CB-CG-CD2	8.29	125.97	121.00
6	5	116	ARG	NE-CZ-NH1	8.28	124.44	120.30
13	E	123	PHE	CB-CG-CD1	8.28	126.59	120.80
21	M	308	ARG	NE-CZ-NH1	8.27	124.43	120.30
1	Z	713	PHE	CB-CG-CD1	8.26	126.58	120.80
12	D	139	ASP	CB-CG-OD2	8.26	125.74	118.30
3	2	132	ARG	NE-CZ-NH2	8.26	124.43	120.30
22	N	49	TYR	CB-CG-CD1	8.26	125.95	121.00
1	Z	217	LEU	CB-CG-CD2	8.25	125.03	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	O	284	ARG	NE-CZ-NH1	-8.25	116.17	120.30
26	R	342	ARG	NE-CZ-NH2	-8.25	116.17	120.30
14	F	126	ARG	NE-CZ-NH2	-8.24	116.18	120.30
19	K	248	ARG	NE-CZ-NH1	-8.23	116.19	120.30
24	P	324	TYR	CB-CG-CD2	-8.22	116.06	121.00
2	1	172	TYR	CB-CG-CD2	8.22	125.93	121.00
3	2	241	ARG	NE-CZ-NH1	-8.21	116.20	120.30
28	T	241	TYR	CB-CG-CD2	-8.20	116.08	121.00
27	S	474	LEU	CB-CG-CD2	8.18	124.91	111.00
1	Z	740	ARG	NE-CZ-NH2	8.18	124.39	120.30
1	Z	62	ARG	NE-CZ-NH2	8.17	124.39	120.30
24	P	199	TYR	CB-CG-CD2	-8.17	116.10	121.00
2	1	99	PHE	CB-CG-CD2	-8.17	115.08	120.80
6	5	171	TYR	CB-CG-CD2	8.17	125.90	121.00
12	D	110	TYR	CB-CG-CD1	-8.16	116.10	121.00
31	W	119	ASP	CB-CG-OD1	-8.16	110.95	118.30
14	F	24	TYR	CB-CG-CD2	-8.16	116.10	121.00
17	I	303	ARG	NE-CZ-NH1	-8.16	116.22	120.30
22	N	590	TYR	CB-CG-CD2	-8.16	116.11	121.00
22	N	900	TYR	CB-CG-CD2	-8.16	116.11	121.00
1	Z	527	VAL	CA-CB-CG2	-8.14	98.69	110.90
9	A	245	ARG	NE-CZ-NH1	-8.14	116.23	120.30
11	C	128	ARG	NE-CZ-NH1	8.14	124.37	120.30
19	K	81	ARG	NE-CZ-NH2	-8.14	116.23	120.30
3	2	167	TYR	CB-CG-CD1	8.13	125.88	121.00
5	4	178	PHE	CB-CG-CD1	-8.13	115.11	120.80
1	Z	181	ARG	NE-CZ-NH1	8.12	124.36	120.30
22	N	253	TYR	CB-CG-CD2	-8.12	116.13	121.00
24	P	304	ASP	CB-CG-OD1	8.12	125.61	118.30
20	L	173	TYR	CB-CG-CD1	-8.11	116.13	121.00
1	Z	816	TYR	CG-CD1-CE1	-8.11	114.81	121.30
21	M	226	TYR	CB-CG-CD1	-8.09	116.14	121.00
19	K	44	TYR	CB-CG-CD2	8.09	125.85	121.00
29	U	211	TYR	CB-CG-CD2	-8.08	116.15	121.00
1	Z	71	TYR	CB-CG-CD1	8.07	125.84	121.00
19	K	417	TYR	CG-CD2-CE2	-8.07	114.84	121.30
10	B	173	PHE	CB-CG-CD2	-8.06	115.16	120.80
29	U	95	TYR	CG-CD1-CE1	-8.06	114.85	121.30
28	T	259	PHE	CB-CG-CD2	-8.06	115.16	120.80
6	5	220	TYR	CB-CG-CD2	-8.06	116.17	121.00
7	6	33	TYR	CB-CG-CD1	-8.06	116.17	121.00
22	N	205	TYR	CG-CD1-CE1	8.05	127.74	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	802	TYR	CB-CG-CD1	-8.05	116.17	121.00
20	L	297	ARG	NE-CZ-NH2	-8.04	116.28	120.30
5	4	95	ARG	NE-CZ-NH2	8.04	124.32	120.30
14	F	107	ARG	NE-CZ-NH1	8.03	124.31	120.30
12	D	55	ASP	CB-CG-OD1	-8.00	111.10	118.30
4	3	147	TYR	CB-CG-CD1	-7.99	116.20	121.00
29	U	239	ASP	CB-CG-OD1	7.99	125.49	118.30
22	N	199	ARG	NE-CZ-NH2	7.98	124.29	120.30
14	F	97	PHE	CB-CG-CD2	7.98	126.39	120.80
23	O	60	TYR	CB-CG-CD2	-7.98	116.21	121.00
20	L	199	VAL	CA-CB-CG2	-7.97	98.94	110.90
19	K	191	TYR	CB-CG-CD2	-7.97	116.22	121.00
20	L	78	ARG	NE-CZ-NH2	7.97	124.28	120.30
2	1	125	ARG	NE-CZ-NH1	7.96	124.28	120.30
25	Q	233	TYR	CB-CG-CD1	7.96	125.77	121.00
14	F	128	TYR	CB-CG-CD2	7.94	125.77	121.00
23	O	70	ARG	NE-CZ-NH1	7.94	124.27	120.30
23	O	349	MET	CG-SD-CE	-7.94	87.49	100.20
16	H	139	ARG	NE-CZ-NH1	7.93	124.27	120.30
28	T	145	ARG	NE-CZ-NH1	-7.93	116.34	120.30
26	R	323	PHE	CB-CG-CD2	7.92	126.34	120.80
14	F	157	ARG	NE-CZ-NH2	-7.91	116.35	120.30
12	D	5	ARG	NE-CZ-NH1	7.89	124.25	120.30
12	D	209	ALA	CB-CA-C	-7.89	98.26	110.10
6	5	171	TYR	CB-CG-CD1	-7.88	116.27	121.00
9	A	95	ARG	NE-CZ-NH2	7.87	124.24	120.30
29	U	267	ARG	NE-CZ-NH2	-7.87	116.36	120.30
24	P	240	TYR	CB-CG-CD1	-7.87	116.28	121.00
24	P	174	TYR	CB-CG-CD1	-7.86	116.28	121.00
26	R	34	ASP	CB-CG-OD2	-7.86	111.23	118.30
15	G	59	TYR	CB-CG-CD1	-7.86	116.29	121.00
7	6	201	ARG	NE-CZ-NH2	-7.85	116.37	120.30
6	5	128	ARG	NE-CZ-NH2	7.85	124.22	120.30
1	Z	432	TYR	CB-CG-CD1	-7.84	116.30	121.00
10	B	13	PHE	CB-CG-CD2	-7.84	115.31	120.80
1	Z	181	ARG	NE-CZ-NH2	-7.83	116.39	120.30
8	7	107	TYR	CB-CG-CD1	7.82	125.69	121.00
4	3	50	TYR	CB-CG-CD2	-7.81	116.31	121.00
28	T	167	TYR	CB-CG-CD1	7.81	125.69	121.00
1	Z	600	TYR	CB-CG-CD1	7.81	125.69	121.00
22	N	579	ARG	NE-CZ-NH1	7.81	124.20	120.30
22	N	889	LEU	CB-CG-CD1	7.80	124.27	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	C	8	ARG	NE-CZ-NH1	7.79	124.20	120.30
26	R	292	TYR	CG-CD1-CE1	7.78	127.52	121.30
25	Q	94	ASP	CB-CG-OD2	7.78	125.30	118.30
11	C	19	TYR	CB-CG-CD2	7.77	125.66	121.00
14	F	153	TYR	CB-CG-CD1	7.77	125.66	121.00
26	R	104	MET	CG-SD-CE	-7.77	87.77	100.20
3	2	51	TYR	CG-CD1-CE1	7.76	127.51	121.30
8	7	227	ARG	NE-CZ-NH1	7.76	124.18	120.30
19	K	149	SER	N-CA-CB	7.76	122.14	110.50
27	S	216	ARG	NE-CZ-NH1	7.76	124.18	120.30
8	7	186	TYR	CG-CD2-CE2	-7.75	115.10	121.30
7	6	133	TYR	CB-CG-CD1	-7.75	116.35	121.00
21	M	168	TYR	CB-CG-CD1	7.74	125.64	121.00
1	Z	489	TYR	CG-CD2-CE2	-7.74	115.11	121.30
6	5	166	ARG	NE-CZ-NH2	-7.74	116.43	120.30
18	J	312	ASP	CB-CG-OD2	7.72	125.25	118.30
17	I	225	TYR	CB-CG-CD2	7.72	125.63	121.00
22	N	140	ARG	NE-CZ-NH1	7.71	124.16	120.30
23	O	283	THR	CA-CB-CG2	-7.71	101.60	112.40
8	7	55	SER	N-CA-CB	7.69	122.04	110.50
5	4	33	ASP	CB-CG-OD2	-7.69	111.38	118.30
13	E	185	TYR	CB-CG-CD2	-7.69	116.39	121.00
22	N	616	ARG	NE-CZ-NH1	7.69	124.14	120.30
31	W	119	ASP	CB-CG-OD2	7.67	125.21	118.30
20	L	372	ARG	NE-CZ-NH2	-7.67	116.47	120.30
17	I	408	ARG	NE-CZ-NH1	7.66	124.13	120.30
21	M	114	ASP	N-CA-CB	7.66	124.39	110.60
23	O	226	ARG	NE-CZ-NH1	7.66	124.13	120.30
27	S	392	TYR	CB-CG-CD1	-7.64	116.41	121.00
29	U	95	TYR	CB-CG-CD1	-7.62	116.43	121.00
8	7	219	ARG	NE-CZ-NH2	7.62	124.11	120.30
16	H	355	PHE	CB-CG-CD1	7.61	126.12	120.80
22	N	875	PHE	CG-CD2-CE2	-7.60	112.44	120.80
27	S	470	ARG	NE-CZ-NH2	7.60	124.10	120.30
3	2	201	ALA	CB-CA-C	-7.60	98.70	110.10
9	A	160	TYR	CB-CG-CD1	7.59	125.56	121.00
19	K	392	TYR	CB-CG-CD1	7.59	125.56	121.00
6	5	156	MET	CG-SD-CE	-7.58	88.07	100.20
22	N	598	ALA	CB-CA-C	-7.58	98.72	110.10
25	Q	243	ASP	CB-CG-OD2	-7.58	111.47	118.30
26	R	24	PHE	CB-CG-CD1	-7.58	115.49	120.80
23	O	280	MET	CG-SD-CE	7.57	112.32	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	1	122	TYR	CB-CG-CD1	-7.55	116.47	121.00
17	I	410	ARG	NE-CZ-NH1	-7.55	116.53	120.30
21	M	133	PHE	CB-CG-CD2	-7.53	115.53	120.80
3	2	170	MET	CG-SD-CE	7.52	112.23	100.20
18	J	49	ARG	NE-CZ-NH1	-7.51	116.55	120.30
10	B	229	TYR	CB-CG-CD2	7.51	125.50	121.00
8	7	107	TYR	CB-CG-CD2	-7.50	116.50	121.00
25	Q	187	ARG	NE-CZ-NH2	-7.50	116.55	120.30
3	2	79	PHE	CB-CG-CD1	7.49	126.04	120.80
27	S	264	TYR	CB-CG-CD2	7.48	125.49	121.00
4	3	198	ARG	CD-NE-CZ	7.47	134.06	123.60
19	K	287	ARG	NE-CZ-NH2	7.47	124.03	120.30
14	F	154	PHE	CB-CG-CD2	-7.46	115.58	120.80
16	H	333	ARG	NE-CZ-NH1	-7.46	116.57	120.30
20	L	216	ARG	NE-CZ-NH2	-7.45	116.57	120.30
16	H	264	ALA	N-CA-CB	7.44	120.51	110.10
14	F	159	MET	CG-SD-CE	-7.43	88.31	100.20
25	Q	141	LYS	N-CA-CB	7.42	123.96	110.60
16	H	124	ASP	CB-CG-OD2	-7.42	111.62	118.30
20	L	221	TYR	CB-CG-CD1	7.40	125.44	121.00
27	S	373	ALA	CB-CA-C	-7.40	99.00	110.10
25	Q	177	TYR	CB-CG-CD2	-7.39	116.56	121.00
1	Z	346	ASP	CB-CG-OD1	-7.39	111.65	118.30
17	I	320	ASP	CB-CG-OD2	7.37	124.93	118.30
5	4	116	TYR	CB-CG-CD2	-7.37	116.58	121.00
28	T	302	TYR	CB-CG-CD2	-7.36	116.59	121.00
22	N	423	MET	CG-SD-CE	-7.35	88.44	100.20
25	Q	310	ARG	NE-CZ-NH1	7.35	123.97	120.30
10	B	77	SER	N-CA-CB	7.34	121.52	110.50
5	4	67	TYR	CB-CG-CD1	7.34	125.40	121.00
8	7	196	ARG	NE-CZ-NH2	7.33	123.97	120.30
7	6	148	ALA	N-CA-CB	7.32	120.35	110.10
19	K	53	PHE	CB-CG-CD1	-7.32	115.67	120.80
28	T	235	TYR	CB-CG-CD1	7.29	125.37	121.00
18	J	78	ARG	NE-CZ-NH2	-7.28	116.66	120.30
24	P	81	ASP	CB-CG-OD2	7.28	124.85	118.30
17	I	272	ARG	NE-CZ-NH1	7.28	123.94	120.30
22	N	676	THR	CA-CB-CG2	-7.28	102.21	112.40
14	F	196	ARG	NE-CZ-NH1	7.27	123.94	120.30
20	L	243	PHE	CB-CG-CD2	-7.27	115.71	120.80
29	U	228	TYR	CD1-CG-CD2	-7.26	109.91	117.90
6	5	222	ALA	N-CA-CB	7.26	120.26	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	83	TYR	CZ-CE2-CD2	-7.24	113.28	119.80
21	M	269	ARG	NE-CZ-NH2	7.24	123.92	120.30
1	Z	489	TYR	CB-CG-CD2	-7.24	116.66	121.00
14	F	82	ARG	NE-CZ-NH2	-7.24	116.68	120.30
28	T	245	PHE	CB-CG-CD1	-7.24	115.73	120.80
19	K	366	ARG	NE-CZ-NH1	7.24	123.92	120.30
26	R	151	TYR	CG-CD1-CE1	-7.23	115.51	121.30
9	A	163	PHE	CB-CG-CD2	7.23	125.86	120.80
26	R	183	TYR	CB-CG-CD2	-7.23	116.66	121.00
1	Z	678	LEU	CB-CG-CD2	7.22	123.28	111.00
18	J	340	ARG	NE-CZ-NH2	-7.22	116.69	120.30
28	T	128	PHE	CB-CG-CD1	7.22	125.86	120.80
28	T	174	TYR	CG-CD1-CE1	-7.21	115.53	121.30
5	4	86	ARG	NE-CZ-NH2	-7.21	116.70	120.30
20	L	269	THR	CA-CB-CG2	-7.20	102.31	112.40
22	N	489	ALA	N-CA-CB	7.19	120.17	110.10
25	Q	338	VAL	CA-CB-CG1	-7.19	100.12	110.90
31	W	21	PHE	CG-CD1-CE1	7.19	128.71	120.80
6	5	179	ARG	NE-CZ-NH2	-7.17	116.72	120.30
1	Z	227	ALA	N-CA-CB	7.16	120.13	110.10
10	B	116	SER	CB-CA-C	-7.16	96.50	110.10
21	M	112	ASP	CB-CG-OD2	7.16	124.74	118.30
8	7	186	TYR	CB-CG-CD2	7.14	125.29	121.00
1	Z	763	ARG	NE-CZ-NH2	-7.14	116.73	120.30
12	D	59	VAL	CA-CB-CG1	-7.14	100.19	110.90
19	K	227	PHE	CB-CG-CD2	7.14	125.80	120.80
7	6	161	ASP	CB-CG-OD2	-7.13	111.88	118.30
11	C	156	TYR	CG-CD2-CE2	-7.13	115.59	121.30
17	I	96	ARG	NE-CZ-NH1	7.12	123.86	120.30
22	N	368	ALA	N-CA-CB	7.12	120.07	110.10
30	V	104	ARG	NE-CZ-NH2	-7.12	116.74	120.30
22	N	494	TYR	CB-CG-CD2	7.12	125.27	121.00
24	P	187	LEU	CB-CA-C	-7.11	96.69	110.20
5	4	107	TYR	CB-CG-CD2	-7.11	116.74	121.00
23	O	330	ARG	NE-CZ-NH2	-7.11	116.75	120.30
16	H	174	TYR	CG-CD1-CE1	-7.10	115.62	121.30
21	M	409	ARG	NE-CZ-NH1	-7.10	116.75	120.30
6	5	83	ALA	N-CA-CB	7.10	120.04	110.10
11	C	80	THR	CA-CB-CG2	-7.10	102.47	112.40
19	K	97	ASP	CB-CG-OD2	-7.10	111.91	118.30
8	7	211	ARG	NE-CZ-NH2	-7.09	116.75	120.30
22	N	246	TYR	CB-CA-C	-7.09	96.21	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	5	81	ALA	N-CA-CB	7.09	120.03	110.10
8	7	177	TYR	CB-CG-CD1	-7.09	116.75	121.00
15	G	132	PHE	CB-CG-CD2	-7.09	115.84	120.80
30	V	161	ARG	NE-CZ-NH2	7.08	123.84	120.30
4	3	100	PHE	CB-CG-CD1	-7.08	115.84	120.80
5	4	161	ARG	NH1-CZ-NH2	-7.08	111.61	119.40
6	5	170	LEU	CB-CA-C	-7.08	96.75	110.20
4	3	45	MET	CG-SD-CE	-7.07	88.89	100.20
17	I	96	ARG	NE-CZ-NH2	-7.06	116.77	120.30
12	D	213	ARG	NE-CZ-NH2	7.06	123.83	120.30
1	Z	614	HIS	CA-CB-CG	7.05	125.59	113.60
7	6	106	SER	CB-CA-C	-7.05	96.70	110.10
17	I	386	ALA	N-CA-CB	7.05	119.97	110.10
30	V	73	PHE	CB-CG-CD2	-7.05	115.87	120.80
15	G	150	TYR	CB-CG-CD1	7.04	125.23	121.00
12	D	125	ARG	NE-CZ-NH1	7.04	123.82	120.30
14	F	3	ARG	NE-CZ-NH1	-7.04	116.78	120.30
9	A	96	TYR	CG-CD2-CE2	-7.03	115.67	121.30
12	D	36	ARG	CB-CA-C	-7.03	96.35	110.40
17	I	294	ARG	NE-CZ-NH2	-7.02	116.79	120.30
7	6	29	ARG	NE-CZ-NH1	7.01	123.80	120.30
28	T	200	LEU	CB-CG-CD2	-7.01	99.08	111.00
15	G	143	VAL	CG1-CB-CG2	7.00	122.10	110.90
29	U	95	TYR	CB-CG-CD2	-7.00	116.80	121.00
22	N	899	ARG	NE-CZ-NH2	-7.00	116.80	120.30
18	J	374	ARG	NE-CZ-NH1	7.00	123.80	120.30
10	B	199	PHE	CB-CG-CD2	6.99	125.69	120.80
30	V	125	VAL	CA-CB-CG2	-6.99	100.42	110.90
2	1	170	TYR	CB-CG-CD1	6.98	125.19	121.00
14	F	226	ASP	N-CA-CB	6.98	123.17	110.60
22	N	644	TYR	CB-CG-CD2	6.98	125.19	121.00
28	T	235	TYR	CB-CG-CD2	-6.98	116.81	121.00
25	Q	194	ARG	NE-CZ-NH2	6.98	123.79	120.30
22	N	783	TYR	CB-CG-CD2	-6.98	116.81	121.00
12	D	118	TYR	CZ-CE2-CD2	6.97	126.07	119.80
26	R	297	ARG	NH1-CZ-NH2	-6.96	111.74	119.40
22	N	246	TYR	CB-CG-CD2	-6.96	116.83	121.00
12	D	176	TYR	CB-CG-CD2	-6.95	116.83	121.00
22	N	765	VAL	CA-CB-CG2	-6.95	100.48	110.90
24	P	420	ASP	CB-CG-OD2	-6.94	112.05	118.30
28	T	118	ARG	NE-CZ-NH2	6.94	123.77	120.30
12	D	38	ARG	NE-CZ-NH1	6.94	123.77	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	713	PHE	CG-CD2-CE2	-6.94	113.17	120.80
19	K	41	TYR	CG-CD1-CE1	-6.94	115.75	121.30
9	A	228	ARG	N-CA-CB	6.93	123.08	110.60
30	V	200	TYR	CB-CG-CD1	-6.93	116.84	121.00
27	S	294	ARG	NE-CZ-NH1	-6.93	116.83	120.30
19	K	53	PHE	CB-CG-CD2	6.91	125.64	120.80
27	S	487	HIS	CA-CB-CG	6.91	125.34	113.60
22	N	147	TYR	CG-CD1-CE1	-6.91	115.78	121.30
11	C	3	ARG	NE-CZ-NH2	-6.90	116.85	120.30
20	L	25	ARG	NE-CZ-NH2	-6.90	116.85	120.30
12	D	106	TYR	CB-CG-CD1	-6.89	116.86	121.00
21	M	182	THR	CA-CB-CG2	-6.89	102.75	112.40
25	Q	344	ARG	N-CA-CB	6.89	123.00	110.60
24	P	55	ARG	NE-CZ-NH2	-6.88	116.86	120.30
1	Z	907	ASP	N-CA-CB	6.88	122.98	110.60
27	S	375	PHE	CB-CG-CD1	6.88	125.61	120.80
27	S	408	ARG	NE-CZ-NH1	6.87	123.74	120.30
10	B	36	VAL	CA-CB-CG1	6.87	121.20	110.90
10	B	121	TYR	CB-CG-CD2	-6.87	116.88	121.00
1	Z	136	GLU	OE1-CD-OE2	6.86	131.53	123.30
3	2	118	ARG	NE-CZ-NH1	6.86	123.73	120.30
13	E	137	PHE	CB-CG-CD1	6.86	125.60	120.80
17	I	186	ASP	CB-CG-OD1	6.86	124.47	118.30
26	R	193	ASP	CB-CG-OD1	-6.86	112.13	118.30
23	O	106	SER	N-CA-CB	6.85	120.78	110.50
9	A	227	PHE	CB-CG-CD2	-6.84	116.01	120.80
14	F	126	ARG	NE-CZ-NH1	6.83	123.72	120.30
8	7	250	THR	CA-CB-CG2	-6.82	102.85	112.40
20	L	213	ARG	NE-CZ-NH1	6.82	123.71	120.30
29	U	38	VAL	CG1-CB-CG2	6.81	121.80	110.90
15	G	159	TYR	CB-CG-CD1	-6.81	116.92	121.00
2	1	133	ILE	N-CA-C	-6.81	92.62	111.00
23	O	43	ASP	CB-CA-C	-6.80	96.80	110.40
20	L	286	ASP	CB-CG-OD2	6.80	124.42	118.30
23	O	175	ASP	CB-CG-OD1	-6.80	112.18	118.30
19	K	339	ARG	NE-CZ-NH1	6.79	123.70	120.30
7	6	64	HIS	CA-CB-CG	-6.79	102.05	113.60
25	Q	96	PHE	CB-CG-CD2	6.79	125.55	120.80
21	M	185	TYR	CG-CD2-CE2	-6.79	115.87	121.30
21	M	169	ASP	CB-CG-OD1	6.78	124.41	118.30
25	Q	282	ARG	NE-CZ-NH2	6.78	123.69	120.30
26	R	291	HIS	CB-CA-C	-6.78	96.84	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	96	TYR	CG-CD2-CE2	-6.78	115.88	121.30
12	D	109	ARG	NE-CZ-NH2	-6.78	116.91	120.30
15	G	119	TYR	CB-CG-CD2	6.78	125.06	121.00
13	E	84	ASP	CB-CG-OD2	6.77	124.39	118.30
26	R	53	TYR	CG-CD1-CE1	-6.77	115.88	121.30
18	J	232	ARG	NE-CZ-NH2	6.77	123.68	120.30
16	H	133	ASP	CB-CG-OD1	-6.76	112.21	118.30
1	Z	695	ALA	N-CA-CB	6.76	119.57	110.10
21	M	394	ALA	CB-CA-C	-6.76	99.96	110.10
11	C	249	ARG	NH1-CZ-NH2	-6.75	111.97	119.40
22	N	771	PHE	CG-CD2-CE2	-6.75	113.37	120.80
23	O	359	ASP	CB-CG-OD1	6.75	124.37	118.30
16	H	249	TYR	CB-CG-CD1	-6.75	116.95	121.00
3	2	85	TYR	CB-CG-CD1	-6.75	116.95	121.00
3	2	188	ASP	CB-CG-OD2	-6.74	112.23	118.30
13	E	103	TYR	CB-CG-CD1	6.74	125.04	121.00
2	1	113	ALA	N-CA-CB	6.74	119.53	110.10
20	L	198	VAL	CA-CB-CG2	-6.73	100.80	110.90
22	N	147	TYR	CB-CG-CD1	-6.73	116.96	121.00
1	Z	143	ARG	NE-CZ-NH2	6.73	123.67	120.30
19	K	399	PHE	CB-CG-CD1	-6.73	116.09	120.80
22	N	376	MET	CG-SD-CE	-6.73	89.43	100.20
25	Q	74	ARG	NE-CZ-NH1	6.73	123.67	120.30
18	J	200	ALA	CB-CA-C	-6.73	100.01	110.10
24	P	377	ARG	NE-CZ-NH1	6.72	123.66	120.30
10	B	100	VAL	CA-CB-CG1	6.72	120.98	110.90
1	Z	310	ASP	CB-CG-OD1	-6.72	112.26	118.30
9	A	160	TYR	CB-CG-CD2	-6.71	116.97	121.00
6	5	185	PHE	CB-CG-CD1	-6.71	116.10	120.80
3	2	139	ALA	N-CA-CB	6.71	119.49	110.10
10	B	60	ARG	NE-CZ-NH1	6.71	123.65	120.30
13	E	184	VAL	CA-CB-CG1	-6.70	100.85	110.90
30	V	90	VAL	CA-CB-CG2	6.70	120.95	110.90
25	Q	166	LEU	CB-CG-CD2	6.70	122.39	111.00
3	2	186	ARG	NE-CZ-NH2	-6.70	116.95	120.30
17	I	87	PRO	N-CA-CB	6.70	111.34	103.30
22	N	644	TYR	C-N-CA	6.69	138.43	121.70
5	4	153	ARG	NE-CZ-NH2	-6.68	116.96	120.30
22	N	260	PHE	CB-CG-CD2	6.68	125.47	120.80
27	S	457	TYR	CB-CG-CD2	-6.68	116.99	121.00
21	M	344	ARG	NE-CZ-NH2	-6.67	116.96	120.30
24	P	199	TYR	CG-CD2-CE2	-6.67	115.96	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	S	382	PHE	CB-CG-CD2	-6.67	116.13	120.80
30	V	302	ALA	CB-CA-C	-6.67	100.10	110.10
14	F	10	VAL	CA-CB-CG1	6.66	120.89	110.90
21	M	134	LEU	CB-CG-CD1	-6.66	99.67	111.00
7	6	222	ARG	NE-CZ-NH2	-6.66	116.97	120.30
19	K	178	ARG	NE-CZ-NH1	6.66	123.63	120.30
20	L	132	TYR	CB-CG-CD1	-6.66	117.00	121.00
1	Z	681	TYR	CB-CA-C	-6.66	97.09	110.40
17	I	422	SER	CB-CA-C	-6.65	97.47	110.10
21	M	133	PHE	CB-CG-CD1	6.65	125.45	120.80
13	E	20	ARG	NE-CZ-NH2	-6.65	116.97	120.30
24	P	151	THR	CA-CB-CG2	-6.65	103.10	112.40
23	O	183	VAL	CA-CB-CG1	6.64	120.86	110.90
6	5	224	TYR	CB-CG-CD2	6.64	124.98	121.00
9	A	85	ALA	CB-CA-C	-6.63	100.15	110.10
29	U	23	PHE	CB-CG-CD2	6.63	125.44	120.80
10	B	145	TYR	CG-CD2-CE2	6.62	126.60	121.30
31	W	159	THR	CA-CB-CG2	6.62	121.67	112.40
20	L	249	ALA	CB-CA-C	-6.62	100.17	110.10
22	N	444	TYR	CG-CD2-CE2	-6.62	116.00	121.30
24	P	436	MET	CG-SD-CE	-6.62	89.61	100.20
12	D	127	PHE	CB-CG-CD2	-6.62	116.17	120.80
15	G	129	VAL	CA-CB-CG1	6.61	120.82	110.90
1	Z	349	TYR	CB-CG-CD1	6.61	124.96	121.00
8	7	259	MET	CG-SD-CE	-6.61	89.63	100.20
4	3	113	ASP	CB-CG-OD2	-6.60	112.36	118.30
5	4	145	ARG	NE-CZ-NH2	-6.60	117.00	120.30
27	S	335	VAL	CA-CB-CG2	-6.59	101.01	110.90
29	U	114	ARG	NE-CZ-NH1	6.59	123.60	120.30
31	W	107	MET	CG-SD-CE	-6.59	89.66	100.20
6	5	239	ARG	NE-CZ-NH1	6.59	123.59	120.30
27	S	335	VAL	CA-CB-CG1	6.59	120.78	110.90
28	T	308	TRP	CB-CG-CD2	-6.58	118.05	126.60
7	6	125	TYR	CB-CG-CD2	6.58	124.95	121.00
11	C	121	TYR	CB-CG-CD1	6.58	124.95	121.00
29	U	270	VAL	CG1-CB-CG2	-6.58	100.38	110.90
19	K	239	TYR	CB-CG-CD1	6.58	124.94	121.00
19	K	227	PHE	CB-CG-CD1	-6.57	116.20	120.80
31	W	130	ARG	NE-CZ-NH1	6.57	123.58	120.30
6	5	84	TYR	CB-CG-CD1	6.57	124.94	121.00
18	J	86	LEU	CB-CG-CD2	6.56	122.15	111.00
20	L	265	ASP	C-N-CA	6.56	136.07	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	I	168	ASP	CB-CG-OD1	-6.55	112.40	118.30
23	O	173	TYR	CZ-CE2-CD2	-6.55	113.90	119.80
28	T	154	TRP	CD1-CG-CD2	-6.55	101.06	106.30
29	U	212	LEU	CB-CG-CD1	6.55	122.13	111.00
5	4	85	ARG	NE-CZ-NH1	-6.55	117.03	120.30
22	N	395	ARG	NE-CZ-NH1	6.55	123.57	120.30
26	R	134	LEU	CB-CA-C	-6.55	97.76	110.20
24	P	341	PHE	CB-CG-CD2	-6.54	116.22	120.80
13	E	123	PHE	CB-CG-CD2	-6.54	116.22	120.80
12	D	176	TYR	CB-CG-CD1	6.54	124.92	121.00
30	V	112	TYR	CB-CG-CD1	6.54	124.92	121.00
28	T	158	ARG	NE-CZ-NH1	6.53	123.57	120.30
3	2	61	THR	O-C-N	6.53	133.15	122.70
21	M	55	MET	CG-SD-CE	-6.53	89.76	100.20
22	N	87	LEU	CB-CG-CD2	6.51	122.07	111.00
25	Q	380	GLN	C-N-CA	6.50	135.95	122.30
13	E	103	TYR	CB-CG-CD2	-6.50	117.10	121.00
24	P	65	ARG	NE-CZ-NH2	-6.50	117.05	120.30
21	M	379	VAL	CA-CB-CG2	-6.50	101.15	110.90
18	J	89	VAL	CA-CB-CG2	-6.50	101.16	110.90
29	U	173	GLU	CB-CA-C	-6.50	97.41	110.40
10	B	13	PHE	CB-CG-CD1	6.49	125.34	120.80
16	H	312	ARG	NE-CZ-NH1	6.49	123.55	120.30
19	K	41	TYR	CB-CA-C	-6.49	97.41	110.40
2	1	220	ARG	NE-CZ-NH2	6.49	123.55	120.30
6	5	123	ARG	NE-CZ-NH2	6.49	123.54	120.30
27	S	207	ALA	N-CA-CB	6.49	119.19	110.10
19	K	241	GLY	N-CA-C	-6.48	96.89	113.10
6	5	187	VAL	CG1-CB-CG2	6.48	121.27	110.90
14	F	75	ALA	N-CA-CB	6.48	119.17	110.10
11	C	159	TRP	CE3-CZ3-CH2	6.48	128.33	121.20
21	M	88	TYR	CD1-CG-CD2	6.48	125.02	117.90
26	R	95	LEU	C-N-CA	6.48	135.90	122.30
19	K	391	ARG	NE-CZ-NH2	-6.47	117.06	120.30
26	R	227	SER	N-CA-CB	6.47	120.21	110.50
13	E	10	ARG	NE-CZ-NH2	-6.47	117.06	120.30
25	Q	121	LYS	N-CA-CB	6.47	122.25	110.60
26	R	101	ARG	NH1-CZ-NH2	6.47	126.51	119.40
22	N	502	TYR	CB-CG-CD2	-6.47	117.12	121.00
28	T	272	ALA	N-CA-CB	-6.47	101.05	110.10
22	N	899	ARG	NE-CZ-NH1	6.46	123.53	120.30
24	P	329	ARG	NE-CZ-NH2	-6.46	117.07	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Q	388	PHE	CB-CG-CD1	-6.46	116.28	120.80
2	1	168	TYR	CB-CG-CD1	6.46	124.87	121.00
27	S	479	ARG	NH1-CZ-NH2	-6.44	112.31	119.40
9	A	83	MET	CB-CA-C	-6.44	97.52	110.40
10	B	121	TYR	CB-CG-CD1	6.44	124.86	121.00
25	Q	187	ARG	NE-CZ-NH1	6.44	123.52	120.30
28	T	124	LEU	CB-CA-C	-6.43	97.98	110.20
26	R	37	VAL	N-CA-C	-6.43	93.64	111.00
7	6	66	ARG	NE-CZ-NH1	-6.43	117.08	120.30
19	K	164	TYR	CZ-CE2-CD2	-6.43	114.01	119.80
18	J	211	PHE	CB-CG-CD1	6.43	125.30	120.80
22	N	193	PHE	CD1-CE1-CZ	-6.42	112.40	120.10
24	P	377	ARG	CG-CD-NE	-6.42	98.33	111.80
27	S	241	ARG	NE-CZ-NH1	6.42	123.51	120.30
24	P	174	TYR	CG-CD1-CE1	-6.41	116.17	121.30
1	Z	688	ARG	NE-CZ-NH2	6.41	123.51	120.30
24	P	324	TYR	CG-CD1-CE1	-6.41	116.17	121.30
26	R	257	ARG	NE-CZ-NH2	-6.40	117.10	120.30
5	4	122	ALA	N-CA-CB	6.40	119.06	110.10
2	1	209	ARG	NE-CZ-NH1	-6.40	117.10	120.30
29	U	70	LEU	CB-CG-CD2	6.40	121.87	111.00
8	7	160	TYR	CG-CD1-CE1	-6.39	116.19	121.30
2	1	77	CYS	CA-CB-SG	6.39	125.51	114.00
14	F	174	ARG	CD-NE-CZ	-6.39	114.65	123.60
21	M	373	MET	CG-SD-CE	-6.39	89.97	100.20
29	U	138	TYR	CG-CD2-CE2	-6.39	116.19	121.30
22	N	797	MET	CG-SD-CE	-6.39	89.98	100.20
22	N	894	MET	CG-SD-CE	-6.39	89.98	100.20
28	T	339	VAL	CA-CB-CG1	6.39	120.48	110.90
8	7	181	SER	N-CA-CB	6.39	120.08	110.50
22	N	627	PHE	CB-CG-CD2	-6.39	116.33	120.80
26	R	151	TYR	CB-CG-CD1	-6.39	117.17	121.00
16	H	256	MET	CB-CA-C	-6.38	97.64	110.40
21	M	112	ASP	N-CA-CB	6.38	122.08	110.60
22	N	269	ARG	N-CA-CB	6.38	122.08	110.60
31	W	15	TYR	CG-CD2-CE2	-6.38	116.20	121.30
3	2	210	LEU	CB-CA-C	-6.37	98.09	110.20
19	K	56	VAL	CB-CA-C	-6.37	99.30	111.40
23	O	339	ARG	NE-CZ-NH2	-6.37	117.12	120.30
25	Q	353	LEU	CB-CG-CD2	6.35	121.80	111.00
3	2	154	TYR	CB-CG-CD2	6.35	124.81	121.00
1	Z	489	TYR	CZ-CE2-CD2	6.34	125.51	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	85	VAL	CA-CB-CG2	-6.34	101.38	110.90
11	C	101	TYR	CB-CG-CD2	6.34	124.80	121.00
19	K	417	TYR	CB-CG-CD2	-6.34	117.20	121.00
22	N	24	LEU	CB-CG-CD2	6.34	121.78	111.00
1	Z	275	MET	CA-CB-CG	6.34	124.07	113.30
29	U	95	TYR	CD1-CG-CD2	6.34	124.87	117.90
7	6	128	ARG	NE-CZ-NH1	6.33	123.47	120.30
18	J	229	ARG	NE-CZ-NH1	6.33	123.47	120.30
23	O	90	PRO	N-CA-CB	6.33	110.90	103.30
27	S	218	TYR	CG-CD1-CE1	6.33	126.36	121.30
22	N	546	ARG	NE-CZ-NH2	-6.33	117.14	120.30
1	Z	674	THR	CA-CB-CG2	-6.33	103.55	112.40
15	G	213	GLU	CB-CA-C	-6.33	97.75	110.40
2	1	99	PHE	CB-CG-CD1	6.32	125.22	120.80
19	K	153	MET	N-CA-CB	6.32	121.97	110.60
21	M	239	ALA	N-CA-CB	-6.32	101.25	110.10
1	Z	554	TYR	CB-CG-CD2	6.31	124.79	121.00
1	Z	591	ALA	N-CA-CB	6.31	118.94	110.10
27	S	241	ARG	NE-CZ-NH2	-6.31	117.14	120.30
27	S	329	HIS	CA-CB-CG	-6.31	102.87	113.60
6	5	146	VAL	CA-CB-CG1	6.30	120.36	110.90
28	T	160	ASP	CB-CG-OD1	-6.30	112.63	118.30
11	C	174	MET	CG-SD-CE	6.30	110.28	100.20
8	7	82	ARG	NE-CZ-NH2	6.29	123.45	120.30
18	J	133	PRO	N-CD-CG	6.29	112.64	103.20
27	S	273	LYS	N-CA-CB	6.29	121.93	110.60
12	D	50	VAL	CG1-CB-CG2	-6.29	100.84	110.90
4	3	205	ASP	CB-CG-OD1	6.29	123.96	118.30
24	P	63	THR	CA-CB-OG1	6.28	122.20	109.00
29	U	104	ASN	CB-CA-C	-6.28	97.83	110.40
6	5	125	TYR	CB-CG-CD2	-6.28	117.23	121.00
9	A	189	TRP	CD1-CG-CD2	-6.28	101.28	106.30
11	C	143	TYR	CG-CD2-CE2	6.28	126.32	121.30
20	L	71	VAL	CA-CB-CG1	-6.28	101.48	110.90
21	M	325	GLN	CB-CA-C	-6.28	97.84	110.40
11	C	44	LEU	CB-CG-CD1	6.27	121.67	111.00
26	R	169	GLU	N-CA-CB	6.27	121.89	110.60
5	4	2	GLU	CB-CA-C	-6.27	97.86	110.40
25	Q	18	THR	CA-CB-CG2	-6.27	103.62	112.40
19	K	43	ARG	NE-CZ-NH1	6.27	123.43	120.30
22	N	362	ASN	N-CA-CB	6.27	121.88	110.60
26	R	216	TYR	CB-CG-CD1	-6.27	117.24	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	S	176	MET	N-CA-CB	6.26	121.88	110.60
2	1	198	MET	CG-SD-CE	6.26	110.21	100.20
3	2	177	ALA	N-CA-CB	6.26	118.86	110.10
19	K	359	ASP	CB-CG-OD1	-6.25	112.67	118.30
14	F	174	ARG	NE-CZ-NH2	6.25	123.42	120.30
27	S	308	THR	CA-CB-CG2	-6.24	103.66	112.40
28	T	259	PHE	CB-CG-CD1	6.24	125.17	120.80
31	W	11	ASP	N-CA-C	-6.24	94.15	111.00
11	C	19	TYR	CD1-CE1-CZ	6.23	125.40	119.80
12	D	139	ASP	N-CA-CB	6.23	121.81	110.60
23	O	98	GLU	CB-CA-C	-6.23	97.95	110.40
20	L	231	PHE	CB-CG-CD1	6.22	125.16	120.80
24	P	347	GLY	C-N-CA	6.22	137.26	121.70
6	5	200	ARG	NE-CZ-NH1	6.22	123.41	120.30
19	K	353	ASN	N-CA-CB	6.22	121.80	110.60
10	B	89	ARG	NE-CZ-NH2	6.22	123.41	120.30
5	4	61	GLN	CB-CA-C	-6.22	97.96	110.40
10	B	127	VAL	CA-CB-CG1	-6.21	101.58	110.90
22	N	706	VAL	CA-CB-CG1	-6.21	101.58	110.90
10	B	127	VAL	CA-CB-CG2	6.21	120.22	110.90
25	Q	161	ASP	CB-CG-OD2	-6.21	112.71	118.30
19	K	363	TYR	CB-CG-CD2	-6.21	117.28	121.00
25	Q	314	ARG	NE-CZ-NH2	6.21	123.40	120.30
2	1	170	TYR	CB-CG-CD2	-6.20	117.28	121.00
14	F	201	ALA	N-CA-CB	6.20	118.78	110.10
21	M	88	TYR	CB-CG-CD2	-6.20	117.28	121.00
28	T	269	ASP	CB-CG-OD2	-6.20	112.72	118.30
15	G	54	VAL	CA-CB-CG2	-6.20	101.60	110.90
14	F	87	PHE	N-CA-CB	6.20	121.75	110.60
25	Q	15	LEU	O-C-N	-6.20	112.78	122.70
18	J	281	ASP	CB-CG-OD1	-6.20	112.72	118.30
19	K	213	THR	CA-CB-CG2	-6.20	103.73	112.40
11	C	111	VAL	CA-CB-CG1	6.19	120.19	110.90
27	S	285	TRP	CD1-CG-CD2	-6.19	101.35	106.30
22	N	375	PHE	CB-CG-CD1	6.19	125.13	120.80
29	U	237	LEU	N-CA-CB	6.19	122.78	110.40
1	Z	817	VAL	CA-CB-CG1	6.19	120.18	110.90
16	H	82	ALA	N-CA-CB	6.19	118.76	110.10
22	N	609	ASP	CB-CG-OD1	-6.19	112.73	118.30
28	T	158	ARG	NE-CZ-NH2	-6.19	117.21	120.30
15	G	115	ARG	NE-CZ-NH1	6.18	123.39	120.30
20	L	221	TYR	CB-CG-CD2	-6.18	117.29	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	68	PHE	CD1-CE1-CZ	-6.18	112.69	120.10
8	7	252	THR	CA-CB-CG2	-6.18	103.75	112.40
10	B	228	ASP	CB-CG-OD1	-6.18	112.74	118.30
11	C	146	GLN	N-CA-CB	6.18	121.72	110.60
17	I	349	ARG	NE-CZ-NH2	6.18	123.39	120.30
1	Z	194	TYR	CB-CG-CD2	6.17	124.70	121.00
8	7	80	ARG	NE-CZ-NH2	-6.17	117.21	120.30
18	J	213	ARG	NE-CZ-NH1	-6.17	117.21	120.30
18	J	247	PHE	CB-CG-CD2	-6.17	116.48	120.80
22	N	682	TYR	CB-CG-CD1	6.17	124.70	121.00
15	G	119	TYR	CG-CD1-CE1	6.17	126.23	121.30
26	R	285	ASP	CB-CG-OD2	-6.16	112.75	118.30
8	7	66	VAL	CA-CB-CG2	-6.15	101.67	110.90
29	U	138	TYR	CA-CB-CG	-6.15	101.72	113.40
8	7	211	ARG	NE-CZ-NH1	6.15	123.37	120.30
19	K	161	ASP	CB-CG-OD2	-6.15	112.77	118.30
21	M	88	TYR	CB-CG-CD1	-6.15	117.31	121.00
20	L	297	ARG	NH1-CZ-NH2	6.14	126.16	119.40
12	D	118	TYR	CB-CG-CD2	6.14	124.69	121.00
15	G	41	ARG	NE-CZ-NH1	6.14	123.37	120.30
16	H	330	ALA	CB-CA-C	-6.14	100.89	110.10
19	K	345	PHE	CB-CG-CD2	-6.14	116.50	120.80
15	G	103	PHE	CB-CG-CD1	-6.14	116.50	120.80
2	1	147	SER	N-CA-CB	6.13	119.70	110.50
19	K	197	ASP	CB-CA-C	-6.13	98.13	110.40
25	Q	76	PHE	CB-CG-CD2	-6.13	116.51	120.80
21	M	324	THR	CA-CB-CG2	-6.13	103.82	112.40
23	O	352	ARG	NE-CZ-NH2	-6.12	117.24	120.30
17	I	272	ARG	NE-CZ-NH2	-6.12	117.24	120.30
25	Q	231	TYR	CD1-CG-CD2	6.12	124.64	117.90
12	D	106	TYR	CZ-CE2-CD2	6.12	125.30	119.80
30	V	201	TYR	CD1-CE1-CZ	6.12	125.30	119.80
1	Z	519	ALA	CB-CA-C	-6.11	100.94	110.10
7	6	241	ASP	CB-CG-OD2	6.11	123.80	118.30
7	6	35	PHE	CB-CG-CD2	-6.11	116.53	120.80
22	N	606	ALA	CB-CA-C	-6.10	100.95	110.10
19	K	270	ILE	CA-CB-CG1	6.09	122.58	111.00
10	B	232	ALA	N-CA-CB	6.09	118.63	110.10
22	N	225	ASP	CB-CG-OD1	-6.09	112.82	118.30
2	1	26	TRP	CZ3-CH2-CZ2	-6.08	114.30	121.60
21	M	80	ILE	CA-CB-CG2	-6.08	98.73	110.90
29	U	155	PHE	CD1-CE1-CZ	-6.08	112.80	120.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	B	118	MET	CG-SD-CE	-6.08	90.47	100.20
21	M	287	GLU	N-CA-CB	6.08	121.54	110.60
21	M	394	ALA	N-CA-CB	6.08	118.61	110.10
6	5	202	TYR	CB-CG-CD1	6.07	124.64	121.00
18	J	286	THR	N-CA-CB	6.07	121.84	110.30
25	Q	360	ASP	CB-CG-OD2	6.07	123.76	118.30
1	Z	239	TYR	CZ-CE2-CD2	6.07	125.26	119.80
24	P	213	PHE	CB-CG-CD1	6.07	125.05	120.80
26	R	295	TYR	CB-CG-CD2	6.07	124.64	121.00
3	2	136	TYR	CB-CG-CD2	-6.06	117.36	121.00
9	A	46	ASP	CB-CG-OD2	-6.06	112.85	118.30
23	O	18	GLN	CB-CA-C	-6.06	98.28	110.40
29	U	105	ASP	CB-CG-OD2	-6.06	112.85	118.30
1	Z	600	TYR	CB-CG-CD2	-6.06	117.36	121.00
10	B	98	TYR	CB-CG-CD1	-6.06	117.36	121.00
14	F	171	TYR	CG-CD1-CE1	6.06	126.14	121.30
8	7	177	TYR	CB-CG-CD2	6.05	124.63	121.00
9	A	33	ASN	N-CA-CB	6.05	121.49	110.60
11	C	60	PHE	CB-CG-CD1	-6.05	116.56	120.80
14	F	125	ARG	NE-CZ-NH2	6.05	123.32	120.30
18	J	214	VAL	CG1-CB-CG2	6.05	120.58	110.90
26	R	146	ARG	NE-CZ-NH2	6.05	123.32	120.30
17	I	183	THR	CA-CB-CG2	-6.04	103.94	112.40
21	M	88	TYR	CG-CD2-CE2	-6.04	116.47	121.30
21	M	130	GLN	CG-CD-OE1	-6.04	109.53	121.60
9	A	113	MET	CG-SD-CE	-6.04	90.54	100.20
4	3	96	TYR	CG-CD1-CE1	-6.03	116.47	121.30
19	K	297	ASP	CB-CG-OD1	6.03	123.73	118.30
22	N	366	HIS	CA-CB-CG	6.03	123.85	113.60
25	Q	262	ASN	N-CA-CB	6.03	121.45	110.60
8	7	189	TYR	CB-CG-CD1	6.03	124.61	121.00
17	I	438	LEU	N-CA-CB	6.03	122.45	110.40
14	F	87	PHE	CB-CA-C	-6.02	98.35	110.40
18	J	150	MET	CG-SD-CE	-6.02	90.56	100.20
29	U	88	ARG	NE-CZ-NH2	6.02	123.31	120.30
21	M	64	HIS	CA-CB-CG	6.02	123.83	113.60
26	R	366	TYR	CG-CD2-CE2	6.02	126.12	121.30
30	V	149	GLN	O-C-N	-6.02	113.07	122.70
7	6	160	ARG	NE-CZ-NH2	-6.01	117.29	120.30
9	A	218	GLY	N-CA-C	-6.01	98.06	113.10
20	L	267	PHE	CB-CG-CD2	-6.01	116.59	120.80
23	O	232	TRP	CB-CG-CD1	6.01	134.82	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	222	PRO	N-CA-CB	6.01	110.51	103.30
16	H	147	TYR	CZ-CE2-CD2	6.01	125.21	119.80
31	W	73	SER	CB-CA-C	-6.01	98.68	110.10
20	L	148	VAL	CA-CB-CG1	6.01	119.92	110.90
1	Z	239	TYR	CB-CG-CD1	6.01	124.61	121.00
8	7	219	ARG	NH1-CZ-NH2	-6.01	112.79	119.40
22	N	572	ARG	CD-NE-CZ	-6.00	115.19	123.60
25	Q	137	TYR	CB-CG-CD1	-6.00	117.40	121.00
19	K	74	HIS	CA-CB-CG	-6.00	103.39	113.60
20	L	297	ARG	NE-CZ-NH1	-6.00	117.30	120.30
1	Z	158	TYR	CB-CG-CD2	-6.00	117.40	121.00
13	E	16	SER	N-CA-CB	6.00	119.50	110.50
14	F	6	TYR	CG-CD2-CE2	6.00	126.10	121.30
21	M	380	ASN	C-N-CA	6.00	136.70	121.70
27	S	178	SER	N-CA-CB	6.00	119.50	110.50
30	V	121	TRP	CA-CB-CG	6.00	125.10	113.70
3	2	57	LEU	N-CA-C	-5.99	94.83	111.00
12	D	13	ASP	CB-CG-OD2	5.99	123.69	118.30
10	B	24	TYR	CD1-CG-CD2	-5.99	111.32	117.90
21	M	173	LYS	N-CA-CB	5.99	121.37	110.60
11	C	96	ARG	NE-CZ-NH2	-5.98	117.31	120.30
19	K	120	ASP	CB-CG-OD2	-5.98	112.92	118.30
9	A	152	TYR	CG-CD1-CE1	5.98	126.08	121.30
22	N	173	VAL	CA-CB-CG2	-5.98	101.93	110.90
25	Q	231	TYR	CG-CD1-CE1	-5.98	116.52	121.30
9	A	23	TYR	CB-CG-CD1	-5.98	117.42	121.00
12	D	96	LEU	CB-CG-CD2	5.97	121.16	111.00
13	E	53	ARG	N-CA-CB	5.97	121.35	110.60
31	W	42	ARG	NE-CZ-NH1	5.97	123.29	120.30
8	7	82	ARG	NE-CZ-NH1	-5.97	117.31	120.30
25	Q	247	ALA	CB-CA-C	-5.97	101.15	110.10
21	M	158	TYR	CZ-CE2-CD2	5.96	125.17	119.80
1	Z	723	TYR	N-CA-CB	5.96	121.33	110.60
21	M	284	PHE	CB-CG-CD2	-5.96	116.63	120.80
28	T	270	GLU	OE1-CD-OE2	5.96	130.45	123.30
7	6	227	THR	CA-CB-OG1	5.96	121.50	109.00
7	6	103	TYR	CG-CD1-CE1	-5.95	116.54	121.30
13	E	147	ASP	CB-CG-OD1	-5.95	112.95	118.30
22	N	194	ARG	NE-CZ-NH2	-5.95	117.33	120.30
26	R	268	TYR	CB-CG-CD2	-5.95	117.43	121.00
27	S	485	ASP	CB-CG-OD1	-5.95	112.95	118.30
5	4	116	TYR	CA-CB-CG	-5.95	102.10	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	174	ASP	N-CA-CB	5.94	121.30	110.60
1	Z	755	ASP	CB-CG-OD1	5.94	123.64	118.30
25	Q	297	ARG	CD-NE-CZ	-5.94	115.28	123.60
1	Z	301	HIS	N-CA-CB	5.94	121.29	110.60
24	P	66	ILE	CG1-CB-CG2	5.94	124.46	111.40
1	Z	760	PHE	CB-CG-CD2	5.93	124.95	120.80
11	C	156	TYR	CB-CG-CD1	5.93	124.56	121.00
4	3	59	ASP	CB-CG-OD2	-5.93	112.96	118.30
26	R	97	GLU	CA-CB-CG	5.93	126.44	113.40
22	N	629	THR	N-CA-C	-5.92	95.00	111.00
10	B	83	TYR	CB-CG-CD2	-5.92	117.45	121.00
28	T	260	ILE	CB-CA-C	-5.92	99.75	111.60
11	C	159	TRP	CZ3-CH2-CZ2	-5.92	114.50	121.60
22	N	600	ARG	NE-CZ-NH2	-5.92	117.34	120.30
5	4	119	ASP	CB-CG-OD1	5.91	123.62	118.30
24	P	231	ILE	CB-CA-C	-5.91	99.77	111.60
26	R	173	ASP	CB-CG-OD1	-5.91	112.98	118.30
17	I	259	TYR	CZ-CE2-CD2	5.91	125.12	119.80
27	S	475	ALA	CB-CA-C	-5.91	101.24	110.10
1	Z	399	LEU	CB-CG-CD2	5.91	121.04	111.00
18	J	349	GLU	OE1-CD-OE2	5.91	130.39	123.30
20	L	283	ASP	CB-CG-OD2	-5.91	112.98	118.30
22	N	400	ALA	N-CA-CB	5.91	118.37	110.10
28	T	315	TYR	CG-CD2-CE2	-5.91	116.58	121.30
14	F	149	PRO	N-CA-CB	5.90	110.39	103.30
27	S	297	ALA	N-CA-CB	5.90	118.36	110.10
16	H	239	ARG	NE-CZ-NH1	-5.90	117.35	120.30
28	T	241	TYR	CG-CD1-CE1	-5.90	116.58	121.30
31	W	15	TYR	CB-CG-CD1	-5.90	117.46	121.00
11	C	139	TRP	CD1-NE1-CE2	-5.90	103.69	109.00
14	F	103	LEU	N-CA-CB	5.90	122.20	110.40
16	H	82	ALA	N-CA-C	-5.90	95.07	111.00
17	I	385	MET	CG-SD-CE	-5.90	90.76	100.20
16	H	408	ASP	CB-CA-C	-5.90	98.60	110.40
22	N	69	TYR	CB-CG-CD1	-5.90	117.46	121.00
5	4	31	ASP	CB-CA-C	-5.89	98.62	110.40
10	B	24	TYR	CG-CD2-CE2	5.89	126.01	121.30
19	K	274	ARG	NE-CZ-NH2	-5.89	117.35	120.30
7	6	33	TYR	CB-CG-CD2	5.89	124.53	121.00
22	N	503	GLN	CB-CA-C	-5.89	98.62	110.40
30	V	275	VAL	CA-CB-CG1	-5.89	102.06	110.90
13	E	229	PHE	CB-CG-CD1	5.89	124.92	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	V	31	VAL	CG1-CB-CG2	-5.89	101.48	110.90
19	K	260	ALA	N-CA-CB	5.89	118.34	110.10
21	M	362	ARG	NE-CZ-NH1	-5.89	117.36	120.30
5	4	53	THR	CA-CB-CG2	-5.88	104.16	112.40
19	K	156	SER	N-CA-C	-5.88	95.11	111.00
23	O	218	MET	CG-SD-CE	-5.88	90.79	100.20
30	V	279	ASP	CB-CG-OD2	5.88	123.59	118.30
1	Z	519	ALA	N-CA-CB	5.88	118.33	110.10
21	M	158	TYR	CG-CD2-CE2	-5.88	116.60	121.30
26	R	357	ASN	N-CA-CB	5.88	121.18	110.60
24	P	174	TYR	CD1-CE1-CZ	5.87	125.09	119.80
28	T	237	MET	CA-CB-CG	5.87	123.28	113.30
29	U	167	ALA	CB-CA-C	-5.87	101.30	110.10
13	E	26	TYR	CB-CG-CD2	-5.87	117.48	121.00
1	Z	367	SER	N-CA-CB	5.87	119.30	110.50
3	2	128	GLN	CA-CB-CG	5.87	126.30	113.40
15	G	136	PHE	CB-CG-CD2	-5.86	116.70	120.80
21	M	90	VAL	CB-CA-C	5.86	122.54	111.40
26	R	24	PHE	CB-CA-C	-5.86	98.68	110.40
4	3	117	PHE	CB-CG-CD2	-5.86	116.70	120.80
10	B	84	ARG	CG-CD-NE	-5.86	99.50	111.80
3	2	232	TYR	CB-CG-CD1	-5.86	117.48	121.00
26	R	323	PHE	CB-CG-CD1	-5.86	116.70	120.80
30	V	263	ASP	CB-CG-OD1	-5.86	113.03	118.30
19	K	362	ASP	CB-CG-OD1	-5.86	113.03	118.30
21	M	401	VAL	CA-CB-CG1	-5.86	102.12	110.90
23	O	70	ARG	NE-CZ-NH2	-5.85	117.37	120.30
22	N	445	ALA	CB-CA-C	-5.85	101.32	110.10
30	V	107	MET	CG-SD-CE	-5.85	90.84	100.20
4	3	133	THR	CA-CB-CG2	-5.85	104.21	112.40
14	F	96	ARG	NE-CZ-NH2	-5.85	117.38	120.30
19	K	112	TYR	CD1-CE1-CZ	5.85	125.06	119.80
27	S	385	LYS	CB-CA-C	-5.84	98.71	110.40
4	3	176	ASP	CB-CG-OD1	-5.84	113.04	118.30
8	7	236	THR	CA-CB-CG2	-5.84	104.23	112.40
3	2	96	ASP	CB-CG-OD1	5.83	123.55	118.30
30	V	151	VAL	CA-CB-CG1	-5.83	102.15	110.90
5	4	161	ARG	NE-CZ-NH2	5.83	123.22	120.30
5	4	172	ILE	CB-CA-C	5.83	123.26	111.60
1	Z	310	ASP	CB-CG-OD2	5.82	123.54	118.30
26	R	218	THR	CA-CB-CG2	-5.82	104.25	112.40
19	K	352	MET	CG-SD-CE	-5.82	90.89	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	J	121	TYR	CG-CD2-CE2	-5.82	116.64	121.30
21	M	140	VAL	CA-CB-CG2	-5.82	102.17	110.90
15	G	203	ASP	CB-CG-OD1	-5.82	113.06	118.30
22	N	772	TRP	CB-CG-CD1	5.82	134.56	127.00
23	O	83	VAL	O-C-N	-5.81	113.40	122.70
19	K	251	PHE	CB-CG-CD2	-5.81	116.73	120.80
23	O	211	PHE	CB-CG-CD2	-5.81	116.73	120.80
22	N	936	GLU	OE1-CD-OE2	-5.81	116.33	123.30
29	U	79	TYR	CB-CG-CD2	5.81	124.49	121.00
26	R	202	LEU	N-CA-CB	-5.81	98.78	110.40
30	V	91	PHE	CD1-CE1-CZ	-5.81	113.13	120.10
16	H	264	ALA	CB-CA-C	-5.81	101.39	110.10
24	P	263	TRP	CA-CB-CG	5.81	124.73	113.70
1	Z	544	GLU	OE1-CD-OE2	-5.80	116.33	123.30
20	L	251	ARG	NE-CZ-NH1	5.80	123.20	120.30
22	N	813	TYR	CB-CG-CD1	-5.80	117.52	121.00
5	4	87	ASN	CB-CA-C	-5.80	98.80	110.40
22	N	771	PHE	CB-CG-CD2	-5.80	116.74	120.80
22	N	634	PRO	N-CA-CB	5.79	110.25	103.30
24	P	340	VAL	CA-CB-CG2	5.79	119.59	110.90
29	U	240	VAL	CG1-CB-CG2	5.79	120.17	110.90
19	K	284	GLU	CB-CA-C	-5.79	98.82	110.40
26	R	137	ARG	NE-CZ-NH2	-5.79	117.41	120.30
19	K	252	ARG	NE-CZ-NH2	-5.79	117.41	120.30
22	N	883	ARG	NE-CZ-NH2	-5.79	117.41	120.30
29	U	69	PHE	CB-CG-CD1	5.79	124.85	120.80
9	A	23	TYR	CG-CD1-CE1	-5.79	116.67	121.30
12	D	71	MET	CG-SD-CE	-5.79	90.94	100.20
21	M	435	LEU	CB-CG-CD2	5.79	120.83	111.00
22	N	548	LEU	O-C-N	5.79	131.96	122.70
5	4	142	ILE	CB-CA-C	-5.78	100.03	111.60
20	L	358	ASP	CA-CB-CG	-5.78	100.67	113.40
14	F	55	GLU	CB-CA-C	-5.78	98.84	110.40
26	R	322	ALA	CB-CA-C	-5.78	101.43	110.10
1	Z	671	ALA	CB-CA-C	-5.78	101.43	110.10
13	E	107	MET	CG-SD-CE	-5.78	90.96	100.20
13	E	94	VAL	CG1-CB-CG2	5.77	120.14	110.90
13	E	236	GLU	CB-CA-C	-5.77	98.86	110.40
23	O	163	TYR	CG-CD1-CE1	-5.77	116.68	121.30
8	7	261	SER	CB-CA-C	-5.77	99.14	110.10
22	N	15	ASP	N-CA-CB	5.77	120.99	110.60
1	Z	892	PRO	N-CA-CB	5.77	110.22	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	K	268	ASP	CB-CG-OD2	-5.77	113.11	118.30
22	N	179	TYR	CB-CG-CD2	-5.77	117.54	121.00
5	4	4	LEU	CB-CA-C	-5.77	99.25	110.20
3	2	127	LYS	CB-CA-C	-5.76	98.87	110.40
7	6	220	ALA	N-CA-CB	5.76	118.17	110.10
30	V	234	TYR	CZ-CE2-CD2	-5.76	114.61	119.80
23	O	108	ASP	N-CA-CB	5.76	120.97	110.60
28	T	224	VAL	CA-CB-CG2	-5.76	102.26	110.90
23	O	3	ASP	CB-CG-OD1	5.76	123.48	118.30
14	F	218	ASP	CB-CG-OD1	5.76	123.48	118.30
1	Z	410	ALA	N-CA-CB	5.76	118.16	110.10
15	G	141	TYR	CG-CD1-CE1	-5.75	116.70	121.30
25	Q	155	ARG	NE-CZ-NH2	-5.75	117.42	120.30
13	E	56	SER	CB-CA-C	-5.75	99.17	110.10
22	N	129	ARG	NE-CZ-NH1	5.75	123.17	120.30
30	V	196	LEU	CA-CB-CG	-5.75	102.07	115.30
15	G	233	ARG	NE-CZ-NH2	-5.75	117.43	120.30
7	6	222	ARG	CD-NE-CZ	-5.75	115.56	123.60
15	G	188	ARG	CD-NE-CZ	5.75	131.64	123.60
20	L	216	ARG	NE-CZ-NH1	-5.74	117.43	120.30
24	P	211	THR	CA-CB-CG2	-5.74	104.36	112.40
5	4	22	ALA	N-CA-C	-5.74	95.50	111.00
20	L	207	TYR	CG-CD1-CE1	-5.74	116.71	121.30
17	I	283	PHE	CB-CG-CD2	-5.74	116.78	120.80
17	I	288	ASP	CB-CG-OD2	-5.74	113.14	118.30
24	P	270	VAL	CA-CB-CG2	-5.74	102.30	110.90
10	B	215	GLU	OE1-CD-OE2	5.73	130.18	123.30
27	S	378	VAL	CA-CB-CG2	5.73	119.50	110.90
5	4	58	GLU	CB-CA-C	-5.73	98.94	110.40
3	2	51	TYR	CZ-CE2-CD2	-5.73	114.64	119.80
29	U	228	TYR	CG-CD1-CE1	5.73	125.88	121.30
14	F	123	TYR	CG-CD1-CE1	-5.73	116.72	121.30
2	1	109	LEU	CB-CG-CD1	5.73	120.73	111.00
9	A	174	GLU	OE1-CD-OE2	5.73	130.17	123.30
29	U	17	LEU	CB-CG-CD2	5.73	120.74	111.00
27	S	269	LYS	CB-CG-CD	5.73	126.49	111.60
1	Z	673	ARG	NH1-CZ-NH2	-5.72	113.10	119.40
18	J	297	ARG	NH1-CZ-NH2	-5.72	113.10	119.40
23	O	240	PHE	N-CA-CB	-5.72	100.29	110.60
24	P	379	ALA	O-C-N	-5.72	113.54	122.70
17	I	343	ARG	NE-CZ-NH2	5.72	123.16	120.30
22	N	931	HIS	CA-CB-CG	5.72	123.33	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Q	16	LEU	CB-CG-CD1	5.72	120.73	111.00
22	N	875	PHE	CZ-CE2-CD2	5.72	126.97	120.10
17	I	408	ARG	NE-CZ-NH2	-5.72	117.44	120.30
21	M	279	ALA	CB-CA-C	-5.72	101.52	110.10
27	S	295	ILE	CB-CA-C	-5.72	100.17	111.60
15	G	56	SER	N-CA-CB	5.72	119.08	110.50
18	J	294	ALA	N-CA-CB	5.72	118.10	110.10
15	G	15	PHE	N-CA-CB	5.71	120.89	110.60
29	U	161	GLU	CB-CA-C	-5.71	98.97	110.40
22	N	579	ARG	NE-CZ-NH2	-5.71	117.45	120.30
24	P	328	LEU	CB-CG-CD1	-5.71	101.30	111.00
30	V	112	TYR	CB-CG-CD2	-5.71	117.58	121.00
12	D	222	PRO	C-N-CA	5.71	135.96	121.70
1	Z	785	ARG	NE-CZ-NH1	5.70	123.15	120.30
21	M	142	ALA	CB-CA-C	-5.70	101.55	110.10
21	M	238	ARG	NE-CZ-NH1	-5.70	117.45	120.30
24	P	190	MET	CG-SD-CE	5.70	109.31	100.20
3	2	227	ASP	CB-CG-OD1	-5.69	113.18	118.30
10	B	112	GLN	CG-CD-OE1	-5.69	110.22	121.60
23	O	34	TRP	N-CA-CB	5.69	120.84	110.60
2	1	172	TYR	CA-CB-CG	-5.69	102.59	113.40
25	Q	113	CYS	N-CA-CB	5.69	120.84	110.60
27	S	317	PRO	O-C-N	5.69	131.80	122.70
14	F	100	ASP	CB-CG-OD1	-5.69	113.18	118.30
17	I	80	ARG	NE-CZ-NH2	5.68	123.14	120.30
24	P	392	PHE	CB-CG-CD1	5.68	124.78	120.80
6	5	154	LEU	O-C-N	5.68	131.79	122.70
15	G	132	PHE	CB-CG-CD1	5.68	124.78	120.80
27	S	236	ARG	NE-CZ-NH1	-5.68	117.46	120.30
4	3	74	TYR	CB-CG-CD1	5.68	124.41	121.00
14	F	153	TYR	CD1-CE1-CZ	-5.67	114.69	119.80
19	K	358	VAL	O-C-N	5.67	131.77	122.70
18	J	310	ARG	NE-CZ-NH1	-5.67	117.47	120.30
19	K	205	TYR	CB-CG-CD1	-5.67	117.60	121.00
8	7	70	ASP	N-CA-CB	5.67	120.80	110.60
23	O	179	PHE	CB-CG-CD2	-5.67	116.83	120.80
20	L	318	GLY	CA-C-O	-5.66	110.41	120.60
29	U	64	ASP	N-CA-CB	5.66	120.79	110.60
15	G	66	ARG	NE-CZ-NH1	5.66	123.13	120.30
21	M	180	ARG	NH1-CZ-NH2	-5.66	113.18	119.40
31	W	50	GLY	N-CA-C	-5.66	98.96	113.10
20	L	40	TYR	CG-CD2-CE2	-5.66	116.78	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	N	181	LEU	CB-CG-CD1	5.66	120.62	111.00
19	K	313	ARG	NE-CZ-NH1	5.66	123.13	120.30
27	S	290	TYR	CG-CD1-CE1	-5.66	116.78	121.30
29	U	71	ASP	CB-CG-OD2	-5.65	113.21	118.30
1	Z	499	THR	CA-CB-CG2	-5.65	104.49	112.40
3	2	51	TYR	CD1-CE1-CZ	-5.65	114.71	119.80
22	N	586	VAL	CA-CB-CG1	5.65	119.38	110.90
2	1	178	ARG	NE-CZ-NH2	-5.65	117.47	120.30
17	I	138	PHE	CB-CG-CD2	-5.65	116.84	120.80
16	H	283	ALA	N-CA-CB	5.65	118.01	110.10
22	N	531	ASP	CB-CG-OD2	-5.65	113.22	118.30
1	Z	294	MET	CA-CB-CG	5.64	122.90	113.30
17	I	307	ARG	CD-NE-CZ	5.64	131.50	123.60
21	M	171	ARG	NE-CZ-NH2	5.64	123.12	120.30
18	J	359	VAL	CA-CB-CG2	-5.64	102.44	110.90
30	V	107	MET	CA-CB-CG	5.64	122.89	113.30
26	R	34	ASP	CB-CG-OD1	5.64	123.38	118.30
12	D	169	ARG	NH1-CZ-NH2	-5.63	113.20	119.40
13	E	156	MET	CG-SD-CE	5.63	109.22	100.20
22	N	217	CYS	CA-CB-SG	-5.63	103.86	114.00
27	S	239	THR	O-C-N	5.63	131.72	122.70
1	Z	788	MET	CG-SD-CE	-5.63	91.19	100.20
31	W	164	ASP	CB-CG-OD1	-5.63	113.23	118.30
1	Z	840	LEU	N-CA-CB	5.63	121.66	110.40
21	M	184	GLN	N-CA-CB	5.63	120.73	110.60
29	U	232	ASP	CB-CG-OD1	5.63	123.37	118.30
22	N	647	HIS	CB-CA-C	-5.63	99.14	110.40
24	P	116	THR	O-C-N	-5.63	113.69	122.70
26	R	201	PHE	CB-CG-CD2	5.63	124.74	120.80
14	F	131	GLY	N-CA-C	-5.63	99.03	113.10
24	P	273	TYR	CB-CG-CD1	-5.63	117.62	121.00
31	W	41	THR	CA-CB-CG2	-5.63	104.52	112.40
23	O	349	MET	N-CA-CB	5.62	120.72	110.60
22	N	770	TRP	CH2-CZ2-CE2	-5.62	111.78	117.40
4	3	124	LEU	CB-CG-CD2	-5.62	101.44	111.00
5	4	107	TYR	CB-CG-CD1	5.62	124.37	121.00
9	A	152	TYR	CB-CG-CD1	5.62	124.37	121.00
1	Z	892	PRO	N-CD-CG	5.62	111.63	103.20
26	R	61	LEU	CB-CG-CD1	-5.62	101.45	111.00
29	U	3	GLU	OE1-CD-OE2	5.61	130.03	123.30
20	L	78	ARG	NH1-CZ-NH2	-5.61	113.23	119.40
2	1	26	TRP	CH2-CZ2-CE2	5.61	123.01	117.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	W	179	LEU	CB-CG-CD2	5.61	120.54	111.00
16	H	312	ARG	NE-CZ-NH2	-5.61	117.50	120.30
19	K	191	TYR	CZ-CE2-CD2	-5.61	114.75	119.80
22	N	882	ALA	CB-CA-C	-5.61	101.69	110.10
24	P	324	TYR	CB-CG-CD1	5.61	124.36	121.00
6	5	225	ARG	NE-CZ-NH1	-5.61	117.50	120.30
11	C	121	TYR	N-CA-CB	5.61	120.69	110.60
29	U	250	TYR	N-CA-CB	5.61	120.69	110.60
10	B	158	TRP	CG-CD2-CE3	-5.60	128.86	133.90
8	7	196	ARG	NE-CZ-NH1	-5.60	117.50	120.30
15	G	141	TYR	CD1-CG-CD2	5.60	124.06	117.90
22	N	88	PHE	CB-CG-CD1	-5.60	116.88	120.80
21	M	88	TYR	CG-CD1-CE1	-5.60	116.82	121.30
14	F	88	MET	CG-SD-CE	-5.60	91.25	100.20
16	H	255	ARG	NE-CZ-NH1	5.59	123.10	120.30
23	O	251	LEU	CB-CG-CD1	5.59	120.51	111.00
28	T	187	TYR	CZ-CE2-CD2	5.59	124.83	119.80
31	W	150	THR	CA-CB-CG2	-5.59	104.57	112.40
28	T	308	TRP	CB-CG-CD1	5.59	134.27	127.00
1	Z	616	CYS	N-CA-CB	5.59	120.67	110.60
22	N	205	TYR	CD1-CE1-CZ	-5.59	114.77	119.80
24	P	182	ARG	NE-CZ-NH2	-5.59	117.50	120.30
26	R	125	ARG	NE-CZ-NH1	5.59	123.09	120.30
20	L	216	ARG	NH1-CZ-NH2	5.59	125.55	119.40
26	R	268	TYR	CG-CD2-CE2	-5.59	116.83	121.30
24	P	316	ARG	NE-CZ-NH2	-5.59	117.51	120.30
19	K	124	LEU	N-CA-C	-5.58	95.92	111.00
9	A	9	PHE	N-CA-CB	5.58	120.65	110.60
10	B	211	GLY	N-CA-C	-5.58	99.14	113.10
12	D	55	ASP	CB-CG-OD2	5.58	123.32	118.30
24	P	120	ILE	CA-CB-CG2	-5.58	99.74	110.90
1	Z	262	PHE	CA-C-O	-5.57	108.40	120.10
4	3	6	TYR	CB-CG-CD1	-5.57	117.66	121.00
13	E	163	VAL	N-CA-C	-5.57	95.95	111.00
28	T	64	MET	N-CA-CB	5.57	120.63	110.60
4	3	135	ASP	CB-CG-OD2	-5.57	113.29	118.30
18	J	189	TYR	CD1-CE1-CZ	-5.57	114.79	119.80
25	Q	89	VAL	O-C-N	-5.57	113.80	122.70
25	Q	324	ALA	CB-CA-C	-5.57	101.75	110.10
8	7	52	THR	CA-CB-CG2	-5.56	104.61	112.40
26	R	207	THR	N-CA-CB	5.56	120.87	110.30
3	2	63	ALA	N-CA-CB	5.56	117.88	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	35	SER	N-CA-CB	-5.56	102.16	110.50
16	H	271	LEU	CB-CG-CD1	5.56	120.45	111.00
27	S	320	THR	CA-CB-CG2	-5.56	104.62	112.40
14	F	228	ASP	CB-CG-OD1	-5.56	113.30	118.30
19	K	331	ILE	N-CA-C	-5.56	96.00	111.00
14	F	196	ARG	NE-CZ-NH2	-5.56	117.52	120.30
1	Z	513	GLU	OE1-CD-OE2	-5.55	116.63	123.30
21	M	252	ALA	N-CA-CB	5.55	117.88	110.10
29	U	7	GLN	N-CA-C	-5.55	96.00	111.00
25	Q	261	LEU	CB-CG-CD2	5.55	120.44	111.00
31	W	136	VAL	CA-CB-CG2	-5.55	102.57	110.90
1	Z	872	VAL	CA-CB-CG2	5.55	119.23	110.90
28	T	140	GLN	N-CA-C	-5.55	96.01	111.00
17	I	149	SER	N-CA-CB	5.55	118.82	110.50
17	I	410	ARG	N-CA-CB	5.55	120.59	110.60
1	Z	100	ARG	NE-CZ-NH2	-5.55	117.53	120.30
5	4	108	ASP	N-CA-CB	5.55	120.58	110.60
17	I	181	GLN	CB-CA-C	-5.55	99.31	110.40
17	I	320	ASP	N-CA-CB	5.55	120.58	110.60
26	R	83	ARG	NE-CZ-NH2	-5.55	117.53	120.30
7	6	117	ALA	N-CA-CB	5.54	117.86	110.10
2	1	35	THR	N-CA-CB	5.54	120.83	110.30
17	I	262	ASP	CB-CG-OD2	-5.54	113.31	118.30
1	Z	349	TYR	CG-CD1-CE1	-5.54	116.87	121.30
7	6	206	VAL	CG1-CB-CG2	-5.54	102.03	110.90
22	N	588	MET	CG-SD-CE	-5.54	91.33	100.20
9	A	48	ALA	N-CA-C	-5.54	96.05	111.00
22	N	783	TYR	N-CA-CB	5.54	120.57	110.60
6	5	147	TYR	CB-CG-CD1	-5.54	117.68	121.00
17	I	369	THR	CA-CB-CG2	-5.54	104.65	112.40
22	N	921	ILE	CA-CB-CG1	5.54	121.52	111.00
16	H	355	PHE	CB-CG-CD2	-5.53	116.93	120.80
2	1	156	ARG	N-CA-CB	5.53	120.56	110.60
19	K	175	GLN	CB-CA-C	-5.53	99.35	110.40
29	U	201	LEU	CB-CG-CD2	5.53	120.40	111.00
10	B	98	TYR	CG-CD1-CE1	-5.53	116.88	121.30
29	U	234	PHE	CB-CG-CD1	5.53	124.67	120.80
30	V	84	VAL	CG1-CB-CG2	5.53	119.74	110.90
15	G	123	TYR	CD1-CE1-CZ	-5.52	114.83	119.80
11	C	61	PHE	CB-CG-CD1	-5.52	116.93	120.80
19	K	363	TYR	CG-CD2-CE2	-5.52	116.88	121.30
8	7	56	VAL	N-CA-C	-5.52	96.09	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	K	310	ALA	N-CA-CB	5.52	117.83	110.10
3	2	182	GLU	CB-CG-CD	-5.52	99.30	114.20
14	F	122	ARG	NE-CZ-NH1	-5.52	117.54	120.30
18	J	241	HIS	CB-CA-C	-5.52	99.36	110.40
24	P	315	MET	N-CA-C	-5.52	96.10	111.00
12	D	86	ARG	NE-CZ-NH1	5.52	123.06	120.30
24	P	420	ASP	O-C-N	-5.52	110.62	121.10
22	N	605	VAL	CA-CB-CG2	5.51	119.17	110.90
5	4	158	GLU	CB-CA-C	-5.51	99.38	110.40
25	Q	220	ALA	CB-CA-C	-5.51	101.83	110.10
19	K	335	LEU	CB-CG-CD1	5.51	120.37	111.00
22	N	202	VAL	CA-CB-CG1	-5.51	102.63	110.90
27	S	261	TYR	CB-CG-CD1	-5.51	117.69	121.00
27	S	453	HIS	CA-CB-CG	5.51	122.97	113.60
8	7	254	TRP	CG-CD2-CE3	-5.51	128.94	133.90
1	Z	760	PHE	CG-CD1-CE1	5.50	126.86	120.80
23	O	284	ARG	CB-CA-C	5.50	121.39	110.40
26	R	383	LEU	CB-CG-CD2	-5.50	101.66	111.00
27	S	221	LEU	N-CA-CB	5.50	121.39	110.40
29	U	152	SER	CB-CA-C	5.50	120.54	110.10
31	W	2	VAL	CG1-CB-CG2	5.50	119.69	110.90
20	L	285	LEU	CB-CG-CD1	5.50	120.34	111.00
20	L	338	PHE	CB-CG-CD1	5.50	124.65	120.80
15	G	159	TYR	CD1-CG-CD2	5.49	123.94	117.90
16	H	232	ARG	NE-CZ-NH2	-5.49	117.55	120.30
17	I	324	ASP	N-CA-CB	5.49	120.49	110.60
22	N	332	GLU	N-CA-CB	5.49	120.49	110.60
26	R	90	ASP	CB-CG-OD1	5.49	123.25	118.30
30	V	281	LYS	CB-CA-C	-5.49	99.42	110.40
1	Z	418	LEU	CB-CG-CD1	5.49	120.33	111.00
1	Z	384	ALA	N-CA-CB	5.49	117.78	110.10
15	G	105	TYR	CZ-CE2-CD2	5.49	124.74	119.80
22	N	147	TYR	CD1-CE1-CZ	5.49	124.74	119.80
2	1	50	ALA	CB-CA-C	-5.49	101.87	110.10
12	D	200	GLN	N-CA-CB	5.49	120.47	110.60
30	V	32	TYR	CB-CG-CD1	-5.49	117.71	121.00
4	3	66	ARG	NE-CZ-NH1	-5.48	117.56	120.30
1	Z	179	VAL	CA-CB-CG2	5.48	119.12	110.90
3	2	241	ARG	NH1-CZ-NH2	5.48	125.43	119.40
28	T	245	PHE	CG-CD2-CE2	-5.48	114.77	120.80
23	O	39	LEU	C-N-CA	5.48	135.40	121.70
26	R	128	TYR	CA-CB-CG	5.48	123.81	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	O	163	TYR	CB-CG-CD1	-5.48	117.71	121.00
12	D	57	ARG	NE-CZ-NH2	5.47	123.04	120.30
15	G	217	VAL	N-CA-C	-5.47	96.23	111.00
8	7	189	TYR	CG-CD2-CE2	-5.47	116.92	121.30
11	C	211	VAL	CG1-CB-CG2	5.47	119.65	110.90
12	D	109	ARG	O-C-N	-5.47	113.95	122.70
1	Z	215	ASP	CB-CG-OD2	5.47	123.22	118.30
5	4	36	PHE	CB-CG-CD1	-5.47	116.97	120.80
7	6	103	TYR	CZ-CE2-CD2	5.47	124.72	119.80
23	O	264	ASN	CB-CA-C	-5.47	99.47	110.40
25	Q	107	VAL	CA-CB-CG2	-5.47	102.70	110.90
9	A	27	TYR	CZ-CE2-CD2	-5.46	114.88	119.80
18	J	113	ARG	CG-CD-NE	-5.46	100.32	111.80
29	U	23	PHE	CB-CG-CD1	-5.46	116.97	120.80
22	N	871	PRO	N-CA-CB	-5.46	96.59	102.60
9	A	151	VAL	O-C-N	-5.46	113.96	122.70
1	Z	215	ASP	CB-CG-OD1	-5.46	113.39	118.30
13	E	126	GLU	OE1-CD-OE2	5.46	129.85	123.30
9	A	14	THR	N-CA-C	-5.46	96.27	111.00
6	5	195	TYR	CB-CG-CD2	-5.46	117.73	121.00
20	L	365	GLU	OE1-CD-OE2	5.45	129.84	123.30
10	B	97	TYR	CB-CG-CD1	5.45	124.27	121.00
19	K	388	ARG	NE-CZ-NH2	5.45	123.03	120.30
28	T	180	GLU	N-CA-CB	5.45	120.41	110.60
6	5	64	ALA	CB-CA-C	-5.45	101.93	110.10
5	4	157	VAL	CA-CB-CG2	-5.44	102.74	110.90
27	S	162	GLU	CB-CA-C	-5.44	99.52	110.40
19	K	154	LEU	N-CA-C	-5.44	96.32	111.00
22	N	794	ASP	CB-CG-OD2	-5.44	113.41	118.30
3	2	129	MET	CG-SD-CE	-5.44	91.50	100.20
27	S	467	TYR	CB-CG-CD2	5.44	124.26	121.00
15	G	164	CYS	N-CA-C	-5.43	96.33	111.00
25	Q	33	ARG	NE-CZ-NH1	-5.43	117.58	120.30
26	R	388	ASN	N-CA-CB	5.43	120.38	110.60
3	2	44	THR	CA-CB-CG2	-5.43	104.80	112.40
27	S	220	PHE	CB-CG-CD2	5.43	124.60	120.80
22	N	253	TYR	CA-CB-CG	-5.43	103.09	113.40
10	B	143	ARG	NE-CZ-NH1	-5.43	117.59	120.30
21	M	132	TYR	CB-CG-CD2	-5.43	117.75	121.00
24	P	393	LEU	CB-CG-CD2	-5.43	101.78	111.00
5	4	107	TYR	CG-CD1-CE1	-5.42	116.96	121.30
11	C	121	TYR	CG-CD1-CE1	-5.42	116.96	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	Q	290	VAL	CG1-CB-CG2	5.42	119.58	110.90
7	6	196	LEU	CB-CG-CD2	5.42	120.21	111.00
27	S	434	ALA	N-CA-C	5.42	125.63	111.00
4	3	27	ARG	NE-CZ-NH1	5.42	123.01	120.30
11	C	5	TYR	CB-CA-C	-5.42	99.57	110.40
12	D	108	THR	CA-CB-CG2	-5.42	104.82	112.40
16	H	215	PHE	CD1-CE1-CZ	5.42	126.60	120.10
22	N	774	PRO	N-CA-CB	5.42	109.80	103.30
26	R	296	VAL	CA-CB-CG1	-5.42	102.78	110.90
22	N	815	ALA	CB-CA-C	-5.42	101.98	110.10
18	J	174	LEU	CB-CA-C	-5.41	99.91	110.20
18	J	192	PRO	O-C-N	5.41	132.41	123.20
7	6	107	ASN	N-CA-C	-5.41	96.40	111.00
22	N	437	TYR	CB-CA-C	-5.41	99.58	110.40
14	F	12	VAL	CG1-CB-CG2	5.41	119.55	110.90
21	M	132	TYR	C-N-CA	5.41	135.22	121.70
27	S	482	PHE	CG-CD1-CE1	5.41	126.75	120.80
6	5	165	LYS	CA-CB-CG	-5.40	101.51	113.40
6	5	232	ALA	CB-CA-C	-5.40	101.99	110.10
2	1	172	TYR	CD1-CE1-CZ	5.40	124.66	119.80
15	G	190	ILE	O-C-N	5.40	131.34	122.70
20	L	73	ALA	CB-CA-C	-5.40	102.00	110.10
23	O	246	GLU	N-CA-CB	5.40	120.32	110.60
1	Z	816	TYR	CG-CD2-CE2	-5.40	116.98	121.30
14	F	128	TYR	CB-CG-CD1	-5.40	117.76	121.00
1	Z	436	SER	N-CA-CB	5.40	118.60	110.50
5	4	173	LEU	CB-CG-CD2	5.40	120.17	111.00
18	J	100	ASP	CB-CG-OD2	-5.39	113.44	118.30
18	J	110	PRO	N-CA-CB	5.39	109.77	103.30
23	O	156	TYR	CG-CD2-CE2	5.39	125.62	121.30
29	U	241	SER	N-CA-C	-5.39	96.44	111.00
8	7	264	GLU	OE1-CD-OE2	-5.39	116.83	123.30
22	N	250	PHE	CB-CG-CD1	-5.39	117.03	120.80
27	S	371	ASN	CB-CG-OD1	-5.39	110.82	121.60
1	Z	247	ALA	N-CA-CB	5.39	117.65	110.10
1	Z	469	TYR	CG-CD1-CE1	-5.39	116.99	121.30
17	I	172	THR	O-C-N	5.39	131.32	122.70
24	P	94	ARG	NE-CZ-NH1	5.39	122.99	120.30
25	Q	239	TYR	CB-CG-CD1	5.39	124.23	121.00
27	S	212	TYR	CB-CG-CD2	-5.39	117.77	121.00
1	Z	727	PHE	CB-CG-CD2	5.38	124.57	120.80
3	2	213	GLY	N-CA-C	-5.38	99.64	113.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	M	133	PHE	N-CA-CB	5.38	120.29	110.60
31	W	9	CYS	CA-CB-SG	-5.38	104.31	114.00
18	J	72	TYR	CB-CG-CD1	5.38	124.23	121.00
1	Z	142	TYR	CZ-CE2-CD2	-5.38	114.96	119.80
7	6	110	ALA	N-CA-CB	5.38	117.64	110.10
20	L	283	ASP	CB-CG-OD1	5.38	123.14	118.30
8	7	219	ARG	NE-CZ-NH1	5.38	122.99	120.30
28	T	342	TYR	CG-CD1-CE1	-5.38	117.00	121.30
10	B	139	TRP	CG-CD2-CE3	-5.38	129.06	133.90
14	F	232	PHE	CB-CG-CD2	-5.38	117.03	120.80
18	J	37	ASP	CB-CA-C	-5.38	99.64	110.40
20	L	205	ASP	CB-CG-OD2	-5.38	113.46	118.30
29	U	211	TYR	CD1-CE1-CZ	-5.38	114.96	119.80
20	L	19	HIS	CA-CB-CG	5.38	122.74	113.60
26	R	249	VAL	CA-CB-CG1	5.38	118.97	110.90
3	2	149	THR	CA-CB-CG2	-5.38	104.88	112.40
14	F	124	GLY	C-N-CA	5.38	135.14	121.70
27	S	211	TYR	CB-CG-CD1	-5.38	117.78	121.00
16	H	237	PHE	N-CA-C	-5.37	96.49	111.00
24	P	254	PRO	N-CD-CG	5.37	111.26	103.20
6	5	187	VAL	N-CA-C	-5.37	96.50	111.00
7	6	156	GLY	N-CA-C	-5.37	99.68	113.10
12	D	143	ARG	NE-CZ-NH2	-5.37	117.62	120.30
4	3	147	TYR	CG-CD1-CE1	-5.37	117.01	121.30
9	A	29	PHE	CB-CG-CD2	-5.37	117.04	120.80
28	T	118	ARG	NE-CZ-NH1	-5.37	117.62	120.30
18	J	223	PHE	CG-CD1-CE1	5.36	126.70	120.80
1	Z	904	PRO	N-CA-CB	5.36	109.73	103.30
26	R	139	ASP	CB-CG-OD2	-5.36	113.48	118.30
31	W	49	VAL	CA-CB-CG1	-5.36	102.86	110.90
11	C	43	VAL	CG1-CB-CG2	5.36	119.47	110.90
20	L	129	ASN	N-CA-CB	5.36	120.24	110.60
26	R	151	TYR	CB-CA-C	-5.36	99.69	110.40
30	V	152	LYS	CA-CB-CG	-5.35	101.62	113.40
30	V	154	LYS	N-CA-CB	5.35	120.24	110.60
7	6	126	SER	N-CA-CB	5.35	118.53	110.50
20	L	124	HIS	CB-CA-C	-5.35	99.71	110.40
31	W	156	PHE	CB-CG-CD2	-5.35	117.06	120.80
32	Y	50	ASP	CB-CG-OD2	-5.35	113.49	118.30
9	A	159	TYR	CB-CG-CD1	-5.34	117.79	121.00
11	C	209	GLU	O-C-N	-5.34	114.15	122.70
16	H	249	TYR	CG-CD1-CE1	-5.34	117.03	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	M	362	ARG	NE-CZ-NH2	5.34	122.97	120.30
20	L	97	ARG	NE-CZ-NH1	-5.34	117.63	120.30
3	2	87	CYS	N-CA-CB	5.34	120.21	110.60
15	G	164	CYS	N-CA-CB	5.34	120.21	110.60
25	Q	302	PHE	CB-CG-CD1	-5.34	117.06	120.80
20	L	286	ASP	CB-CG-OD1	-5.34	113.50	118.30
22	N	880	ASN	CA-C-N	5.34	132.04	117.10
29	U	120	VAL	CA-CB-CG2	5.34	118.91	110.90
9	A	219	VAL	CA-CB-CG1	-5.33	102.90	110.90
18	J	92	GLU	C-N-CA	5.33	133.50	122.30
15	G	15	PHE	CB-CG-CD1	5.33	124.53	120.80
19	K	300	ASP	N-CA-CB	5.33	120.19	110.60
30	V	109	VAL	CA-CB-CG2	5.33	118.89	110.90
22	N	57	ARG	NE-CZ-NH1	-5.33	117.64	120.30
11	C	71	ASP	CB-CG-OD1	-5.33	113.51	118.30
14	F	39	LYS	N-CA-CB	5.33	120.19	110.60
19	K	392	TYR	CD1-CE1-CZ	5.33	124.59	119.80
24	P	366	MET	CG-SD-CE	-5.33	91.68	100.20
13	E	237	VAL	CA-CB-CG2	-5.32	102.92	110.90
11	C	49	ARG	NE-CZ-NH1	5.32	122.96	120.30
16	H	413	VAL	CA-CB-CG2	-5.32	102.92	110.90
27	S	311	ASN	CB-CG-OD1	-5.32	110.96	121.60
19	K	97	ASP	CB-CG-OD1	5.32	123.09	118.30
25	Q	124	PHE	CD1-CE1-CZ	5.32	126.48	120.10
4	3	147	TYR	CG-CD2-CE2	-5.32	117.05	121.30
15	G	59	TYR	CG-CD1-CE1	-5.32	117.05	121.30
15	G	100	ARG	NE-CZ-NH1	5.32	122.96	120.30
4	3	87	LEU	CB-CG-CD1	-5.32	101.96	111.00
8	7	186	TYR	CG-CD1-CE1	5.32	125.55	121.30
15	G	188	ARG	NE-CZ-NH1	5.32	122.96	120.30
1	Z	502	LEU	CA-C-N	5.31	131.98	117.10
19	K	310	ALA	CB-CA-C	-5.31	102.13	110.10
22	N	923	GLU	CB-CA-C	-5.31	99.78	110.40
28	T	131	THR	C-N-CA	5.31	134.98	121.70
10	B	131	GLY	O-C-N	5.31	131.19	122.70
22	N	535	TYR	CG-CD2-CE2	5.31	125.55	121.30
23	O	293	PHE	CB-CA-C	-5.31	99.78	110.40
1	Z	420	TRP	NE1-CE2-CZ2	5.30	136.23	130.40
4	3	149	MET	N-CA-CB	5.30	120.15	110.60
8	7	128	TYR	CA-CB-CG	5.30	123.48	113.40
9	A	229	ILE	N-CA-C	-5.30	96.67	111.00
21	M	223	VAL	CG1-CB-CG2	-5.30	102.41	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	P	426	ASN	CB-CA-C	-5.30	99.79	110.40
16	H	318	LEU	CB-CG-CD1	-5.30	101.98	111.00
22	N	437	TYR	CD1-CE1-CZ	5.30	124.57	119.80
14	F	135	ALA	N-CA-CB	-5.30	102.68	110.10
17	I	114	GLU	OE1-CD-OE2	5.30	129.66	123.30
21	M	115	SER	N-CA-CB	5.30	118.45	110.50
12	D	134	VAL	CB-CA-C	-5.30	101.34	111.40
19	K	41	TYR	CB-CG-CD2	-5.30	117.82	121.00
22	N	920	ASP	C-N-CA	5.30	134.94	121.70
29	U	88	ARG	NE-CZ-NH1	5.30	122.95	120.30
14	F	152	ASN	N-CA-CB	5.29	120.13	110.60
24	P	268	LYS	CB-CG-CD	5.29	125.36	111.60
1	Z	524	MET	N-CA-CB	-5.29	101.08	110.60
10	B	219	ARG	NE-CZ-NH1	-5.29	117.66	120.30
13	E	216	GLU	N-CA-CB	5.29	120.12	110.60
17	I	335	GLU	O-C-N	5.29	131.16	122.70
4	3	149	MET	CG-SD-CE	-5.29	91.74	100.20
11	C	1	MET	CG-SD-CE	-5.29	91.74	100.20
28	T	164	PHE	CB-CG-CD2	-5.29	117.10	120.80
28	T	187	TYR	CB-CG-CD1	-5.29	117.83	121.00
12	D	35	VAL	CA-CB-CG2	-5.29	102.97	110.90
22	N	745	THR	CA-CB-OG1	5.29	120.10	109.00
3	2	238	LYS	CA-C-N	5.28	126.77	116.20
4	3	90	MET	CG-SD-CE	-5.28	91.75	100.20
20	L	53	VAL	CA-CB-CG1	5.28	118.83	110.90
24	P	240	TYR	CB-CG-CD2	5.28	124.17	121.00
26	R	175	ASP	CB-CG-OD1	5.28	123.06	118.30
26	R	194	PHE	CB-CG-CD1	5.28	124.50	120.80
11	C	146	GLN	CB-CA-C	-5.28	99.84	110.40
21	M	350	ARG	NE-CZ-NH2	-5.28	117.66	120.30
1	Z	760	PHE	CB-CG-CD1	-5.28	117.11	120.80
8	7	242	VAL	CG1-CB-CG2	5.28	119.34	110.90
17	I	382	ASP	CB-CA-C	-5.28	99.84	110.40
8	7	80	ARG	NE-CZ-NH1	5.28	122.94	120.30
14	F	153	TYR	CZ-CE2-CD2	-5.28	115.05	119.80
20	L	114	GLU	N-CA-C	-5.28	96.76	111.00
22	N	167	ILE	CA-CB-CG1	-5.28	100.97	111.00
14	F	72	ILE	CA-C-N	-5.27	105.60	117.20
22	N	200	VAL	CA-CB-CG1	5.27	118.81	110.90
1	Z	816	TYR	CB-CG-CD2	5.27	124.16	121.00
21	M	347	ARG	NE-CZ-NH1	5.27	122.93	120.30
30	V	140	ALA	N-CA-CB	5.27	117.48	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	64	ILE	CA-CB-CG1	5.27	121.01	111.00
13	E	153	LEU	CB-CG-CD2	-5.27	102.05	111.00
16	H	412	ALA	N-CA-CB	5.26	117.47	110.10
18	J	189	TYR	CB-CG-CD1	-5.26	117.84	121.00
25	Q	1	MET	CG-SD-CE	-5.26	91.78	100.20
16	H	320	ALA	N-CA-CB	-5.26	102.73	110.10
24	P	358	VAL	CA-CB-CG2	5.26	118.79	110.90
4	3	96	TYR	CB-CG-CD2	-5.26	117.84	121.00
10	B	145	TYR	C-N-CA	5.26	134.85	121.70
13	E	100	TRP	CB-CG-CD2	-5.26	119.76	126.60
18	J	334	ARG	NE-CZ-NH2	-5.26	117.67	120.30
19	K	417	TYR	CZ-CE2-CD2	5.26	124.53	119.80
10	B	179	ASN	C-N-CA	5.26	134.84	121.70
18	J	74	GLY	CA-C-O	5.26	130.06	120.60
1	Z	828	ARG	N-CA-C	-5.25	96.81	111.00
9	A	23	TYR	CB-CA-C	-5.25	99.89	110.40
9	A	9	PHE	N-CA-C	-5.25	96.82	111.00
18	J	105	ILE	CA-CB-CG2	-5.25	100.39	110.90
2	1	83	ALA	CB-CA-C	-5.25	102.22	110.10
22	N	385	PHE	CB-CG-CD1	5.25	124.48	120.80
29	U	117	PRO	N-CA-CB	5.25	109.60	103.30
11	C	8	ARG	NE-CZ-NH2	-5.25	117.67	120.30
1	Z	749	ALA	CB-CA-C	-5.25	102.23	110.10
3	2	57	LEU	CB-CA-C	-5.25	100.23	110.20
5	4	170	ARG	N-CA-CB	5.25	120.04	110.60
21	M	236	LEU	CB-CA-C	-5.25	100.23	110.20
27	S	166	TYR	CD1-CE1-CZ	5.25	124.52	119.80
5	4	36	PHE	N-CA-C	-5.24	96.84	111.00
20	L	69	PHE	CG-CD1-CE1	-5.24	115.03	120.80
8	7	145	ARG	NE-CZ-NH1	5.24	122.92	120.30
15	G	21	VAL	CA-CB-CG1	-5.24	103.04	110.90
21	M	344	ARG	NE-CZ-NH1	5.24	122.92	120.30
17	I	283	PHE	CG-CD1-CE1	-5.24	115.04	120.80
1	Z	192	VAL	CA-C-N	5.24	131.76	117.10
1	Z	592	ASN	CB-CG-OD1	-5.24	111.13	121.60
6	5	243	TRP	CG-CD2-CE3	-5.24	129.19	133.90
15	G	15	PHE	CB-CG-CD2	-5.24	117.13	120.80
1	Z	533	ASP	CB-CG-OD1	5.24	123.01	118.30
21	M	174	ALA	N-CA-CB	5.24	117.43	110.10
26	R	156	LEU	CB-CA-C	-5.24	100.25	110.20
27	S	470	ARG	NH1-CZ-NH2	-5.24	113.64	119.40
13	E	84	ASP	CB-CG-OD1	-5.23	113.59	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	H	119	ALA	N-CA-CB	5.23	117.43	110.10
31	W	41	THR	N-CA-CB	5.23	120.24	110.30
5	4	153	ARG	NE-CZ-NH1	5.23	122.92	120.30
20	L	269	THR	N-CA-C	-5.23	96.88	111.00
21	M	171	ARG	NH1-CZ-NH2	-5.23	113.64	119.40
24	P	96	GLN	CB-CA-C	5.23	120.86	110.40
25	Q	147	LEU	CB-CG-CD2	5.23	119.88	111.00
16	H	167	GLU	CB-CA-C	5.22	120.85	110.40
20	L	99	ALA	N-CA-CB	5.22	117.42	110.10
29	U	284	ASP	CB-CG-OD2	-5.22	113.60	118.30
10	B	83	TYR	CD1-CG-CD2	5.22	123.64	117.90
8	7	214	VAL	CA-CB-CG1	-5.22	103.07	110.90
14	F	128	TYR	CG-CD2-CE2	5.22	125.47	121.30
19	K	235	PHE	N-CA-CB	5.22	120.00	110.60
26	R	255	ALA	N-CA-CB	5.22	117.41	110.10
11	C	91	ARG	NE-CZ-NH1	-5.22	117.69	120.30
21	M	251	LEU	N-CA-CB	5.22	120.84	110.40
7	6	115	ALA	N-CA-CB	5.22	117.40	110.10
25	Q	181	SER	CB-CA-C	5.22	120.01	110.10
29	U	270	VAL	O-C-N	-5.22	114.35	122.70
13	E	218	ALA	N-CA-CB	5.21	117.40	110.10
17	I	276	GLU	CB-CA-C	-5.21	99.97	110.40
20	L	242	ARG	NE-CZ-NH1	-5.21	117.69	120.30
25	Q	363	ARG	NE-CZ-NH2	5.21	122.91	120.30
26	R	261	PHE	CB-CG-CD1	-5.21	117.15	120.80
6	5	106	GLY	N-CA-C	-5.21	100.07	113.10
14	F	67	ASP	CB-CG-OD1	5.21	122.99	118.30
16	H	95	VAL	CG1-CB-CG2	5.21	119.24	110.90
1	Z	326	LEU	CB-CA-C	-5.21	100.30	110.20
5	4	30	ASP	CB-CG-OD2	-5.21	113.61	118.30
26	R	313	SER	N-CA-C	-5.21	96.93	111.00
1	Z	374	SER	CB-CA-C	-5.21	100.21	110.10
2	1	117	PHE	CB-CG-CD2	5.21	124.44	120.80
4	3	72	ASN	CB-CA-C	-5.21	99.99	110.40
4	3	154	TRP	CA-CB-CG	5.21	123.59	113.70
22	N	116	ALA	CB-CA-C	-5.21	102.29	110.10
24	P	263	TRP	CB-CG-CD2	-5.21	119.83	126.60
1	Z	593	THR	CA-CB-CG2	-5.20	105.12	112.40
10	B	113	ARG	NE-CZ-NH2	-5.20	117.70	120.30
28	T	324	LYS	N-CA-CB	5.20	119.96	110.60
2	1	178	ARG	NE-CZ-NH1	5.20	122.90	120.30
26	R	92	GLU	OE1-CD-OE2	-5.20	117.06	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	826	GLN	CB-CA-C	-5.20	100.01	110.40
8	7	147	LYS	C-N-CA	5.20	134.69	121.70
10	B	3	GLU	CA-CB-CG	5.20	124.83	113.40
5	4	131	ALA	CB-CA-C	-5.19	102.31	110.10
16	H	418	LYS	CB-CA-C	-5.19	100.01	110.40
11	C	112	THR	CA-CB-CG2	-5.19	105.13	112.40
11	C	258	GLU	C-N-CA	5.19	134.68	121.70
18	J	326	LEU	CB-CA-C	-5.19	100.33	110.20
23	O	374	ILE	N-CA-C	-5.19	96.99	111.00
22	N	900	TYR	CB-CG-CD1	5.19	124.11	121.00
25	Q	420	LYS	N-CA-CB	5.19	119.94	110.60
27	S	361	PHE	CB-CG-CD2	-5.19	117.17	120.80
29	U	139	ILE	N-CA-C	-5.19	96.99	111.00
27	S	201	ARG	NE-CZ-NH2	5.19	122.89	120.30
1	Z	193	PRO	N-CD-CG	5.18	110.98	103.20
1	Z	208	LEU	CB-CG-CD2	5.18	119.81	111.00
1	Z	268	LEU	CB-CG-CD2	5.18	119.81	111.00
22	N	49	TYR	CG-CD2-CE2	5.18	125.45	121.30
10	B	99	LEU	CB-CG-CD1	5.18	119.81	111.00
26	R	157	ILE	CA-CB-CG1	5.18	120.84	111.00
14	F	24	TYR	CZ-CE2-CD2	-5.18	115.14	119.80
3	2	221	ILE	CA-CB-CG1	5.18	120.84	111.00
20	L	148	VAL	CA-CB-CG2	-5.18	103.14	110.90
24	P	317	TRP	CG-CD2-CE3	-5.18	129.24	133.90
1	Z	745	LEU	O-C-N	-5.17	114.42	122.70
6	5	247	SER	N-CA-CB	5.17	118.26	110.50
20	L	40	TYR	CZ-CE2-CD2	5.17	124.46	119.80
30	V	133	PHE	CB-CG-CD1	-5.17	117.18	120.80
10	B	91	ARG	NE-CZ-NH2	-5.17	117.71	120.30
4	3	126	LEU	CB-CG-CD2	-5.17	102.21	111.00
17	I	159	VAL	CG1-CB-CG2	5.17	119.17	110.90
22	N	502	TYR	N-CA-CB	5.17	119.90	110.60
26	R	323	PHE	N-CA-CB	5.17	119.90	110.60
4	3	150	CYS	N-CA-CB	5.17	119.90	110.60
7	6	224	CYS	N-CA-CB	5.17	119.90	110.60
18	J	336	MET	CA-CB-CG	5.17	122.08	113.30
4	3	131	MET	CG-SD-CE	-5.16	91.94	100.20
29	U	257	MET	CG-SD-CE	-5.16	91.94	100.20
9	A	176	THR	OG1-CB-CG2	-5.16	98.14	110.00
15	G	127	SER	CB-CA-C	-5.16	100.30	110.10
1	Z	377	VAL	C-N-CA	5.15	134.59	121.70
1	Z	882	LEU	CB-CG-CD2	5.15	119.76	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	Z	421	ASP	CB-CG-OD1	-5.15	113.66	118.30
6	5	112	SER	CB-CA-C	-5.15	100.31	110.10
15	G	63	SER	N-CA-CB	5.15	118.23	110.50
22	N	478	SER	CB-CA-C	-5.15	100.31	110.10
10	B	130	PHE	N-CA-CB	5.15	119.87	110.60
29	U	88	ARG	NH1-CZ-NH2	-5.15	113.74	119.40
21	M	436	GLN	O-C-N	5.15	130.93	122.70
10	B	52	GLN	N-CA-CB	5.14	119.86	110.60
13	E	109	VAL	CA-CB-CG1	5.14	118.61	110.90
1	Z	828	ARG	CG-CD-NE	-5.14	101.00	111.80
2	1	124	TYR	CB-CG-CD1	5.14	124.08	121.00
15	G	18	ASP	O-C-N	-5.14	114.46	123.20
21	M	149	ASP	CA-CB-CG	-5.14	102.09	113.40
4	3	34	MET	CG-SD-CE	-5.14	91.98	100.20
9	A	88	ARG	NE-CZ-NH1	-5.14	117.73	120.30
17	I	426	VAL	CG1-CB-CG2	-5.14	102.68	110.90
18	J	87	VAL	CA-CB-CG2	-5.14	103.19	110.90
10	B	28	ALA	N-CA-CB	5.14	117.29	110.10
11	C	83	ALA	CB-CA-C	-5.14	102.40	110.10
22	N	88	PHE	CB-CG-CD2	5.14	124.39	120.80
22	N	460	TYR	CG-CD2-CE2	-5.14	117.19	121.30
25	Q	12	ALA	CB-CA-C	-5.14	102.39	110.10
1	Z	483	PHE	CB-CG-CD1	-5.13	117.21	120.80
27	S	211	TYR	CG-CD1-CE1	-5.13	117.19	121.30
20	L	192	ASP	N-CA-CB	5.13	119.84	110.60
22	N	706	VAL	CA-CB-CG2	5.13	118.60	110.90
27	S	378	VAL	CA-CB-CG1	-5.13	103.20	110.90
27	S	409	MET	CA-CB-CG	5.13	122.03	113.30
4	3	27	ARG	NH1-CZ-NH2	5.13	125.04	119.40
16	H	108	ASP	CB-CG-OD2	-5.13	113.68	118.30
26	R	169	GLU	OE1-CD-OE2	-5.13	117.15	123.30
19	K	356	GLU	OE1-CD-OE2	-5.13	117.15	123.30
20	L	207	TYR	N-CA-CB	5.13	119.83	110.60
23	O	280	MET	CB-CA-C	-5.13	100.15	110.40
5	4	141	SER	CB-CA-C	-5.12	100.36	110.10
19	K	121	ARG	NH1-CZ-NH2	-5.12	113.76	119.40
29	U	292	GLU	N-CA-C	-5.12	97.17	111.00
22	N	663	THR	CA-CB-CG2	5.12	119.57	112.40
28	T	219	ASP	CB-CG-OD2	5.12	122.91	118.30
11	C	12	PHE	CG-CD1-CE1	5.12	126.43	120.80
11	C	72	MET	CG-SD-CE	-5.12	92.01	100.20
12	D	125	ARG	NH1-CZ-NH2	-5.12	113.77	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	K	287	ARG	NE-CZ-NH1	-5.12	117.74	120.30
22	N	261	LEU	CB-CG-CD2	5.12	119.70	111.00
22	N	675	MET	N-CA-CB	5.12	119.81	110.60
28	T	178	TYR	CD1-CG-CD2	5.12	123.53	117.90
25	Q	340	GLU	CA-C-N	5.11	131.42	117.10
30	V	108	VAL	CA-CB-CG1	5.11	118.57	110.90
1	Z	124	ASP	CB-CG-OD2	5.11	122.90	118.30
26	R	201	PHE	N-CA-CB	5.11	119.80	110.60
30	V	261	GLU	OE1-CD-OE2	-5.11	117.17	123.30
31	W	112	PHE	CB-CG-CD2	5.11	124.38	120.80
18	J	189	TYR	CG-CD1-CE1	5.11	125.39	121.30
23	O	9	GLN	CA-CB-CG	5.11	124.64	113.40
4	3	39	PHE	CB-CG-CD2	-5.11	117.23	120.80
9	A	31	ALA	N-CA-C	-5.11	97.22	111.00
10	B	229	TYR	CB-CG-CD1	-5.11	117.94	121.00
28	T	303	ALA	CB-CA-C	-5.11	102.44	110.10
30	V	161	ARG	N-CA-C	-5.11	97.21	111.00
1	Z	483	PHE	CZ-CE2-CD2	5.10	126.22	120.10
4	3	29	GLY	N-CA-C	-5.10	100.35	113.10
7	6	141	LEU	CB-CG-CD1	-5.10	102.33	111.00
26	R	325	VAL	CA-CB-CG1	5.10	118.56	110.90
12	D	156	TRP	CD1-CG-CD2	-5.10	102.22	106.30
26	R	283	LYS	N-CA-CB	5.10	119.78	110.60
11	C	245	ALA	CB-CA-C	-5.10	102.46	110.10
16	H	147	TYR	CB-CG-CD1	-5.10	117.94	121.00
13	E	40	ILE	N-CA-C	-5.09	97.24	111.00
23	O	102	GLU	OE1-CD-OE2	5.09	129.41	123.30
9	A	138	MET	CG-SD-CE	-5.09	92.05	100.20
18	J	228	ALA	N-CA-CB	-5.09	102.97	110.10
9	A	73	THR	N-CA-C	-5.09	97.26	111.00
10	B	29	VAL	CA-CB-CG2	-5.09	103.26	110.90
18	J	139	MET	CG-SD-CE	-5.09	92.05	100.20
19	K	132	LEU	CB-CG-CD1	5.09	119.66	111.00
25	Q	342	PHE	N-CA-CB	5.09	119.76	110.60
27	S	313	LEU	CB-CA-C	-5.09	100.53	110.20
7	6	194	LEU	CB-CA-C	-5.09	100.53	110.20
13	E	46	VAL	CB-CA-C	-5.09	101.73	111.40
16	H	330	ALA	N-CA-CB	5.09	117.23	110.10
1	Z	674	THR	CA-CB-OG1	5.09	119.68	109.00
28	T	128	PHE	CD1-CG-CD2	-5.09	111.69	118.30
16	H	336	ARG	N-CA-CB	5.08	119.75	110.60
18	J	66	LEU	CB-CA-C	-5.08	100.54	110.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	E	137	PHE	CG-CD1-CE1	5.08	126.39	120.80
9	A	120	ASP	CB-CG-OD2	5.08	122.87	118.30
4	3	6	TYR	CG-CD2-CE2	-5.08	117.24	121.30
15	G	224	ARG	NE-CZ-NH1	-5.08	117.76	120.30
18	J	260	GLU	N-CA-C	-5.08	97.29	111.00
22	N	601	ARG	NE-CZ-NH2	-5.08	117.76	120.30
27	S	489	MET	CG-SD-CE	-5.08	92.07	100.20
22	N	173	VAL	CA-CB-CG1	5.08	118.52	110.90
5	4	171	PHE	CG-CD2-CE2	5.08	126.38	120.80
17	I	394	ASP	CB-CA-C	-5.08	100.25	110.40
31	W	59	GLU	CA-CB-CG	5.08	124.57	113.40
17	I	302	GLU	CA-C-N	-5.07	106.04	117.20
12	D	183	THR	CA-CB-OG1	5.07	119.65	109.00
22	N	900	TYR	N-CA-CB	5.07	119.73	110.60
18	J	54	ALA	CB-CA-C	-5.07	102.50	110.10
18	J	223	PHE	CD1-CG-CD2	-5.07	111.71	118.30
26	R	28	LEU	CA-C-N	5.07	131.29	117.10
19	K	277	ALA	N-CA-CB	5.07	117.20	110.10
29	U	291	GLN	N-CA-CB	5.07	119.72	110.60
24	P	97	LEU	CB-CG-CD2	5.07	119.62	111.00
31	W	92	VAL	CA-CB-CG1	-5.07	103.30	110.90
1	Z	136	GLU	CG-CD-OE2	-5.07	108.17	118.30
1	Z	576	ILE	CA-CB-CG1	5.07	120.62	111.00
19	K	414	HIS	CA-CB-CG	5.07	122.21	113.60
12	D	16	LEU	CB-CG-CD2	5.06	119.61	111.00
1	Z	304	PHE	CB-CA-C	-5.06	100.28	110.40
3	2	170	MET	N-CA-C	-5.06	97.33	111.00
11	C	101	TYR	C-N-CA	5.06	134.35	121.70
19	K	392	TYR	CG-CD2-CE2	5.06	125.35	121.30
6	5	82	GLY	CA-C-O	-5.06	111.49	120.60
11	C	151	ASP	N-CA-C	-5.06	97.34	111.00
29	U	54	PHE	CB-CG-CD1	5.06	124.34	120.80
4	3	20	VAL	CG1-CB-CG2	5.06	118.99	110.90
26	R	355	GLU	N-CA-CB	5.06	119.70	110.60
27	S	196	SER	CB-CA-C	-5.06	100.49	110.10
30	V	54	MET	CG-SD-CE	5.06	108.29	100.20
7	6	213	ARG	NE-CZ-NH1	-5.06	117.77	120.30
3	2	108	LEU	CB-CA-C	-5.05	100.60	110.20
4	3	38	ASP	CA-CB-CG	-5.05	102.28	113.40
13	E	37	ALA	CB-CA-C	-5.05	102.52	110.10
16	H	363	SER	N-CA-CB	5.05	118.08	110.50
19	K	43	ARG	CB-CG-CD	5.05	124.74	111.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	M	90	VAL	N-CA-C	-5.05	97.35	111.00
29	U	82	PHE	CB-CG-CD1	5.05	124.34	120.80
6	5	225	ARG	CB-CA-C	-5.05	100.30	110.40
13	E	26	TYR	CD1-CE1-CZ	5.05	124.35	119.80
7	6	140	GLY	N-CA-C	-5.05	100.47	113.10
10	B	113	ARG	NE-CZ-NH1	5.05	122.83	120.30
12	D	124	ARG	NE-CZ-NH2	5.05	122.83	120.30
30	V	292	MET	CA-CB-CG	5.05	121.88	113.30
3	2	85	TYR	CA-CB-CG	-5.05	103.81	113.40
8	7	52	THR	C-N-CA	5.05	132.90	122.30
8	7	229	TYR	CB-CG-CD1	-5.05	117.97	121.00
19	K	243	GLY	N-CA-C	-5.05	100.48	113.10
1	Z	72	ARG	NH1-CZ-NH2	-5.04	113.85	119.40
3	2	227	ASP	CB-CG-OD2	5.04	122.84	118.30
19	K	326	ARG	NH1-CZ-NH2	5.04	124.95	119.40
21	M	236	LEU	CA-CB-CG	-5.04	103.70	115.30
25	Q	93	LEU	CB-CG-CD2	5.04	119.57	111.00
8	7	212	ASP	CB-CG-OD1	-5.04	113.76	118.30
26	R	286	TRP	CG-CD1-NE1	5.04	115.14	110.10
27	S	314	ARG	NE-CZ-NH1	5.04	122.82	120.30
21	M	204	LEU	CA-C-N	5.04	131.21	117.10
21	M	293	THR	N-CA-C	-5.04	97.39	111.00
4	3	121	ILE	CA-CB-CG2	-5.04	100.82	110.90
5	4	103	LEU	CB-CG-CD2	5.04	119.57	111.00
15	G	15	PHE	CB-CA-C	-5.04	100.33	110.40
20	L	269	THR	N-CA-CB	5.04	119.87	110.30
24	P	263	TRP	CB-CG-CD1	5.04	133.55	127.00
18	J	172	PRO	N-CD-CG	5.04	110.76	103.20
19	K	191	TYR	CD1-CE1-CZ	-5.04	115.27	119.80
19	K	200	ARG	NE-CZ-NH2	-5.04	117.78	120.30
20	L	65	THR	CA-CB-CG2	-5.04	105.35	112.40
22	N	460	TYR	CB-CG-CD1	-5.04	117.98	121.00
9	A	227	PHE	CB-CG-CD1	5.03	124.32	120.80
30	V	36	LEU	CB-CA-C	-5.03	100.64	110.20
14	F	147	THR	N-CA-C	-5.03	97.41	111.00
8	7	139	ARG	CB-CG-CD	5.03	124.67	111.60
20	L	294	ARG	CA-CB-CG	5.03	124.46	113.40
30	V	135	ALA	N-CA-CB	5.03	117.14	110.10
23	O	335	TRP	CB-CG-CD1	5.03	133.53	127.00
14	F	97	PHE	CB-CG-CD1	-5.02	117.28	120.80
2	1	218	VAL	CA-CB-CG2	5.02	118.44	110.90
18	J	325	ARG	NH1-CZ-NH2	-5.02	113.88	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	K	76	GLN	N-CA-CB	5.02	119.64	110.60
22	N	891	VAL	N-CA-CB	5.02	122.55	111.50
26	R	142	PHE	CG-CD1-CE1	5.02	126.32	120.80
22	N	628	ARG	NE-CZ-NH1	5.02	122.81	120.30
24	P	370	TYR	CB-CA-C	-5.02	100.36	110.40
13	E	168	ARG	NE-CZ-NH2	5.02	122.81	120.30
22	N	893	THR	CA-CB-OG1	5.02	119.54	109.00
9	A	71	LYS	N-CA-C	-5.02	97.45	111.00
22	N	246	TYR	CB-CG-CD1	5.02	124.01	121.00
23	O	311	VAL	CG1-CB-CG2	5.02	118.93	110.90
1	Z	300	ARG	NE-CZ-NH1	5.01	122.81	120.30
2	1	105	ASN	C-N-CA	5.01	134.23	121.70
17	I	439	TYR	CD1-CE1-CZ	-5.01	115.29	119.80
29	U	190	ARG	NE-CZ-NH2	-5.01	117.79	120.30
19	K	316	THR	CA-CB-OG1	5.01	119.52	109.00
20	L	173	TYR	CB-CG-CD2	5.01	124.01	121.00
24	P	358	VAL	CA-CB-CG1	-5.01	103.38	110.90
30	V	297	VAL	CA-CB-CG1	-5.01	103.38	110.90
10	B	57	TYR	CG-CD1-CE1	-5.01	117.29	121.30
22	N	900	TYR	CZ-CE2-CD2	-5.01	115.29	119.80
15	G	151	MET	CG-SD-CE	-5.01	92.19	100.20
10	B	169	ASN	CB-CA-C	-5.01	100.39	110.40
11	C	50	ARG	NE-CZ-NH2	-5.01	117.80	120.30
14	F	154	PHE	CB-CG-CD1	5.01	124.30	120.80
20	L	211	SER	CB-CA-C	-5.01	100.59	110.10
22	N	493	VAL	CA-CB-CG1	-5.01	103.39	110.90
22	N	557	TYR	CG-CD2-CE2	-5.01	117.30	121.30
20	L	264	MET	CG-SD-CE	-5.00	92.19	100.20
20	L	311	ASP	CB-CG-OD1	5.00	122.80	118.30
25	Q	340	GLU	O-C-N	-5.00	111.59	121.10
32	Y	50	ASP	CB-CG-OD1	5.00	122.80	118.30

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
16	H	311	PRO	CA
22	N	752	THR	CA

All (269) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	1	124	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	1	178	ARG	Sidechain
2	1	59	TYR	Sidechain
3	2	115	ARG	Sidechain
3	2	157	TYR	Sidechain
3	2	167	TYR	Sidechain
3	2	186	ARG	Sidechain
3	2	207	PHE	Sidechain
4	3	100	PHE	Sidechain
4	3	6	TYR	Sidechain
4	3	80	ARG	Sidechain
5	4	117	TYR	Sidechain
5	4	12	TYR	Sidechain
5	4	129	PHE	Sidechain
5	4	145	ARG	Sidechain
5	4	85	ARG	Sidechain
5	4	93	ARG	Sidechain
5	4	98	TYR	Sidechain
6	5	147	TYR	Sidechain
6	5	179	ARG	Sidechain
6	5	204	TYR	Sidechain
6	5	209	GLU	Sidechain
6	5	245	ARG	Sidechain
6	5	99	TYR	Sidechain
7	6	125	TYR	Sidechain
7	6	133	TYR	Sidechain
7	6	152	PHE	Sidechain
7	6	198	ARG	Sidechain
7	6	201	ARG	Sidechain
7	6	222	ARG	Sidechain
7	6	30	PHE	Sidechain
7	6	61	PHE	Sidechain
7	6	72	TYR	Sidechain
8	7	139	ARG	Sidechain
8	7	142	TYR	Sidechain
8	7	160	TYR	Sidechain
8	7	169	TYR	Sidechain
8	7	177	TYR	Sidechain
8	7	189	TYR	Sidechain
8	7	222	TYR	Sidechain
8	7	223	TYR	Sidechain
8	7	229	TYR	Sidechain
9	A	107	TYR	Sidechain

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Mol	Chain	Res	Type	Group
9	A	125	TYR	Sidechain
9	A	132	ARG	Sidechain
9	A	152	TYR	Sidechain
9	A	160	TYR	Sidechain
9	A	23	TYR	Sidechain
9	A	245	ARG	Sidechain
9	A	43	ARG	Sidechain
9	A	93	ARG	Sidechain
9	A	96	TYR	Sidechain
10	B	156	PHE	Sidechain
10	B	229	TYR	Sidechain
10	B	60	ARG	Sidechain
11	C	101	TYR	Sidechain
11	C	121	TYR	Sidechain
11	C	130	PHE	Sidechain
11	C	156	TYR	Sidechain
11	C	218	ARG	Sidechain
11	C	23	TYR	Sidechain
11	C	4	ARG	Sidechain
11	C	60	PHE	Sidechain
11	C	61	PHE	Sidechain
12	D	118	TYR	Sidechain
12	D	21	TYR	Sidechain
12	D	213	ARG	Sidechain
12	D	228	TYR	Sidechain
12	D	60	ARG	Sidechain
14	F	125	ARG	Sidechain
14	F	154	PHE	Sidechain
14	F	157	ARG	Sidechain
14	F	174	ARG	Sidechain
14	F	196	ARG	Sidechain
14	F	3	ARG	Sidechain
14	F	6	TYR	Sidechain
14	F	89	ARG	Sidechain
15	G	141	TYR	Sidechain
15	G	170	ARG	Sidechain
15	G	20	ARG	Sidechain
15	G	26	TYR	Sidechain
16	H	107	GLU	Peptide
16	H	111	TYR	Sidechain
16	H	139	ARG	Sidechain
16	H	232	ARG	Sidechain

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Mol	Chain	Res	Type	Group
16	H	255	ARG	Sidechain
16	H	258	ARG	Sidechain
16	H	283	ALA	Peptide
16	H	333	ARG	Sidechain
16	H	351	ARG	Sidechain
16	H	358	HIS	Sidechain
16	H	360	ARG	Sidechain
16	H	75	PRO	Peptide
17	I	184	TYR	Sidechain
17	I	225	TYR	Sidechain
17	I	272	ARG	Sidechain
17	I	295	TYR	Sidechain
17	I	428	TYR	Sidechain
18	J	104	ASP	Mainchain
18	J	121	TYR	Sidechain
18	J	258	ARG	Sidechain
18	J	271	ARG	Sidechain
18	J	310	ARG	Sidechain
18	J	313	ARG	Sidechain
18	J	325	ARG	Sidechain
18	J	332	HIS	Sidechain
18	J	49	ARG	Sidechain
18	J	72	TYR	Sidechain
19	K	135	HIS	Sidechain
19	K	178	ARG	Sidechain
19	K	191	TYR	Sidechain
19	K	205	TYR	Sidechain
19	K	221	HIS	Sidechain
19	K	239	TYR	Sidechain
19	K	251	PHE	Sidechain
19	K	283	ARG	Sidechain
19	K	339	ARG	Sidechain
19	K	342	ARG	Sidechain
19	K	366	ARG	Sidechain
19	K	392	TYR	Sidechain
19	K	403	TYR	Sidechain
19	K	409	LYS	Peptide
19	K	41	TYR	Sidechain
19	K	414	HIS	Sidechain
19	K	417	TYR	Sidechain
19	K	44	TYR	Sidechain
19	K	92	PHE	Sidechain

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Mol	Chain	Res	Type	Group
20	L	120	TYR	Sidechain
20	L	173	TYR	Sidechain
20	L	185	ARG	Sidechain
20	L	241	ARG	Sidechain
20	L	251	ARG	Sidechain
20	L	291	ARG	Sidechain
20	L	309	ARG	Sidechain
20	L	338	PHE	Sidechain
20	L	344	ARG	Sidechain
20	L	356	ARG	Sidechain
20	L	79	TYR	Sidechain
21	M	121	CYS	Peptide
21	M	133	PHE	Sidechain
21	M	158	TYR	Sidechain
21	M	168	TYR	Sidechain
21	M	238	ARG	Sidechain
21	M	321	GLN	Peptide
21	M	344	ARG	Sidechain
21	M	350	ARG	Sidechain
21	M	376	SER	Peptide
21	M	386	ARG	Sidechain
21	M	391	PHE	Sidechain
21	M	88	TYR	Sidechain
22	N	140	ARG	Sidechain
22	N	147	TYR	Sidechain
22	N	158	ARG	Sidechain
22	N	210	LYS	Peptide
22	N	246	TYR	Sidechain
22	N	250	PHE	Sidechain
22	N	260	PHE	Sidechain
22	N	375	PHE	Sidechain
22	N	402	PHE	Sidechain
22	N	490	ARG	Sidechain
22	N	557	TYR	Sidechain
22	N	590	TYR	Sidechain
22	N	644	TYR	Sidechain
22	N	647	HIS	Sidechain
22	N	650	TYR	Sidechain
22	N	802	TYR	Sidechain
23	O	110	ALA	Mainchain
23	O	173	TYR	Sidechain
23	O	178	ARG	Sidechain

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Mol	Chain	Res	Type	Group
23	O	208	GLU	Peptide
23	O	289	ARG	Sidechain
23	O	339	ARG	Sidechain
23	O	342	ASP	Peptide
23	O	355	PHE	Sidechain
24	P	123	ARG	Sidechain
24	P	129	ARG	Sidechain
24	P	142	ARG	Sidechain
24	P	174	TYR	Sidechain
24	P	199	TYR	Sidechain
24	P	213	PHE	Sidechain
24	P	214	PHE	Sidechain
24	P	226	TYR	Sidechain
24	P	247	TYR	Sidechain
24	P	248	ARG	Sidechain
24	P	364	ARG	Sidechain
24	P	392	PHE	Sidechain
24	P	75	TYR	Sidechain
25	Q	11	ARG	Sidechain
25	Q	122	ARG	Sidechain
25	Q	142	ARG	Sidechain
25	Q	143	TYR	Sidechain
25	Q	201	TYR	Sidechain
25	Q	229	TYR	Sidechain
25	Q	253	TYR	Sidechain
25	Q	297	ARG	Sidechain
25	Q	314	ARG	Sidechain
25	Q	327	TYR	Sidechain
25	Q	349	HIS	Sidechain
25	Q	76	PHE	Sidechain
26	R	113	ARG	Sidechain
26	R	124	PHE	Sidechain
26	R	125	ARG	Sidechain
26	R	128	TYR	Sidechain
26	R	177	ARG	Sidechain
26	R	183	TYR	Sidechain
26	R	211	TYR	Sidechain
26	R	259	TYR	Sidechain
26	R	288	PHE	Sidechain
26	R	293	ARG	Sidechain
26	R	295	TYR	Sidechain
26	R	300	ARG	Sidechain

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Mol	Chain	Res	Type	Group
26	R	312	ARG	Sidechain
26	R	32	ARG	Sidechain
26	R	336	ARG	Sidechain
26	R	366	TYR	Sidechain
26	R	379	ARG	Sidechain
26	R	38	ARG	Sidechain
27	S	166	TYR	Sidechain
27	S	181	TYR	Sidechain
27	S	228	ARG	Sidechain
27	S	241	ARG	Sidechain
27	S	288	TYR	Sidechain
27	S	302	TYR	Sidechain
27	S	355	ARG	Sidechain
27	S	397	ARG	Sidechain
27	S	436	PHE	Sidechain
27	S	443	ARG	Sidechain
27	S	479	ARG	Sidechain
28	T	118	ARG	Sidechain
28	T	145	ARG	Sidechain
28	T	174	TYR	Sidechain
28	T	214	ARG	Sidechain
28	T	225	TYR	Sidechain
28	T	292	PHE	Sidechain
28	T	315	TYR	Sidechain
28	T	316	TYR	Sidechain
29	U	114	ARG	Sidechain
29	U	115	TYR	Sidechain
29	U	209	ARG	Sidechain
29	U	224	HIS	Sidechain
29	U	261	TYR	Sidechain
29	U	68	TRP	Mainchain
29	U	90	ARG	Sidechain
30	V	115	HIS	Sidechain
30	V	237	HIS	Mainchain
30	V	68	ARG	Sidechain
31	W	17	ARG	Sidechain
31	W	25	ARG	Sidechain
31	W	70	ARG	Sidechain
32	Y	65	TYR	Sidechain
1	Z	110	TYR	Sidechain
1	Z	120	ARG	Sidechain
1	Z	143	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	Z	239	TYR	Sidechain
1	Z	341	GLU	Peptide
1	Z	434	TYR	Sidechain
1	Z	439	TYR	Sidechain
1	Z	469	TYR	Sidechain
1	Z	587	PHE	Sidechain
1	Z	62	ARG	Sidechain
1	Z	713	PHE	Sidechain
1	Z	740	ARG	Sidechain
1	Z	746	ARG	Sidechain
1	Z	751	TYR	Sidechain
1	Z	763	ARG	Sidechain
1	Z	781	TYR	Sidechain
1	Z	79	ARG	Sidechain
1	Z	816	TYR	Sidechain
1	Z	828	ARG	Sidechain

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	Z	6146	0	6189	24	0
2	1	1607	0	1567	2	0
3	2	1676	0	1695	5	0
4	3	1599	0	1621	10	0
5	4	1554	0	1559	8	0
6	5	1509	0	1477	3	0
7	6	1654	0	1653	3	0
8	7	1705	0	1674	3	0
9	A	1874	0	1879	10	0
10	B	1826	0	1823	11	0
11	C	2069	0	2099	9	0
12	D	1961	0	2000	3	0
13	E	1770	0	1760	8	0
14	F	1837	0	1834	10	0
15	G	1894	0	1877	12	0
16	H	2962	0	3027	12	0
17	I	2840	0	2881	12	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
18	J	2929	0	3044	8	0
19	K	3032	0	3072	8	0
20	L	2862	0	2924	14	0
21	M	3046	0	3116	14	0
22	N	6508	0	6533	17	0
23	O	3020	0	3041	11	0
24	P	3447	0	3567	6	0
25	Q	3335	0	3435	8	0
26	R	3084	0	3086	16	0
27	S	2757	0	2819	7	0
28	T	2056	0	2096	4	0
29	U	2183	0	2223	9	0
30	V	1986	0	2014	8	0
31	W	1420	0	1463	4	0
32	Y	175	0	159	0	0
All	All	78323	0	79207	256	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 2.

All (256) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:O:128:LEU:H	23:O:128:LEU:HD22	1.58	0.68
20:L:85:ARG:HE	30:V:47:ALA:HA	1.59	0.67
1:Z:261:ARG:HH21	1:Z:267:ARG:HH12	1.43	0.65
17:I:303:ARG:HE	17:I:307:ARG:HH22	1.43	0.65
29:U:254:ASN:HA	29:U:257:MET:HE2	1.78	0.64
17:I:409:GLU:HG3	17:I:411:ARG:HH21	1.62	0.64
18:J:147:THR:H	18:J:150:MET:HB2	1.64	0.63
23:O:103:LYS:H	23:O:111:VAL:HG13	1.64	0.62
9:A:12:HIS:CD2	11:C:4:ARG:HH22	2.18	0.61
1:Z:463:LEU:H	1:Z:463:LEU:HD12	1.66	0.61
21:M:120:LYS:HG2	21:M:121:CYS:H	1.66	0.60
19:K:252:ARG:HH21	19:K:255:LYS:HB2	1.65	0.60
16:H:157:ILE:HG23	16:H:265:ARG:HB3	1.84	0.60
22:N:791:LEU:H	22:N:798:PRO:HD2	1.70	0.57
1:Z:828:ARG:HH22	1:Z:883:ALA:H	1.52	0.57
30:V:137:SER:HB3	30:V:139:ARG:H	1.71	0.56
13:E:161:THR:HG22	13:E:162:PHE:H	1.71	0.56
16:H:111:TYR:HE2	16:H:124:ASP:H	1.53	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
30:V:169:VAL:HG11	30:V:194:HIS:CE1	2.41	0.55
22:N:218:GLN:HA	22:N:221:ILE:HD12	1.88	0.55
13:E:96:THR:HA	13:E:107:MET:SD	2.48	0.54
18:J:114:VAL:HG21	18:J:123:LEU:HD23	1.90	0.54
22:N:749:GLN:HE22	22:N:752:THR:HG23	1.72	0.54
15:G:10:LEU:H	15:G:10:LEU:HD22	1.73	0.54
23:O:223:GLU:H	23:O:223:GLU:CD	2.12	0.53
5:4:138:LEU:H	5:4:138:LEU:HD12	1.73	0.53
6:5:132:ARG:HA	6:5:132:ARG:HH11	1.73	0.53
10:B:60:ARG:HH21	10:B:223:PRO:HG2	1.73	0.53
1:Z:891:THR:H	1:Z:892:PRO:CD	2.22	0.53
23:O:229:ASP:HA	23:O:232:TRP:CD2	2.44	0.53
14:F:38:LEU:HD21	14:F:179:PHE:CZ	2.44	0.53
13:E:161:THR:HG22	13:E:162:PHE:N	2.25	0.52
21:M:231:THR:HG22	21:M:392:ASN:HB3	1.91	0.52
23:O:5:PRO:HA	23:O:39:LEU:HD21	1.91	0.52
29:U:12:HIS:HB2	29:U:15:VAL:HG23	1.90	0.52
19:K:404:LYS:HA	19:K:407:ILE:HG22	1.91	0.52
27:S:443:ARG:HD2	28:T:274:CYS:SG	2.50	0.51
4:3:47:ASP:H	4:3:48:ARG:NH2	2.09	0.51
1:Z:90:THR:HA	1:Z:98:PHE:CE1	2.45	0.51
7:6:195:SER:HB2	7:6:198:ARG:HB3	1.91	0.51
19:K:221:HIS:CE1	19:K:222:HIS:CE1	2.98	0.51
20:L:312:ILE:HG22	20:L:316:HIS:CE1	2.45	0.51
18:J:340:ARG:HD3	26:R:208:PHE:H	1.76	0.50
27:S:319:HIS:CG	27:S:320:THR:H	2.29	0.50
13:E:176:GLY:H	16:H:375:ARG:HH22	1.58	0.50
27:S:334:VAL:HG11	27:S:394:LEU:HD22	1.93	0.50
21:M:150:LEU:HD21	21:M:168:TYR:CD1	2.46	0.50
22:N:592:GLY:H	22:N:625:ILE:HA	1.76	0.50
16:H:150:HIS:CD2	16:H:152:PRO:HD3	2.47	0.50
11:C:60:PHE:HB3	11:C:62:SER:H	1.77	0.50
3:2:63:ALA:HB3	3:2:71:ASP:HB2	1.93	0.49
6:5:203:SER:HB3	6:5:205:ASP:H	1.78	0.49
1:Z:267:ARG:HH21	1:Z:894:LEU:HD12	1.77	0.49
10:B:189:HIS:HE1	10:B:229:TYR:CD2	2.30	0.49
16:H:95:VAL:HG22	16:H:139:ARG:HH21	1.77	0.49
26:R:304:TYR:CE1	26:R:334:LEU:HD13	2.48	0.49
5:4:181:ARG:HH21	5:4:188:ILE:HG22	1.78	0.49
7:6:199:ALA:O	7:6:203:VAL:HG23	2.13	0.48
13:E:155:HIS:CE1	13:E:170:ILE:HG21	2.47	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:F:79:ALA:HA	14:F:82:ARG:HE	1.77	0.48
21:M:86:LEU:HA	21:M:87:PRO:C	2.34	0.48
5:4:29:LYS:NZ	6:5:183:ALA:H	2.12	0.48
14:F:74:ILE:HD11	14:F:130:VAL:HB	1.95	0.48
26:R:141:VAL:HG13	26:R:161:THR:HG23	1.96	0.48
1:Z:102:HIS:CE1	1:Z:105:LYS:HB3	2.49	0.48
21:M:362:ARG:HA	21:M:365:ILE:HD12	1.96	0.48
26:R:286:TRP:CE2	26:R:287:LEU:HG	2.49	0.48
20:L:281:ARG:HH12	21:M:294:LYS:HD2	1.80	0.47
1:Z:589:SER:HB3	1:Z:615:ILE:HD12	1.95	0.47
21:M:246:ALA:HA	21:M:280:PRO:HG2	1.96	0.47
15:G:70:VAL:HB	15:G:74:VAL:HB	1.97	0.47
26:R:80:GLU:HA	26:R:83:ARG:HE	1.79	0.47
1:Z:408:LEU:HD22	1:Z:442:SER:HB2	1.96	0.47
22:N:772:TRP:CD1	22:N:774:PRO:HD2	2.50	0.47
1:Z:466:LEU:HD23	1:Z:500:LEU:HG	1.97	0.47
9:A:42:VAL:HG23	9:A:49:VAL:HG22	1.96	0.47
16:H:119:ALA:HA	16:H:121:PHE:CE1	2.49	0.47
17:I:364:ILE:CG2	17:I:368:HIS:CE1	2.98	0.47
24:P:443:THR:HG21	29:U:157:HIS:HE1	1.79	0.47
27:S:214:HIS:CE1	27:S:224:LEU:HD22	2.49	0.47
4:3:72:ASN:HD22	11:C:95:GLN:HE22	1.61	0.47
21:M:344:ARG:HH21	21:M:347:ARG:HG3	1.80	0.47
21:M:416:THR:HG22	21:M:419:ASP:OD2	2.15	0.47
8:7:69:ALA:HB1	8:7:86:ARG:HD2	1.97	0.46
1:Z:122:ALA:O	1:Z:125:ILE:HG22	2.16	0.46
22:N:749:GLN:HA	22:N:756:HIS:CG	2.51	0.46
5:4:49:GLU:O	5:4:53:THR:HG23	2.15	0.46
20:L:323:HIS:CG	20:L:324:GLY:N	2.78	0.46
9:A:125:TYR:HA	9:A:128:ASN:HD22	1.81	0.46
10:B:183:GLU:H	10:B:186:ASP:HB2	1.81	0.46
14:F:65:HIS:CD2	14:F:65:HIS:O	2.69	0.46
5:4:13:VAL:HB	5:4:183:ILE:HG23	1.97	0.46
21:M:204:LEU:HD22	21:M:208:HIS:CE1	2.51	0.45
3:2:61:THR:HG23	3:2:74:CYS:H	1.80	0.45
17:I:131:HIS:CE1	17:I:155:LYS:O	2.69	0.45
17:I:364:ILE:HG23	17:I:368:HIS:CE1	2.52	0.45
24:P:191:ARG:HH21	24:P:192:LEU:HA	1.81	0.45
26:R:137:ARG:HE	26:R:168:ILE:CG2	2.29	0.45
26:R:137:ARG:HE	26:R:168:ILE:HG21	1.81	0.45
14:F:37:GLY:HA2	14:F:46:LEU:HG	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:2:237:LYS:H	3:2:237:LYS:HD3	1.82	0.45
4:3:121:ILE:HD11	4:3:135:ASP:H	1.81	0.45
17:I:163:LEU:HG	17:I:165:ASP:H	1.82	0.45
20:L:33:LEU:HD22	21:M:66:LEU:HD22	1.98	0.45
28:T:224:VAL:O	28:T:228:HIS:CE1	2.70	0.45
15:G:108:PRO:HB2	15:G:111:HIS:H	1.81	0.45
16:H:78:TRP:CD1	17:I:132:TYR:CE1	3.04	0.45
19:K:268:ASP:HA	19:K:271:ALA:HB3	1.99	0.45
23:O:128:LEU:H	23:O:128:LEU:CD2	2.27	0.45
9:A:186:LYS:HA	9:A:189:TRP:CE2	2.51	0.45
15:G:10:LEU:H	15:G:10:LEU:CD2	2.29	0.45
30:V:83:SER:HB2	30:V:86:ALA:HB2	1.99	0.45
13:E:202:LEU:HD13	13:E:215:ILE:HD11	1.98	0.45
20:L:29:LEU:O	20:L:33:LEU:HG	2.17	0.45
23:O:81:LEU:HD13	23:O:96:PHE:CD2	2.52	0.45
29:U:214:LYS:HG2	29:U:219:LYS:HD3	1.99	0.45
4:3:122:CYS:HA	4:3:133:THR:H	1.81	0.44
10:B:39:LYS:HG2	10:B:41:ALA:H	1.82	0.44
10:B:148:GLN:HE21	10:B:163:MET:CE	2.30	0.44
18:J:309:GLY:H	18:J:311:ILE:HG12	1.83	0.44
20:L:169:GLY:HA2	20:L:275:MET:HB3	1.99	0.44
21:M:382:GLU:CD	21:M:382:GLU:H	2.20	0.44
26:R:152:MET:HA	26:R:152:MET:HE3	1.98	0.44
10:B:60:ARG:HH21	10:B:223:PRO:CG	2.31	0.44
15:G:194:VAL:HA	15:G:197:ILE:HD12	2.00	0.44
24:P:220:GLU:HB2	24:P:257:GLN:HG2	1.99	0.44
15:G:181:GLN:CD	15:G:181:GLN:H	2.21	0.44
1:Z:296:PHE:CD2	1:Z:339:ILE:HG21	2.52	0.44
15:G:79:ALA:CB	15:G:166:ILE:HD12	2.48	0.44
15:G:79:ALA:HB2	15:G:166:ILE:HD12	1.99	0.44
20:L:104:THR:HG22	20:L:106:THR:HG23	1.99	0.44
20:L:195:PHE:CE2	20:L:229:ILE:HG13	2.53	0.44
22:N:449:ILE:HG13	22:N:450:HIS:CD2	2.53	0.44
25:Q:28:HIS:CE1	25:Q:53:LEU:HB2	2.53	0.44
4:3:29:GLY:HA2	4:3:35:VAL:H	1.83	0.44
22:N:478:SER:HB2	22:N:511:ALA:HB1	1.99	0.44
30:V:113:HIS:CE1	30:V:115:HIS:CE1	3.06	0.44
19:K:233:SER:HA	19:K:269:ALA:HB3	1.99	0.43
31:W:125:VAL:HG22	31:W:159:THR:HG21	1.99	0.43
1:Z:262:PHE:CG	1:Z:290:VAL:HG11	2.53	0.43
26:R:254:PRO:HG3	26:R:257:ARG:HH11	1.82	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
28:T:282:ILE:HG23	28:T:314:ASN:HD22	1.83	0.43
5:4:37:LYS:HA	5:4:43:LEU:HD12	2.01	0.43
23:O:244:ASN:HD22	23:O:247:ARG:HG3	1.84	0.43
25:Q:372:LYS:O	25:Q:375:HIS:CE1	2.71	0.43
26:R:308:LEU:HD23	26:R:314:LEU:HD23	2.00	0.43
31:W:7:MET:HG2	31:W:97:LEU:HD21	2.01	0.43
1:Z:159:VAL:HB	1:Z:191:ILE:HG23	2.01	0.43
17:I:229:GLY:CA	18:J:310:ARG:HH22	2.31	0.43
20:L:83:CYS:SG	20:L:107:ILE:HB	2.58	0.43
25:Q:154:LEU:HD11	25:Q:170:GLN:HE21	1.83	0.43
27:S:228:ARG:O	27:S:232:HIS:CD2	2.72	0.43
13:E:154:PHE:CZ	13:E:164:GLN:HG2	2.54	0.43
14:F:38:LEU:HD13	14:F:39:LYS:N	2.33	0.43
16:H:321:THR:HG21	16:H:324:PRO:HA	1.99	0.43
23:O:336:VAL:HG22	23:O:336:VAL:O	2.19	0.43
16:H:172:VAL:O	16:H:173:THR:HG23	2.16	0.43
22:N:373:ASN:O	22:N:377:HIS:CD2	2.72	0.43
31:W:173:VAL:HG21	31:W:183:LEU:HD23	2.01	0.43
13:E:127:ASP:H	14:F:125:ARG:H	1.66	0.43
16:H:107:GLU:HG3	16:H:125:LEU:HD23	2.01	0.43
17:I:223:ILE:HG12	17:I:329:MET:HB2	2.00	0.43
29:U:18:SER:O	29:U:22:HIS:CG	2.72	0.43
3:2:230:ARG:HB3	3:2:231:PRO:HD2	2.00	0.43
25:Q:82:LYS:HE3	25:Q:120:GLU:HB3	2.01	0.43
9:A:15:ILE:HB	10:B:21:GLN:HE22	1.83	0.42
19:K:85:ILE:HA	19:K:86:PRO:C	2.39	0.42
20:L:370:ALA:O	20:L:374:VAL:HG23	2.19	0.42
27:S:298:ILE:HA	27:S:397:ARG:HH12	1.84	0.42
29:U:41:GLY:HA2	29:U:51:SER:HB2	2.01	0.42
1:Z:613:LEU:HD21	1:Z:677:HIS:CD2	2.54	0.42
17:I:131:HIS:HE1	17:I:155:LYS:O	2.02	0.42
26:R:104:MET:HA	26:R:107:LYS:HB2	2.01	0.42
14:F:13:TRP:HE1	15:G:131:PRO:HD2	1.84	0.42
24:P:97:LEU:HB2	24:P:100:ALA:H	1.83	0.42
26:R:157:ILE:C	26:R:157:ILE:HD12	2.40	0.42
9:A:18:PRO:HD3	10:B:24:TYR:CE1	2.55	0.42
16:H:73:ALA:HB3	17:I:131:HIS:HA	2.00	0.42
22:N:378:CYS:HA	22:N:410:VAL:HG12	2.01	0.42
22:N:699:THR:HB	22:N:700:GLU:H	1.67	0.42
9:A:186:LYS:HB2	9:A:189:TRP:CZ3	2.55	0.42
2:1:110:VAL:HG13	2:1:111:HIS:H	1.84	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:3:26:ARG:HE	4:3:39:PHE:H	1.67	0.42
4:3:35:VAL:HG13	4:3:36:THR:HG22	2.02	0.42
21:M:215:LEU:HD12	21:M:217:ILE:HG23	2.02	0.42
24:P:242:SER:HB3	24:P:246:HIS:CE1	2.55	0.42
1:Z:348:ILE:O	1:Z:352:HIS:CD2	2.72	0.42
11:C:69:ASN:ND2	11:C:70:GLU:H	2.17	0.42
21:M:188:ILE:HG12	21:M:191:LEU:HD12	2.02	0.42
22:N:44:LYS:H	22:N:44:LYS:HD2	1.85	0.42
25:Q:171:LEU:HD12	25:Q:213:GLN:HE22	1.85	0.42
8:7:100:GLY:HA3	8:7:153:ASN:HA	2.02	0.41
14:F:219:LEU:HD13	14:F:219:LEU:HA	1.87	0.41
18:J:90:HIS:HB2	18:J:91:PRO:HD3	2.02	0.41
4:3:25:ASP:HA	4:3:185:VAL:HG12	2.01	0.41
18:J:57:ARG:HH22	22:N:649:ARG:CZ	2.33	0.41
17:I:229:GLY:HA3	18:J:310:ARG:HH22	1.86	0.41
19:K:221:HIS:CD2	19:K:221:HIS:C	2.93	0.41
31:W:88:THR:HA	31:W:91:ARG:HE	1.86	0.41
1:Z:82:ILE:O	1:Z:82:ILE:HG22	2.20	0.41
1:Z:168:LYS:O	1:Z:171:GLN:HG2	2.20	0.41
2:1:170:TYR:O	2:1:173:VAL:HG22	2.21	0.41
4:3:82:ILE:C	4:3:82:ILE:HD12	2.41	0.41
5:4:5:ILE:HG22	5:4:6:GLY:N	2.35	0.41
16:H:131:PRO:HB3	16:H:140:VAL:HG22	2.03	0.41
20:L:289:LEU:HD13	20:L:295:LEU:HD12	2.02	0.41
22:N:731:ILE:HG23	22:N:732:LEU:N	2.35	0.41
25:Q:244:SER:HB3	25:Q:245:PRO:HD2	2.03	0.41
19:K:154:LEU:HD23	19:K:229:ARG:O	2.21	0.41
20:L:58:GLY:HA3	20:L:100:LEU:HD11	2.01	0.41
26:R:124:PHE:CE2	26:R:143:TYR:CD1	3.08	0.41
28:T:295:THR:HG22	28:T:297:LYS:H	1.85	0.41
29:U:14:LEU:HD13	30:V:39:LEU:HB3	2.02	0.41
5:4:62:LYS:HG3	12:D:92:GLN:HB3	2.03	0.41
9:A:192:GLU:OE2	9:A:238:HIS:CE1	2.74	0.41
10:B:1:MET:HB3	10:B:4:ARG:HB2	2.01	0.41
22:N:701:ILE:HG22	22:N:701:ILE:O	2.21	0.41
26:R:229:ILE:HD12	26:R:299:MET:HG3	2.02	0.41
15:G:38:ILE:HD13	15:G:38:ILE:HG21	1.86	0.41
20:L:97:ARG:HH11	20:L:114:GLU:H	1.68	0.41
25:Q:103:THR:O	25:Q:107:VAL:HG23	2.21	0.41
1:Z:62:ARG:HH21	1:Z:70:LEU:HD22	1.85	0.41
1:Z:285:CYS:HB2	1:Z:291:GLN:HE21	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:A:43:ARG:HH21	9:A:164:LYS:HG2	1.86	0.41
10:B:123:GLN:HA	11:C:128:ARG:HE	1.85	0.41
10:B:139:TRP:HA	10:B:145:TYR:CE1	2.55	0.41
11:C:42:GLY:H	11:C:218:ARG:HH12	1.69	0.41
11:C:88:ASN:HD22	11:C:91:ARG:HH21	1.67	0.41
15:G:10:LEU:HD22	15:G:10:LEU:N	2.36	0.41
23:O:166:ILE:HG13	23:O:168:ASN:H	1.84	0.41
24:P:225:LYS:O	24:P:229:LEU:HD23	2.20	0.41
25:Q:306:LEU:HD23	25:Q:310:ARG:HH22	1.86	0.41
29:U:30:GLY:HA2	29:U:32:GLN:HE22	1.85	0.41
30:V:155:VAL:H	30:V:155:VAL:HG12	1.66	0.41
1:Z:874:LEU:HD21	1:Z:879:ARG:O	2.20	0.41
8:7:131:ARG:H	8:7:131:ARG:HD2	1.86	0.41
26:R:287:LEU:HA	26:R:287:LEU:HD23	1.90	0.41
1:Z:249:LEU:HD12	1:Z:249:LEU:H	1.85	0.40
11:C:30:HIS:N	11:C:30:HIS:CD2	2.87	0.40
14:F:226:ASP:O	14:F:229:VAL:HG22	2.21	0.40
29:U:79:TYR:CE2	29:U:83:LYS:HD3	2.56	0.40
12:D:35:VAL:HG11	12:D:187:THR:CG2	2.50	0.40
12:D:76:LEU:HD12	12:D:79:ASP:OD2	2.20	0.40
22:N:461:LEU:O	22:N:461:LEU:HD23	2.21	0.40
1:Z:63:LEU:HD22	1:Z:125:ILE:HD12	2.03	0.40
1:Z:412:ALA:HA	1:Z:447:ALA:HB2	2.03	0.40
26:R:101:ARG:HH21	26:R:132:VAL:H	1.69	0.40
30:V:161:ARG:HD2	30:V:161:ARG:HA	1.94	0.40
7:6:149:VAL:H	7:6:160:ARG:NH2	2.19	0.40
15:G:192:LYS:HA	15:G:236:ALA:HB1	2.03	0.40
3:2:258:LYS:O	4:3:196:THR:HG23	2.21	0.40
9:A:73:THR:HG23	9:A:76:ILE:H	1.86	0.40
11:C:42:GLY:HA3	11:C:186:LEU:HD21	2.03	0.40
22:N:210:LYS:HB2	22:N:210:LYS:HZ2	1.86	0.40
23:O:149:THR:HG23	23:O:151:VAL:HG13	2.03	0.40
27:S:267:ALA:O	27:S:271:VAL:HG23	2.22	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	Z	788/908 (87%)	698 (89%)	66 (8%)	24 (3%)	4 28
2	1	212/239 (89%)	187 (88%)	19 (9%)	6 (3%)	5 30
3	2	220/277 (79%)	206 (94%)	9 (4%)	5 (2%)	6 34
4	3	203/205 (99%)	184 (91%)	14 (7%)	5 (2%)	5 32
5	4	192/201 (96%)	173 (90%)	13 (7%)	6 (3%)	4 27
6	5	193/263 (73%)	177 (92%)	12 (6%)	4 (2%)	7 36
7	6	211/241 (88%)	185 (88%)	15 (7%)	11 (5%)	2 19
8	7	216/264 (82%)	193 (89%)	17 (8%)	6 (3%)	5 30
9	A	237/246 (96%)	219 (92%)	15 (6%)	3 (1%)	12 48
10	B	232/234 (99%)	210 (90%)	14 (6%)	8 (3%)	3 26
11	C	259/261 (99%)	239 (92%)	11 (4%)	9 (4%)	3 25
12	D	246/248 (99%)	221 (90%)	21 (8%)	4 (2%)	9 44
13	E	230/241 (95%)	210 (91%)	13 (6%)	7 (3%)	4 28
14	F	231/263 (88%)	213 (92%)	12 (5%)	6 (3%)	5 31
15	G	240/255 (94%)	217 (90%)	18 (8%)	5 (2%)	7 36
16	H	376/433 (87%)	320 (85%)	32 (8%)	24 (6%)	1 16
17	I	360/440 (82%)	331 (92%)	18 (5%)	11 (3%)	4 27
18	J	371/406 (91%)	342 (92%)	18 (5%)	11 (3%)	4 28
19	K	377/418 (90%)	328 (87%)	39 (10%)	10 (3%)	5 31
20	L	359/389 (92%)	319 (89%)	32 (9%)	8 (2%)	6 35
21	M	387/439 (88%)	336 (87%)	37 (10%)	14 (4%)	3 25
22	N	830/953 (87%)	758 (91%)	50 (6%)	22 (3%)	5 31
23	O	374/376 (100%)	331 (88%)	26 (7%)	17 (4%)	2 22
24	P	420/456 (92%)	390 (93%)	21 (5%)	9 (2%)	7 36
25	Q	420/422 (100%)	389 (93%)	23 (6%)	8 (2%)	8 38

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	R	372/389 (96%)	338 (91%)	26 (7%)	8 (2%)	6 35
27	S	336/534 (63%)	305 (91%)	20 (6%)	11 (3%)	4 26
28	T	249/350 (71%)	226 (91%)	14 (6%)	9 (4%)	3 25
29	U	266/324 (82%)	252 (95%)	12 (4%)	2 (1%)	19 60
30	V	246/310 (79%)	227 (92%)	15 (6%)	4 (2%)	9 44
31	W	183/377 (48%)	170 (93%)	7 (4%)	6 (3%)	4 26
32	Y	19/70 (27%)	18 (95%)	1 (5%)	0	100 100
All	All	9855/11432 (86%)	8912 (90%)	660 (7%)	283 (3%)	7 29

All (283) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	Z	303	VAL
1	Z	306	GLU
1	Z	365	VAL
1	Z	891	THR
2	1	110	VAL
3	2	136	TYR
3	2	231	PRO
3	2	244	ARG
4	3	39	PHE
5	4	25	ILE
6	5	247	SER
7	6	75	THR
10	B	2	ALA
10	B	61	SER
10	B	180	GLU
10	B	233	ILE
11	C	2	SER
11	C	259	LYS
12	D	58	THR
13	E	16	SER
15	G	229	PRO
16	H	311	PRO
17	I	286	GLU
19	K	162	VAL
19	K	409	LYS
21	M	110	ASN
21	M	112	ASP
22	N	212	ASP

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Mol	Chain	Res	Type
22	N	362	ASN
22	N	429	LYS
22	N	645	ASN
22	N	801	GLN
23	O	51	ALA
23	O	80	ILE
23	O	336	VAL
23	O	343	LEU
24	P	130	MET
25	Q	121	LYS
25	Q	342	PHE
25	Q	420	LYS
26	R	94	ASN
26	R	169	GLU
27	S	182	LYS
27	S	221	LEU
27	S	316	ALA
27	S	318	GLN
27	S	414	TYR
28	T	182	LEU
28	T	183	PRO
28	T	319	ALA
1	Z	260	SER
1	Z	836	GLU
2	1	233	VAL
3	2	62	ARG
3	2	235	PRO
5	4	21	ALA
5	4	22	ALA
5	4	177	THR
6	5	81	ALA
6	5	90	VAL
7	6	47	ASP
7	6	183	PHE
9	A	165	ALA
10	B	53	LYS
10	B	146	LEU
11	C	4	ARG
11	C	124	PHE
11	C	125	GLY
11	C	219	GLU
12	D	200	GLN

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Mol	Chain	Res	Type
13	E	132	ALA
13	E	214	ASN
14	F	33	SER
16	H	139	ARG
17	I	229	GLY
18	J	127	LEU
19	K	147	ALA
20	L	127	PRO
21	M	172	VAL
21	M	336	ASP
21	M	436	GLN
22	N	557	TYR
22	N	752	THR
22	N	791	LEU
23	O	104	VAL
23	O	221	VAL
24	P	115	ILE
24	P	176	SER
24	P	326	MET
24	P	346	GLU
25	Q	262	ASN
26	R	96	GLY
26	R	255	ALA
27	S	240	LEU
27	S	263	LEU
27	S	322	VAL
27	S	432	GLU
28	T	203	ASN
29	U	222	ILE
31	W	168	SER
1	Z	94	LYS
1	Z	116	GLY
1	Z	174	ASP
1	Z	513	GLU
1	Z	753	ALA
2	1	236	LEU
4	3	27	ARG
5	4	97	PRO
7	6	32	PRO
7	6	68	SER
8	7	91	ASN
8	7	163	GLY

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Mol	Chain	Res	Type
8	7	247	PRO
9	A	186	LYS
9	A	225	PRO
12	D	67	ASP
12	D	149	PRO
13	E	35	SER
13	E	53	ARG
13	E	126	GLU
14	F	164	ARG
14	F	183	ASN
15	G	34	SER
16	H	81	ALA
16	H	130	ALA
16	H	133	ASP
16	H	157	ILE
16	H	268	LYS
16	H	283	ALA
16	H	367	ASP
16	H	400	ARG
17	I	231	GLY
17	I	323	GLY
17	I	438	LEU
18	J	195	GLY
18	J	252	ASP
18	J	259	LEU
19	K	334	PRO
20	L	77	PRO
20	L	128	GLY
20	L	283	ASP
21	M	437	TYR
22	N	661	ALA
22	N	701	ILE
22	N	756	HIS
22	N	871	PRO
22	N	921	ILE
23	O	34	TRP
23	O	73	PRO
23	O	101	ARG
23	O	187	ASP
23	O	288	HIS
24	P	62	SER
25	Q	391	PRO

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Mol	Chain	Res	Type
26	R	271	PHE
28	T	216	PRO
28	T	324	LYS
28	T	347	GLU
29	U	158	VAL
30	V	139	ARG
30	V	151	VAL
30	V	222	LYS
31	W	56	ASN
31	W	66	PRO
31	W	162	GLY
1	Z	147	SER
1	Z	153	SER
1	Z	367	SER
1	Z	419	LEU
1	Z	718	ASP
1	Z	878	GLU
1	Z	892	PRO
2	1	106	GLU
2	1	234	ALA
5	4	39	SER
6	5	253	ASP
7	6	157	SER
8	7	92	ASN
11	C	3	ARG
11	C	50	ARG
14	F	103	LEU
15	G	62	GLY
16	H	116	LYS
16	H	174	TYR
16	H	276	GLU
16	H	289	ALA
16	H	290	GLY
17	I	173	VAL
17	I	228	PRO
18	J	265	GLY
18	J	288	ASN
18	J	354	ALA
19	K	153	MET
19	K	393	ILE
20	L	324	GLY
21	M	102	ASN

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Mol	Chain	Res	Type
21	M	156	ASP
21	M	158	TYR
21	M	279	ALA
21	M	287	GLU
21	M	295	ARG
21	M	300	LYS
21	M	428	GLN
22	N	16	GLU
22	N	414	GLY
22	N	704	PRO
22	N	774	PRO
22	N	878	LEU
22	N	899	ARG
23	O	57	ILE
23	O	226	ARG
23	O	284	ARG
23	O	327	VAL
23	O	371	ALA
24	P	41	GLN
24	P	296	LEU
25	Q	421	LEU
28	T	133	GLY
1	Z	271	MET
1	Z	549	GLU
1	Z	717	ALA
4	3	31	GLN
4	3	44	PRO
4	3	114	PRO
7	6	109	LYS
8	7	77	SER
10	B	3	GLU
10	B	199	PHE
13	E	225	ASN
14	F	41	LYS
15	G	12	ALA
15	G	63	SER
16	H	75	PRO
16	H	101	ILE
16	H	176	ASP
16	H	308	GLY
16	H	322	ASN
17	I	337	LEU

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Mol	Chain	Res	Type
17	I	343	ARG
18	J	69	GLN
19	K	224	THR
19	K	414	HIS
20	L	323	HIS
22	N	432	SER
23	O	259	PRO
24	P	96	GLN
26	R	132	VAL
26	R	192	ARG
27	S	300	LEU
27	S	352	SER
28	T	180	GLU
30	V	166	ASN
31	W	145	GLU
1	Z	316	ASP
7	6	107	ASN
7	6	219	ASP
8	7	161	ALA
14	F	125	ARG
16	H	141	GLY
17	I	128	GLY
18	J	251	ILE
19	K	118	THR
19	K	367	PRO
22	N	935	ILE
25	Q	243	ASP
7	6	155	VAL
16	H	109	PRO
20	L	167	PRO
11	C	103	GLU
16	H	115	VAL
1	Z	359	GLY
16	H	137	GLY
17	I	127	VAL
18	J	110	PRO
22	N	592	GLY
26	R	290	PRO
1	Z	779	CYS
2	1	238	PRO
20	L	282	PRO
25	Q	390	GLU

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Mol	Chain	Res	Type
31	W	148	VAL
7	6	182	GLY
18	J	255	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	Z	670/763 (88%)	642 (96%)	28 (4%)	30	54
2	1	167/181 (92%)	158 (95%)	9 (5%)	22	47
3	2	183/228 (80%)	174 (95%)	9 (5%)	25	50
4	3	174/174 (100%)	161 (92%)	13 (8%)	13	38
5	4	165/171 (96%)	157 (95%)	8 (5%)	25	51
6	5	151/202 (75%)	144 (95%)	7 (5%)	27	52
7	6	178/199 (89%)	169 (95%)	9 (5%)	24	48
8	7	180/215 (84%)	170 (94%)	10 (6%)	21	46
9	A	205/210 (98%)	193 (94%)	12 (6%)	19	45
10	B	191/191 (100%)	182 (95%)	9 (5%)	26	51
11	C	221/221 (100%)	203 (92%)	18 (8%)	11	35
12	D	211/211 (100%)	200 (95%)	11 (5%)	23	48
13	E	194/203 (96%)	186 (96%)	8 (4%)	30	55
14	F	200/224 (89%)	194 (97%)	6 (3%)	41	63
15	G	199/212 (94%)	185 (93%)	14 (7%)	15	40
16	H	324/372 (87%)	298 (92%)	26 (8%)	12	35
17	I	318/385 (83%)	302 (95%)	16 (5%)	24	49
18	J	325/352 (92%)	309 (95%)	16 (5%)	25	50
19	K	332/366 (91%)	310 (93%)	22 (7%)	16	41
20	L	315/341 (92%)	303 (96%)	12 (4%)	33	57
21	M	333/379 (88%)	318 (96%)	15 (4%)	27	52

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
22	N	710/816 (87%)	678 (96%)	32 (4%)	27	52
23	O	336/336 (100%)	320 (95%)	16 (5%)	25	51
24	P	389/416 (94%)	370 (95%)	19 (5%)	25	50
25	Q	362/362 (100%)	353 (98%)	9 (2%)	47	68
26	R	330/344 (96%)	307 (93%)	23 (7%)	15	40
27	S	299/460 (65%)	290 (97%)	9 (3%)	41	63
28	T	222/294 (76%)	215 (97%)	7 (3%)	39	61
29	U	245/295 (83%)	233 (95%)	12 (5%)	25	50
30	V	221/268 (82%)	214 (97%)	7 (3%)	39	61
31	W	163/312 (52%)	155 (95%)	8 (5%)	25	50
32	Y	19/63 (30%)	19 (100%)	0	100	100
All	All	8532/9766 (87%)	8112 (95%)	420 (5%)	29	50

All (420) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	Z	100	ARG
1	Z	118	ASN
1	Z	174	ASP
1	Z	178	LYS
1	Z	212	GLU
1	Z	223	GLU
1	Z	231	LEU
1	Z	236	CYS
1	Z	272	LEU
1	Z	275	MET
1	Z	289	VAL
1	Z	306	GLU
1	Z	364	GLN
1	Z	370	MET
1	Z	376	PHE
1	Z	418	LEU
1	Z	435	SER
1	Z	456	ARG
1	Z	498	LEU
1	Z	554	TYR
1	Z	576	ILE
1	Z	614	HIS

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Mol	Chain	Res	Type
1	Z	659	LEU
1	Z	686	LEU
1	Z	714	SER
1	Z	741	LEU
1	Z	752	HIS
1	Z	895	GLU
2	1	35	THR
2	1	123	ARG
2	1	125	ARG
2	1	126	GLU
2	1	138	ASP
2	1	179	GLU
2	1	189	PHE
2	1	210	LEU
2	1	215	GLU
3	2	102	ILE
3	2	146	VAL
3	2	207	PHE
3	2	210	LEU
3	2	230	ARG
3	2	231	PRO
3	2	237	LYS
3	2	246	ARG
3	2	258	LYS
4	3	48	ARG
4	3	85	TYR
4	3	88	MET
4	3	95	LEU
4	3	121	ILE
4	3	124	LEU
4	3	125	ASP
4	3	126	LEU
4	3	131	MET
4	3	178	ASP
4	3	185	VAL
4	3	192	LYS
4	3	193	ASP
5	4	12	TYR
5	4	19	ARG
5	4	27	GLN
5	4	40	GLU
5	4	82	ASN

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Mol	Chain	Res	Type
5	4	108	ASP
5	4	160	LEU
5	4	183	ILE
6	5	132	ARG
6	5	142	LEU
6	5	156	MET
6	5	166	ARG
6	5	195	TYR
6	5	202	TYR
6	5	220	TYR
7	6	75	THR
7	6	128	ARG
7	6	134	VAL
7	6	154	PRO
7	6	192	VAL
7	6	201	ARG
7	6	221	LEU
7	6	236	VAL
7	6	240	LYS
8	7	74	SER
8	7	87	ILE
8	7	107	TYR
8	7	131	ARG
8	7	202	GLN
8	7	211	ARG
8	7	212	ASP
8	7	230	ASN
8	7	240	LYS
8	7	247	PRO
9	A	96	TYR
9	A	101	TRP
9	A	109	ILE
9	A	132	ARG
9	A	140	LEU
9	A	144	ASP
9	A	147	GLN
9	A	152	TYR
9	A	160	TYR
9	A	183	VAL
9	A	184	LYS
9	A	226	LYS
10	B	6	TYR

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Mol	Chain	Res	Type
10	B	11	THR
10	B	46	LEU
10	B	70	LYS
10	B	112	GLN
10	B	122	THR
10	B	134	LEU
10	B	202	GLN
10	B	212	ILE
11	C	4	ARG
11	C	19	TYR
11	C	45	LEU
11	C	48	GLU
11	C	63	GLU
11	C	69	ASN
11	C	99	LEU
11	C	104	PRO
11	C	112	THR
11	C	117	ILE
11	C	141	LYS
11	C	156	TYR
11	C	187	LYS
11	C	192	LEU
11	C	218	ARG
11	C	239	LYS
11	C	251	LYS
11	C	261	LYS
12	D	13	ASP
12	D	38	ARG
12	D	79	ASP
12	D	106	TYR
12	D	148	ASP
12	D	172	LEU
12	D	181	ILE
12	D	184	ASP
12	D	196	LEU
12	D	201	SER
12	D	213	ARG
13	E	35	SER
13	E	41	GLN
13	E	43	SER
13	E	184	VAL
13	E	199	LEU

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Mol	Chain	Res	Type
13	E	208	GLU
13	E	225	ASN
13	E	228	MET
14	F	42	THR
14	F	65	HIS
14	F	69	HIS
14	F	120	THR
14	F	153	TYR
14	F	231	PRO
15	G	10	LEU
15	G	20	ARG
15	G	35	SER
15	G	69	ASN
15	G	76	MET
15	G	110	LYS
15	G	138	LEU
15	G	168	LYS
15	G	171	GLN
15	G	216	TRP
15	G	230	LYS
15	G	234	GLU
15	G	237	GLU
15	G	246	GLU
16	H	53	GLN
16	H	58	LYS
16	H	63	THR
16	H	72	LEU
16	H	93	LEU
16	H	95	VAL
16	H	109	PRO
16	H	120	LYS
16	H	164	MET
16	H	168	GLU
16	H	169	LYS
16	H	171	ASP
16	H	199	GLU
16	H	222	LYS
16	H	247	GLN
16	H	261	PHE
16	H	268	LYS
16	H	285	PHE
16	H	307	ASP

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Mol	Chain	Res	Type
16	H	334	PRO
16	H	339	ARG
16	H	342	GLU
16	H	360	ARG
16	H	367	ASP
16	H	402	LYS
16	H	416	VAL
17	I	139	VAL
17	I	141	LYS
17	I	162	VAL
17	I	174	MET
17	I	209	GLU
17	I	239	VAL
17	I	250	VAL
17	I	287	ILE
17	I	295	TYR
17	I	298	ASN
17	I	326	LYS
17	I	341	LEU
17	I	346	ARG
17	I	374	LEU
17	I	412	MET
17	I	415	THR
18	J	49	ARG
18	J	67	GLN
18	J	69	GLN
18	J	86	LEU
18	J	107	ASP
18	J	124	HIS
18	J	138	MET
18	J	144	PRO
18	J	145	ASP
18	J	155	ASP
18	J	191	PRO
18	J	245	ILE
18	J	299	ASP
18	J	336	MET
18	J	345	ARG
18	J	364	THR
19	K	62	LYS
19	K	79	VAL
19	K	82	ILE

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Mol	Chain	Res	Type
19	K	86	PRO
19	K	110	ASN
19	K	115	ILE
19	K	120	ASP
19	K	148	ASP
19	K	158	GLN
19	K	221	HIS
19	K	245	ARG
19	K	246	MET
19	K	252	ARG
19	K	276	ASP
19	K	287	ARG
19	K	303	VAL
19	K	318	ASP
19	K	330	LYS
19	K	364	VAL
19	K	392	TYR
19	K	410	ASP
19	K	417	TYR
20	L	31	GLU
20	L	92	LEU
20	L	111	LEU
20	L	120	TYR
20	L	121	ASN
20	L	144	GLU
20	L	155	ASN
20	L	213	ARG
20	L	226	GLN
20	L	269	THR
20	L	294	ARG
20	L	346	VAL
21	M	57	SER
21	M	81	LYS
21	M	117	ARG
21	M	121	CYS
21	M	132	TYR
21	M	134	LEU
21	M	137	ILE
21	M	180	ARG
21	M	215	LEU
21	M	219	PRO
21	M	233	LYS

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Mol	Chain	Res	Type
21	M	293	THR
21	M	342	LEU
21	M	349	ASP
21	M	382	GLU
22	N	15	ASP
22	N	24	LEU
22	N	71	LEU
22	N	90	VAL
22	N	95	GLU
22	N	106	ASP
22	N	172	ASP
22	N	194	ARG
22	N	210	LYS
22	N	234	GLU
22	N	357	LYS
22	N	366	HIS
22	N	428	PRO
22	N	473	VAL
22	N	494	TYR
22	N	546	ARG
22	N	561	GLU
22	N	567	ILE
22	N	580	ARG
22	N	585	THR
22	N	702	THR
22	N	709	PHE
22	N	722	ASP
22	N	746	ILE
22	N	747	SER
22	N	786	THR
22	N	797	MET
22	N	814	PRO
22	N	871	PRO
22	N	895	PRO
22	N	925	VAL
22	N	926	GLU
23	O	5	PRO
23	O	31	LYS
23	O	52	GLN
23	O	54	ASP
23	O	76	LEU
23	O	128	LEU

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Mol	Chain	Res	Type
23	O	133	GLU
23	O	198	PHE
23	O	205	LEU
23	O	223	GLU
23	O	225	LEU
23	O	226	ARG
23	O	230	ARG
23	O	247	ARG
23	O	251	LEU
23	O	284	ARG
24	P	93	ARG
24	P	104	MET
24	P	123	ARG
24	P	126	ASP
24	P	155	GLN
24	P	170	GLN
24	P	177	MET
24	P	202	THR
24	P	217	GLU
24	P	253	THR
24	P	257	GLN
24	P	268	LYS
24	P	297	GLU
24	P	314	LEU
24	P	326	MET
24	P	388	GLU
24	P	408	ARG
24	P	438	LEU
24	P	445	LEU
25	Q	20	ARG
25	Q	24	ILE
25	Q	74	ARG
25	Q	77	LEU
25	Q	81	SER
25	Q	93	LEU
25	Q	144	GLN
25	Q	285	GLU
25	Q	382	GLU
26	R	31	HIS
26	R	34	ASP
26	R	42	MET
26	R	73	MET

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Mol	Chain	Res	Type
26	R	87	GLU
26	R	97	GLU
26	R	104	MET
26	R	124	PHE
26	R	132	VAL
26	R	142	PHE
26	R	145	LEU
26	R	157	ILE
26	R	159	ARG
26	R	168	ILE
26	R	177	ARG
26	R	195	LYS
26	R	214	MET
26	R	253	LEU
26	R	254	PRO
26	R	261	PHE
26	R	350	VAL
26	R	356	THR
26	R	372	LYS
27	S	181	TYR
27	S	182	LYS
27	S	194	LYS
27	S	258	TYR
27	S	319	HIS
27	S	414	TYR
27	S	432	GLU
27	S	459	GLN
27	S	478	GLN
28	T	62	ARG
28	T	154	TRP
28	T	223	ASN
28	T	236	LEU
28	T	257	THR
28	T	281	LYS
28	T	348	MET
29	U	38	VAL
29	U	77	ASN
29	U	113	LYS
29	U	193	ASN
29	U	215	VAL
29	U	220	LEU
29	U	228	TYR

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Mol	Chain	Res	Type
29	U	232	ASP
29	U	233	VAL
29	U	246	VAL
29	U	247	LYS
29	U	252	LYS
30	V	87	VAL
30	V	107	MET
30	V	108	VAL
30	V	113	HIS
30	V	138	GLU
30	V	205	ILE
30	V	279	ASP
31	W	26	LEU
31	W	45	PRO
31	W	61	LEU
31	W	62	THR
31	W	70	ARG
31	W	88	THR
31	W	100	ARG
31	W	129	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (109) such sidechains are listed below:

Mol	Chain	Res	Type
1	Z	102	HIS
1	Z	195	ASN
1	Z	198	HIS
1	Z	291	GLN
1	Z	301	HIS
1	Z	352	HIS
1	Z	371	ASN
1	Z	566	HIS
1	Z	724	ASN
1	Z	815	HIS
1	Z	903	ASN
6	5	69	HIS
7	6	36	ASN
8	7	149	ASN
8	7	207	GLN
9	A	12	HIS
9	A	75	ASN
9	A	128	ASN

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Mol	Chain	Res	Type
9	A	147	GLN
9	A	238	HIS
10	B	21	GLN
10	B	71	HIS
10	B	148	GLN
10	B	189	HIS
11	C	53	HIS
11	C	69	ASN
11	C	88	ASN
11	C	95	GLN
11	C	123	GLN
13	E	99	HIS
13	E	155	HIS
14	F	65	HIS
14	F	183	ASN
15	G	181	GLN
16	H	150	HIS
17	I	81	ASN
17	I	131	HIS
17	I	368	HIS
17	I	416	ASN
18	J	48	GLN
18	J	53	ASN
18	J	106	ASN
19	K	133	HIS
19	K	221	HIS
19	K	222	HIS
19	K	312	ASN
20	L	75	ASN
20	L	155	ASN
20	L	190	GLN
20	L	305	ASN
20	L	316	HIS
21	M	83	ASN
21	M	184	GLN
21	M	321	GLN
21	M	417	HIS
22	N	70	HIS
22	N	91	ASN
22	N	377	HIS
22	N	632	GLN
22	N	708	GLN

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Mol	Chain	Res	Type
22	N	749	GLN
22	N	756	HIS
23	O	12	GLN
23	O	23	HIS
23	O	35	HIS
23	O	69	HIS
23	O	193	GLN
23	O	244	ASN
24	P	189	GLN
24	P	210	ASN
24	P	246	HIS
24	P	265	GLN
24	P	440	ASN
24	P	456	GLN
25	Q	10	GLN
25	Q	28	HIS
25	Q	170	GLN
25	Q	322	HIS
25	Q	375	HIS
26	R	291	HIS
26	R	302	HIS
27	S	214	HIS
27	S	232	HIS
27	S	260	HIS
27	S	326	GLN
27	S	381	GLN
27	S	477	HIS
27	S	478	GLN
28	T	221	GLN
28	T	314	ASN
29	U	7	GLN
29	U	31	ASN
29	U	32	GLN
29	U	72	HIS
29	U	77	ASN
29	U	157	HIS
29	U	224	HIS
30	V	113	HIS
30	V	115	HIS
30	V	194	HIS
30	V	199	HIS
30	V	240	HIS

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Mol	Chain	Res	Type
30	V	241	ASN
30	V	254	ASN
30	V	274	ASN
30	V	278	GLN
30	V	298	GLN
31	W	99	HIS
31	W	158	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

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.

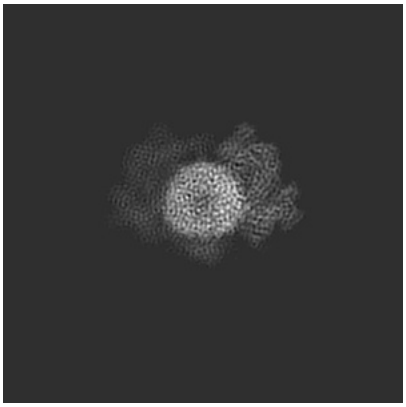
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-4089. These allow visual inspection of the internal detail of the map and identification of artifacts.

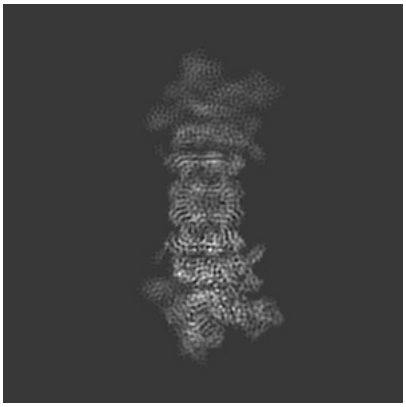
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

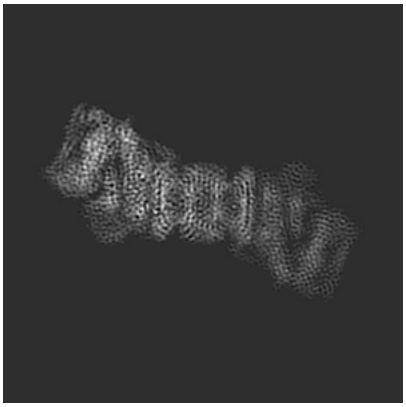
6.1.1 Primary map



X



Y

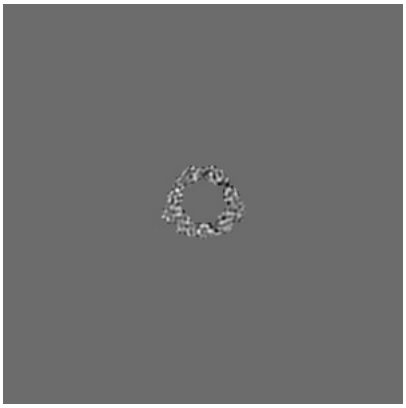


Z

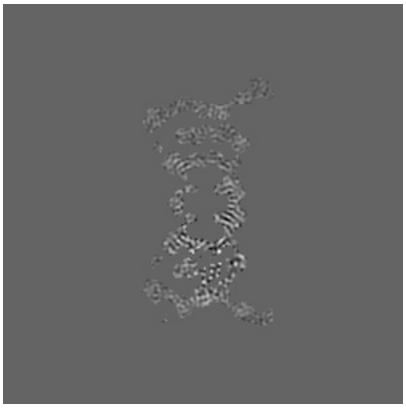
The images above show the map projected in three orthogonal directions.

6.2 Central slices

6.2.1 Primary map



X Index: 140



Y Index: 140

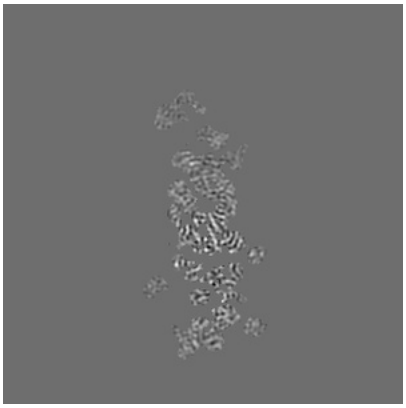
Z Index: 140

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: 111



Y Index: 153

Z Index: 134

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

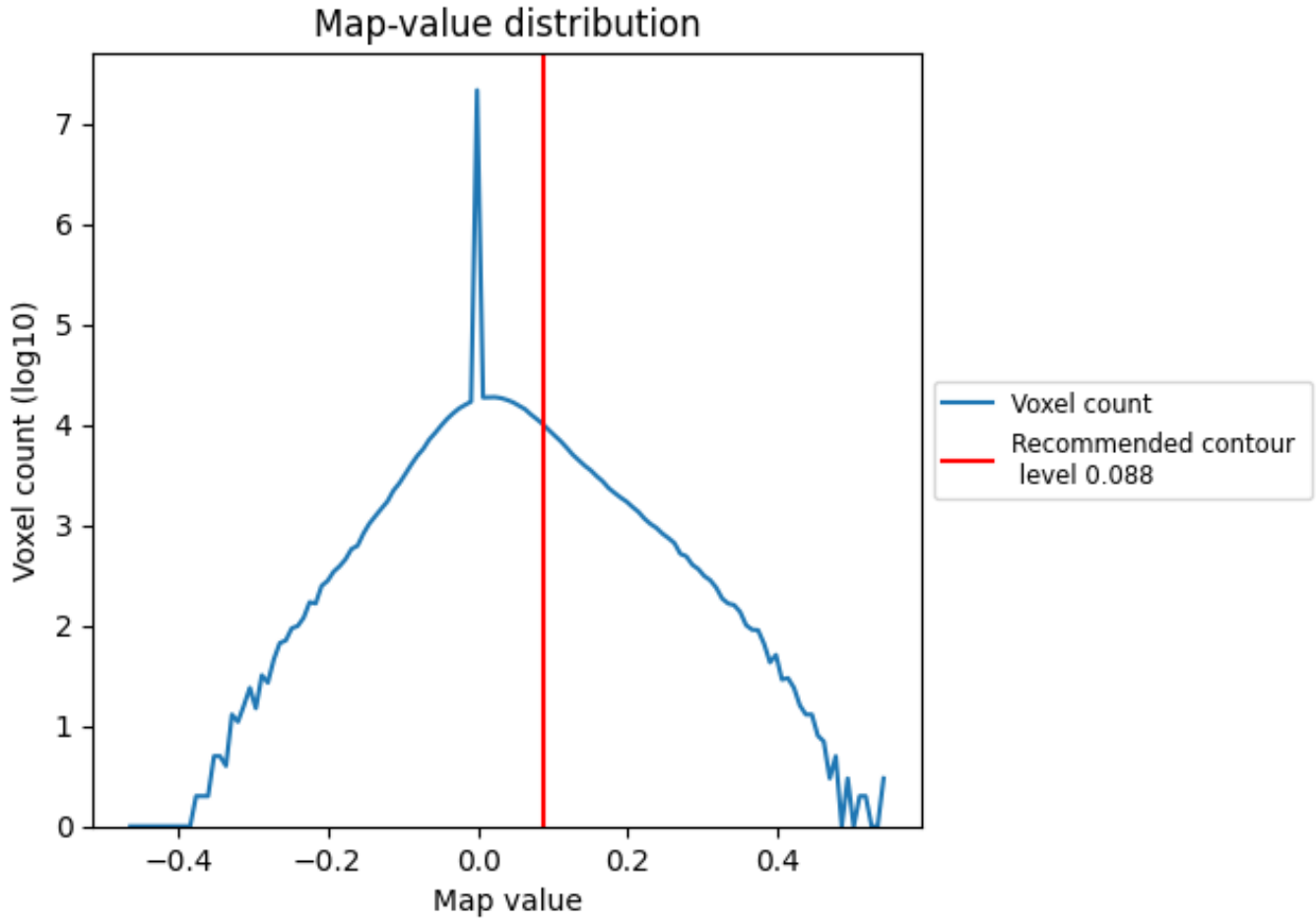
6.5 Mask visualisation (i)

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

7 Map analysis

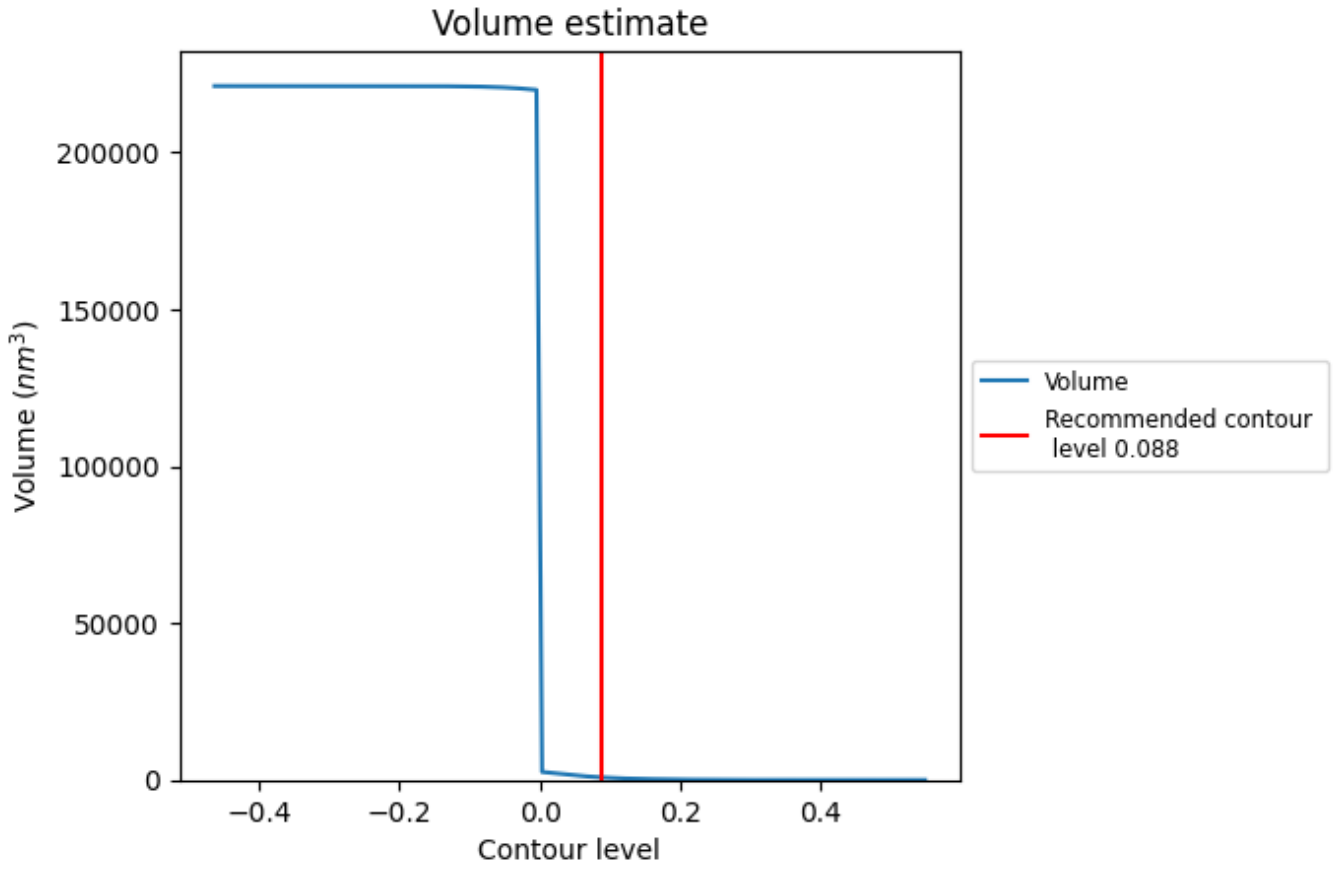
This section contains the results of statistical analysis of the map.

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.

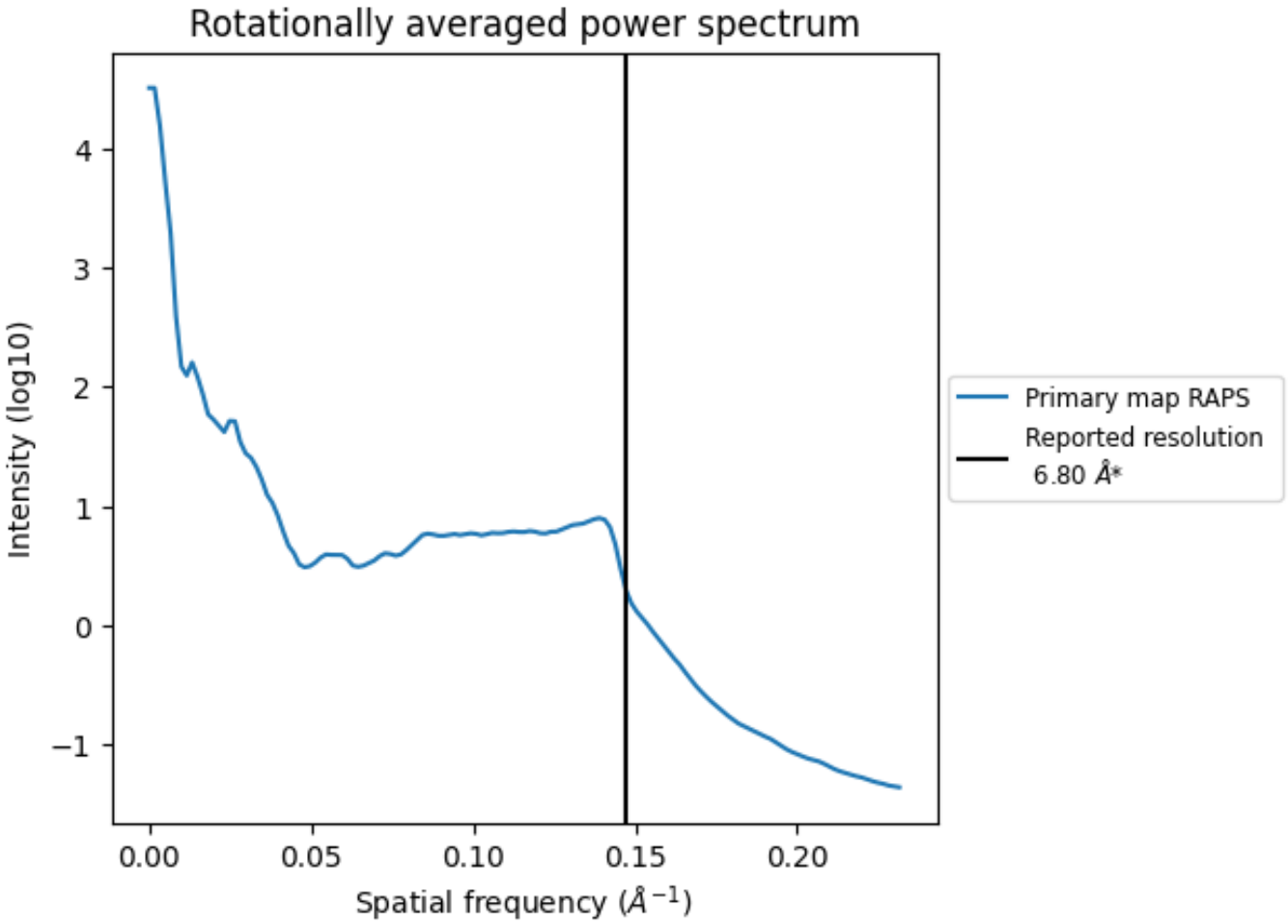
7.2 Volume estimate



The volume at the recommended contour level is 815 nm^3; this corresponds to an approximate mass of 737 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 0.147 $Å^{-1}$

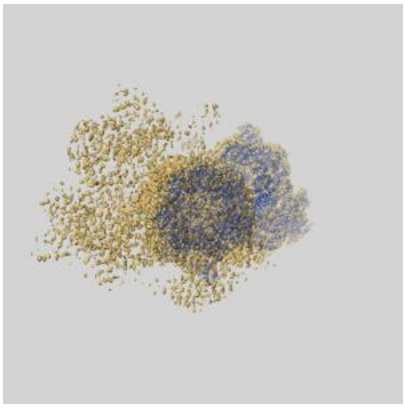
8 Fourier-Shell correlation (i)

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

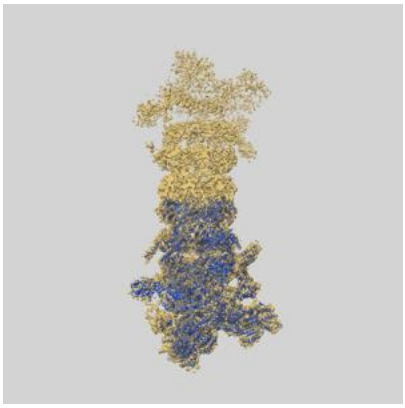
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-4089 and PDB model 5LN3. Per-residue inclusion information can be found in section 3 on page 9.

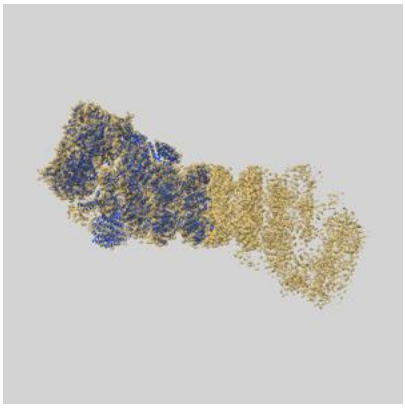
9.1 Map-model overlay



X



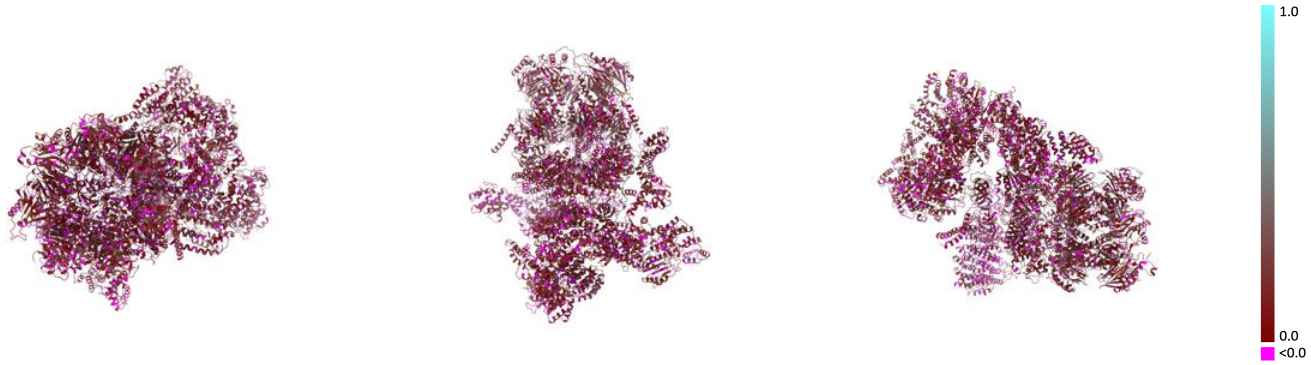
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.088 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.

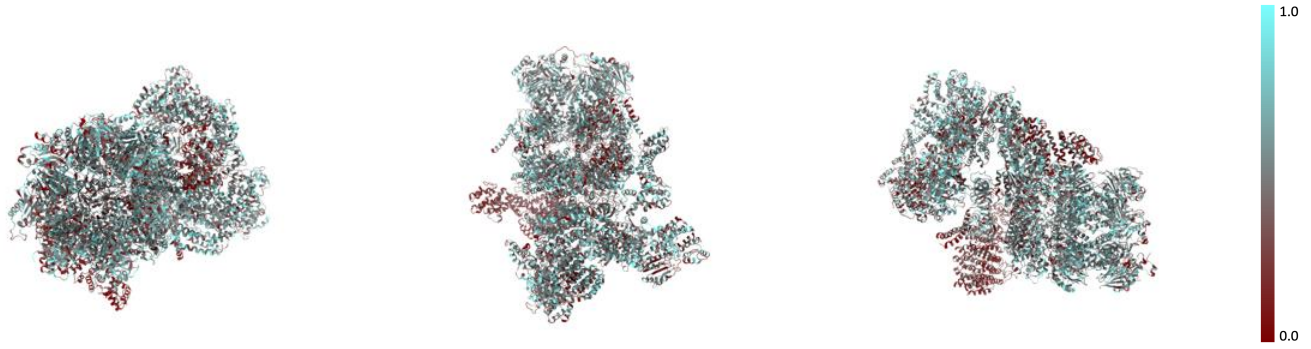
9.2 Q-score mapped to coordinate model



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.

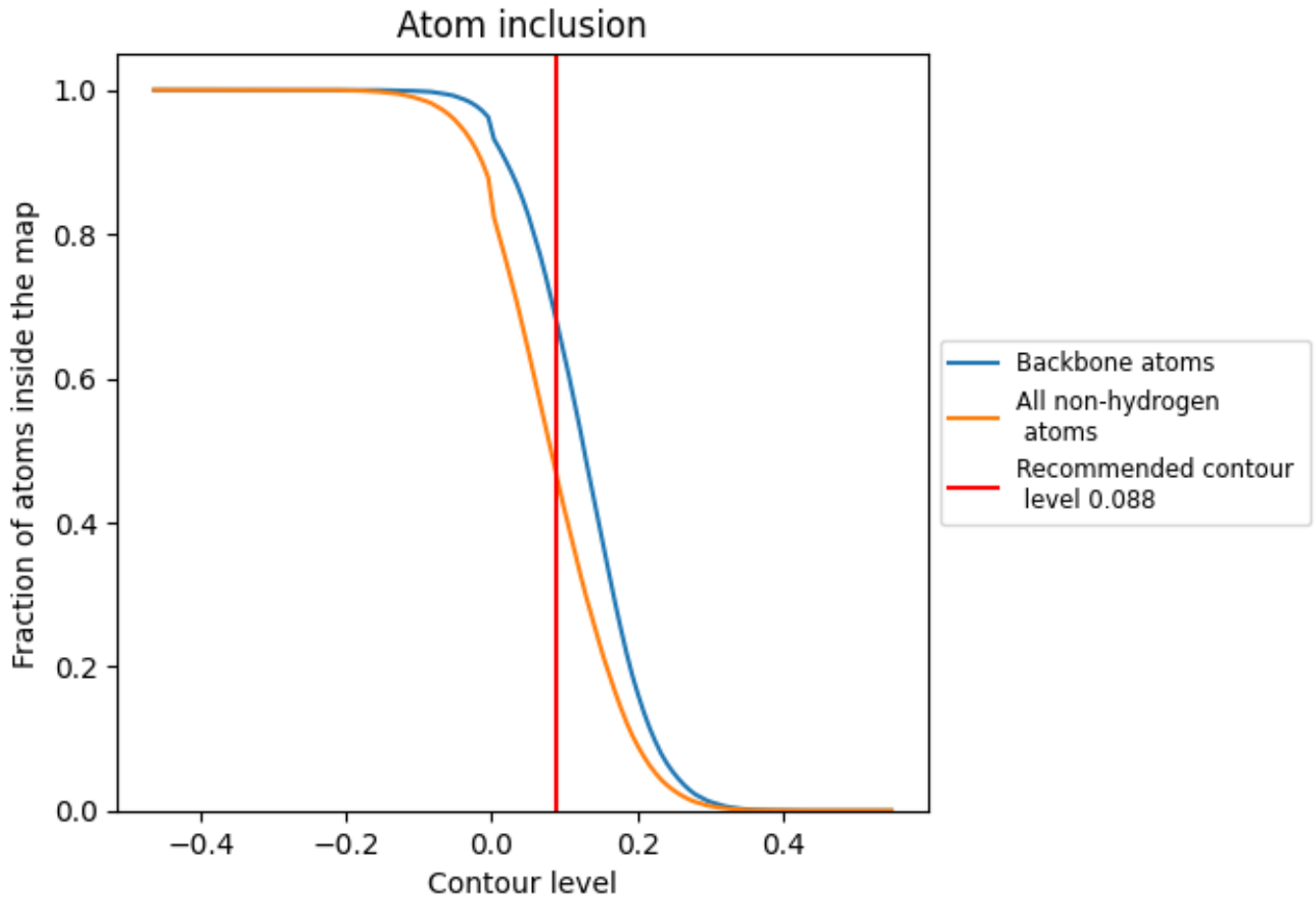
9.3 Atom inclusion mapped to coordinate model



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 (0.088).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 47% 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 (0.088) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4692	0.1410
1	0.5057	0.1550
2	0.5598	0.1950
3	0.4987	0.1550
4	0.5603	0.1640
5	0.5637	0.1700
6	0.5025	0.1640
7	0.5166	0.1590
A	0.5950	0.1790
B	0.5610	0.1630
C	0.5372	0.1670
D	0.5358	0.1720
E	0.5462	0.1610
F	0.5463	0.1660
G	0.5310	0.1520
H	0.4645	0.1340
I	0.4551	0.1290
J	0.5024	0.1470
K	0.5103	0.1440
L	0.4880	0.1450
M	0.4553	0.1340
N	0.4455	0.1440
O	0.5266	0.1330
P	0.5203	0.1320
Q	0.3147	0.1120
R	0.5370	0.1380
S	0.5004	0.1440
T	0.5109	0.1360
U	0.5416	0.1560
V	0.5214	0.1530
W	0.4298	0.1420
Y	0.4419	0.1600
Z	0.1146	0.0640