Full wwPDB EM Validation Report ⓘ

Nov 19, 2022 – 09:07 pm GMT

PDB ID	:	6EPD
EMDB ID	:	EMD-3914
Title	:	Substrate processing state 26S proteasome (SPS1)
Authors	:	Guo, Q.; Lehmer, C.; Martinez-Sanchez, A.; Rudack, T.; Beck, F.; Hartmann, H.; Hipp, M.S.; Hartl, F.U.; Edbauer, D.; Baumeister, W.; Fernandez-Busna diego, R.
Deposited on	:	2017-10-11
Resolution	:	15.40 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:

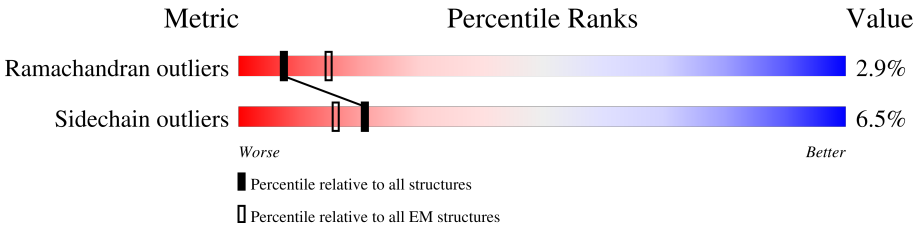
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance

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

The reported resolution of this entry is 15.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	246	13% 76% 21%
2	B	234	10% 71% 24% 5%
3	C	261	10% 68% 25% 5%
4	D	254	12% 69% 22% 6%
5	E	241	6% 76% 18%
6	F	263	67% 21% 10%
7	G	255	9% 72% 21%
8	1	238	11% 57% 22% 6% 15%
9	2	277	16% 53% 22% 21%

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Mol	Chain	Length	Quality of chain
10	3	205	14% 64% 31% 5%
11	4	201	14% 65% 27% 5%
12	5	263	7% 47% 24% 5% 24%
13	6	240	16% 58% 23% 7% 11%
14	7	263	11% 53% 25% 18%
15	W	377	8% 41% 10% 48%
16	V	310	5% 73% 18% 7%
17	T	353	15% 52% 18% 25%
18	Y	70	13% 27% 7% 66%
19	Z	908	29% 74% 21%
20	N	953	13% 73% 19% 5%
21	S	530	13% 66% 19% 10%
22	P	456	23% 75% 21%
23	Q	422	28% 77% 20%
24	R	389	21% 72% 21% 5%
25	U	320	15% 69% 17% 10%
26	O	376	26% 76% 20%
27	H	433	11% 67% 23% 9%
28	I	440	12% 66% 18% 12%
29	K	418	16% 65% 26% 6%
30	L	403	16% 74% 17% 6%
31	M	442	9% 69% 21% 6%
32	J	406	16% 76% 20%

2 Entry composition (i)

There are 32 unique types of molecules in this entry. The entry contains 82757 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Proteasome subunit alpha type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	246	1920	1215	322	369	14	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	234	1828	1166	311	344	7	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	249	1960	1238	337	374	11	0	0

- Molecule 4 is a protein called Proteasome subunit alpha type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	246	1926	1209	340	371	6	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	233	1778	1114	296	358	10	0	0

- Molecule 6 is a protein called Proteasome subunit alpha type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	238	1871	1170	337	353	11	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	245	Total	C	N	O	S	0	0
			1912	1212	326	362	12		

- Molecule 8 is a protein called Proteasome subunit beta type-6.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	1	202	Total	C	N	O	S	0	0
			1516	948	259	297	12		

- Molecule 9 is a protein called Proteasome subunit beta type-7.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	2	219	Total	C	N	O	S	0	0
			1651	1042	281	316	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	3	205	Total	C	N	O	S	0	0
			1600	1018	266	296	20		

- Molecule 11 is a protein called Proteasome subunit beta type-2.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	4	196	Total	C	N	O	S	0	0
			1572	1007	267	289	9		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	5	201	Total	C	N	O	S	0	0
			1560	984	272	295	9		

- Molecule 13 is a protein called Proteasome subunit beta type-1.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	6	213	Total	C	N	O	S	0	0
			1659	1050	284	315	10		

- Molecule 14 is a protein called Proteasome subunit beta type-4.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	7	216	Total	C	N	O	S	0	0
			1686	1065	292	317	12		

- Molecule 15 is a protein called 26S proteasome subunit S5a.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	W	195	Total	C	N	O	S	0	0
			1480	922	265	285	8		

- Molecule 16 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 14.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	V	289	Total	C	N	O	S	0	0
			2272	1438	391	424	19		

- Molecule 17 is a protein called Proteasome 26S subunit, non-ATPase 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	T	263	Total	C	N	O	S	0	0
			2149	1390	351	398	10		

- Molecule 18 is a protein called RCG28037.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	Y	24	Total	C	N	O	S	0	0
			199	120	34	44	1		

- Molecule 19 is a protein called 26S proteasome non-ATPase regulatory subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	896	Total	C	N	O	S	0	0
			6913	4342	1178	1346	47		

- Molecule 20 is a protein called 26S proteasome non-ATPase regulatory subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	905	Total	C	N	O	S	0	0
			7082	4487	1193	1356	46		

- Molecule 21 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	S	476	Total	C	N	O	S	0	0
			3844	2438	685	707	14		

- Molecule 22 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 12.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	P	456	Total	C	N	O	S	0	0
			3706	2338	635	709	24		

- Molecule 23 is a protein called 26S proteasome non-ATPase regulatory subunit 11.

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

- Molecule 24 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	R	389	Total	C	N	O	S	0	0
			3204	2042	542	600	20		

- Molecule 25 is a protein called Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 7 (Predicted).

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	288	Total	C	N	O	S	0	0
			2299	1470	395	428	6		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
26	O	376	Total	C	N	O	S	0	0
			3011	1918	514	564	15		

- Molecule 27 is a protein called 26S proteasome regulatory subunit 7.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	H	396	Total	C	N	O	S	0	0
			3113	1960	546	589	18		

- Molecule 28 is a protein called 26S proteasome regulatory subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	I	385	Total	C	N	O	S	0	0
			3042	1913	516	598	15		

- Molecule 29 is a protein called 26S proteasome regulatory subunit 6B.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	K	391	Total	C	N	O	S	0	0
			3125	1978	535	599	13		

- Molecule 30 is a protein called Proteasome 26S subunit, ATPase 6.

Mol	Chain	Residues	Atoms					AltConf	Trace
30	L	389	Total	C	N	O	S	0	0
			3098	1947	552	582	17		

- Molecule 31 is a protein called 26S proteasome regulatory subunit 6A.

Mol	Chain	Residues	Atoms					AltConf	Trace
31	M	415	Total	C	N	O	S	0	0
			3252	2038	561	635	18		

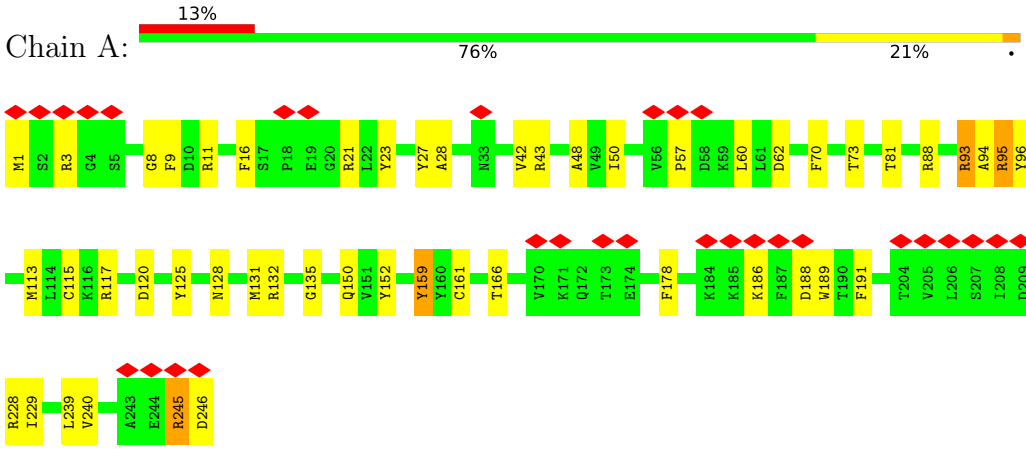
- Molecule 32 is a protein called 26S proteasome regulatory subunit 8.

Mol	Chain	Residues	Atoms					AltConf	Trace
32	J	406	Total	C	N	O	S	0	0
			3194	2006	569	599	20		

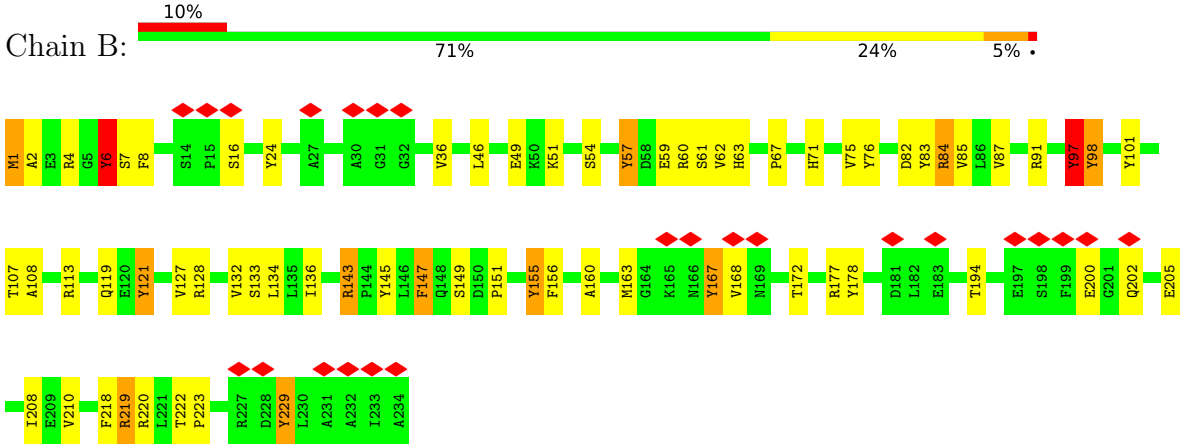
3 Residue-property plots (i)

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

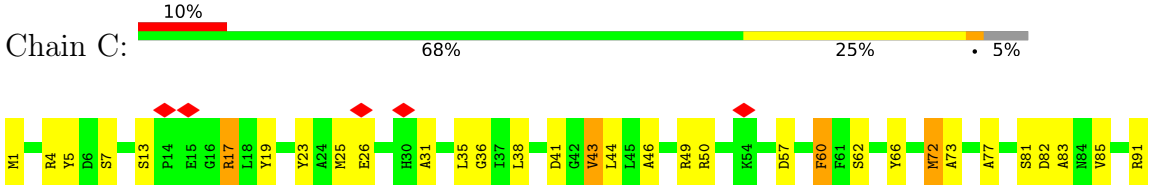
• Molecule 1: Proteasome subunit alpha type-6

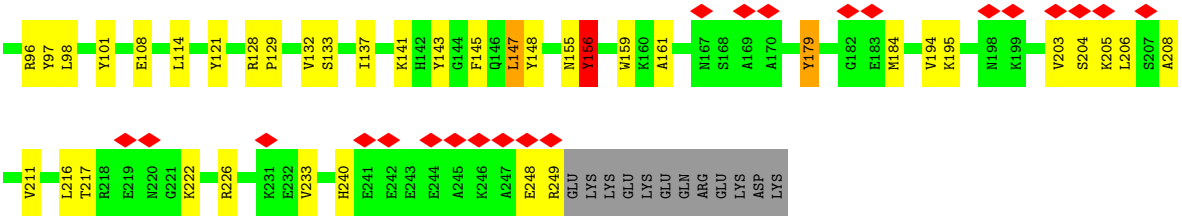


• Molecule 2: Proteasome subunit alpha type-2

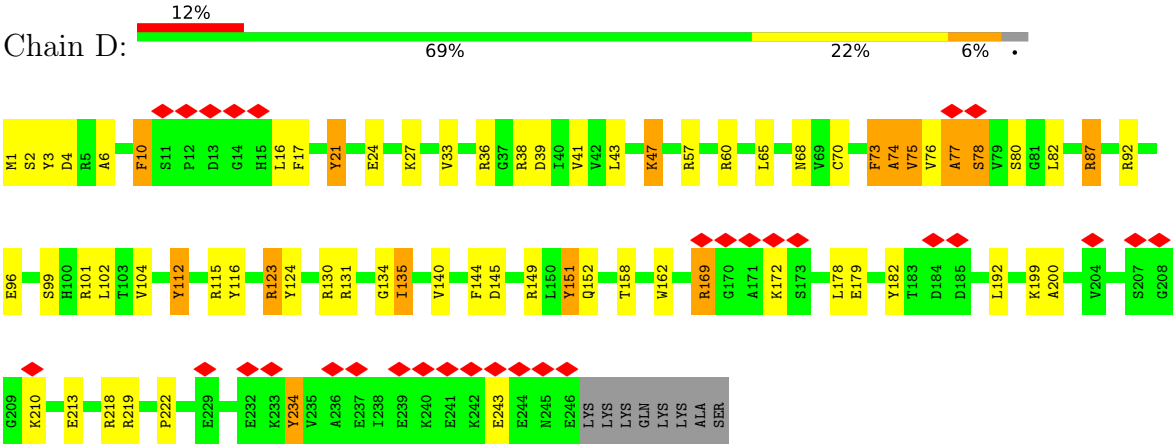


• Molecule 3: Proteasome subunit alpha type-4

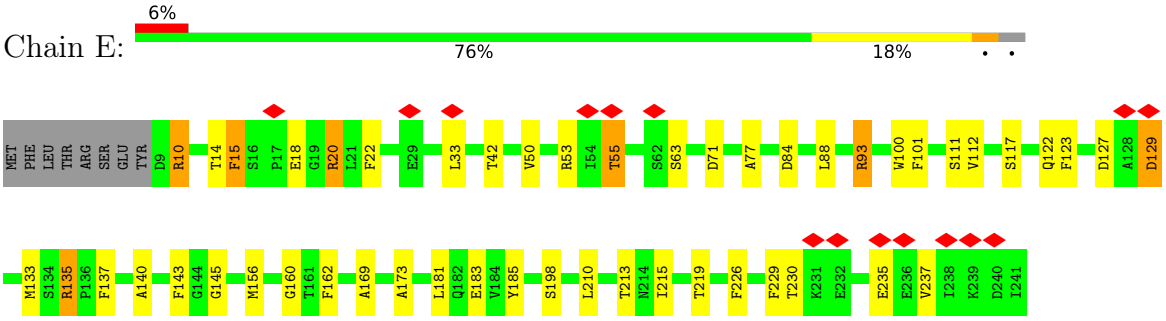




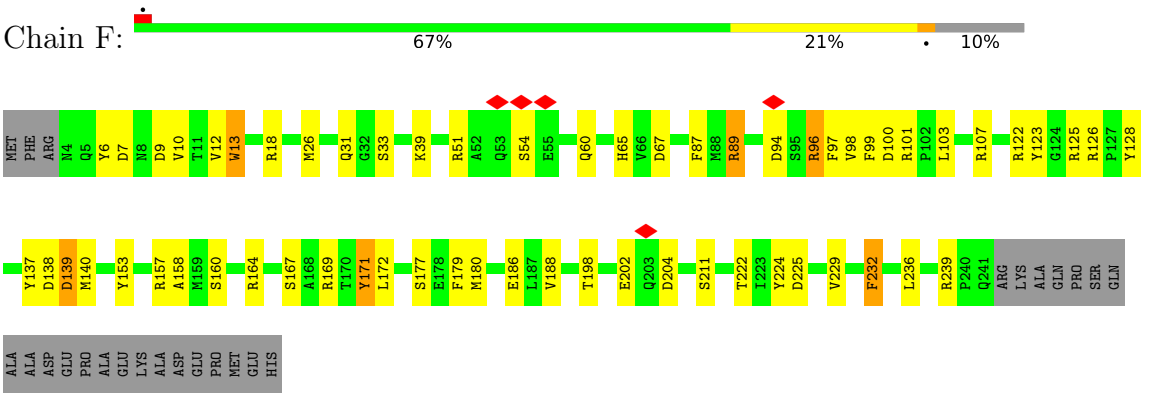
• Molecule 4: Proteasome subunit alpha type-7



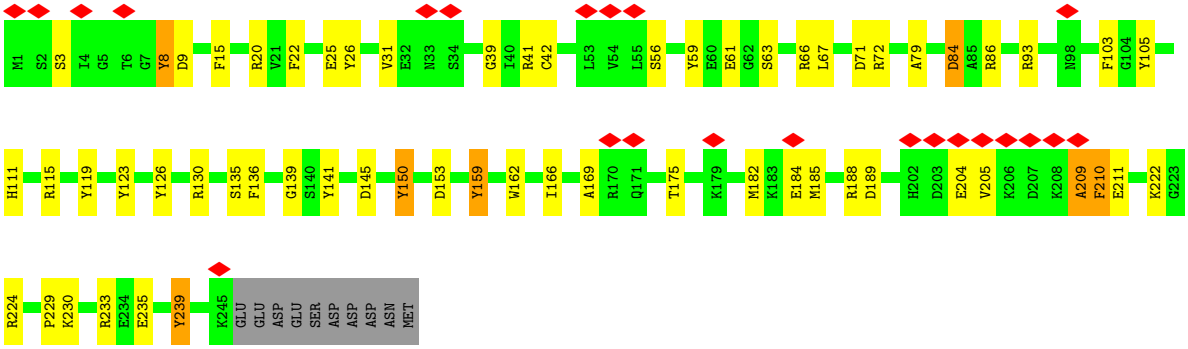
• Molecule 5: Proteasome subunit alpha type-5



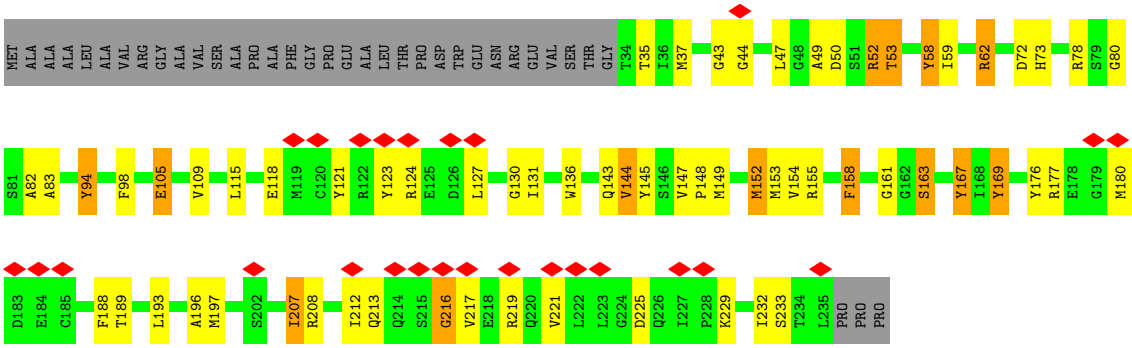
• Molecule 6: Proteasome subunit alpha type-1



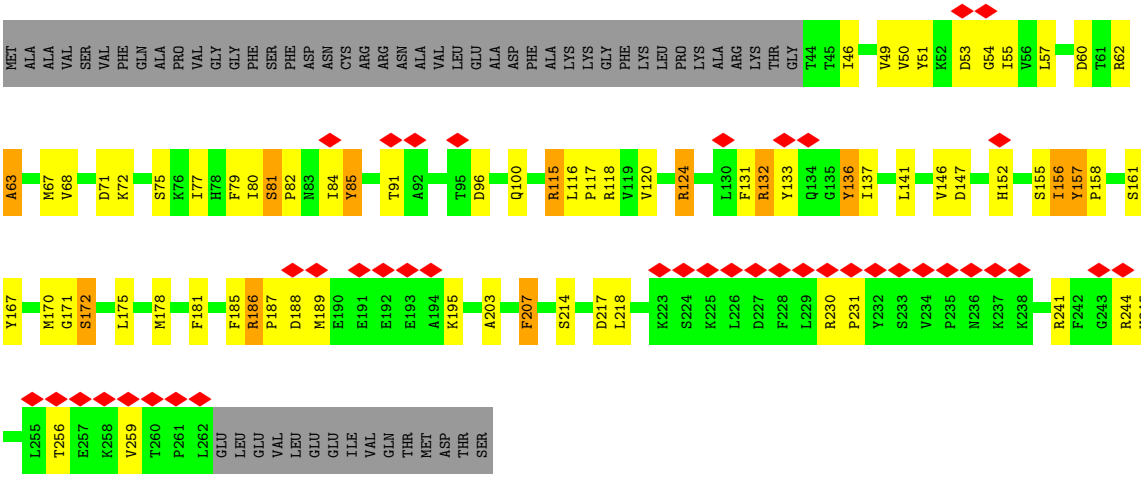
• Molecule 7: Proteasome subunit alpha type-3



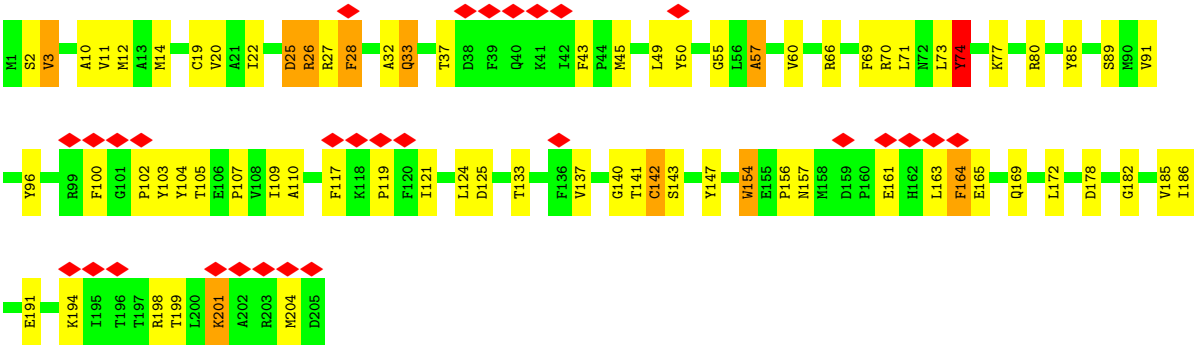
• Molecule 8: Proteasome subunit beta type-6



• Molecule 9: Proteasome subunit beta type-7

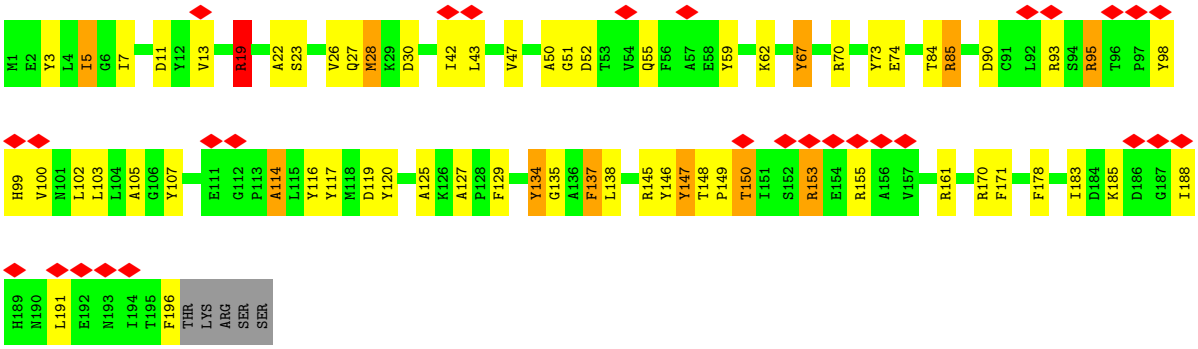


• Molecule 10: Proteasome subunit beta type-3



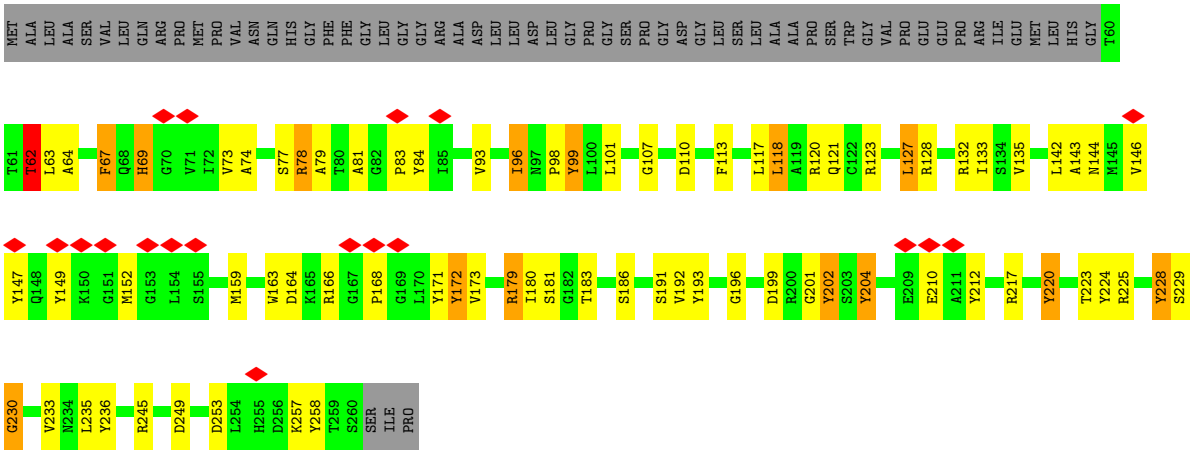
• Molecule 11: Proteasome subunit beta type-2

Chain 4:



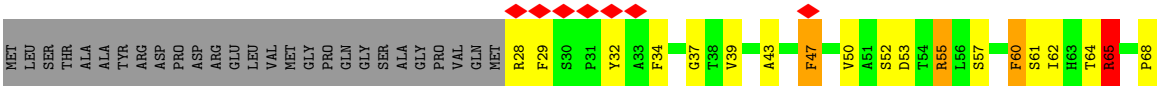
• Molecule 12: Proteasome subunit beta type-5

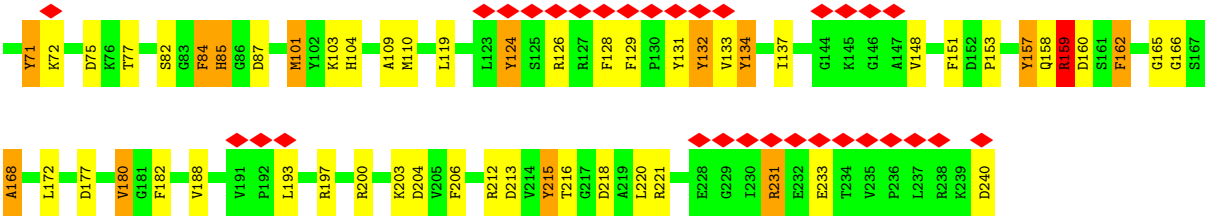
Chain 5:



• Molecule 13: Proteasome subunit beta type-1

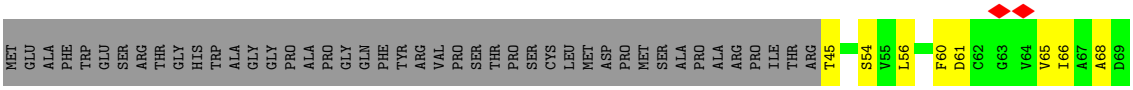
Chain 6:

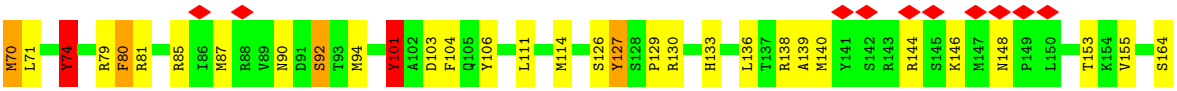


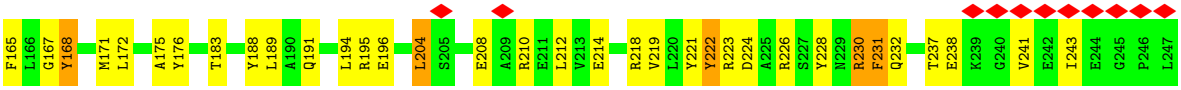


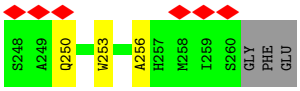
• Molecule 14: Proteasome subunit beta type-4

Chain 7:



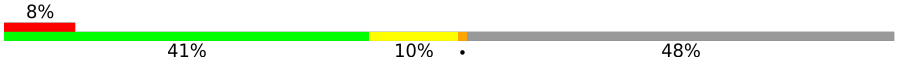


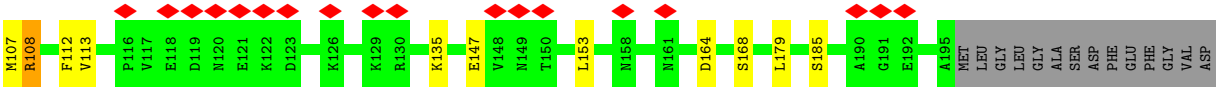


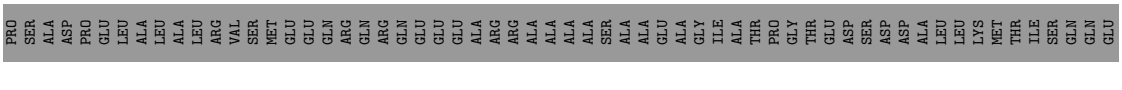


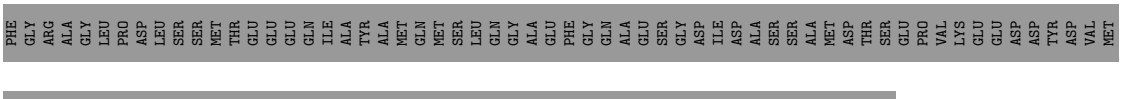
• Molecule 15: 26S proteasome subunit S5a

Chain W:



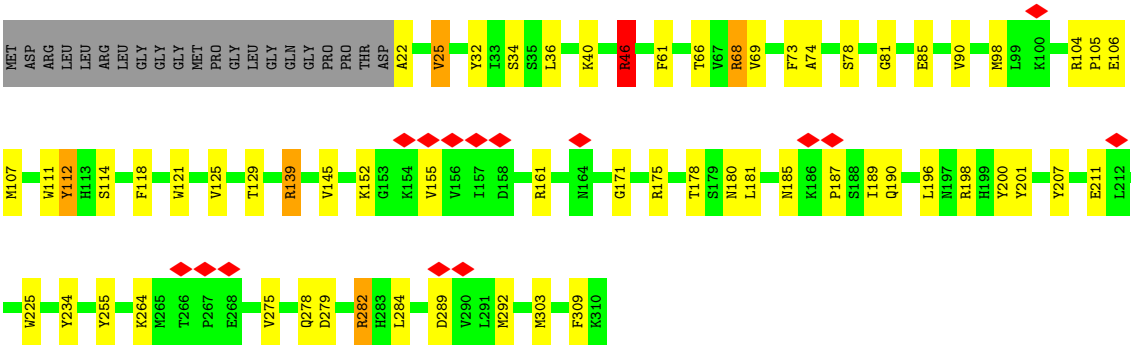


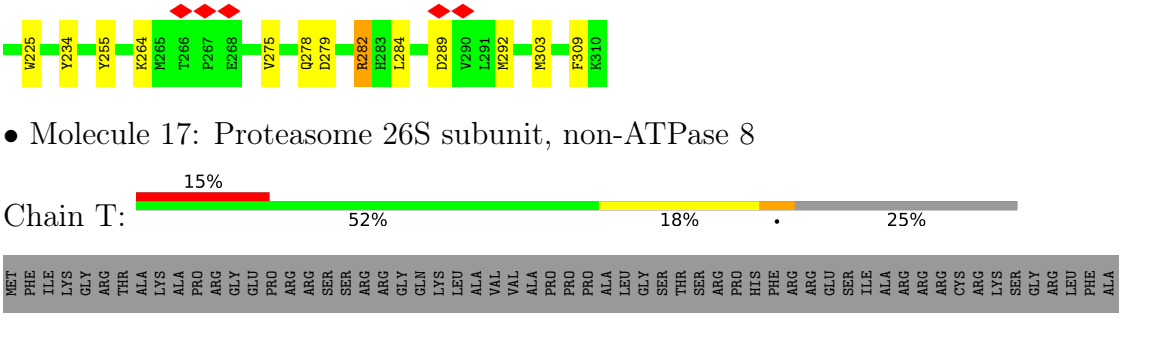




• Molecule 16: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 14

Chain V:



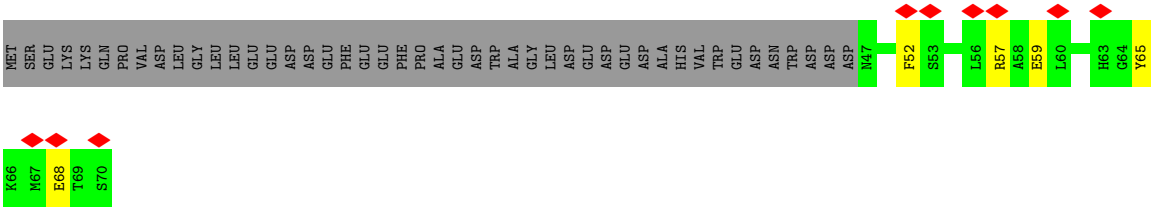


• Molecule 17: Proteasome 26S subunit, non-ATPase 8

Chain T:

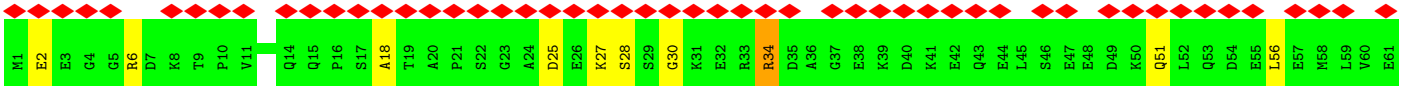
• Molecule 18: RCG28037

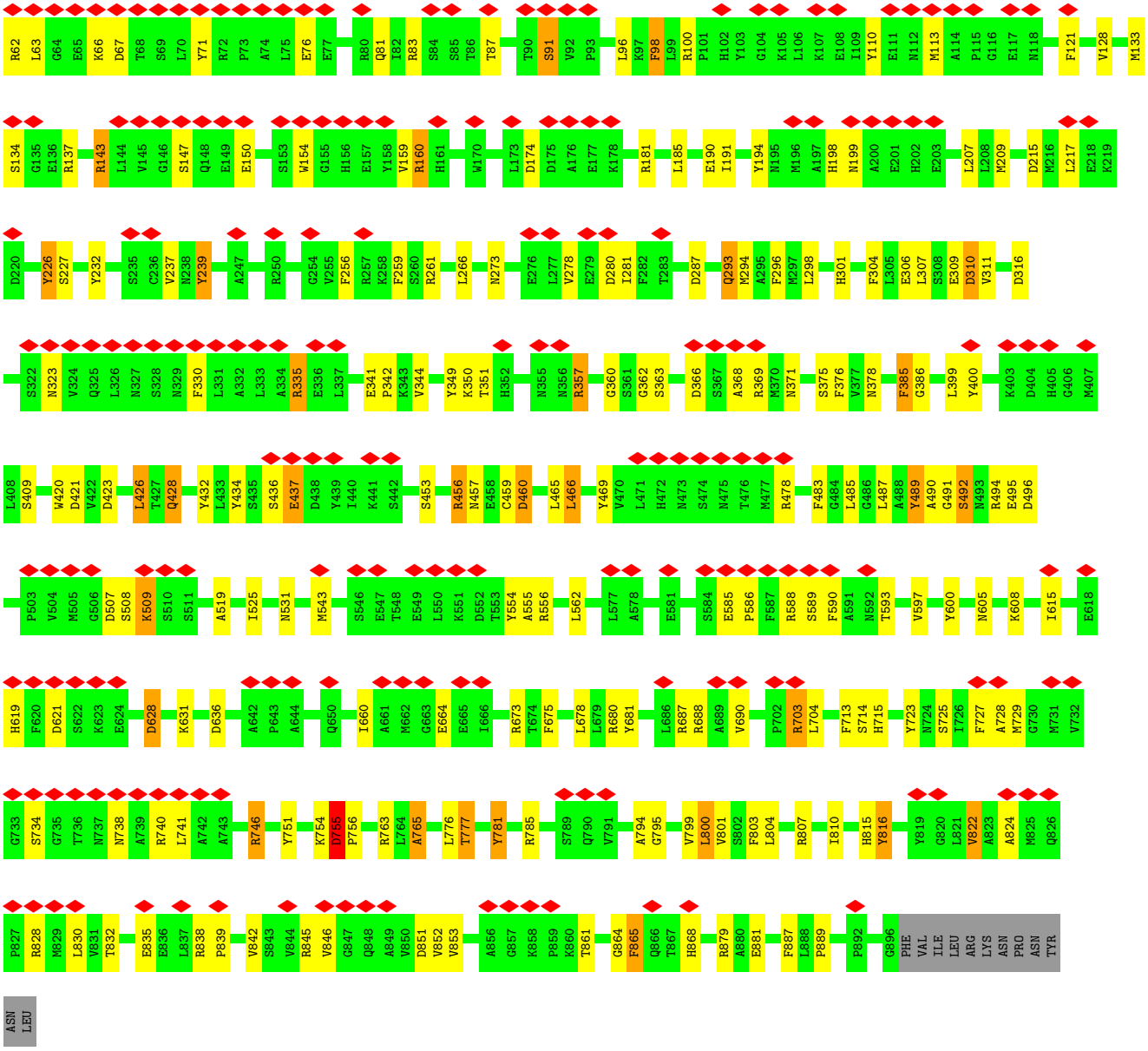
Chain Y:



• Molecule 19: 26S proteasome non-ATPase regulatory subunit 2

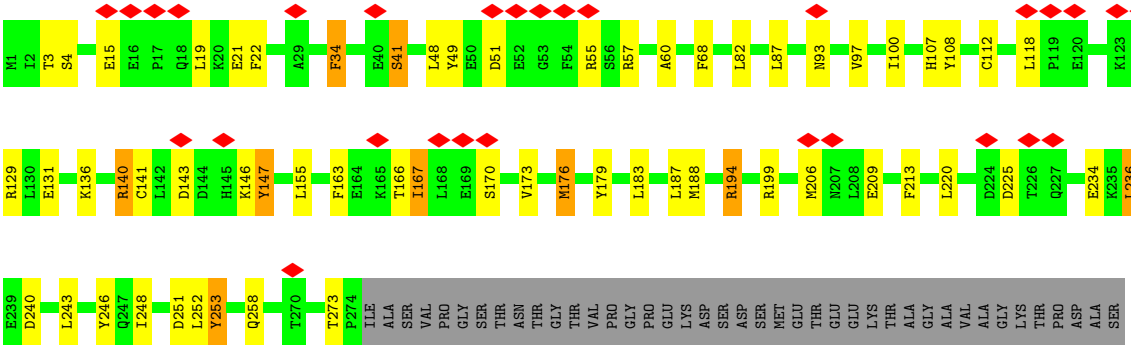
Chain Z:

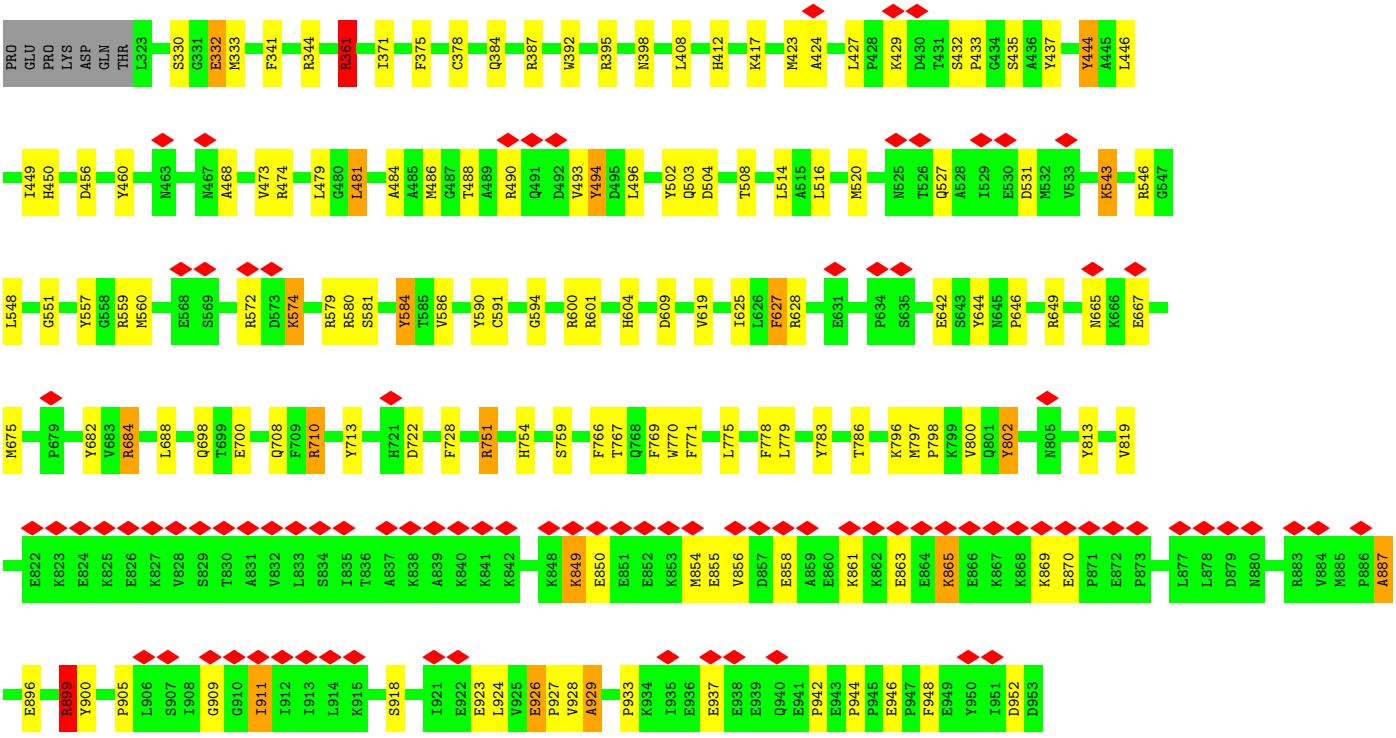




• Molecule 20: 26S proteasome non-ATPase regulatory subunit 1

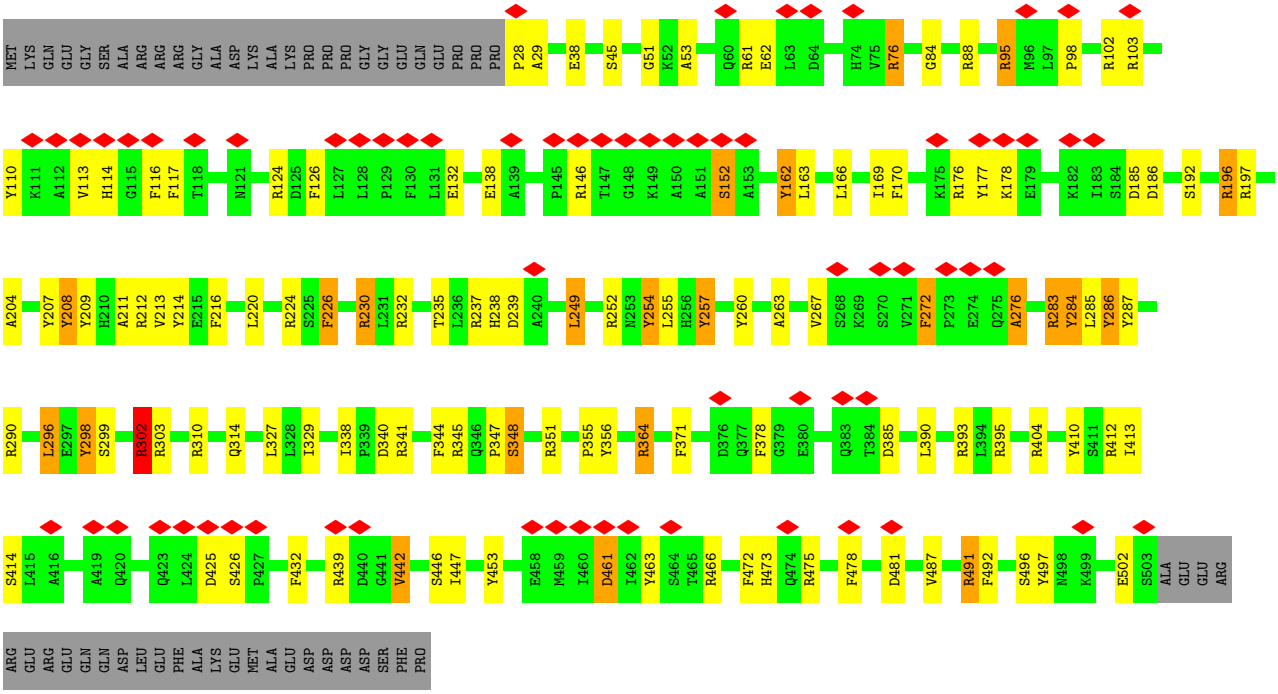
Chain N:





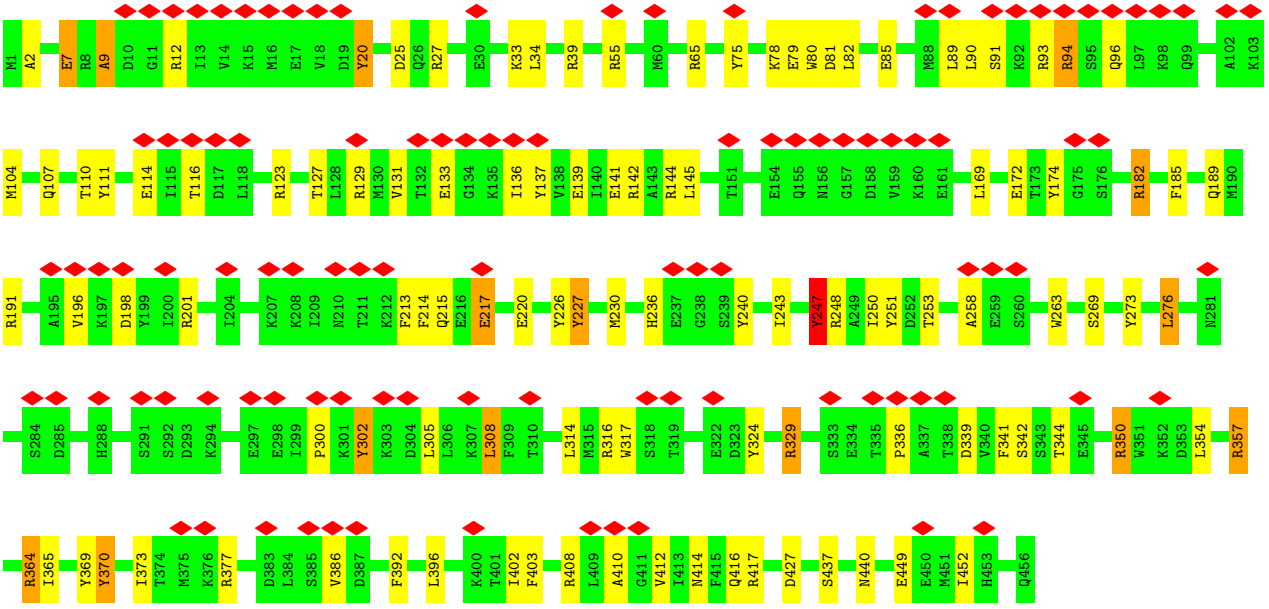
• Molecule 21: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 3

Chain S:



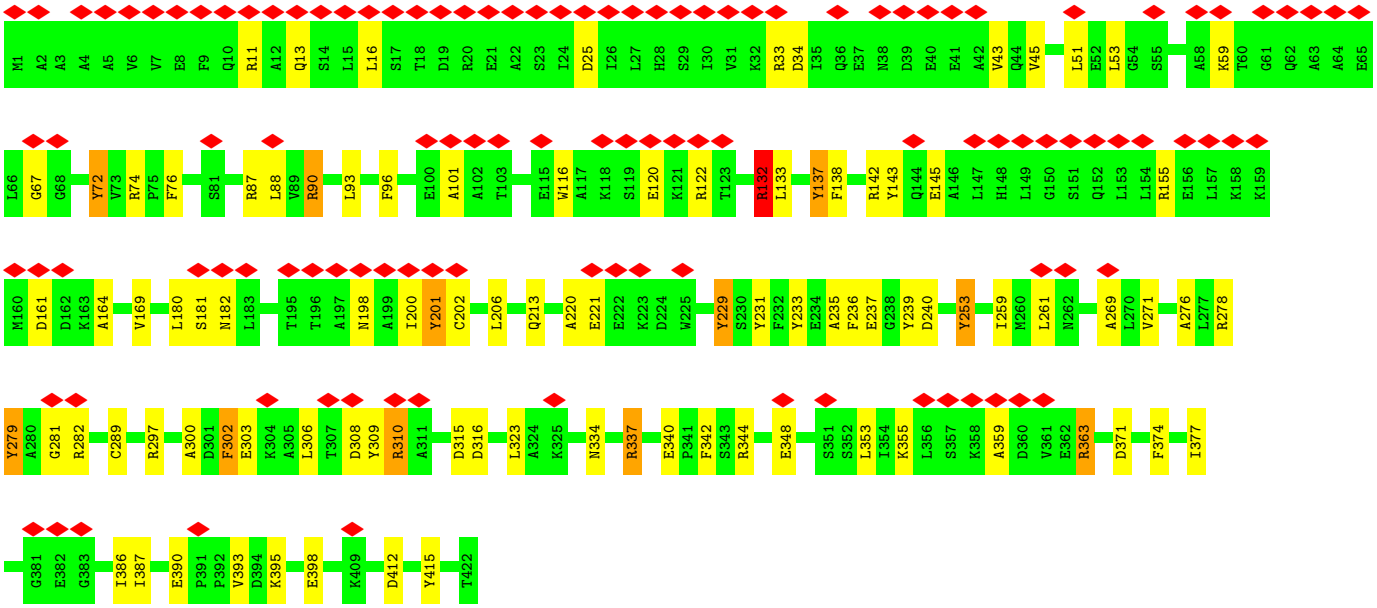
• Molecule 22: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 12

Chain P:



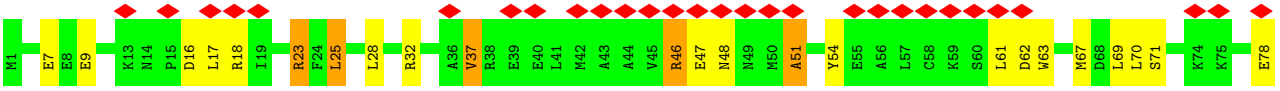
• Molecule 23: 26S proteasome non-ATPase regulatory subunit 11

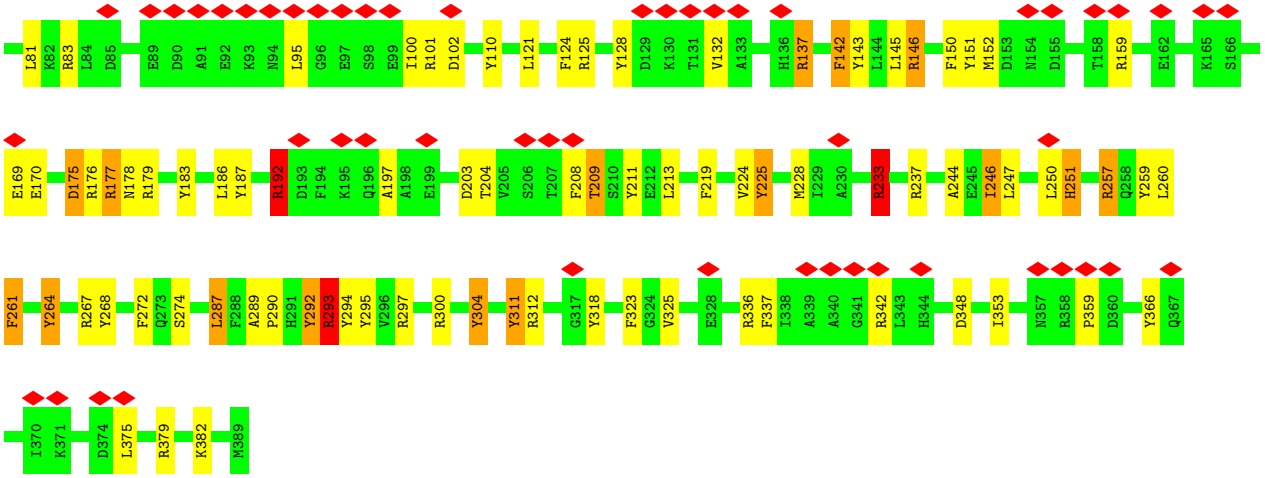
Chain Q:



• Molecule 24: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 6

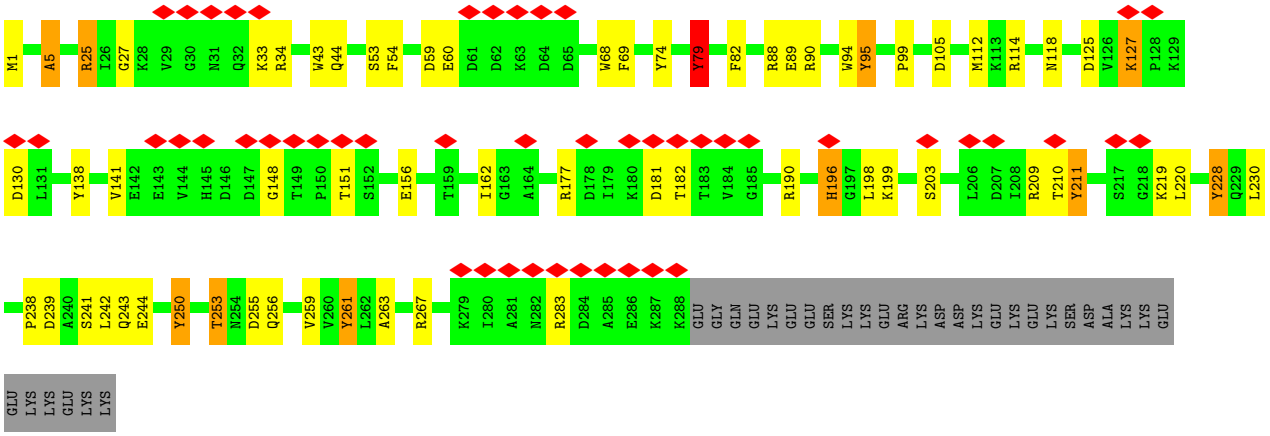
Chain R:





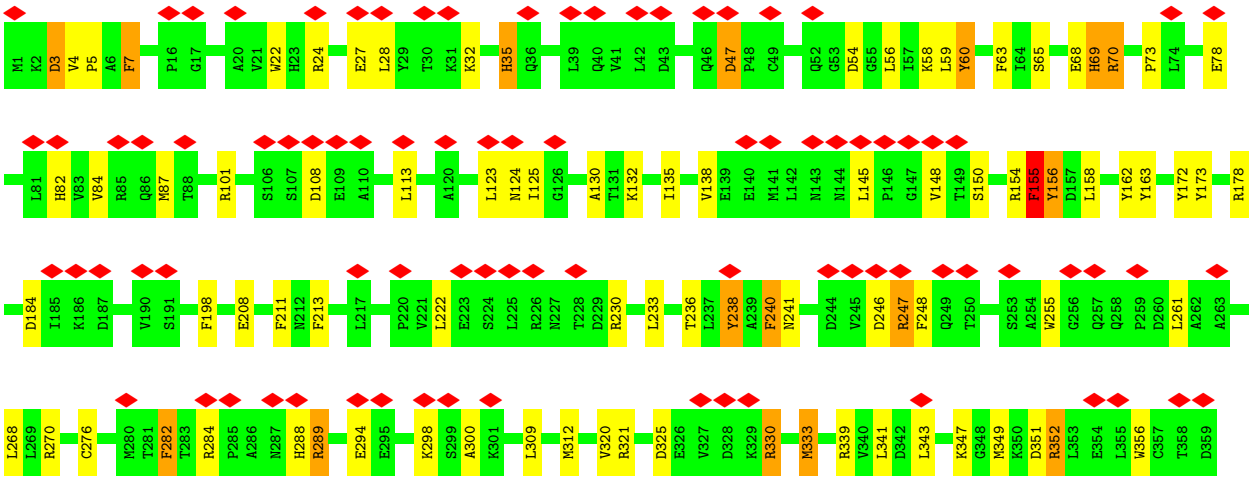
• Molecule 25: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 7 (Predicted)

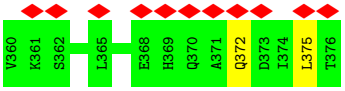
Chain U:



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

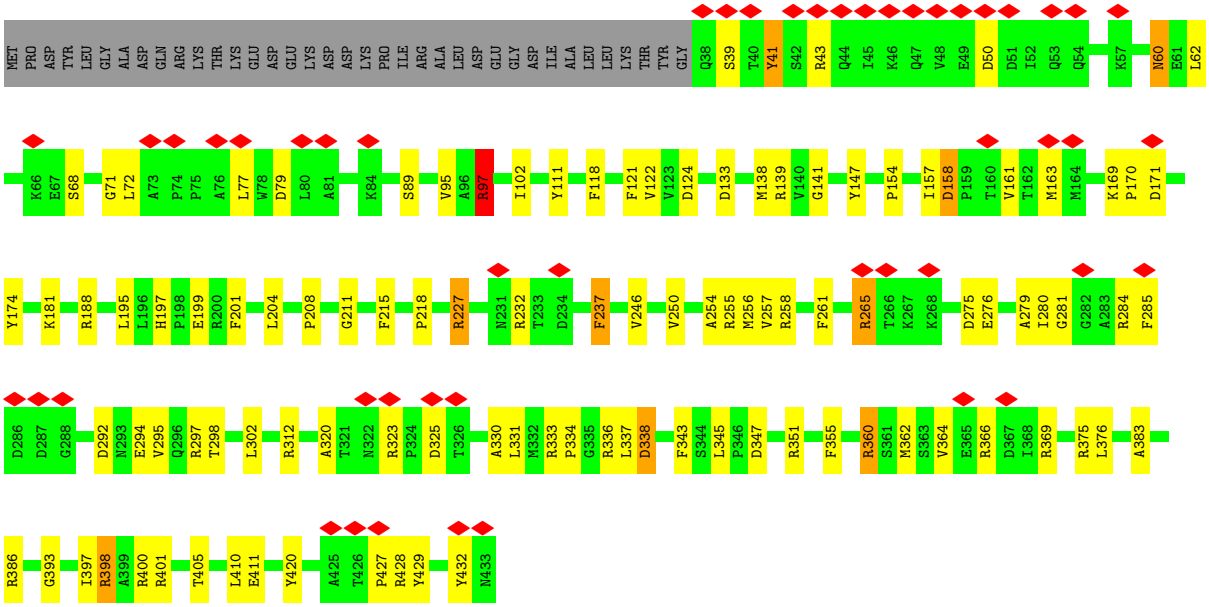
Chain O:





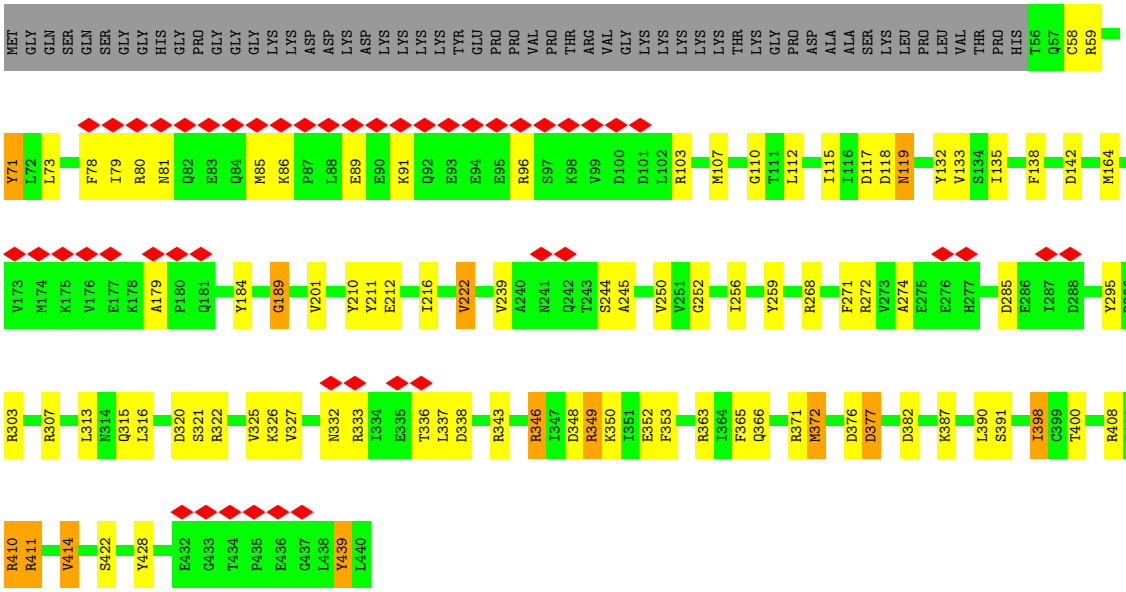
• Molecule 27: 26S proteasome regulatory subunit 7

Chain H:



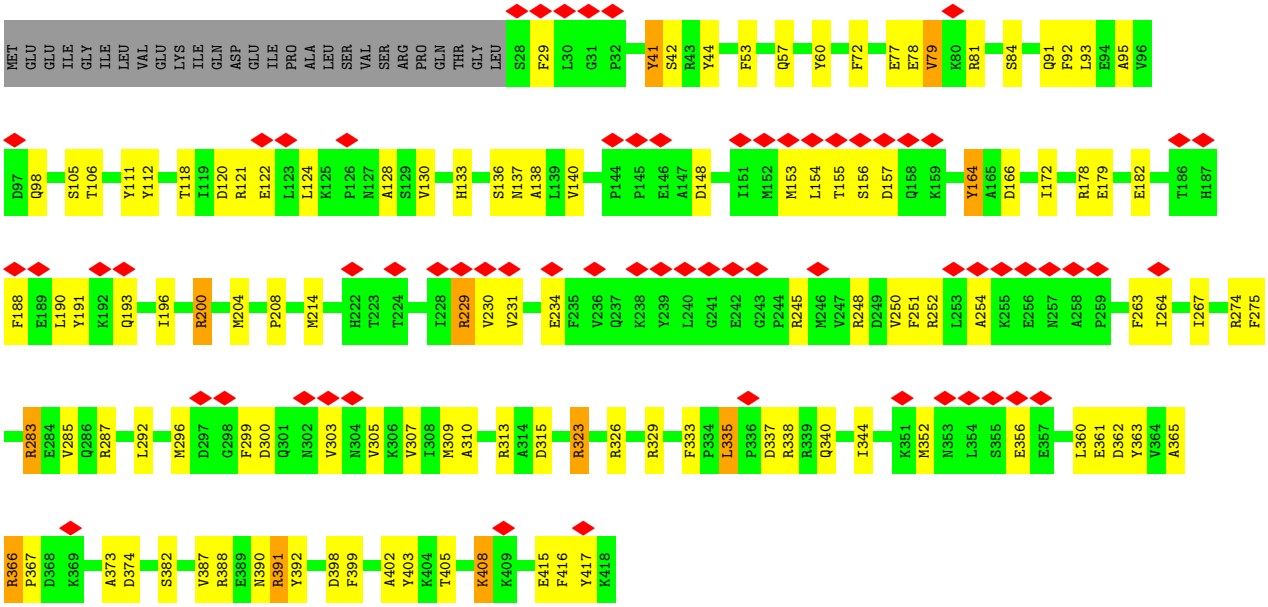
• Molecule 28: 26S proteasome regulatory subunit 4

Chain I:



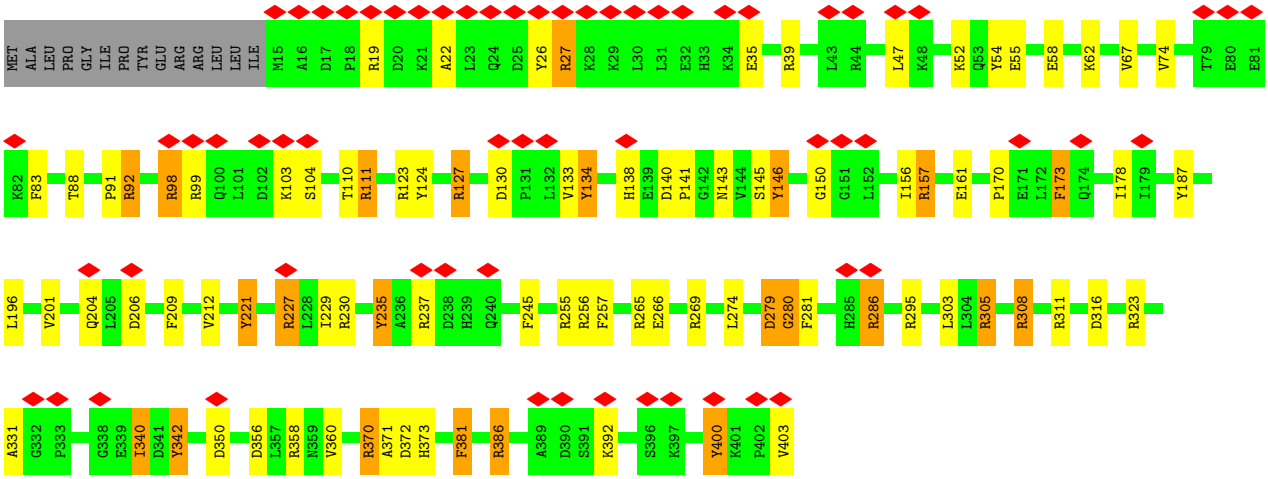
• Molecule 29: 26S proteasome regulatory subunit 6B

Chain K:



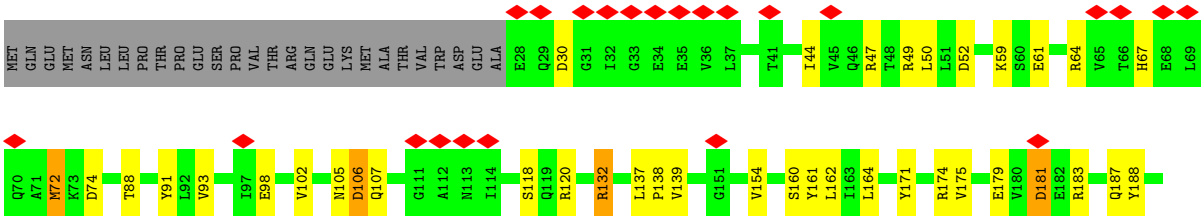
• Molecule 30: Proteasome 26S subunit, ATPase 6

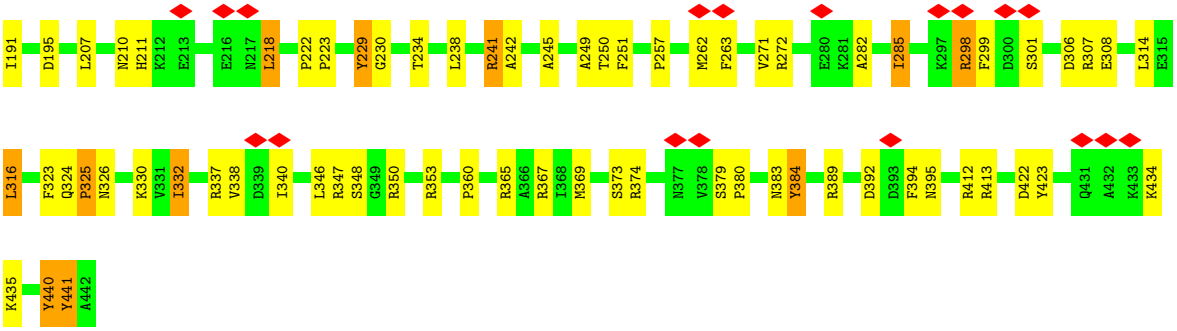
Chain L:



• Molecule 31: 26S proteasome regulatory subunit 6A

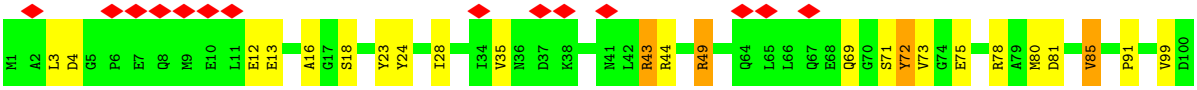
Chain M:

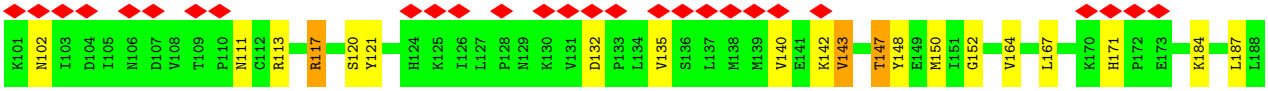


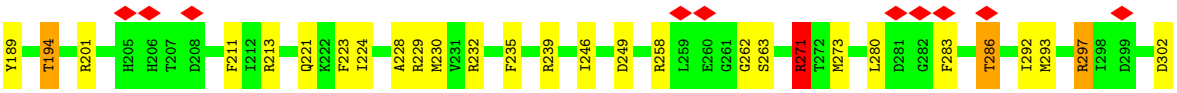


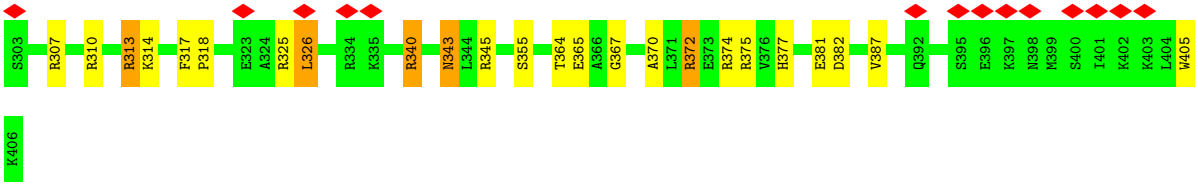
• Molecule 32: 26S proteasome regulatory subunit 8

Chain J:









4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	2136	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 ($e^-/Å^2$)	1.8	Depositor
Minimum defocus (nm)	5000	Depositor
Maximum defocus (nm)	7000	Depositor
Magnification	42000	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.810	Depositor
Minimum map value	-0.432	Depositor
Average map value	-0.034	Depositor
Map value standard deviation	0.175	Depositor
Recommended contour level	0.4	Depositor
Map size (Å)	307.80002, 307.80002, 307.80002	wwPDB
Map dimensions	90, 90, 90	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	3.4200003, 3.4200003, 3.4200003	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	1.72	24/1954 (1.2%)	1.92	40/2638 (1.5%)
2	B	1.75	15/1867 (0.8%)	2.13	59/2527 (2.3%)
3	C	1.71	14/1990 (0.7%)	2.03	65/2680 (2.4%)
4	D	1.69	14/1953 (0.7%)	2.08	61/2637 (2.3%)
5	E	2.03	22/1806 (1.2%)	1.86	33/2439 (1.4%)
6	F	1.75	19/1906 (1.0%)	1.96	51/2577 (2.0%)
7	G	1.74	18/1947 (0.9%)	1.96	48/2620 (1.8%)
8	1	1.73	14/1542 (0.9%)	2.13	54/2089 (2.6%)
9	2	1.74	11/1679 (0.7%)	2.13	55/2271 (2.4%)
10	3	1.66	12/1629 (0.7%)	2.08	51/2195 (2.3%)
11	4	1.74	18/1604 (1.1%)	2.09	56/2170 (2.6%)
12	5	2.74	20/1592 (1.3%)	2.12	58/2152 (2.7%)
13	6	1.72	16/1690 (0.9%)	2.17	66/2278 (2.9%)
14	7	1.76	19/1720 (1.1%)	2.06	58/2327 (2.5%)
15	W	1.64	12/1500 (0.8%)	1.83	26/2030 (1.3%)
16	V	1.67	20/2315 (0.9%)	1.92	51/3129 (1.6%)
17	T	1.80	24/2195 (1.1%)	1.94	56/2964 (1.9%)
18	Y	1.70	1/201 (0.5%)	1.94	6/266 (2.3%)
19	Z	1.73	65/7026 (0.9%)	1.95	158/9495 (1.7%)
20	N	1.69	57/7206 (0.8%)	1.86	138/9738 (1.4%)
21	S	1.76	40/3918 (1.0%)	1.95	108/5287 (2.0%)
22	P	1.74	36/3754 (1.0%)	1.92	99/5049 (2.0%)
23	Q	1.69	26/3381 (0.8%)	1.91	72/4558 (1.6%)
24	R	1.79	42/3263 (1.3%)	2.07	94/4393 (2.1%)
25	U	1.62	14/2344 (0.6%)	1.92	55/3178 (1.7%)
26	O	1.71	22/3066 (0.7%)	1.91	65/4148 (1.6%)
27	H	1.75	39/3166 (1.2%)	1.99	91/4275 (2.1%)
28	I	1.71	27/3085 (0.9%)	2.00	85/4158 (2.0%)
29	K	1.72	30/3178 (0.9%)	1.95	95/4290 (2.2%)
30	L	1.74	35/3146 (1.1%)	2.01	87/4233 (2.1%)
31	M	1.71	35/3293 (1.1%)	2.00	88/4436 (2.0%)
32	J	1.72	27/3236 (0.8%)	1.93	78/4347 (1.8%)
All	All	1.75	788/84152 (0.9%)	1.98	2207/113574 (1.9%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	8
2	B	0	9
3	C	0	4
4	D	0	9
5	E	0	5
6	F	0	7
7	G	0	7
8	1	0	6
9	2	1	6
10	3	0	1
11	4	0	10
12	5	0	11
13	6	0	5
14	7	0	9
15	W	0	3
16	V	0	7
17	T	0	12
18	Y	0	1
19	Z	0	21
20	N	0	16
21	S	0	17
22	P	0	10
23	Q	0	8
24	R	0	14
25	U	0	6
26	O	0	13
27	H	0	9
28	I	0	6
29	K	0	9
30	L	0	17
31	M	0	5
32	J	0	11
All	All	1	282

All (788) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	118	LEU	CA-CB	82.05	3.42	1.53
5	E	101	PHE	CG-CD1	22.43	1.72	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	101	PHE	CG-CD2	22.32	1.72	1.38
5	E	101	PHE	CD2-CE2	17.82	1.74	1.39
5	E	101	PHE	CE2-CZ	17.35	1.70	1.37
5	E	101	PHE	CE1-CZ	15.76	1.67	1.37
5	E	101	PHE	CD1-CE1	14.19	1.67	1.39
28	I	268	ARG	NE-CZ	10.65	1.46	1.33
27	H	265	ARG	CZ-NH1	8.74	1.44	1.33
26	O	294	GLU	CG-CD	8.63	1.64	1.51
19	Z	588	ARG	CZ-NH2	8.62	1.44	1.33
5	E	93	ARG	CZ-NH1	8.57	1.44	1.33
9	2	115	ARG	CZ-NH1	8.55	1.44	1.33
16	V	46	ARG	CZ-NH1	8.45	1.44	1.33
6	F	157	ARG	CD-NE	8.42	1.60	1.46
25	U	99	PRO	N-CD	-8.39	1.36	1.47
30	L	221	TYR	CE1-CZ	8.19	1.49	1.38
4	D	131	ARG	NE-CZ	8.18	1.43	1.33
29	K	60	TYR	CE2-CZ	8.10	1.49	1.38
29	K	323	ARG	CD-NE	8.09	1.60	1.46
30	L	26	TYR	CB-CG	8.08	1.63	1.51
6	F	224	TYR	CG-CD2	8.06	1.49	1.39
19	Z	687	ARG	CD-NE	8.02	1.60	1.46
20	N	594	GLY	CA-C	-8.02	1.39	1.51
21	S	232	ARG	CD-NE	8.00	1.60	1.46
24	R	274	SER	CA-CB	7.96	1.64	1.52
32	J	213	ARG	NE-CZ	7.95	1.43	1.33
17	T	107	ARG	CZ-NH1	7.94	1.43	1.33
7	G	184	GLU	CD-OE1	7.93	1.34	1.25
24	R	300	ARG	CZ-NH1	7.90	1.43	1.33
1	A	125	TYR	CE1-CZ	7.90	1.48	1.38
19	Z	680	ARG	NE-CZ	7.88	1.43	1.33
24	R	63	TRP	NE1-CE2	7.86	1.47	1.37
29	K	392	TYR	CE1-CZ	7.86	1.48	1.38
19	Z	845	ARG	CD-NE	7.84	1.59	1.46
24	R	176	ARG	CZ-NH2	7.79	1.43	1.33
32	J	43	ARG	NE-CZ	7.73	1.43	1.33
32	J	75	GLU	CD-OE2	7.71	1.34	1.25
21	S	28	PRO	N-CD	7.70	1.58	1.47
22	P	111	TYR	CE1-CZ	7.69	1.48	1.38
13	6	157	TYR	CG-CD2	7.67	1.49	1.39
16	V	161	ARG	CZ-NH2	7.66	1.43	1.33
7	G	235	GLU	CD-OE2	7.64	1.34	1.25
29	K	164	TYR	CB-CG	7.64	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	159	ARG	NE-CZ	7.61	1.43	1.33
22	P	27	ARG	CZ-NH1	7.57	1.42	1.33
19	Z	688	ARG	CZ-NH1	7.56	1.42	1.33
19	Z	100	ARG	CD-NE	7.54	1.59	1.46
21	S	177	TYR	CE1-CZ	7.54	1.48	1.38
23	Q	310	ARG	CZ-NH1	7.47	1.42	1.33
21	S	207	TYR	CG-CD2	7.45	1.48	1.39
26	O	321	ARG	NE-CZ	7.45	1.42	1.33
19	Z	828	ARG	CZ-NH1	7.44	1.42	1.33
31	M	367	ARG	CD-NE	7.43	1.59	1.46
19	Z	409	SER	CA-CB	7.40	1.64	1.52
23	Q	155	ARG	CZ-NH1	7.40	1.42	1.33
32	J	365	GLU	CD-OE2	7.40	1.33	1.25
17	T	292	ARG	CZ-NH1	7.39	1.42	1.33
17	T	258	SER	CA-CB	7.38	1.64	1.52
26	O	5	PRO	CA-C	-7.38	1.38	1.52
19	Z	304	PHE	CG-CD1	7.36	1.49	1.38
31	M	64	ARG	NE-CZ	7.34	1.42	1.33
19	Z	181	ARG	CD-NE	7.33	1.58	1.46
4	D	169	ARG	CD-NE	7.32	1.58	1.46
21	S	299	SER	CA-CB	7.32	1.64	1.52
14	7	138	ARG	NE-CZ	7.30	1.42	1.33
16	V	68	ARG	CZ-NH1	7.29	1.42	1.33
17	T	161	CYS	CB-SG	-7.29	1.69	1.82
13	6	126	ARG	CZ-NH2	7.28	1.42	1.33
22	P	39	ARG	CZ-NH2	7.27	1.42	1.33
25	U	177	ARG	CD-NE	7.25	1.58	1.46
30	L	305	ARG	NE-CZ	7.24	1.42	1.33
32	J	375	ARG	NE-CZ	7.24	1.42	1.33
26	O	270	ARG	NE-CZ	7.22	1.42	1.33
21	S	395	ARG	CD-NE	7.22	1.58	1.46
12	5	181	SER	CA-CB	7.15	1.63	1.52
31	M	299	PHE	CG-CD1	7.09	1.49	1.38
5	E	185	TYR	CE2-CZ	7.08	1.47	1.38
31	M	98	GLU	CG-CD	7.06	1.62	1.51
6	F	177	SER	CA-CB	7.04	1.63	1.52
4	D	99	SER	CA-CB	7.03	1.63	1.52
1	A	103	TYR	CE2-CZ	7.03	1.47	1.38
32	J	148	TYR	CE1-CZ	7.02	1.47	1.38
2	B	220	ARG	CZ-NH2	7.00	1.42	1.33
20	N	642	GLU	CD-OE1	-6.99	1.18	1.25
16	V	68	ARG	NE-CZ	6.97	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	194	ARG	CD-NE	6.97	1.58	1.46
10	3	89	SER	CA-CB	6.96	1.63	1.52
31	M	183	ARG	CZ-NH1	6.96	1.42	1.33
19	Z	150	GLU	CD-OE1	6.93	1.33	1.25
3	C	248	GLU	CD-OE1	6.91	1.33	1.25
24	R	54	TYR	CG-CD1	6.91	1.48	1.39
17	T	168	GLU	CB-CG	6.91	1.65	1.52
23	Q	253	TYR	CG-CD2	6.90	1.48	1.39
10	3	165	GLU	CG-CD	6.88	1.62	1.51
20	N	559	ARG	CZ-NH2	6.85	1.42	1.33
27	H	312	ARG	NE-CZ	6.84	1.42	1.33
30	L	358	ARG	NE-CZ	6.84	1.42	1.33
24	R	336	ARG	CZ-NH2	6.83	1.42	1.33
26	O	238	TYR	CE1-CZ	6.80	1.47	1.38
12	5	123	ARG	NE-CZ	6.74	1.41	1.33
19	Z	589	SER	CA-CB	6.74	1.63	1.52
20	N	330	SER	CA-CB	6.72	1.63	1.52
27	H	218	PRO	N-CD	-6.71	1.38	1.47
20	N	557	TYR	CB-CG	-6.70	1.41	1.51
27	H	147	TYR	CZ-OH	6.69	1.49	1.37
28	I	71	TYR	CZ-OH	6.68	1.49	1.37
16	V	207	TYR	CE2-CZ	6.66	1.47	1.38
23	Q	398	GLU	CB-CG	6.65	1.64	1.52
12	5	191	SER	CA-CB	6.65	1.62	1.52
28	I	322	ARG	CZ-NH1	6.65	1.41	1.33
23	Q	236	PHE	CG-CD2	6.63	1.48	1.38
17	T	148	ARG	CD-NE	6.63	1.57	1.46
11	4	155	ARG	CZ-NH2	6.63	1.41	1.33
29	K	366	ARG	CZ-NH2	6.63	1.41	1.33
31	M	307	ARG	CD-NE	6.63	1.57	1.46
3	C	50	ARG	NE-CZ	6.62	1.41	1.33
31	M	61	GLU	CD-OE1	6.62	1.32	1.25
29	K	326	ARG	NE-CZ	6.62	1.41	1.33
7	G	239	TYR	CZ-OH	6.60	1.49	1.37
21	S	95	ARG	NE-CZ	6.60	1.41	1.33
24	R	318	TYR	CB-CG	6.60	1.61	1.51
27	H	199	GLU	CA-CB	6.60	1.68	1.53
22	P	201	ARG	CZ-NH1	6.60	1.41	1.33
5	E	145	GLY	N-CA	-6.59	1.36	1.46
19	Z	478	ARG	CZ-NH2	6.59	1.41	1.33
4	D	112	TYR	CE1-CZ	6.59	1.47	1.38
27	H	39	SER	CA-CB	6.58	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	S	196	ARG	NE-CZ	6.56	1.41	1.33
21	S	491	ARG	CZ-NH1	6.56	1.41	1.33
19	Z	137	ARG	CZ-NH2	6.54	1.41	1.33
29	K	382	SER	CA-CB	6.53	1.62	1.52
31	M	179	GLU	CD-OE2	6.53	1.32	1.25
19	Z	688	ARG	NE-CZ	6.53	1.41	1.33
24	R	187	TYR	CE1-CZ	6.52	1.47	1.38
30	L	342	TYR	CD1-CE1	6.51	1.49	1.39
8	1	177	ARG	NE-CZ	6.51	1.41	1.33
31	M	120	ARG	CZ-NH1	6.51	1.41	1.33
17	T	187	GLU	CD-OE1	6.49	1.32	1.25
26	O	65	SER	CA-CB	-6.49	1.43	1.52
32	J	374	ARG	CZ-NH1	6.48	1.41	1.33
28	I	322	ARG	NE-CZ	6.47	1.41	1.33
11	4	135	GLY	CA-C	-6.47	1.41	1.51
14	7	214	GLU	CG-CD	-6.47	1.42	1.51
10	3	70	ARG	CZ-NH1	6.46	1.41	1.33
11	4	67	TYR	CE1-CZ	6.46	1.47	1.38
3	C	145	PHE	CG-CD1	6.45	1.48	1.38
27	H	276	GLU	CG-CD	6.45	1.61	1.51
9	2	157	TYR	CE2-CZ	6.45	1.47	1.38
15	W	42	ARG	NE-CZ	6.45	1.41	1.33
11	4	95	ARG	NE-CZ	6.44	1.41	1.33
21	S	453	TYR	CE2-CZ	6.44	1.47	1.38
21	S	351	ARG	CZ-NH1	6.44	1.41	1.33
6	F	122	ARG	CZ-NH2	6.43	1.41	1.33
13	6	221	ARG	CD-NE	6.43	1.57	1.46
14	7	208	GLU	CD-OE2	6.42	1.32	1.25
16	V	161	ARG	CD-NE	6.41	1.57	1.46
32	J	201	ARG	NE-CZ	6.41	1.41	1.33
5	E	185	TYR	CZ-OH	6.41	1.48	1.37
28	I	212	GLU	CG-CD	6.41	1.61	1.51
22	P	123	ARG	CZ-NH2	6.41	1.41	1.33
4	D	144	PHE	CE2-CZ	6.40	1.49	1.37
20	N	107	HIS	CB-CG	6.39	1.61	1.50
1	A	128	ASN	CB-CG	6.39	1.65	1.51
11	4	116	TYR	CZ-OH	6.38	1.48	1.37
30	L	227	ARG	CZ-NH1	6.38	1.41	1.33
24	R	83	ARG	CD-NE	6.38	1.57	1.46
17	T	345	TYR	CE1-CZ	6.37	1.46	1.38
20	N	41	SER	CA-CB	6.37	1.62	1.52
20	N	332	GLU	CG-CD	6.37	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O	247	ARG	NE-CZ	6.36	1.41	1.33
9	2	54	GLY	CA-C	-6.36	1.41	1.51
19	Z	259	PHE	CG-CD2	6.36	1.48	1.38
9	2	85	TYR	CE1-CZ	6.36	1.46	1.38
11	4	51	GLY	N-CA	-6.36	1.36	1.46
24	R	259	TYR	CB-CG	6.34	1.61	1.51
23	Q	143	TYR	CE2-CZ	6.33	1.46	1.38
22	P	196	VAL	CB-CG2	6.32	1.66	1.52
24	R	151	TYR	CE2-CZ	6.32	1.46	1.38
16	V	69	VAL	CB-CG1	6.32	1.66	1.52
5	E	213	THR	C-N	6.31	1.48	1.34
31	M	188	TYR	CE2-CZ	6.31	1.46	1.38
29	K	274	ARG	CZ-NH2	6.30	1.41	1.33
7	G	211	GLU	CD-OE1	6.29	1.32	1.25
11	4	134	TYR	CG-CD1	6.29	1.47	1.39
15	W	102	GLY	N-CA	-6.29	1.36	1.46
24	R	71	SER	CA-CB	6.29	1.62	1.52
23	Q	221	GLU	CD-OE1	6.29	1.32	1.25
30	L	311	ARG	CZ-NH1	6.29	1.41	1.33
6	F	171	TYR	CE2-CZ	6.28	1.46	1.38
1	A	27	TYR	CE1-CZ	6.28	1.46	1.38
12	5	258	TYR	CZ-OH	6.27	1.48	1.37
3	C	128	ARG	CD-NE	6.26	1.57	1.46
8	1	80	GLY	CA-C	-6.25	1.41	1.51
17	T	104	GLU	CG-CD	6.25	1.61	1.51
3	C	50	ARG	CZ-NH2	6.24	1.41	1.33
12	5	258	TYR	CE1-CZ	6.24	1.46	1.38
20	N	246	TYR	CE1-CZ	6.24	1.46	1.38
23	Q	76	PHE	CG-CD1	6.24	1.48	1.38
19	Z	190	GLU	CD-OE2	6.23	1.32	1.25
30	L	295	ARG	CD-NE	6.22	1.57	1.46
30	L	127	ARG	CD-NE	6.22	1.57	1.46
28	I	59	ARG	CZ-NH1	6.22	1.41	1.33
32	J	310	ARG	CD-NE	6.22	1.57	1.46
24	R	101	ARG	CZ-NH1	6.20	1.41	1.33
14	7	231	PHE	CG-CD2	6.19	1.48	1.38
20	N	474	ARG	CD-NE	6.19	1.56	1.46
29	K	251	PHE	CG-CD1	6.18	1.48	1.38
12	5	230	GLY	CA-C	-6.18	1.42	1.51
19	Z	437	GLU	CD-OE2	6.18	1.32	1.25
27	H	197	HIS	CB-CG	6.17	1.61	1.50
32	J	273	MET	CA-CB	6.17	1.67	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	155	TYR	CG-CD1	6.16	1.47	1.39
23	Q	297	ARG	CZ-NH2	6.16	1.41	1.33
4	D	130	ARG	CZ-NH1	6.15	1.41	1.33
7	G	79	ALA	C-N	6.15	1.44	1.33
21	S	487	VAL	CB-CG1	6.15	1.65	1.52
19	Z	436	SER	CA-CB	6.15	1.62	1.52
29	K	367	PRO	N-CD	6.15	1.56	1.47
1	A	132	ARG	NE-CZ	6.14	1.41	1.33
31	M	229	TYR	CG-CD2	6.14	1.47	1.39
2	B	178	TYR	CZ-OH	6.14	1.48	1.37
13	6	28	ARG	NE-CZ	6.13	1.41	1.33
11	4	153	ARG	CZ-NH1	6.13	1.41	1.33
25	U	105	ASP	CB-CG	6.13	1.64	1.51
27	H	97	ARG	NE-CZ	6.13	1.41	1.33
22	P	137	TYR	CG-CD2	6.12	1.47	1.39
24	R	183	TYR	CG-CD1	6.12	1.47	1.39
30	L	157	ARG	CD-NE	6.11	1.56	1.46
20	N	580	ARG	NE-CZ	6.11	1.41	1.33
21	S	290	ARG	CZ-NH2	6.10	1.41	1.33
23	Q	87	ARG	CZ-NH1	6.10	1.41	1.33
21	S	232	ARG	NE-CZ	6.10	1.41	1.33
32	J	271	ARG	CZ-NH1	6.09	1.41	1.33
19	Z	881	GLU	CG-CD	6.08	1.61	1.51
16	V	211	GLU	CG-CD	6.07	1.61	1.51
2	B	113	ARG	CZ-NH2	6.07	1.41	1.33
1	A	223	GLU	CD-OE2	6.07	1.32	1.25
23	Q	142	ARG	CZ-NH2	6.06	1.41	1.33
24	R	379	ARG	NE-CZ	6.05	1.41	1.33
32	J	318	PRO	N-CD	-6.05	1.39	1.47
14	7	168	TYR	CG-CD2	6.04	1.47	1.39
9	2	214	SER	CA-CB	6.04	1.62	1.52
14	7	223	ARG	CZ-NH2	6.04	1.41	1.33
27	H	355	PHE	CG-CD1	6.04	1.47	1.38
3	C	41	ASP	CB-CG	6.03	1.64	1.51
5	E	237	VAL	CB-CG2	6.02	1.65	1.52
11	4	93	ARG	CZ-NH2	6.02	1.40	1.33
3	C	248	GLU	CG-CD	-6.01	1.43	1.51
20	N	57	ARG	CD-NE	6.01	1.56	1.46
22	P	139	GLU	CD-OE2	6.01	1.32	1.25
16	V	207	TYR	CG-CD2	6.01	1.47	1.39
20	N	108	TYR	CD1-CE1	6.01	1.48	1.39
25	U	250	TYR	CE1-CZ	6.00	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	34	ARG	CD-NE	6.00	1.56	1.46
27	H	43	ARG	CZ-NH2	5.99	1.40	1.33
19	Z	434	TYR	CG-CD1	5.99	1.47	1.39
24	R	32	ARG	NE-CZ	5.99	1.40	1.33
14	7	210	ARG	CZ-NH1	5.99	1.40	1.33
23	Q	279	TYR	CE1-CZ	5.99	1.46	1.38
24	R	267	ARG	NE-CZ	5.98	1.40	1.33
7	G	26	TYR	CE1-CZ	5.98	1.46	1.38
24	R	293	ARG	CA-CB	5.97	1.67	1.53
20	N	581	SER	CB-OG	5.97	1.50	1.42
28	I	184	TYR	CE2-CZ	5.97	1.46	1.38
1	A	135	GLY	N-CA	-5.97	1.37	1.46
13	6	82	SER	CB-OG	-5.97	1.34	1.42
20	N	858	GLU	CB-CG	5.96	1.63	1.52
29	K	391	ARG	NE-CZ	5.96	1.40	1.33
20	N	209	GLU	CD-OE1	5.95	1.32	1.25
28	I	333	ARG	NE-CZ	5.95	1.40	1.33
20	N	140	ARG	NE-CZ	5.95	1.40	1.33
8	1	155	ARG	NE-CZ	5.94	1.40	1.33
11	4	137	PHE	CG-CD1	5.94	1.47	1.38
29	K	248	ARG	NE-CZ	5.94	1.40	1.33
1	A	178	PHE	CG-CD1	5.94	1.47	1.38
5	E	117	SER	CA-CB	5.93	1.61	1.52
12	5	149	TYR	CG-CD1	5.93	1.46	1.39
17	T	279	GLU	CD-OE1	5.93	1.32	1.25
6	F	107	ARG	CD-NE	5.91	1.56	1.46
13	6	101	MET	N-CA	-5.91	1.34	1.46
30	L	67	VAL	C-N	5.91	1.43	1.33
19	Z	194	TYR	CB-CG	5.91	1.60	1.51
19	Z	110	TYR	CE1-CZ	5.90	1.46	1.38
31	M	120	ARG	CD-NE	5.90	1.56	1.46
1	A	159	TYR	CZ-OH	5.89	1.47	1.37
21	S	341	ARG	NE-CZ	5.89	1.40	1.33
22	P	172	GLU	CD-OE2	5.89	1.32	1.25
11	4	95	ARG	CD-NE	5.89	1.56	1.46
20	N	417	LYS	N-CA	-5.89	1.34	1.46
21	S	439	ARG	CZ-NH1	5.89	1.40	1.33
31	M	218	LEU	C-N	5.89	1.43	1.33
20	N	234	GLU	CG-CD	5.88	1.60	1.51
29	K	391	ARG	CD-NE	5.88	1.56	1.46
22	P	220	GLU	CD-OE1	5.87	1.32	1.25
12	5	78	ARG	CZ-NH1	5.86	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	673	ARG	CD-NE	5.85	1.56	1.46
8	1	130	GLY	CA-C	5.85	1.61	1.51
14	7	221	TYR	CG-CD2	5.85	1.46	1.39
14	7	79	ARG	NE-CZ	5.85	1.40	1.33
20	N	682	TYR	CE1-CZ	5.85	1.46	1.38
19	Z	816	TYR	CG-CD1	5.84	1.46	1.39
5	E	53	ARG	NE-CZ	5.84	1.40	1.33
5	E	135	ARG	CZ-NH1	5.84	1.40	1.33
14	7	230	ARG	CZ-NH2	5.84	1.40	1.33
26	O	178	ARG	CZ-NH2	5.84	1.40	1.33
6	F	186	GLU	CB-CG	5.83	1.63	1.52
4	D	60	ARG	CZ-NH2	5.83	1.40	1.33
22	P	141	GLU	CD-OE1	-5.83	1.19	1.25
32	J	355	SER	CA-CB	5.83	1.61	1.52
19	Z	746	ARG	CZ-NH1	5.82	1.40	1.33
24	R	110	TYR	CE2-CZ	5.82	1.46	1.38
1	A	214	GLU	CG-CD	5.82	1.60	1.51
22	P	263	TRP	NE1-CE2	5.81	1.45	1.37
30	L	54	TYR	CE1-CZ	5.81	1.46	1.38
20	N	57	ARG	CZ-NH2	5.80	1.40	1.33
30	L	295	ARG	CZ-NH2	5.80	1.40	1.33
6	F	33	SER	CB-OG	-5.80	1.34	1.42
12	5	99	TYR	CZ-OH	5.80	1.47	1.37
27	H	336	ARG	CZ-NH1	5.79	1.40	1.33
30	L	19	ARG	NE-CZ	5.79	1.40	1.33
9	2	136	TYR	CB-CG	5.79	1.60	1.51
19	Z	519	ALA	CA-CB	5.79	1.64	1.52
22	P	94	ARG	NE-CZ	5.79	1.40	1.33
8	1	136	TRP	NE1-CE2	5.79	1.45	1.37
27	H	360	ARG	CZ-NH2	5.79	1.40	1.33
20	N	361	ARG	CZ-NH1	5.78	1.40	1.33
19	Z	360	GLY	N-CA	-5.78	1.37	1.46
19	Z	400	TYR	CG-CD1	5.78	1.46	1.39
29	K	81	ARG	NE-CZ	5.78	1.40	1.33
25	U	190	ARG	NE-CZ	5.77	1.40	1.33
30	L	403	VAL	CB-CG2	5.77	1.65	1.52
22	P	263	TRP	CE2-CZ2	5.76	1.49	1.39
27	H	215	PHE	CG-CD2	5.76	1.47	1.38
28	I	189	GLY	N-CA	-5.76	1.37	1.46
9	2	161	SER	CA-CB	5.76	1.61	1.52
14	7	106	TYR	CD2-CE2	5.76	1.48	1.39
26	O	330	ARG	CZ-NH1	5.76	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Q	142	ARG	CD-NE	5.76	1.56	1.46
10	3	143	SER	CB-OG	5.76	1.49	1.42
27	H	68	SER	CB-OG	5.76	1.49	1.42
2	B	219	ARG	CD-NE	5.75	1.56	1.46
15	W	25	ARG	CD-NE	5.75	1.56	1.46
15	W	91	ARG	NE-CZ	5.75	1.40	1.33
26	O	27	GLU	CD-OE1	5.75	1.31	1.25
31	M	91	TYR	CB-CG	5.75	1.60	1.51
20	N	199	ARG	CZ-NH2	5.75	1.40	1.33
19	Z	879	ARG	CZ-NH1	5.74	1.40	1.33
20	N	361	ARG	NE-CZ	5.74	1.40	1.33
22	P	191	ARG	CZ-NH2	5.73	1.40	1.33
17	T	178	TYR	CG-CD2	5.73	1.46	1.39
31	M	394	PHE	CG-CD1	5.73	1.47	1.38
25	U	283	ARG	CD-NE	5.72	1.56	1.46
22	P	129	ARG	NE-CZ	5.72	1.40	1.33
20	N	504	ASP	CA-CB	5.72	1.66	1.53
13	6	82	SER	CA-CB	5.71	1.61	1.52
12	5	159	MET	N-CA	-5.71	1.34	1.46
20	N	490	ARG	CZ-NH1	5.71	1.40	1.33
15	W	15	TYR	CE2-CZ	5.71	1.46	1.38
12	5	224	TYR	CE1-CZ	5.70	1.46	1.38
26	O	289	ARG	NE-CZ	5.70	1.40	1.33
29	K	263	PHE	CG-CD2	5.69	1.47	1.38
31	M	389	ARG	CZ-NH1	5.69	1.40	1.33
24	R	250	LEU	N-CA	-5.68	1.34	1.46
23	Q	309	TYR	N-CA	-5.68	1.34	1.46
20	N	129	ARG	NE-CZ	5.68	1.40	1.33
22	P	93	ARG	CZ-NH2	5.67	1.40	1.33
31	M	230	GLY	CA-C	-5.67	1.42	1.51
7	G	93	ARG	CD-NE	5.67	1.56	1.46
1	A	8	GLY	N-CA	-5.67	1.37	1.46
11	4	67	TYR	CG-CD1	5.67	1.46	1.39
25	U	53	SER	CB-OG	5.67	1.49	1.42
23	Q	281	GLY	N-CA	-5.67	1.37	1.46
23	Q	11	ARG	CZ-NH2	5.67	1.40	1.33
31	M	337	ARG	CZ-NH2	5.67	1.40	1.33
12	5	186	SER	CA-CB	5.66	1.61	1.52
20	N	490	ARG	CZ-NH2	5.66	1.40	1.33
3	C	155	ASN	N-CA	-5.66	1.35	1.46
2	B	219	ARG	NE-CZ	5.66	1.40	1.33
13	6	165	GLY	C-N	5.66	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	145	TYR	CE1-CZ	5.65	1.45	1.38
20	N	682	TYR	CG-CD1	5.65	1.46	1.39
27	H	211	GLY	CA-C	-5.65	1.42	1.51
2	B	128	ARG	CZ-NH2	5.65	1.40	1.33
6	F	202	GLU	CD-OE1	5.64	1.31	1.25
27	H	294	GLU	CD-OE1	5.64	1.31	1.25
21	S	446	SER	CB-OG	-5.64	1.34	1.42
11	4	147	TYR	CG-CD1	5.64	1.46	1.39
14	7	126	SER	CA-CB	5.64	1.61	1.52
7	G	93	ARG	CZ-NH2	5.63	1.40	1.33
2	B	6	TYR	CE1-CZ	5.63	1.45	1.38
8	1	123	TYR	CG-CD1	5.63	1.46	1.39
13	6	215	TYR	CE2-CZ	5.63	1.45	1.38
30	L	19	ARG	CZ-NH1	5.63	1.40	1.33
31	M	365	ARG	CZ-NH2	5.62	1.40	1.33
19	Z	763	ARG	CZ-NH2	5.62	1.40	1.33
20	N	700	GLU	CG-CD	5.61	1.60	1.51
24	R	233	ARG	NE-CZ	5.61	1.40	1.33
29	K	329	ARG	NE-CZ	5.61	1.40	1.33
24	R	225	TYR	CD2-CE2	5.61	1.47	1.39
25	U	89	GLU	CA-CB	5.61	1.66	1.53
30	L	386	ARG	CD-NE	5.60	1.55	1.46
1	A	228	ARG	NE-CZ	5.60	1.40	1.33
19	Z	110	TYR	CZ-OH	5.60	1.47	1.37
24	R	312	ARG	CZ-NH1	5.60	1.40	1.33
8	1	225	ASP	CA-CB	5.59	1.66	1.53
19	Z	386	GLY	CA-C	-5.59	1.43	1.51
20	N	946	GLU	CA-CB	5.59	1.66	1.53
31	M	308	GLU	CD-OE2	5.59	1.31	1.25
19	Z	400	TYR	CZ-OH	5.58	1.47	1.37
11	4	19	ARG	CD-NE	5.58	1.55	1.46
4	D	102	LEU	CA-CB	5.58	1.66	1.53
5	E	160	GLY	CA-C	-5.58	1.43	1.51
7	G	56	SER	CA-CB	5.57	1.61	1.52
17	T	217	ARG	CZ-NH2	5.57	1.40	1.33
21	S	162	TYR	CE1-CZ	5.57	1.45	1.38
22	P	82	LEU	CA-CB	5.57	1.66	1.53
10	3	28	PHE	CG-CD2	5.56	1.47	1.38
31	M	285	ILE	N-CA	-5.56	1.35	1.46
32	J	307	ARG	CD-NE	5.56	1.55	1.46
20	N	494	TYR	CZ-OH	5.55	1.47	1.37
32	J	18	SER	CB-OG	5.55	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	H	360	ARG	CD-NE	5.55	1.55	1.46
13	6	233	GLU	CD-OE1	5.54	1.31	1.25
30	L	392	LYS	CD-CE	5.54	1.65	1.51
6	F	169	ARG	CD-NE	5.54	1.55	1.46
24	R	9	GLU	CB-CG	5.54	1.62	1.52
24	R	63	TRP	CZ3-CH2	5.54	1.49	1.40
29	K	403	TYR	CG-CD2	5.54	1.46	1.39
1	A	117	ARG	CZ-NH2	5.54	1.40	1.33
21	S	466	ARG	CZ-NH1	5.54	1.40	1.33
6	F	164	ARG	CZ-NH2	5.53	1.40	1.33
10	3	2	SER	CA-CB	5.53	1.61	1.52
27	H	147	TYR	CE1-CZ	5.53	1.45	1.38
7	G	222	LYS	CE-NZ	-5.53	1.35	1.49
22	P	39	ARG	CD-NE	5.53	1.55	1.46
8	1	121	TYR	CB-CG	-5.52	1.43	1.51
26	O	288	HIS	CB-CG	5.52	1.59	1.50
17	T	319	TYR	CE2-CZ	5.52	1.45	1.38
22	P	142	ARG	CZ-NH1	5.52	1.40	1.33
28	I	346	ARG	CZ-NH2	5.51	1.40	1.33
28	I	110	GLY	N-CA	-5.51	1.37	1.46
21	S	88	ARG	CZ-NH1	5.51	1.40	1.33
19	Z	740	ARG	NE-CZ	5.51	1.40	1.33
21	S	257	TYR	CB-CG	5.51	1.59	1.51
28	I	132	TYR	CE1-CZ	5.51	1.45	1.38
13	6	159	ARG	NE-CZ	5.50	1.40	1.33
3	C	249	ARG	CZ-NH2	5.50	1.40	1.33
12	5	229	SER	C-N	5.50	1.43	1.33
5	E	183	GLU	CB-CG	5.50	1.62	1.52
27	H	333	ARG	CZ-NH1	5.50	1.40	1.33
24	R	337	PHE	CG-CD1	5.50	1.47	1.38
21	S	298	TYR	CG-CD2	5.50	1.46	1.39
3	C	203	VAL	CB-CG1	5.49	1.64	1.52
25	U	79	TYR	CG-CD2	5.49	1.46	1.39
12	5	107	GLY	N-CA	-5.49	1.37	1.46
30	L	323	ARG	NE-CZ	5.49	1.40	1.33
20	N	68	PHE	CG-CD1	5.49	1.47	1.38
24	R	297	ARG	CZ-NH2	5.49	1.40	1.33
21	S	211	ALA	CA-CB	5.48	1.64	1.52
30	L	235	TYR	CZ-OH	5.48	1.47	1.37
3	C	195	LYS	CA-CB	-5.48	1.41	1.53
21	S	252	ARG	CZ-NH1	5.48	1.40	1.33
24	R	293	ARG	CZ-NH1	5.48	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	M	367	ARG	CZ-NH1	5.48	1.40	1.33
1	A	3	ARG	CZ-NH2	5.48	1.40	1.33
20	N	361	ARG	CZ-NH2	5.47	1.40	1.33
32	J	367	GLY	N-CA	-5.47	1.37	1.46
14	7	54	SER	CA-CB	5.47	1.61	1.52
29	K	164	TYR	CE2-CZ	5.47	1.45	1.38
29	K	287	ARG	CZ-NH2	5.47	1.40	1.33
19	Z	585	GLU	CD-OE2	5.47	1.31	1.25
20	N	759	SER	CA-CB	5.47	1.61	1.52
21	S	412	ARG	NE-CZ	5.46	1.40	1.33
14	7	230	ARG	NE-CZ	5.46	1.40	1.33
21	S	176	ARG	CZ-NH2	5.46	1.40	1.33
32	J	24	TYR	CE2-CZ	5.46	1.45	1.38
17	T	105	TRP	CD2-CE2	-5.46	1.34	1.41
21	S	356	TYR	CD2-CE2	5.46	1.47	1.39
22	P	377	ARG	CZ-NH1	5.45	1.40	1.33
32	J	258	ARG	CZ-NH2	5.45	1.40	1.33
19	Z	342	PRO	CA-CB	-5.45	1.42	1.53
22	P	114	GLU	CD-OE1	5.45	1.31	1.25
24	R	325	VAL	CA-C	-5.44	1.38	1.52
24	R	233	ARG	CZ-NH2	5.44	1.40	1.33
24	R	268	TYR	CB-CG	-5.44	1.43	1.51
1	A	11	ARG	CZ-NH1	5.43	1.40	1.33
19	Z	6	ARG	CZ-NH1	5.43	1.40	1.33
20	N	896	GLU	CB-CG	5.43	1.62	1.52
28	I	244	SER	CA-CB	5.43	1.61	1.52
19	Z	725	SER	CA-CB	5.43	1.61	1.52
28	I	80	ARG	CD-NE	5.43	1.55	1.46
14	7	188	TYR	CE1-CZ	5.43	1.45	1.38
19	Z	456	ARG	CD-NE	5.43	1.55	1.46
22	P	104	MET	N-CA	-5.43	1.35	1.46
3	C	66	TYR	CE1-CZ	5.42	1.45	1.38
24	R	137	ARG	CZ-NH2	5.42	1.40	1.33
32	J	184	LYS	CD-CE	5.42	1.64	1.51
8	1	163	SER	CA-CB	5.42	1.61	1.52
9	2	124	ARG	CD-NE	5.42	1.55	1.46
19	Z	362	GLY	CA-C	-5.41	1.43	1.51
21	S	103	ARG	CZ-NH1	5.41	1.40	1.33
28	I	169	PRO	CA-C	-5.41	1.42	1.52
31	M	249	ALA	CA-CB	5.41	1.63	1.52
11	4	73	TYR	CE2-CZ	5.41	1.45	1.38
31	M	251	PHE	CD2-CE2	5.41	1.50	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O	132	LYS	CA-CB	5.40	1.65	1.53
22	P	251	TYR	CE2-CZ	5.40	1.45	1.38
12	5	225	ARG	CA-CB	5.40	1.65	1.53
13	6	134	TYR	CE2-CZ	5.40	1.45	1.38
20	N	770	TRP	CD2-CE3	-5.39	1.32	1.40
31	M	210	ASN	CA-CB	5.39	1.67	1.53
20	N	850	GLU	CG-CD	5.39	1.60	1.51
12	5	123	ARG	CZ-NH2	5.39	1.40	1.33
21	S	303	ARG	NE-CZ	5.39	1.40	1.33
22	P	65	ARG	CZ-NH2	5.39	1.40	1.33
22	P	247	TYR	CD2-CE2	5.38	1.47	1.39
19	Z	681	TYR	CE1-CZ	5.38	1.45	1.38
6	F	101	ARG	CZ-NH2	5.38	1.40	1.33
19	Z	494	ARG	CZ-NH2	5.38	1.40	1.33
15	W	79	GLN	CG-CD	5.38	1.63	1.51
19	Z	531	ASN	CB-CG	5.38	1.63	1.51
19	Z	239	TYR	CZ-OH	5.38	1.47	1.37
19	Z	785	ARG	NE-CZ	5.38	1.40	1.33
29	K	42	SER	CA-CB	5.37	1.61	1.52
32	J	229	ARG	NE-CZ	5.37	1.40	1.33
1	A	191	PHE	CG-CD2	5.37	1.46	1.38
31	M	423	TYR	CE2-CZ	5.37	1.45	1.38
21	S	51	GLY	CA-C	5.37	1.60	1.51
24	R	259	TYR	CZ-OH	5.37	1.47	1.37
5	E	20	ARG	NE-CZ	5.36	1.40	1.33
8	1	73	HIS	CB-CG	5.36	1.59	1.50
19	Z	67	ASP	N-CA	-5.36	1.35	1.46
4	D	179	GLU	CG-CD	5.36	1.59	1.51
7	G	20	ARG	CD-NE	5.36	1.55	1.46
19	Z	71	TYR	CE1-CZ	5.36	1.45	1.38
24	R	211	TYR	CE2-CZ	5.36	1.45	1.38
29	K	252	ARG	NE-CZ	5.36	1.40	1.33
11	4	70	ARG	CZ-NH1	5.35	1.40	1.33
16	V	282	ARG	CZ-NH1	5.35	1.40	1.33
21	S	348	SER	CA-CB	5.35	1.60	1.52
20	N	412	HIS	CA-CB	5.35	1.65	1.53
19	Z	154	TRP	CG-CD1	5.35	1.44	1.36
5	E	235	GLU	CB-CG	5.35	1.62	1.52
23	Q	87	ARG	NE-CZ	5.35	1.40	1.33
9	2	167	TYR	CD2-CE2	5.34	1.47	1.39
16	V	200	TYR	CD2-CE2	5.34	1.47	1.39
29	K	179	GLU	CD-OE1	5.34	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	150	GLY	CA-C	-5.34	1.43	1.51
31	M	174	ARG	NE-CZ	5.34	1.40	1.33
26	O	60	TYR	CG-CD1	5.34	1.46	1.39
27	H	41	TYR	CZ-OH	5.34	1.47	1.37
6	F	164	ARG	CZ-NH1	5.33	1.40	1.33
16	V	121	TRP	CB-CG	5.33	1.59	1.50
8	1	121	TYR	CG-CD2	5.33	1.46	1.39
22	P	248	ARG	NE-CZ	5.33	1.40	1.33
27	H	366	ARG	CZ-NH1	5.33	1.40	1.33
30	L	143	ASN	N-CA	-5.33	1.35	1.46
26	O	150	SER	CA-CB	5.33	1.60	1.52
2	B	143	ARG	CZ-NH1	5.32	1.40	1.33
19	Z	853	VAL	C-N	5.32	1.42	1.33
21	S	62	GLU	CG-CD	5.32	1.59	1.51
21	S	84	GLY	N-CA	-5.32	1.38	1.46
30	L	370	ARG	CZ-NH1	5.32	1.40	1.33
23	Q	278	ARG	NE-CZ	5.32	1.40	1.33
16	V	34	SER	CA-CB	5.31	1.60	1.52
19	Z	341	GLU	CD-OE1	5.31	1.31	1.25
27	H	400	ARG	CZ-NH2	5.31	1.40	1.33
4	D	218	ARG	NE-CZ	5.31	1.40	1.33
27	H	351	ARG	CZ-NH2	5.31	1.40	1.33
30	L	91	PRO	N-CD	-5.31	1.40	1.47
10	3	66	ARG	CD-NE	5.31	1.55	1.46
10	3	26	ARG	CA-C	-5.30	1.39	1.52
26	O	155	PHE	CG-CD1	5.30	1.46	1.38
13	6	65	ARG	NE-CZ	5.30	1.40	1.33
23	Q	239	TYR	CE2-CZ	5.30	1.45	1.38
30	L	206	ASP	CA-CB	5.30	1.65	1.53
23	Q	76	PHE	CG-CD2	5.30	1.46	1.38
23	Q	337	ARG	CD-NE	5.29	1.55	1.46
4	D	96	GLU	CB-CG	5.29	1.62	1.52
20	N	800	VAL	CB-CG1	5.29	1.64	1.52
25	U	148	GLY	CA-C	-5.29	1.43	1.51
26	O	173	TYR	CD1-CE1	5.29	1.47	1.39
9	2	246	ARG	NE-CZ	5.29	1.40	1.33
31	M	257	PRO	CA-C	-5.29	1.42	1.52
2	B	54	SER	CA-CB	5.28	1.60	1.52
27	H	169	LYS	C-N	-5.28	1.24	1.34
20	N	551	GLY	N-CA	5.28	1.53	1.46
27	H	71	GLY	N-CA	5.28	1.53	1.46
30	L	156	ILE	CA-CB	-5.28	1.42	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	I	272	ARG	NE-CZ	5.28	1.40	1.33
15	W	70	ARG	CZ-NH1	5.28	1.40	1.33
17	T	305	TYR	CG-CD2	5.28	1.46	1.39
1	A	28	ALA	CA-CB	5.27	1.63	1.52
29	K	366	ARG	CZ-NH1	5.27	1.40	1.33
17	T	347	ARG	CZ-NH2	5.27	1.40	1.33
22	P	133	GLU	CG-CD	5.27	1.59	1.51
5	E	55	THR	N-CA	-5.27	1.35	1.46
15	W	17	ARG	CZ-NH1	5.26	1.39	1.33
26	O	240	PHE	CG-CD2	5.26	1.46	1.38
2	B	145	TYR	CD2-CE2	5.26	1.47	1.39
20	N	199	ARG	CD-NE	5.26	1.55	1.46
2	B	210	VAL	C-N	5.26	1.42	1.33
10	3	201	LYS	CA-CB	5.26	1.65	1.53
31	M	348	SER	CA-CB	5.26	1.60	1.52
14	7	226	ARG	CZ-NH2	5.25	1.39	1.33
15	W	147	GLU	CD-OE1	-5.25	1.19	1.25
19	Z	801	VAL	CB-CG1	5.25	1.63	1.52
16	V	201	TYR	CG-CD1	5.25	1.46	1.39
6	F	97	PHE	CG-CD2	5.25	1.46	1.38
12	5	179	ARG	CZ-NH2	5.25	1.39	1.33
19	Z	781	TYR	CE2-CZ	5.25	1.45	1.38
20	N	112	CYS	N-CA	-5.25	1.35	1.46
19	Z	143	ARG	CZ-NH1	5.24	1.39	1.33
29	K	112	TYR	CE1-CZ	5.24	1.45	1.38
17	T	342	VAL	CA-CB	-5.24	1.43	1.54
21	S	426	SER	CA-CB	5.24	1.60	1.52
6	F	123	TYR	CG-CD1	5.23	1.46	1.39
12	5	236	TYR	CG-CD1	5.23	1.46	1.39
20	N	474	ARG	CZ-NH1	5.23	1.39	1.33
1	A	88	ARG	CZ-NH2	5.23	1.39	1.33
20	N	3	THR	N-CA	-5.23	1.35	1.46
20	N	546	ARG	CD-NE	5.23	1.55	1.46
22	P	437	SER	CA-CB	5.23	1.60	1.52
13	6	52	SER	CA-CB	5.23	1.60	1.52
27	H	258	ARG	NE-CZ	5.23	1.39	1.33
22	P	392	PHE	CA-C	-5.22	1.39	1.52
20	N	437	TYR	CZ-OH	5.22	1.46	1.37
20	N	870	GLU	CB-CG	5.22	1.62	1.52
32	J	232	ARG	CD-NE	5.22	1.55	1.46
25	U	177	ARG	CZ-NH2	5.22	1.39	1.33
6	F	54	SER	CA-CB	5.22	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	U	203	SER	CA-CB	5.22	1.60	1.52
29	K	78	GLU	CD-OE2	5.21	1.31	1.25
31	M	188	TYR	CZ-OH	5.21	1.46	1.37
10	3	26	ARG	C-O	5.21	1.33	1.23
24	R	336	ARG	CD-NE	5.21	1.55	1.46
15	W	73	SER	CA-CB	5.21	1.60	1.52
30	L	256	ARG	NE-CZ	5.21	1.39	1.33
17	T	282	TYR	CE1-CZ	5.21	1.45	1.38
22	P	329	ARG	CZ-NH1	5.21	1.39	1.33
17	T	292	ARG	N-CA	-5.21	1.35	1.46
11	4	98	TYR	CZ-OH	5.20	1.46	1.37
30	L	204	GLN	N-CA	-5.20	1.35	1.46
19	Z	495	GLU	CB-CG	5.20	1.62	1.52
22	P	227	TYR	CB-CG	5.20	1.59	1.51
19	Z	261	ARG	NE-CZ	5.19	1.39	1.33
27	H	323	ARG	NE-CZ	5.19	1.39	1.33
11	4	170	ARG	CD-NE	5.19	1.55	1.46
21	S	283	ARG	CD-NE	5.19	1.55	1.46
21	S	192	SER	CB-OG	5.19	1.49	1.42
23	Q	132	ARG	CZ-NH2	5.19	1.39	1.33
1	A	11	ARG	CD-NE	5.19	1.55	1.46
17	T	238	TYR	CG-CD1	5.19	1.45	1.39
6	F	60	GLN	CG-CD	5.18	1.62	1.51
30	L	99	ARG	CD-NE	5.18	1.55	1.46
31	M	59	LYS	C-N	5.18	1.46	1.34
24	R	237	ARG	CD-NE	5.18	1.55	1.46
28	I	411	ARG	CZ-NH1	5.18	1.39	1.33
28	I	352	GLU	CB-CG	5.18	1.61	1.52
21	S	76	ARG	CZ-NH2	5.17	1.39	1.33
25	U	25	ARG	CZ-NH2	5.17	1.39	1.33
30	L	104	SER	CA-CB	5.17	1.60	1.52
2	B	98	TYR	CZ-OH	5.17	1.46	1.37
23	Q	237	GLU	CG-CD	-5.17	1.44	1.51
30	L	308	ARG	CZ-NH1	5.16	1.39	1.33
7	G	63	SER	CA-CB	5.16	1.60	1.52
6	F	171	TYR	CG-CD2	5.16	1.45	1.39
17	T	142	GLN	CG-CD	5.16	1.62	1.51
22	P	94	ARG	CZ-NH1	5.16	1.39	1.33
20	N	778	PHE	CG-CD1	5.15	1.46	1.38
31	M	241	ARG	CZ-NH2	5.15	1.39	1.33
21	S	237	ARG	NE-CZ	5.15	1.39	1.33
26	O	68	GLU	CD-OE2	5.15	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	M	188	TYR	CE1-CZ	5.15	1.45	1.38
22	P	214	PHE	N-CA	-5.15	1.36	1.46
29	K	193	GLN	N-CA	-5.15	1.36	1.46
23	Q	138	PHE	CG-CD1	5.15	1.46	1.38
3	C	128	ARG	NE-CZ	5.14	1.39	1.33
7	G	233	ARG	NE-CZ	5.14	1.39	1.33
18	Y	59	GLU	CB-CG	5.14	1.61	1.52
6	F	99	PHE	CE2-CZ	5.14	1.47	1.37
29	K	105	SER	CA-CB	5.13	1.60	1.52
17	T	164	ILE	N-CA	-5.13	1.36	1.46
8	1	78	ARG	CZ-NH2	5.13	1.39	1.33
30	L	111	ARG	CZ-NH1	5.13	1.39	1.33
32	J	49	ARG	CZ-NH2	5.13	1.39	1.33
2	B	67	PRO	CA-C	-5.12	1.42	1.52
19	Z	815	HIS	CA-CB	5.12	1.65	1.53
24	R	336	ARG	CZ-NH1	5.12	1.39	1.33
1	A	21	ARG	CZ-NH1	5.12	1.39	1.33
14	7	195	ARG	NE-CZ	5.12	1.39	1.33
28	I	349	ARG	CZ-NH2	5.12	1.39	1.33
27	H	333	ARG	CZ-NH2	5.12	1.39	1.33
16	V	279	ASP	C-N	-5.12	1.24	1.34
28	I	80	ARG	CZ-NH1	5.12	1.39	1.33
19	Z	554	TYR	CG-CD2	5.12	1.45	1.39
27	H	60	ASN	CA-CB	5.12	1.66	1.53
28	I	169	PRO	N-CA	5.12	1.55	1.47
24	R	257	ARG	NE-CZ	5.11	1.39	1.33
27	H	360	ARG	NE-CZ	5.11	1.39	1.33
19	Z	714	SER	CA-CB	5.11	1.60	1.52
29	K	287	ARG	CD-NE	5.11	1.55	1.46
20	N	55	ARG	CA-CB	5.11	1.65	1.53
20	N	944	PRO	N-CD	-5.11	1.40	1.47
28	I	285	ASP	CB-CG	5.11	1.62	1.51
15	W	28	ALA	CA-C	-5.10	1.39	1.52
13	6	197	ARG	CZ-NH2	5.09	1.39	1.33
26	O	78	GLU	CB-CG	5.09	1.61	1.52
27	H	393	GLY	CA-C	5.09	1.60	1.51
4	D	134	GLY	N-CA	-5.09	1.38	1.46
20	N	21	GLU	CG-CD	5.09	1.59	1.51
28	I	315	GLN	CA-CB	5.09	1.65	1.53
8	1	233	SER	CA-CB	5.09	1.60	1.52
14	7	81	ARG	NE-CZ	5.09	1.39	1.33
21	S	497	TYR	CE1-CZ	5.09	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	O	211	PHE	CG-CD2	5.09	1.46	1.38
29	K	122	GLU	CB-CG	5.09	1.61	1.52
27	H	95	VAL	CB-CG2	5.08	1.63	1.52
19	Z	492	SER	CA-CB	5.08	1.60	1.52
27	H	330	ALA	CA-CB	5.08	1.63	1.52
27	H	369	ARG	CD-NE	5.08	1.55	1.46
9	2	68	VAL	CB-CG2	5.08	1.63	1.52
1	A	43	ARG	NE-CZ	5.07	1.39	1.33
7	G	139	GLY	N-CA	-5.07	1.38	1.46
1	A	125	TYR	CZ-OH	5.07	1.46	1.37
10	3	27	ARG	CZ-NH1	5.07	1.39	1.33
22	P	85	GLU	CD-OE2	-5.07	1.20	1.25
23	Q	67	GLY	C-N	5.07	1.42	1.33
30	L	161	GLU	N-CA	-5.07	1.36	1.46
10	3	85	TYR	CG-CD1	5.06	1.45	1.39
20	N	155	LEU	CA-CB	5.06	1.65	1.53
20	N	688	LEU	N-CA	-5.06	1.36	1.46
27	H	312	ARG	CZ-NH2	5.06	1.39	1.33
27	H	401	ARG	CZ-NH1	5.06	1.39	1.33
7	G	25	GLU	CG-CD	5.06	1.59	1.51
29	K	200	ARG	CZ-NH1	5.06	1.39	1.33
32	J	121	TYR	CG-CD2	5.06	1.45	1.39
15	W	42	ARG	CZ-NH2	5.06	1.39	1.33
19	Z	703	ARG	NE-CZ	5.05	1.39	1.33
1	A	94	ALA	N-CA	-5.05	1.36	1.46
32	J	73	VAL	CB-CG2	5.05	1.63	1.52
16	V	185	ASN	CB-CG	5.05	1.62	1.51
32	J	381	GLU	CD-OE1	5.05	1.31	1.25
24	R	292	TYR	CD2-CE2	5.05	1.47	1.39
24	R	110	TYR	N-CA	-5.05	1.36	1.46
22	P	217	GLU	CG-CD	5.04	1.59	1.51
26	O	208	GLU	CD-OE2	5.04	1.31	1.25
32	J	405	TRP	CD2-CE2	5.04	1.47	1.41
13	6	134	TYR	CD1-CE1	5.04	1.47	1.39
19	Z	628	ASP	CB-CG	5.04	1.62	1.51
24	R	186	LEU	CA-CB	5.04	1.65	1.53
25	U	263	ALA	CA-CB	5.04	1.63	1.52
5	E	111	SER	CA-CB	5.04	1.60	1.52
16	V	32	TYR	CE1-CZ	5.04	1.45	1.38
28	I	252	GLY	N-CA	-5.04	1.38	1.46
27	H	201	PHE	CG-CD1	5.04	1.46	1.38
27	H	411	GLU	CB-CG	5.04	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	96	TYR	CG-CD1	5.03	1.45	1.39
16	V	81	GLY	N-CA	-5.03	1.38	1.46
4	D	149	ARG	CZ-NH1	5.03	1.39	1.33
7	G	229	PRO	CA-CB	5.03	1.63	1.53
21	S	209	TYR	CE1-CZ	5.03	1.45	1.38
30	L	55	GLU	CG-CD	5.03	1.59	1.51
14	7	130	ARG	CZ-NH1	5.02	1.39	1.33
17	T	196	GLY	CA-C	-5.02	1.43	1.51
20	N	644	TYR	CZ-OH	5.02	1.46	1.37
23	Q	122	ARG	CZ-NH2	5.02	1.39	1.33
28	I	422	SER	CB-OG	5.02	1.48	1.42
30	L	269	ARG	NE-CZ	5.02	1.39	1.33
7	G	119	TYR	CE1-CZ	5.02	1.45	1.38
16	V	85	GLU	CD-OE1	5.02	1.31	1.25
16	V	104	ARG	NE-CZ	5.02	1.39	1.33
5	E	18	GLU	CD-OE1	-5.01	1.20	1.25
31	M	263	PHE	CG-CD1	5.01	1.46	1.38
8	1	47	LEU	CA-CB	5.01	1.65	1.53
28	I	333	ARG	CZ-NH2	5.01	1.39	1.33
19	Z	400	TYR	CG-CD2	-5.01	1.32	1.39
20	N	911	ILE	CA-CB	-5.01	1.43	1.54
32	J	246	ILE	CA-C	-5.01	1.40	1.52
4	D	60	ARG	NE-CZ	5.01	1.39	1.33
7	G	150	TYR	CB-CG	5.01	1.59	1.51
17	T	259	TYR	CB-CG	5.01	1.59	1.51
28	I	71	TYR	CD2-CE2	5.00	1.46	1.39
3	C	96	ARG	CZ-NH1	5.00	1.39	1.33
12	5	217	ARG	NE-CZ	5.00	1.39	1.33
19	Z	688	ARG	CD-NE	5.00	1.54	1.46
31	M	412	ARG	CZ-NH2	5.00	1.39	1.33

All (2207) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	84	ARG	NE-CZ-NH1	21.94	131.27	120.30
30	L	98	ARG	NE-CZ-NH1	20.64	130.62	120.30
13	6	197	ARG	NE-CZ-NH2	-19.58	110.51	120.30
32	J	325	ARG	NE-CZ-NH2	-19.08	110.76	120.30
24	R	177	ARG	NE-CZ-NH2	-18.09	111.25	120.30
19	Z	763	ARG	NE-CZ-NH2	-17.92	111.34	120.30
8	1	208	ARG	NE-CZ-NH2	-16.72	111.94	120.30
28	I	333	ARG	NE-CZ-NH1	16.48	128.54	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	20	TYR	CB-CG-CD2	-16.34	111.20	121.00
4	D	124	TYR	CB-CG-CD2	-16.19	111.29	121.00
27	H	255	ARG	NE-CZ-NH2	-16.19	112.21	120.30
19	Z	489	TYR	CB-CG-CD2	-16.03	111.38	121.00
22	P	144	ARG	NE-CZ-NH1	15.77	128.19	120.30
2	B	219	ARG	NE-CZ-NH2	-15.59	112.51	120.30
10	3	85	TYR	CB-CG-CD2	15.51	130.31	121.00
19	Z	687	ARG	NE-CZ-NH1	15.51	128.05	120.30
10	3	80	ARG	NE-CZ-NH2	-15.48	112.56	120.30
30	L	99	ARG	NE-CZ-NH1	15.26	127.93	120.30
21	S	197	ARG	NE-CZ-NH2	-15.13	112.74	120.30
4	D	218	ARG	NE-CZ-NH2	-15.11	112.74	120.30
6	F	171	TYR	CB-CG-CD1	-15.04	111.97	121.00
25	U	114	ARG	NE-CZ-NH1	14.97	127.79	120.30
11	4	129	PHE	CB-CG-CD1	14.95	131.27	120.80
19	Z	478	ARG	NE-CZ-NH1	14.94	127.77	120.30
1	A	27	TYR	CB-CG-CD1	14.87	129.92	121.00
2	B	84	ARG	NE-CZ-NH2	-14.76	112.92	120.30
24	R	177	ARG	NE-CZ-NH1	14.68	127.64	120.30
19	Z	71	TYR	CB-CG-CD1	14.63	129.78	121.00
7	G	59	TYR	CB-CG-CD1	14.61	129.77	121.00
9	2	51	TYR	CB-CG-CD2	-14.53	112.28	121.00
4	D	169	ARG	NE-CZ-NH1	14.46	127.53	120.30
19	Z	688	ARG	NE-CZ-NH1	-14.33	113.14	120.30
28	I	322	ARG	NE-CZ-NH2	-14.20	113.20	120.30
28	I	333	ARG	NE-CZ-NH2	-14.20	113.20	120.30
24	R	295	TYR	CB-CG-CD2	-14.09	112.55	121.00
27	H	43	ARG	NE-CZ-NH2	-14.00	113.30	120.30
21	S	491	ARG	NE-CZ-NH1	13.98	127.29	120.30
19	Z	489	TYR	CB-CG-CD1	13.97	129.38	121.00
14	7	144	ARG	NE-CZ-NH2	13.96	127.28	120.30
11	4	145	ARG	NE-CZ-NH1	13.76	127.18	120.30
31	M	423	TYR	CB-CG-CD1	-13.67	112.80	121.00
19	Z	478	ARG	NE-CZ-NH2	-13.60	113.50	120.30
32	J	375	ARG	NE-CZ-NH2	-13.60	113.50	120.30
24	R	137	ARG	NE-CZ-NH1	13.56	127.08	120.30
27	H	333	ARG	NE-CZ-NH1	13.54	127.07	120.30
24	R	23	ARG	NE-CZ-NH1	13.54	127.07	120.30
12	5	236	TYR	CB-CG-CD1	-13.53	112.88	121.00
25	U	114	ARG	NE-CZ-NH2	-13.49	113.56	120.30
15	W	112	PHE	CB-CG-CD2	13.35	130.15	120.80
30	L	342	TYR	CB-CG-CD1	13.29	128.98	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Z	687	ARG	NE-CZ-NH2	-13.19	113.71	120.30
28	I	96	ARG	NE-CZ-NH2	-13.10	113.75	120.30
24	R	23	ARG	NE-CZ-NH2	-13.06	113.77	120.30
3	C	143	TYR	CB-CG-CD2	-13.04	113.18	121.00
31	M	298	ARG	NE-CZ-NH2	-12.99	113.81	120.30
9	2	132	ARG	NE-CZ-NH2	-12.96	113.82	120.30
2	B	24	TYR	CB-CG-CD2	-12.88	113.27	121.00
12	5	123	ARG	NE-CZ-NH2	-12.78	113.91	120.30
28	I	343	ARG	NE-CZ-NH1	12.78	126.69	120.30
24	R	183	TYR	CB-CG-CD1	12.71	128.63	121.00
26	O	156	TYR	CB-CG-CD1	12.69	128.62	121.00
9	2	118	ARG	NE-CZ-NH2	-12.65	113.98	120.30
26	O	240	PHE	CB-CG-CD1	12.63	129.64	120.80
21	S	102	ARG	NE-CZ-NH2	-12.57	114.01	120.30
22	P	417	ARG	NE-CZ-NH2	-12.56	114.02	120.30
9	2	131	PHE	CB-CG-CD1	-12.55	112.01	120.80
13	6	134	TYR	CB-CG-CD1	12.53	128.52	121.00
16	V	46	ARG	NE-CZ-NH2	12.48	126.54	120.30
6	F	171	TYR	CB-CG-CD2	12.42	128.45	121.00
1	A	27	TYR	CB-CG-CD2	-12.34	113.60	121.00
19	Z	121	PHE	CB-CG-CD2	-12.34	112.16	120.80
15	W	112	PHE	CB-CG-CD1	-12.31	112.18	120.80
29	K	274	ARG	NE-CZ-NH1	12.28	126.44	120.30
29	K	178	ARG	NE-CZ-NH2	-12.27	114.16	120.30
18	Y	65	TYR	CB-CG-CD2	-12.23	113.66	121.00
7	G	141	TYR	CB-CG-CD1	-12.21	113.67	121.00
13	6	29	PHE	CB-CG-CD1	12.20	129.34	120.80
27	H	43	ARG	NE-CZ-NH1	12.17	126.39	120.30
23	Q	415	TYR	CB-CG-CD2	-12.17	113.70	121.00
10	3	103	TYR	CB-CG-CD2	12.06	128.24	121.00
26	O	70	ARG	NE-CZ-NH2	12.02	126.31	120.30
3	C	19	TYR	CB-CG-CD2	-12.00	113.80	121.00
20	N	783	TYR	CB-CG-CD1	11.99	128.19	121.00
1	A	245	ARG	NE-CZ-NH2	-11.98	114.31	120.30
22	P	182	ARG	NE-CZ-NH2	-11.94	114.33	120.30
24	R	295	TYR	CB-CG-CD1	11.94	128.16	121.00
19	Z	181	ARG	NE-CZ-NH2	-11.93	114.33	120.30
2	B	60	ARG	NE-CZ-NH1	11.93	126.27	120.30
11	4	145	ARG	NE-CZ-NH2	-11.83	114.39	120.30
6	F	18	ARG	NE-CZ-NH1	11.73	126.17	120.30
21	S	102	ARG	NE-CZ-NH1	11.73	126.17	120.30
24	R	304	TYR	CB-CG-CD2	-11.67	114.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	76	TYR	CB-CG-CD2	11.66	128.00	121.00
2	B	76	TYR	CB-CG-CD1	-11.66	114.01	121.00
24	R	142	PHE	CB-CG-CD2	-11.65	112.65	120.80
23	Q	76	PHE	CB-CG-CD1	11.64	128.95	120.80
25	U	267	ARG	NE-CZ-NH2	-11.63	114.49	120.30
29	K	188	PHE	CB-CG-CD1	11.62	128.94	120.80
13	6	29	PHE	CB-CG-CD2	-11.59	112.69	120.80
31	M	241	ARG	NE-CZ-NH1	11.58	126.09	120.30
10	3	85	TYR	CB-CG-CD1	-11.57	114.06	121.00
30	L	311	ARG	NE-CZ-NH1	11.56	126.08	120.30
24	R	267	ARG	NE-CZ-NH2	-11.55	114.52	120.30
30	L	269	ARG	NE-CZ-NH2	-11.50	114.55	120.30
30	L	342	TYR	CB-CG-CD2	-11.49	114.10	121.00
8	1	158	PHE	CB-CG-CD1	-11.49	112.75	120.80
31	M	423	TYR	CB-CG-CD2	11.48	127.89	121.00
24	R	297	ARG	NE-CZ-NH2	-11.44	114.58	120.30
30	L	381	PHE	CB-CG-CD1	-11.44	112.80	120.80
4	D	124	TYR	CB-CG-CD1	11.39	127.83	121.00
11	4	129	PHE	CB-CG-CD2	-11.34	112.87	120.80
8	1	176	TYR	CB-CG-CD2	11.33	127.80	121.00
28	I	268	ARG	NE-CZ-NH2	-11.27	114.67	120.30
6	F	96	ARG	NE-CZ-NH1	11.23	125.92	120.30
2	B	229	TYR	CB-CG-CD1	-11.23	114.26	121.00
20	N	628	ARG	NE-CZ-NH1	11.23	125.92	120.30
14	7	85	ARG	NE-CZ-NH1	11.23	125.91	120.30
7	G	72	ARG	NE-CZ-NH2	-11.22	114.69	120.30
31	M	394	PHE	CB-CG-CD1	11.20	128.64	120.80
20	N	502	TYR	CB-CG-CD1	11.19	127.71	121.00
14	7	81	ARG	NE-CZ-NH1	11.18	125.89	120.30
26	O	156	TYR	CB-CG-CD2	-11.18	114.30	121.00
11	4	93	ARG	NE-CZ-NH1	11.15	125.87	120.30
24	R	264	TYR	CB-CG-CD2	-11.12	114.33	121.00
2	B	220	ARG	NE-CZ-NH1	11.11	125.85	120.30
29	K	283	ARG	NE-CZ-NH2	-11.10	114.75	120.30
16	V	207	TYR	CB-CG-CD1	11.10	127.66	121.00
32	J	239	ARG	NE-CZ-NH2	-11.10	114.75	120.30
10	3	125	ASP	CB-CG-OD1	11.08	128.28	118.30
5	E	93	ARG	NE-CZ-NH2	11.06	125.83	120.30
19	Z	137	ARG	NE-CZ-NH2	-11.05	114.78	120.30
31	M	91	TYR	CB-CG-CD1	-11.02	114.39	121.00
26	O	240	PHE	CB-CG-CD2	-11.01	113.09	120.80
10	3	178	ASP	CB-CG-OD1	10.99	128.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	4	ARG	NE-CZ-NH1	10.98	125.79	120.30
27	H	265	ARG	NE-CZ-NH1	10.98	125.79	120.30
1	A	105	TYR	CB-CG-CD1	-10.98	114.41	121.00
11	4	116	TYR	CB-CG-CD2	-10.98	114.41	121.00
19	Z	554	TYR	CB-CG-CD1	10.97	127.58	121.00
31	M	394	PHE	CB-CG-CD2	-10.97	113.12	120.80
28	I	271	PHE	CB-CG-CD2	-10.91	113.16	120.80
22	P	191	ARG	NE-CZ-NH2	-10.90	114.85	120.30
6	F	123	TYR	CB-CG-CD2	-10.82	114.51	121.00
23	Q	76	PHE	CB-CG-CD2	-10.78	113.25	120.80
32	J	317	PHE	CB-CG-CD1	10.73	128.31	120.80
13	6	197	ARG	NE-CZ-NH1	10.72	125.66	120.30
9	2	245	TYR	CB-CG-CD1	-10.72	114.57	121.00
24	R	300	ARG	NE-CZ-NH1	10.70	125.65	120.30
15	W	91	ARG	NE-CZ-NH2	-10.69	114.95	120.30
17	T	345	TYR	CB-CG-CD1	-10.66	114.60	121.00
19	Z	71	TYR	CB-CG-CD2	-10.66	114.61	121.00
19	Z	483	PHE	CB-CG-CD1	10.66	128.26	120.80
23	Q	132	ARG	NE-CZ-NH2	-10.62	114.99	120.30
9	2	185	PHE	CB-CG-CD2	10.62	128.23	120.80
9	2	62	ARG	NE-CZ-NH1	10.61	125.60	120.30
11	4	155	ARG	NE-CZ-NH1	10.59	125.60	120.30
7	G	59	TYR	CB-CG-CD2	-10.59	114.65	121.00
22	P	185	PHE	CB-CG-CD2	-10.59	113.39	120.80
14	7	127	TYR	CB-CG-CD1	-10.56	114.67	121.00
21	S	214	TYR	CB-CG-CD1	-10.54	114.67	121.00
24	R	323	PHE	CB-CG-CD2	-10.54	113.42	120.80
7	G	72	ARG	NE-CZ-NH1	10.48	125.54	120.30
19	Z	239	TYR	CB-CG-CD2	10.47	127.28	121.00
24	R	183	TYR	CB-CG-CD2	-10.43	114.74	121.00
27	H	323	ARG	NE-CZ-NH1	10.41	125.50	120.30
23	Q	90	ARG	NE-CZ-NH2	-10.40	115.10	120.30
24	R	342	ARG	NE-CZ-NH1	10.39	125.50	120.30
12	5	67	PHE	CB-CG-CD2	10.39	128.07	120.80
11	4	93	ARG	NE-CZ-NH2	-10.35	115.12	120.30
26	O	248	PHE	CB-CG-CD1	-10.34	113.56	120.80
3	C	17	ARG	NE-CZ-NH2	-10.30	115.15	120.30
10	3	104	TYR	CB-CG-CD2	-10.29	114.82	121.00
11	4	161	ARG	NE-CZ-NH2	-10.29	115.16	120.30
1	A	152	TYR	CB-CG-CD1	10.25	127.15	121.00
19	Z	160	ARG	NE-CZ-NH1	-10.25	115.18	120.30
27	H	400	ARG	NE-CZ-NH1	10.25	125.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	4	3	TYR	CB-CG-CD1	-10.23	114.86	121.00
22	P	39	ARG	NE-CZ-NH2	-10.21	115.19	120.30
23	Q	310	ARG	NE-CZ-NH2	10.21	125.41	120.30
16	V	61	PHE	CB-CG-CD2	-10.20	113.66	120.80
21	S	197	ARG	NE-CZ-NH1	10.20	125.40	120.30
24	R	83	ARG	NE-CZ-NH2	-10.19	115.20	120.30
27	H	41	TYR	CB-CG-CD2	-10.19	114.89	121.00
28	I	363	ARG	NE-CZ-NH1	10.14	125.37	120.30
31	M	353	ARG	NE-CZ-NH1	10.13	125.36	120.30
31	M	272	ARG	NE-CZ-NH1	-10.12	115.24	120.30
23	Q	132	ARG	NE-CZ-NH1	10.10	125.35	120.30
26	O	162	TYR	CB-CG-CD2	-10.10	114.94	121.00
3	C	72	MET	CG-SD-CE	-10.09	84.06	100.20
8	1	176	TYR	CB-CG-CD1	-10.09	114.95	121.00
20	N	751	ARG	NE-CZ-NH2	-10.08	115.26	120.30
19	Z	816	TYR	CB-CG-CD2	-10.05	114.97	121.00
29	K	283	ARG	NE-CZ-NH1	10.03	125.32	120.30
22	P	55	ARG	NE-CZ-NH2	-10.02	115.29	120.30
16	V	61	PHE	CB-CG-CD1	10.01	127.81	120.80
20	N	55	ARG	NE-CZ-NH2	-10.01	115.30	120.30
17	T	179	PHE	CB-CG-CD2	-9.97	113.82	120.80
4	D	77	ALA	N-CA-CB	9.95	124.03	110.10
31	M	440	TYR	CB-CG-CD2	-9.93	115.04	121.00
14	7	222	TYR	CB-CG-CD1	-9.87	115.08	121.00
30	L	99	ARG	NE-CZ-NH2	-9.85	115.37	120.30
16	V	175	ARG	NE-CZ-NH1	-9.85	115.38	120.30
20	N	802	TYR	CB-CG-CD1	-9.85	115.09	121.00
14	7	226	ARG	NE-CZ-NH1	9.83	125.22	120.30
17	T	211	PHE	CB-CG-CD1	-9.82	113.93	120.80
29	K	391	ARG	NE-CZ-NH2	-9.81	115.39	120.30
13	6	162	PHE	CB-CG-CD2	-9.80	113.94	120.80
17	T	201	PHE	CB-CG-CD1	9.80	127.66	120.80
23	Q	231	TYR	CB-CG-CD2	-9.80	115.12	121.00
28	I	303	ARG	NE-CZ-NH1	9.76	125.18	120.30
7	G	103	PHE	CB-CG-CD1	9.75	127.63	120.80
20	N	584	TYR	CB-CG-CD2	-9.75	115.15	121.00
28	I	142	ASP	CB-CG-OD2	9.74	127.07	118.30
8	1	78	ARG	NE-CZ-NH1	9.74	125.17	120.30
9	2	51	TYR	CB-CG-CD1	9.73	126.84	121.00
9	2	131	PHE	CB-CG-CD2	9.71	127.60	120.80
32	J	317	PHE	CB-CG-CD2	-9.71	114.00	120.80
5	E	93	ARG	NE-CZ-NH1	-9.69	115.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	H	297	ARG	NE-CZ-NH1	9.67	125.14	120.30
23	Q	310	ARG	NE-CZ-NH1	-9.66	115.47	120.30
27	H	401	ARG	NE-CZ-NH1	9.66	125.13	120.30
7	G	66	ARG	NE-CZ-NH1	9.65	125.12	120.30
20	N	887	ALA	N-CA-CB	9.64	123.60	110.10
6	F	157	ARG	NE-CZ-NH1	-9.64	115.48	120.30
31	M	441	TYR	CB-CG-CD1	9.63	126.78	121.00
19	Z	763	ARG	NE-CZ-NH1	9.62	125.11	120.30
26	O	282	PHE	CB-CG-CD1	9.60	127.52	120.80
26	O	352	ARG	NE-CZ-NH2	-9.60	115.50	120.30
2	B	91	ARG	NE-CZ-NH2	-9.58	115.51	120.30
7	G	233	ARG	NE-CZ-NH2	-9.57	115.51	120.30
6	F	9	ASP	CB-CG-OD1	-9.57	109.69	118.30
20	N	502	TYR	CB-CG-CD2	-9.55	115.27	121.00
2	B	178	TYR	CB-CG-CD1	-9.54	115.28	121.00
32	J	148	TYR	CB-CG-CD1	-9.52	115.29	121.00
30	L	316	ASP	CB-CG-OD2	-9.50	109.75	118.30
6	F	107	ARG	NE-CZ-NH1	9.45	125.03	120.30
22	P	226	TYR	CB-CG-CD2	-9.45	115.33	121.00
25	U	190	ARG	NE-CZ-NH2	-9.44	115.58	120.30
10	3	66	ARG	NE-CZ-NH2	9.43	125.02	120.30
19	Z	432	TYR	CB-CG-CD2	-9.42	115.35	121.00
23	Q	33	ARG	NE-CZ-NH1	-9.42	115.59	120.30
4	D	234	TYR	CB-CG-CD1	9.41	126.65	121.00
25	U	250	TYR	CB-CG-CD2	-9.39	115.37	121.00
10	3	80	ARG	NE-CZ-NH1	9.39	124.99	120.30
12	5	67	PHE	CB-CG-CD1	-9.38	114.24	120.80
11	4	155	ARG	NE-CZ-NH2	-9.37	115.61	120.30
30	L	286	ARG	NE-CZ-NH1	9.36	124.98	120.30
13	6	221	ARG	NE-CZ-NH1	9.36	124.98	120.30
9	2	118	ARG	NE-CZ-NH1	9.35	124.97	120.30
24	R	267	ARG	NE-CZ-NH1	9.35	124.98	120.30
7	G	22	PHE	CB-CG-CD1	9.33	127.33	120.80
25	U	267	ARG	NE-CZ-NH1	9.31	124.96	120.30
24	R	300	ARG	NE-CZ-NH2	-9.31	115.64	120.30
13	6	134	TYR	CB-CG-CD2	-9.30	115.42	121.00
21	S	432	PHE	CB-CG-CD1	-9.30	114.29	120.80
22	P	39	ARG	NE-CZ-NH1	9.29	124.95	120.30
16	V	98	MET	CG-SD-CE	-9.28	85.35	100.20
28	I	303	ARG	NE-CZ-NH2	-9.28	115.66	120.30
29	K	416	PHE	CB-CG-CD2	9.28	127.30	120.80
24	R	233	ARG	NE-CZ-NH1	9.28	124.94	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	S	207	TYR	CB-CG-CD1	9.27	126.56	121.00
22	P	364	ARG	NE-CZ-NH1	-9.26	115.67	120.30
20	N	444	TYR	CB-CG-CD1	9.24	126.55	121.00
8	1	62	ARG	NE-CZ-NH1	9.24	124.92	120.30
26	O	60	TYR	CB-CG-CD2	-9.22	115.47	121.00
15	W	108	ARG	NE-CZ-NH1	9.22	124.91	120.30
4	D	115	ARG	NE-CZ-NH1	9.19	124.90	120.30
16	V	289	ASP	CB-CG-OD1	9.19	126.57	118.30
28	I	307	ARG	NE-CZ-NH2	-9.15	115.72	120.30
24	R	294	TYR	CB-CG-CD1	9.14	126.49	121.00
27	H	227	ARG	NE-CZ-NH2	-9.14	115.73	120.30
31	M	389	ARG	NE-CZ-NH2	-9.14	115.73	120.30
32	J	72	TYR	CB-CG-CD1	9.14	126.48	121.00
26	O	230	ARG	NE-CZ-NH1	9.07	124.83	120.30
30	L	281	PHE	CB-CG-CD1	-9.07	114.45	120.80
3	C	60	PHE	CB-CG-CD1	9.06	127.14	120.80
7	G	22	PHE	CB-CG-CD2	-9.04	114.47	120.80
24	R	366	TYR	CB-CG-CD2	-9.04	115.58	121.00
21	S	298	TYR	CB-CG-CD2	8.99	126.39	121.00
22	P	20	TYR	CB-CG-CD1	8.98	126.39	121.00
10	3	178	ASP	CB-CG-OD2	-8.95	110.24	118.30
31	M	183	ARG	NE-CZ-NH2	8.95	124.78	120.30
25	U	211	TYR	CB-CG-CD2	-8.93	115.64	121.00
22	P	302	TYR	CB-CG-CD2	-8.93	115.64	121.00
13	6	60	PHE	CB-CG-CD1	8.92	127.04	120.80
22	P	324	TYR	CB-CG-CD2	-8.91	115.65	121.00
3	C	143	TYR	CB-CG-CD1	8.90	126.34	121.00
30	L	157	ARG	NE-CZ-NH1	-8.90	115.85	120.30
26	O	238	TYR	CB-CG-CD2	-8.88	115.67	121.00
29	K	323	ARG	NE-CZ-NH2	-8.88	115.86	120.30
32	J	72	TYR	CB-CG-CD2	-8.87	115.68	121.00
19	Z	494	ARG	NE-CZ-NH1	8.86	124.73	120.30
19	Z	785	ARG	NE-CZ-NH2	-8.86	115.87	120.30
13	6	182	PHE	CB-CG-CD1	-8.86	114.60	120.80
10	3	26	ARG	NE-CZ-NH2	-8.84	115.88	120.30
17	T	177	TYR	CB-CG-CD2	-8.84	115.70	121.00
20	N	253	TYR	CB-CG-CD1	-8.83	115.70	121.00
26	O	7	PHE	CB-CG-CD1	-8.82	114.63	120.80
28	I	408	ARG	NE-CZ-NH1	8.82	124.71	120.30
25	U	228	TYR	CB-CG-CD1	8.82	126.29	121.00
2	B	83	TYR	CB-CG-CD2	-8.81	115.71	121.00
29	K	44	TYR	CB-CG-CD1	8.81	126.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	L	286	ARG	NE-CZ-NH2	-8.80	115.90	120.30
24	R	142	PHE	CB-CG-CD1	8.79	126.96	120.80
32	J	81	ASP	CB-CG-OD2	-8.78	110.40	118.30
17	T	178	TYR	CG-CD2-CE2	-8.78	114.28	121.30
24	R	233	ARG	NE-CZ-NH2	-8.77	115.91	120.30
2	B	132	VAL	CA-CB-CG1	8.77	124.05	110.90
29	K	229	ARG	NE-CZ-NH2	-8.77	115.92	120.30
18	Y	52	PHE	CB-CG-CD2	8.76	126.93	120.80
21	S	124	ARG	NE-CZ-NH2	-8.76	115.92	120.30
21	S	28	PRO	CA-N-CD	-8.75	99.25	111.50
31	M	337	ARG	NE-CZ-NH1	8.75	124.67	120.30
26	O	330	ARG	NE-CZ-NH1	8.74	124.67	120.30
30	L	370	ARG	NE-CZ-NH2	8.74	124.67	120.30
4	D	145	ASP	CB-CG-OD2	-8.72	110.45	118.30
1	A	1	MET	CG-SD-CE	-8.72	86.25	100.20
24	R	125	ARG	NE-CZ-NH2	-8.70	115.95	120.30
13	6	124	TYR	CB-CG-CD2	-8.69	115.79	121.00
12	5	149	TYR	CD1-CE1-CZ	8.68	127.61	119.80
21	S	432	PHE	CB-CG-CD2	8.67	126.87	120.80
3	C	91	ARG	NE-CZ-NH1	8.67	124.63	120.30
2	B	98	TYR	CB-CG-CD1	-8.66	115.80	121.00
19	Z	494	ARG	NE-CZ-NH2	-8.65	115.97	120.30
13	6	43	ALA	N-CA-CB	8.64	122.20	110.10
20	N	387	ARG	NE-CZ-NH2	-8.63	115.98	120.30
22	P	316	ARG	NE-CZ-NH2	-8.61	115.99	120.30
20	N	900	TYR	CG-CD1-CE1	-8.61	114.42	121.30
30	L	209	PHE	CB-CG-CD1	-8.61	114.78	120.80
8	1	35	THR	CA-CB-CG2	-8.59	100.37	112.40
27	H	386	ARG	NE-CZ-NH2	8.59	124.60	120.30
2	B	219	ARG	NE-CZ-NH1	8.58	124.59	120.30
29	K	416	PHE	CB-CG-CD1	-8.57	114.80	120.80
30	L	127	ARG	NE-CZ-NH1	8.56	124.58	120.30
24	R	54	TYR	CB-CG-CD1	8.56	126.14	121.00
7	G	239	TYR	CB-CG-CD2	-8.55	115.87	121.00
27	H	398	ARG	NE-CZ-NH1	8.55	124.58	120.30
28	I	272	ARG	NE-CZ-NH1	8.55	124.58	120.30
8	1	188	PHE	CB-CG-CD1	8.55	126.78	120.80
27	H	174	TYR	CB-CG-CD1	-8.55	115.87	121.00
19	Z	777	THR	CA-CB-CG2	-8.54	100.45	112.40
24	R	183	TYR	CD1-CE1-CZ	8.53	127.47	119.80
12	5	236	TYR	CB-CG-CD2	8.52	126.11	121.00
6	F	51	ARG	NE-CZ-NH1	8.51	124.56	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	128	ARG	NE-CZ-NH1	8.50	124.55	120.30
6	F	224	TYR	CB-CG-CD2	8.49	126.09	121.00
32	J	78	ARG	NE-CZ-NH1	8.48	124.54	120.30
22	P	357	ARG	NE-CZ-NH1	8.48	124.54	120.30
22	P	247	TYR	CB-CG-CD1	-8.47	115.92	121.00
17	T	217	ARG	NE-CZ-NH2	-8.46	116.07	120.30
12	5	220	TYR	CB-CG-CD1	8.46	126.08	121.00
27	H	79	ASP	CB-CG-OD2	-8.44	110.70	118.30
22	P	247	TYR	CB-CG-CD2	8.42	126.05	121.00
31	M	347	ARG	NE-CZ-NH1	8.41	124.50	120.30
11	4	59	TYR	CB-CG-CD2	8.40	126.04	121.00
26	O	178	ARG	NE-CZ-NH2	-8.40	116.10	120.30
13	6	60	PHE	CB-CG-CD2	-8.39	114.92	120.80
31	M	195	ASP	CB-CG-OD2	-8.39	110.75	118.30
20	N	444	TYR	CB-CG-CD2	-8.39	115.97	121.00
23	Q	231	TYR	CB-CG-CD1	8.38	126.03	121.00
21	S	284	TYR	CB-CG-CD1	-8.38	115.97	121.00
19	Z	385	PHE	CB-CG-CD1	8.38	126.67	120.80
14	7	138	ARG	NE-CZ-NH2	-8.38	116.11	120.30
32	J	326	LEU	CB-CG-CD1	8.37	125.23	111.00
8	1	229	LYS	N-CA-CB	8.37	125.66	110.60
9	2	246	ARG	NE-CZ-NH2	-8.36	116.12	120.30
22	P	240	TYR	CB-CG-CD1	-8.35	115.99	121.00
6	F	157	ARG	NE-CZ-NH2	8.35	124.47	120.30
13	6	55	ARG	NE-CZ-NH2	-8.34	116.13	120.30
16	V	207	TYR	CB-CG-CD2	-8.34	115.99	121.00
1	A	21	ARG	NE-CZ-NH2	8.34	124.47	120.30
21	S	237	ARG	NE-CZ-NH2	-8.33	116.13	120.30
21	S	95	ARG	NE-CZ-NH2	-8.32	116.14	120.30
21	S	385	ASP	CB-CG-OD2	-8.31	110.82	118.30
24	R	18	ARG	NE-CZ-NH1	8.30	124.45	120.30
22	P	240	TYR	CB-CG-CD2	8.29	125.98	121.00
11	4	134	TYR	CB-CG-CD2	8.29	125.97	121.00
27	H	312	ARG	NE-CZ-NH2	-8.29	116.16	120.30
23	Q	116	TRP	CB-CG-CD2	-8.28	115.83	126.60
21	S	283	ARG	NE-CZ-NH1	8.28	124.44	120.30
14	7	127	TYR	CB-CG-CD2	8.28	125.97	121.00
13	6	124	TYR	CB-CG-CD1	8.27	125.96	121.00
31	M	365	ARG	NE-CZ-NH2	-8.25	116.17	120.30
17	T	167	PHE	CB-CG-CD2	-8.24	115.03	120.80
19	Z	34	ARG	NE-CZ-NH2	-8.23	116.19	120.30
31	M	64	ARG	NE-CZ-NH1	8.23	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	S	214	TYR	CG-CD2-CE2	-8.22	114.72	121.30
20	N	675	MET	CG-SD-CE	-8.22	87.05	100.20
10	3	103	TYR	CB-CG-CD1	-8.21	116.07	121.00
23	Q	315	ASP	CB-CG-OD1	8.21	125.69	118.30
24	R	304	TYR	CG-CD1-CE1	-8.21	114.73	121.30
29	K	338	ARG	NE-CZ-NH2	-8.21	116.20	120.30
29	K	188	PHE	CB-CG-CD2	-8.20	115.06	120.80
8	1	53	THR	N-CA-CB	8.20	125.87	110.30
21	S	230	ARG	N-CA-CB	8.20	125.35	110.60
29	K	120	ASP	CB-CG-OD2	-8.20	110.92	118.30
8	1	153	MET	CG-SD-CE	-8.19	87.09	100.20
2	B	121	TYR	CB-CG-CD2	-8.19	116.09	121.00
9	2	217	ASP	CB-CG-OD1	8.18	125.66	118.30
19	Z	741	LEU	CB-CG-CD1	8.18	124.91	111.00
19	Z	688	ARG	NE-CZ-NH2	8.18	124.39	120.30
19	Z	781	TYR	CB-CG-CD2	-8.18	116.09	121.00
20	N	710	ARG	NE-CZ-NH2	-8.18	116.21	120.30
9	2	186	ARG	NE-CZ-NH2	-8.17	116.22	120.30
12	5	228	TYR	CB-CG-CD2	8.17	125.90	121.00
26	O	154	ARG	NE-CZ-NH1	8.14	124.37	120.30
20	N	684	ARG	NE-CZ-NH2	-8.13	116.23	120.30
30	L	92	ARG	NE-CZ-NH2	8.13	124.36	120.30
32	J	81	ASP	CB-CG-OD1	8.12	125.61	118.30
31	M	353	ARG	NE-CZ-NH2	-8.12	116.24	120.30
13	6	65	ARG	NE-CZ-NH2	8.11	124.35	120.30
24	R	176	ARG	NE-CZ-NH1	8.10	124.35	120.30
13	6	231	ARG	NE-CZ-NH1	8.10	124.35	120.30
21	S	216	PHE	CB-CG-CD2	8.10	126.47	120.80
5	E	84	ASP	CB-CG-OD1	8.10	125.59	118.30
32	J	13	GLU	OE1-CD-OE2	8.10	133.01	123.30
19	Z	755	ASP	CB-CG-OD1	8.08	125.57	118.30
31	M	171	TYR	CB-CG-CD1	-8.07	116.16	121.00
9	2	136	TYR	CB-CG-CD2	-8.07	116.16	121.00
9	2	244	ARG	NE-CZ-NH2	8.06	124.33	120.30
7	G	145	ASP	CB-CG-OD1	-8.05	111.05	118.30
21	S	207	TYR	CB-CG-CD2	-8.05	116.17	121.00
1	A	228	ARG	NE-CZ-NH2	-8.05	116.28	120.30
3	C	4	ARG	NE-CZ-NH1	8.04	124.32	120.30
7	G	41	ARG	NE-CZ-NH1	8.03	124.32	120.30
31	M	413	ARG	NE-CZ-NH1	8.03	124.31	120.30
20	N	460	TYR	CB-CG-CD1	8.03	125.81	121.00
27	H	432	TYR	CD1-CE1-CZ	-8.02	112.58	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	128	ARG	NE-CZ-NH2	-8.02	116.29	120.30
10	3	125	ASP	CB-CG-OD2	-8.02	111.08	118.30
30	L	308	ARG	NE-CZ-NH2	-8.02	116.29	120.30
30	L	98	ARG	NH1-CZ-NH2	-8.02	110.58	119.40
31	M	174	ARG	NE-CZ-NH1	8.01	124.31	120.30
13	6	28	ARG	NE-CZ-NH2	-8.01	116.29	120.30
3	C	60	PHE	CB-CG-CD2	-8.01	115.19	120.80
26	O	325	ASP	CB-CG-OD1	-8.01	111.09	118.30
4	D	87	ARG	NE-CZ-NH2	-8.00	116.30	120.30
17	T	178	TYR	CB-CG-CD2	-7.99	116.20	121.00
20	N	129	ARG	NE-CZ-NH1	-7.99	116.31	120.30
23	Q	137	TYR	CB-CG-CD2	-7.99	116.21	121.00
19	Z	816	TYR	CB-CG-CD1	7.98	125.78	121.00
9	2	75	SER	C-N-CA	7.97	141.63	121.70
13	6	168	ALA	N-CA-CB	7.96	121.25	110.10
27	H	111	TYR	CB-CG-CD1	-7.96	116.22	121.00
17	T	211	PHE	CB-CG-CD2	7.95	126.36	120.80
3	C	97	TYR	CG-CD2-CE2	-7.95	114.94	121.30
32	J	372	ARG	NE-CZ-NH2	7.93	124.27	120.30
23	Q	279	TYR	CB-CG-CD2	-7.93	116.24	121.00
25	U	74	TYR	CB-CG-CD1	-7.92	116.25	121.00
17	T	177	TYR	CB-CG-CD1	7.91	125.74	121.00
23	Q	72	TYR	CB-CG-CD2	-7.89	116.26	121.00
31	M	132	ARG	N-CA-CB	7.89	124.81	110.60
8	1	58	TYR	CB-CG-CD2	7.89	125.73	121.00
19	Z	368	ALA	N-CA-CB	7.88	121.13	110.10
16	V	90	VAL	CA-CB-CG2	7.88	122.71	110.90
22	P	350	ARG	NE-CZ-NH1	7.87	124.24	120.30
20	N	502	TYR	CG-CD1-CE1	7.87	127.60	121.30
27	H	139	ARG	NE-CZ-NH2	-7.86	116.37	120.30
1	A	23	TYR	CB-CG-CD2	-7.86	116.28	121.00
29	K	352	MET	CG-SD-CE	7.86	112.77	100.20
4	D	140	VAL	CA-CB-CG1	7.85	122.68	110.90
31	M	299	PHE	CB-CG-CD1	-7.85	115.30	120.80
11	4	125	ALA	CB-CA-C	-7.84	98.35	110.10
17	T	292	ARG	NE-CZ-NH1	7.83	124.22	120.30
2	B	60	ARG	NE-CZ-NH2	-7.83	116.39	120.30
2	B	147	PHE	CB-CG-CD1	7.83	126.28	120.80
32	J	313	ARG	NE-CZ-NH2	-7.83	116.39	120.30
19	Z	330	PHE	CB-CG-CD1	7.82	126.27	120.80
22	P	191	ARG	NE-CZ-NH1	7.81	124.21	120.30
1	A	152	TYR	CG-CD2-CE2	7.81	127.55	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	188	PHE	CB-CG-CD2	-7.79	115.34	120.80
22	P	144	ARG	NE-CZ-NH2	-7.79	116.40	120.30
27	H	429	TYR	CB-CG-CD2	-7.79	116.33	121.00
30	L	74	VAL	CA-CB-CG2	-7.79	99.22	110.90
30	L	381	PHE	CB-CG-CD2	7.79	126.25	120.80
12	5	123	ARG	NE-CZ-NH1	7.78	124.19	120.30
12	5	193	TYR	CZ-CE2-CD2	7.78	126.80	119.80
29	K	329	ARG	NE-CZ-NH2	-7.77	116.41	120.30
22	P	20	TYR	CG-CD1-CE1	-7.77	115.09	121.30
23	Q	282	ARG	NE-CZ-NH1	7.77	124.18	120.30
22	P	273	TYR	CB-CG-CD2	-7.76	116.34	121.00
32	J	80	MET	CG-SD-CE	-7.76	87.79	100.20
25	U	253	THR	CA-CB-CG2	-7.76	101.54	112.40
21	S	286	TYR	CB-CG-CD1	-7.75	116.35	121.00
19	Z	256	PHE	CB-CG-CD2	-7.75	115.38	120.80
10	3	185	VAL	CA-CB-CG2	-7.74	99.29	110.90
26	O	172	TYR	CB-CG-CD1	7.74	125.65	121.00
31	M	188	TYR	CB-CG-CD2	-7.74	116.35	121.00
10	3	154	TRP	CB-CG-CD1	7.74	137.06	127.00
13	6	200	ARG	NE-CZ-NH2	-7.74	116.43	120.30
23	Q	308	ASP	CB-CG-OD2	7.74	125.26	118.30
20	N	649	ARG	NE-CZ-NH2	-7.73	116.44	120.30
20	N	728	PHE	CB-CG-CD2	-7.73	115.39	120.80
30	L	230	ARG	NE-CZ-NH2	-7.72	116.44	120.30
19	Z	25	ASP	CB-CG-OD1	-7.70	111.37	118.30
30	L	130	ASP	CB-CG-OD2	-7.69	111.38	118.30
27	H	420	TYR	CB-CG-CD2	-7.69	116.39	121.00
32	J	78	ARG	NE-CZ-NH2	-7.68	116.46	120.30
28	I	346	ARG	NE-CZ-NH2	-7.68	116.46	120.30
20	N	129	ARG	NE-CZ-NH2	-7.67	116.47	120.30
20	N	22	PHE	CB-CG-CD2	-7.66	115.44	120.80
13	6	87	ASP	CB-CG-OD1	7.66	125.19	118.30
13	6	131	TYR	CB-CG-CD2	-7.66	116.41	121.00
32	J	49	ARG	NE-CZ-NH1	7.66	124.13	120.30
2	B	83	TYR	CB-CG-CD1	7.66	125.59	121.00
27	H	432	TYR	CB-CG-CD2	-7.65	116.41	121.00
3	C	19	TYR	CB-CG-CD1	7.64	125.58	121.00
26	O	349	MET	CG-SD-CE	-7.64	87.97	100.20
22	P	369	TYR	CB-CG-CD1	-7.64	116.42	121.00
8	1	155	ARG	NE-CZ-NH2	-7.64	116.48	120.30
11	4	161	ARG	NE-CZ-NH1	7.64	124.12	120.30
19	Z	287	ASP	CB-CG-OD2	7.64	125.17	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	L	111	ARG	NE-CZ-NH2	-7.63	116.48	120.30
12	5	118	LEU	CB-CA-C	7.63	124.70	110.20
16	V	198	ARG	NE-CZ-NH1	7.62	124.11	120.30
30	L	257	PHE	CB-CG-CD2	-7.62	115.46	120.80
7	G	153	ASP	CB-CG-OD1	-7.62	111.44	118.30
3	C	145	PHE	CB-CG-CD2	-7.62	115.47	120.80
29	K	388	ARG	NE-CZ-NH2	-7.62	116.49	120.30
17	T	179	PHE	CB-CG-CD1	7.61	126.13	120.80
32	J	310	ARG	NE-CZ-NH2	-7.60	116.50	120.30
4	D	92	ARG	NE-CZ-NH1	-7.60	116.50	120.30
2	B	91	ARG	CD-NE-CZ	-7.60	112.96	123.60
4	D	234	TYR	CB-CG-CD2	-7.60	116.44	121.00
29	K	337	ASP	CB-CG-OD2	-7.60	111.46	118.30
28	I	411	ARG	NE-CZ-NH1	7.58	124.09	120.30
14	7	45	THR	CA-CB-CG2	-7.58	101.79	112.40
9	2	81	SER	CA-C-N	7.58	138.31	117.10
17	T	167	PHE	CB-CG-CD1	7.58	126.10	120.80
20	N	520	MET	CA-CB-CG	-7.57	100.43	113.30
13	6	65	ARG	NE-CZ-NH1	-7.57	116.52	120.30
11	4	107	TYR	CB-CG-CD2	-7.56	116.46	121.00
10	3	50	TYR	CB-CG-CD2	-7.56	116.47	121.00
3	C	145	PHE	CB-CG-CD1	7.55	126.09	120.80
10	3	103	TYR	CG-CD2-CE2	7.55	127.34	121.30
21	S	491	ARG	NE-CZ-NH2	-7.55	116.52	120.30
26	O	54	ASP	CB-CG-OD2	-7.54	111.51	118.30
9	2	217	ASP	CB-CG-OD2	-7.54	111.52	118.30
1	A	103	TYR	CG-CD1-CE1	-7.54	115.27	121.30
20	N	199	ARG	NE-CZ-NH2	-7.53	116.53	120.30
19	Z	259	PHE	CB-CG-CD2	-7.53	115.53	120.80
30	L	323	ARG	NE-CZ-NH1	7.53	124.06	120.30
11	4	146	TYR	CB-CG-CD2	-7.52	116.49	121.00
14	7	81	ARG	NE-CZ-NH2	-7.51	116.54	120.30
11	4	116	TYR	CB-CG-CD1	7.51	125.51	121.00
4	D	3	TYR	CZ-CE2-CD2	7.51	126.56	119.80
12	5	149	TYR	CB-CG-CD2	-7.51	116.50	121.00
4	D	218	ARG	NE-CZ-NH1	7.50	124.05	120.30
12	5	118	LEU	CA-CB-CG	7.50	132.54	115.30
23	Q	53	LEU	C-N-CA	7.49	138.03	122.30
1	A	120	ASP	CB-CG-OD2	-7.49	111.56	118.30
32	J	239	ARG	NE-CZ-NH1	7.49	124.04	120.30
3	C	23	TYR	CB-CG-CD2	-7.49	116.51	121.00
21	S	284	TYR	CG-CD2-CE2	-7.49	115.31	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	L	187	TYR	CG-CD1-CE1	-7.49	115.31	121.30
15	W	100	ARG	CG-CD-NE	-7.47	96.11	111.80
24	R	32	ARG	NE-CZ-NH2	7.47	124.04	120.30
14	7	61	ASP	CB-CG-OD1	7.47	125.02	118.30
29	K	313	ARG	NE-CZ-NH2	-7.46	116.57	120.30
13	6	84	PHE	CB-CG-CD1	-7.46	115.58	120.80
21	S	463	TYR	CB-CG-CD2	7.46	125.48	121.00
31	M	47	ARG	NE-CZ-NH2	-7.45	116.57	120.30
21	S	226	PHE	CB-CG-CD2	7.45	126.02	120.80
6	F	225	ASP	CB-CG-OD2	-7.45	111.60	118.30
20	N	710	ARG	NE-CZ-NH1	7.44	124.02	120.30
19	Z	703	ARG	NE-CZ-NH2	-7.44	116.58	120.30
20	N	387	ARG	NE-CZ-NH1	7.44	124.02	120.30
28	I	184	TYR	CB-CG-CD1	7.44	125.46	121.00
7	G	210	PHE	CB-CG-CD2	-7.43	115.60	120.80
15	W	179	LEU	CB-CG-CD1	-7.43	98.37	111.00
23	Q	344	ARG	NE-CZ-NH1	7.43	124.02	120.30
28	I	297	SER	N-CA-CB	7.43	121.64	110.50
31	M	298	ARG	NE-CZ-NH1	7.42	124.01	120.30
7	G	141	TYR	CB-CG-CD2	7.42	125.45	121.00
7	G	150	TYR	CB-CG-CD2	-7.42	116.55	121.00
10	3	60	VAL	CA-CB-CG1	7.42	122.02	110.90
24	R	244	ALA	CB-CA-C	-7.41	98.99	110.10
22	P	248	ARG	NE-CZ-NH1	-7.40	116.60	120.30
29	K	326	ARG	NE-CZ-NH1	7.40	124.00	120.30
23	Q	43	VAL	CA-CB-CG2	-7.39	99.81	110.90
10	3	100	PHE	CB-CG-CD1	-7.38	115.63	120.80
12	5	224	TYR	CB-CG-CD1	7.38	125.43	121.00
27	H	246	VAL	CA-CB-CG1	-7.38	99.83	110.90
19	Z	713	PHE	CB-CG-CD1	7.37	125.96	120.80
28	I	271	PHE	CB-CG-CD1	7.37	125.96	120.80
26	O	289	ARG	N-CA-CB	7.37	123.86	110.60
27	H	297	ARG	NE-CZ-NH2	-7.37	116.62	120.30
30	L	356	ASP	CB-CG-OD2	-7.36	111.68	118.30
3	C	41	ASP	CB-CG-OD1	-7.35	111.68	118.30
31	M	138	PRO	N-CA-CB	7.35	112.12	103.30
31	M	161	TYR	CB-CG-CD2	7.35	125.41	121.00
29	K	344	ILE	CA-CB-CG1	7.35	124.96	111.00
32	J	340	ARG	NE-CZ-NH1	7.35	123.97	120.30
21	S	209	TYR	CB-CG-CD1	-7.34	116.60	121.00
28	I	96	ARG	NE-CZ-NH1	7.34	123.97	120.30
17	T	222	ASP	CB-CG-OD2	7.33	124.90	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	L	123	ARG	NE-CZ-NH1	7.33	123.96	120.30
19	Z	554	TYR	CB-CG-CD2	-7.32	116.61	121.00
5	E	22	PHE	CB-CG-CD2	7.32	125.92	120.80
23	Q	90	ARG	NE-CZ-NH1	7.31	123.95	120.30
13	6	212	ARG	NE-CZ-NH2	-7.30	116.65	120.30
8	1	52	ARG	NE-CZ-NH1	-7.30	116.65	120.30
3	C	184	MET	CG-SD-CE	-7.30	88.52	100.20
8	1	37	MET	CG-SD-CE	-7.30	88.52	100.20
25	U	79	TYR	CB-CG-CD1	7.30	125.38	121.00
16	V	139	ARG	NE-CZ-NH1	7.30	123.95	120.30
24	R	192	ARG	NE-CZ-NH1	7.30	123.95	120.30
20	N	628	ARG	NE-CZ-NH2	-7.30	116.65	120.30
14	7	230	ARG	NE-CZ-NH1	7.29	123.95	120.30
10	3	57	ALA	N-CA-CB	7.29	120.31	110.10
2	B	178	TYR	CG-CD2-CE2	-7.28	115.47	121.30
8	1	167	TYR	CB-CG-CD2	-7.27	116.64	121.00
25	U	250	TYR	CB-CG-CD1	7.26	125.36	121.00
30	L	157	ARG	NE-CZ-NH2	7.26	123.93	120.30
31	M	374	ARG	NE-CZ-NH1	7.25	123.93	120.30
2	B	218	PHE	CB-CG-CD1	-7.25	115.72	120.80
19	Z	456	ARG	NE-CZ-NH2	-7.25	116.67	120.30
24	R	208	PHE	CB-CG-CD1	-7.25	115.72	120.80
20	N	341	PHE	CB-CG-CD1	7.24	125.87	120.80
8	1	163	SER	N-CA-CB	7.24	121.36	110.50
29	K	44	TYR	CB-CG-CD2	-7.24	116.66	121.00
17	T	259	TYR	CB-CG-CD1	-7.24	116.66	121.00
30	L	58	GLU	N-CA-CB	7.24	123.62	110.60
8	1	121	TYR	CG-CD1-CE1	7.23	127.08	121.30
19	Z	159	VAL	CA-CB-CG2	7.23	121.74	110.90
27	H	124	ASP	CB-CG-OD1	7.23	124.81	118.30
13	6	221	ARG	NE-CZ-NH2	-7.22	116.69	120.30
28	I	320	ASP	CB-CG-OD2	-7.22	111.80	118.30
27	H	139	ARG	NE-CZ-NH1	7.22	123.91	120.30
20	N	783	TYR	CB-CG-CD2	-7.21	116.67	121.00
9	2	244	ARG	NE-CZ-NH1	-7.21	116.70	120.30
31	M	174	ARG	NE-CZ-NH2	-7.20	116.70	120.30
12	5	225	ARG	NE-CZ-NH2	-7.20	116.70	120.30
32	J	167	LEU	CB-CG-CD1	7.20	123.23	111.00
11	4	98	TYR	CB-CG-CD1	7.19	125.32	121.00
30	L	134	TYR	CB-CG-CD2	7.19	125.32	121.00
21	S	224	ARG	NE-CZ-NH1	7.19	123.90	120.30
12	5	149	TYR	CG-CD1-CE1	-7.19	115.55	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Q	363	ARG	NE-CZ-NH1	7.18	123.89	120.30
24	R	51	ALA	N-CA-CB	7.18	120.15	110.10
6	F	96	ARG	NH1-CZ-NH2	-7.18	111.50	119.40
22	P	25	ASP	CB-CG-OD1	-7.18	111.84	118.30
19	Z	807	ARG	NE-CZ-NH1	7.17	123.89	120.30
27	H	257	VAL	CA-CB-CG1	7.17	121.66	110.90
30	L	27	ARG	NE-CZ-NH1	7.17	123.88	120.30
13	6	160	ASP	CB-CG-OD2	-7.16	111.86	118.30
21	S	116	PHE	CB-CG-CD2	-7.16	115.79	120.80
5	E	162	PHE	CB-CG-CD2	-7.15	115.79	120.80
20	N	494	TYR	CB-CG-CD1	7.15	125.29	121.00
23	Q	164	ALA	CB-CA-C	-7.14	99.39	110.10
32	J	374	ARG	NE-CZ-NH1	7.14	123.87	120.30
27	H	325	ASP	CB-CG-OD2	7.14	124.72	118.30
19	Z	385	PHE	CB-CG-CD2	-7.14	115.81	120.80
29	K	229	ARG	NE-CZ-NH1	7.14	123.87	120.30
29	K	417	TYR	CB-CG-CD2	-7.14	116.72	121.00
29	K	274	ARG	NE-CZ-NH2	-7.13	116.73	120.30
4	D	21	TYR	CG-CD1-CE1	-7.13	115.59	121.30
27	H	428	ARG	NE-CZ-NH2	7.13	123.87	120.30
4	D	17	PHE	CB-CG-CD2	7.13	125.79	120.80
1	A	11	ARG	NE-CZ-NH1	-7.12	116.74	120.30
17	T	148	ARG	NE-CZ-NH2	-7.12	116.74	120.30
20	N	722	ASP	CB-CG-OD1	7.12	124.71	118.30
28	I	132	TYR	CB-CG-CD2	7.12	125.27	121.00
6	F	204	ASP	CB-CG-OD2	-7.12	111.89	118.30
28	I	295	TYR	CB-CG-CD2	7.11	125.27	121.00
6	F	123	TYR	CG-CD1-CE1	-7.11	115.61	121.30
23	Q	282	ARG	NE-CZ-NH2	-7.11	116.74	120.30
7	G	115	ARG	NE-CZ-NH1	-7.11	116.75	120.30
24	R	203	ASP	CB-CG-OD2	-7.11	111.91	118.30
28	I	363	ARG	NH1-CZ-NH2	-7.11	111.58	119.40
20	N	460	TYR	CB-CG-CD2	-7.09	116.75	121.00
8	1	109	VAL	CA-CB-CG2	-7.08	100.28	110.90
32	J	43	ARG	NE-CZ-NH1	-7.08	116.76	120.30
20	N	129	ARG	NH1-CZ-NH2	7.08	127.19	119.40
20	N	378	CYS	CA-CB-SG	7.08	126.73	114.00
21	S	340	ASP	CB-CG-OD1	7.07	124.67	118.30
27	H	279	ALA	N-CA-CB	7.07	120.00	110.10
19	Z	496	ASP	CB-CG-OD2	-7.07	111.94	118.30
9	2	185	PHE	CB-CG-CD1	-7.07	115.85	120.80
17	T	261	PHE	CB-CG-CD1	7.07	125.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	J	258	ARG	NE-CZ-NH1	7.07	123.83	120.30
19	Z	239	TYR	N-CA-CB	7.07	123.32	110.60
5	E	101	PHE	CB-CG-CD2	-7.06	115.86	120.80
12	5	64	ALA	N-CA-C	-7.05	91.96	111.00
3	C	77	ALA	N-CA-CB	7.05	119.97	110.10
31	M	440	TYR	CG-CD1-CE1	-7.05	115.66	121.30
3	C	129	PRO	N-CA-CB	7.04	111.75	103.30
20	N	494	TYR	CB-CG-CD2	-7.04	116.78	121.00
8	1	121	TYR	CB-CG-CD2	7.04	125.22	121.00
19	Z	832	THR	CA-CB-CG2	-7.04	102.55	112.40
14	7	85	ARG	NE-CZ-NH2	-7.04	116.78	120.30
28	I	211	TYR	CG-CD2-CE2	-7.04	115.67	121.30
9	2	181	PHE	CB-CG-CD2	7.03	125.72	120.80
12	5	199	ASP	CB-CG-OD1	7.03	124.63	118.30
17	T	287	PHE	CB-CG-CD2	7.03	125.72	120.80
20	N	194	ARG	NE-CZ-NH2	7.03	123.81	120.30
23	Q	87	ARG	NE-CZ-NH1	-7.02	116.79	120.30
4	D	144	PHE	CB-CG-CD1	-7.02	115.89	120.80
4	D	57	ARG	NE-CZ-NH1	7.02	123.81	120.30
5	E	169	ALA	N-CA-CB	7.01	119.92	110.10
4	D	57	ARG	NE-CZ-NH2	-7.01	116.80	120.30
4	D	73	PHE	CB-CG-CD2	-6.99	115.90	120.80
1	A	23	TYR	CB-CG-CD1	6.99	125.19	121.00
13	6	206	PHE	CG-CD2-CE2	6.99	128.49	120.80
29	K	200	ARG	NE-CZ-NH1	6.99	123.79	120.30
30	L	230	ARG	NE-CZ-NH1	6.98	123.79	120.30
8	1	144	VAL	CA-CB-CG1	-6.98	100.43	110.90
1	A	131	MET	CG-SD-CE	-6.96	89.06	100.20
27	H	195	LEU	CB-CA-C	-6.96	96.97	110.20
27	H	261	PHE	CB-CG-CD1	-6.96	115.92	120.80
19	Z	879	ARG	NE-CZ-NH1	6.96	123.78	120.30
8	1	221	VAL	CA-CB-CG1	-6.96	100.46	110.90
25	U	220	LEU	CB-CG-CD2	6.96	122.83	111.00
27	H	360	ARG	NE-CZ-NH2	-6.96	116.82	120.30
13	6	160	ASP	CB-CG-OD1	6.95	124.56	118.30
28	I	138	PHE	CB-CG-CD2	-6.95	115.93	120.80
32	J	171	HIS	N-CA-CB	6.95	123.11	110.60
20	N	899	ARG	NE-CZ-NH1	6.95	123.78	120.30
26	O	282	PHE	CB-CG-CD2	-6.95	115.94	120.80
30	L	27	ARG	NE-CZ-NH2	-6.93	116.83	120.30
6	F	179	PHE	CB-CG-CD2	-6.93	115.95	120.80
19	Z	76	GLU	N-CA-CB	6.93	123.08	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	N	682	TYR	CG-CD2-CE2	6.93	126.85	121.30
32	J	345	ARG	NE-CZ-NH2	6.93	123.77	120.30
32	J	235	PHE	CB-CG-CD2	-6.93	115.95	120.80
24	R	192	ARG	NE-CZ-NH2	-6.93	116.84	120.30
12	5	62	THR	CA-CB-CG2	6.92	122.09	112.40
10	3	110	ALA	N-CA-CB	6.92	119.79	110.10
3	C	5	TYR	CB-CG-CD2	-6.92	116.85	121.00
11	4	52	ASP	CB-CG-OD2	6.91	124.52	118.30
27	H	298	THR	CA-CB-CG2	-6.91	102.73	112.40
21	S	463	TYR	CB-CG-CD1	-6.91	116.86	121.00
6	F	167	SER	N-CA-CB	6.90	120.85	110.50
1	A	246	ASP	CB-CG-OD2	6.89	124.51	118.30
25	U	5	ALA	N-CA-CB	6.89	119.75	110.10
20	N	187	LEU	CB-CG-CD1	6.89	122.71	111.00
16	V	303	MET	CG-SD-CE	-6.89	89.18	100.20
19	Z	226	TYR	CB-CG-CD2	-6.88	116.87	121.00
6	F	31	GLN	N-CA-CB	6.88	122.99	110.60
1	A	103	TYR	CD1-CE1-CZ	6.88	125.99	119.80
16	V	196	LEU	CB-CG-CD2	6.88	122.69	111.00
31	M	74	ASP	CB-CG-OD1	-6.88	112.11	118.30
20	N	531	ASP	CB-CG-OD1	-6.87	112.11	118.30
9	2	147	ASP	CB-CG-OD2	-6.86	112.12	118.30
25	U	90	ARG	NE-CZ-NH1	6.85	123.73	120.30
19	Z	273	ASN	N-CA-CB	6.85	122.94	110.60
19	Z	239	TYR	CG-CD1-CE1	6.85	126.78	121.30
3	C	159	TRP	CG-CD2-CE3	-6.85	127.74	133.90
20	N	580	ARG	NE-CZ-NH2	-6.85	116.88	120.30
21	S	364	ARG	NE-CZ-NH1	-6.84	116.88	120.30
2	B	46	LEU	CB-CG-CD2	6.84	122.63	111.00
22	P	182	ARG	NE-CZ-NH1	6.84	123.72	120.30
27	H	174	TYR	CA-CB-CG	-6.84	100.40	113.40
24	R	257	ARG	NE-CZ-NH2	-6.84	116.88	120.30
30	L	26	TYR	CB-CG-CD2	6.83	125.10	121.00
32	J	117	ARG	NE-CZ-NH1	-6.83	116.88	120.30
5	E	71	ASP	CB-CG-OD2	-6.83	112.15	118.30
23	Q	161	ASP	CB-CG-OD1	-6.83	112.16	118.30
30	L	371	ALA	C-N-CA	6.83	138.77	121.70
20	N	557	TYR	CB-CG-CD2	-6.83	116.91	121.00
23	Q	239	TYR	CB-CG-CD2	-6.82	116.91	121.00
31	M	323	PHE	CB-CG-CD2	-6.82	116.02	120.80
30	L	311	ARG	NE-CZ-NH2	-6.82	116.89	120.30
20	N	778	PHE	CB-CG-CD1	6.81	125.57	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	E	229	PHE	CB-CG-CD2	-6.81	116.03	120.80
8	1	189	THR	CA-CB-CG2	-6.81	102.87	112.40
11	4	74	GLU	N-CA-CB	6.81	122.86	110.60
12	5	132	ARG	NE-CZ-NH1	6.81	123.70	120.30
27	H	124	ASP	CB-CG-OD2	-6.80	112.18	118.30
28	I	313	LEU	CB-CG-CD2	6.80	122.56	111.00
29	K	374	ASP	CB-CG-OD1	6.79	124.41	118.30
25	U	82	PHE	CB-CA-C	-6.79	96.83	110.40
10	3	25	ASP	CB-CG-OD1	-6.79	112.19	118.30
11	4	119	ASP	CB-CG-OD1	-6.79	112.19	118.30
31	M	423	TYR	CD1-CE1-CZ	-6.79	113.69	119.80
6	F	225	ASP	CB-CG-OD1	6.78	124.40	118.30
1	A	159	TYR	CB-CG-CD2	-6.78	116.93	121.00
4	D	10	PHE	CB-CG-CD1	6.77	125.54	120.80
32	J	325	ARG	NH1-CZ-NH2	6.77	126.85	119.40
12	5	159	MET	N-CA-CB	6.77	122.79	110.60
23	Q	315	ASP	CB-CG-OD2	-6.77	112.21	118.30
20	N	900	TYR	CB-CG-CD2	-6.76	116.94	121.00
25	U	95	TYR	CG-CD2-CE2	-6.76	115.89	121.30
6	F	98	VAL	CA-CB-CG2	6.76	121.04	110.90
13	6	85	HIS	N-CA-CB	6.75	122.75	110.60
19	Z	98	PHE	CB-CG-CD2	-6.75	116.07	120.80
13	6	128	PHE	CB-CG-CD1	6.74	125.52	120.80
30	L	83	PHE	CB-CG-CD1	-6.74	116.08	120.80
9	2	96	ASP	CB-CG-OD1	-6.74	112.24	118.30
13	6	132	TYR	CB-CG-CD2	6.73	125.04	121.00
3	C	91	ARG	NE-CZ-NH2	-6.73	116.94	120.30
6	F	232	PHE	CB-CG-CD2	-6.73	116.09	120.80
23	Q	33	ARG	NH1-CZ-NH2	6.73	126.80	119.40
24	R	323	PHE	CB-CG-CD1	6.72	125.51	120.80
20	N	627	PHE	CB-CG-CD2	-6.72	116.10	120.80
19	Z	113	MET	CG-SD-CE	-6.71	89.47	100.20
7	G	126	TYR	CD1-CE1-CZ	6.71	125.83	119.80
21	S	272	PHE	CB-CG-CD1	-6.70	116.11	120.80
32	J	343	ASN	N-CA-CB	6.70	122.66	110.60
26	O	178	ARG	NE-CZ-NH1	6.70	123.65	120.30
32	J	135	VAL	CA-CB-CG2	6.69	120.94	110.90
14	7	70	MET	CG-SD-CE	-6.69	89.49	100.20
10	3	198	ARG	NE-CZ-NH1	6.69	123.64	120.30
25	U	228	TYR	CB-CG-CD2	-6.69	116.99	121.00
1	A	188	ASP	CB-CG-OD1	-6.68	112.28	118.30
12	5	229	SER	CB-CA-C	-6.68	97.40	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Z	751	TYR	CB-CG-CD1	-6.68	116.99	121.00
19	Z	865	PHE	CB-CG-CD1	-6.68	116.12	120.80
4	D	101	ARG	NE-CZ-NH1	6.68	123.64	120.30
19	Z	100	ARG	NE-CZ-NH1	6.68	123.64	120.30
4	D	75	VAL	N-CA-CB	6.67	126.19	111.50
14	7	231	PHE	CB-CG-CD1	6.67	125.47	120.80
19	Z	369	ARG	NE-CZ-NH2	-6.67	116.96	120.30
24	R	209	THR	CA-CB-CG2	-6.67	103.06	112.40
20	N	344	ARG	NE-CZ-NH1	6.67	123.64	120.30
19	Z	83	ARG	NE-CZ-NH1	6.67	123.63	120.30
24	R	178	ASN	N-CA-CB	6.67	122.60	110.60
24	R	203	ASP	CB-CG-OD1	6.67	124.30	118.30
12	5	118	LEU	N-CA-CB	6.66	123.72	110.40
28	I	58	CYS	CA-CB-SG	6.66	125.98	114.00
21	S	341	ARG	NE-CZ-NH2	-6.65	116.97	120.30
9	2	157	TYR	CA-CB-CG	-6.64	100.78	113.40
22	P	258	ALA	CB-CA-C	-6.64	100.14	110.10
25	U	239	ASP	CB-CG-OD1	6.64	124.28	118.30
32	J	132	ASP	CB-CG-OD2	-6.64	112.32	118.30
23	Q	33	ARG	NE-CZ-NH2	-6.64	116.98	120.30
27	H	158	ASP	CB-CG-OD1	6.64	124.27	118.30
7	G	185	MET	CG-SD-CE	-6.63	89.59	100.20
21	S	254	TYR	CZ-CE2-CD2	-6.63	113.83	119.80
29	K	402	ALA	N-CA-CB	6.62	119.37	110.10
4	D	47	LYS	N-CA-CB	6.62	122.51	110.60
15	W	70	ARG	NE-CZ-NH2	6.61	123.61	120.30
29	K	91	GLN	N-CA-C	-6.61	93.14	111.00
19	Z	727	PHE	CB-CG-CD2	-6.61	116.17	120.80
21	S	341	ARG	NE-CZ-NH1	6.61	123.60	120.30
10	3	25	ASP	CB-CG-OD2	6.61	124.25	118.30
12	5	202	TYR	CB-CG-CD2	-6.61	117.04	121.00
27	H	351	ARG	NE-CZ-NH2	-6.60	117.00	120.30
16	V	25	VAL	CA-CB-CG2	6.59	120.79	110.90
8	1	180	MET	CG-SD-CE	6.59	110.74	100.20
4	D	39	ASP	CB-CG-OD2	-6.59	112.37	118.30
2	B	229	TYR	CB-CG-CD2	6.58	124.95	121.00
5	E	230	THR	CA-CB-CG2	-6.58	103.18	112.40
29	K	398	ASP	CB-CG-OD2	6.58	124.22	118.30
23	Q	155	ARG	NE-CZ-NH1	6.58	123.59	120.30
11	4	73	TYR	CB-CG-CD1	-6.58	117.06	121.00
21	S	213	VAL	CA-CB-CG1	-6.58	101.04	110.90
3	C	17	ARG	NH1-CZ-NH2	6.57	126.63	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	L	124	TYR	CB-CG-CD1	-6.57	117.06	121.00
17	T	207	ARG	CD-NE-CZ	-6.57	114.40	123.60
27	H	250	VAL	CG1-CB-CG2	6.57	121.41	110.90
32	J	35	VAL	CG1-CB-CG2	6.57	121.41	110.90
9	2	115	ARG	NE-CZ-NH2	6.56	123.58	120.30
28	I	382	ASP	CB-CG-OD1	-6.56	112.39	118.30
31	M	441	TYR	CB-CG-CD2	-6.56	117.07	121.00
16	V	32	TYR	CB-CG-CD1	-6.55	117.07	121.00
2	B	91	ARG	NE-CZ-NH1	6.55	123.57	120.30
28	I	372	MET	CG-SD-CE	-6.55	89.73	100.20
26	O	24	ARG	NE-CZ-NH1	6.54	123.57	120.30
30	L	19	ARG	NE-CZ-NH2	-6.54	117.03	120.30
29	K	138	ALA	N-CA-CB	6.54	119.26	110.10
20	N	179	TYR	CB-CG-CD2	-6.54	117.08	121.00
26	O	87	MET	CG-SD-CE	-6.54	89.74	100.20
2	B	1	MET	CG-SD-CE	-6.53	89.75	100.20
8	1	149	MET	CG-SD-CE	-6.53	89.75	100.20
19	Z	25	ASP	CB-CG-OD2	6.53	124.17	118.30
25	U	88	ARG	NE-CZ-NH1	6.52	123.56	120.30
19	Z	207	LEU	CB-CG-CD2	6.52	122.09	111.00
23	Q	11	ARG	NE-CZ-NH1	6.52	123.56	120.30
20	N	424	ALA	N-CA-CB	6.52	119.22	110.10
7	G	84	ASP	CB-CG-OD2	6.51	124.16	118.30
22	P	9	ALA	CB-CA-C	-6.51	100.33	110.10
22	P	273	TYR	CB-CG-CD1	6.51	124.91	121.00
15	W	15	TYR	CB-CG-CD1	-6.51	117.09	121.00
7	G	136	PHE	CB-CG-CD2	-6.51	116.25	120.80
11	4	117	TYR	CG-CD2-CE2	-6.50	116.10	121.30
14	7	71	LEU	CB-CA-C	-6.50	97.85	110.20
31	M	98	GLU	OE1-CD-OE2	6.50	131.10	123.30
27	H	347	ASP	CB-CG-OD1	6.50	124.15	118.30
26	O	248	PHE	CB-CG-CD2	6.50	125.35	120.80
25	U	181	ASP	CB-CG-OD1	6.49	124.14	118.30
27	H	41	TYR	CB-CG-CD1	6.49	124.90	121.00
17	T	202	LEU	CB-CG-CD2	6.49	122.03	111.00
22	P	408	ARG	NE-CZ-NH2	-6.49	117.06	120.30
17	T	188	SER	N-CA-CB	6.49	120.23	110.50
29	K	178	ARG	NH1-CZ-NH2	6.49	126.54	119.40
8	1	94	TYR	CB-CG-CD2	-6.49	117.11	121.00
24	R	152	MET	CG-SD-CE	-6.49	89.82	100.20
29	K	254	ALA	CB-CA-C	-6.49	100.37	110.10
3	C	96	ARG	NE-CZ-NH1	-6.48	117.06	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	62	ASP	CB-CG-OD2	-6.48	112.47	118.30
19	Z	71	TYR	CG-CD1-CE1	6.48	126.48	121.30
19	Z	256	PHE	CB-CG-CD1	6.48	125.33	120.80
23	Q	16	LEU	CB-CG-CD1	6.48	122.01	111.00
20	N	167	ILE	CA-CB-CG1	6.47	123.30	111.00
20	N	473	VAL	CG1-CB-CG2	-6.47	100.55	110.90
32	J	194	THR	CA-CB-CG2	-6.47	103.35	112.40
19	Z	483	PHE	CB-CG-CD2	-6.46	116.28	120.80
24	R	224	VAL	CA-CB-CG2	-6.46	101.21	110.90
27	H	401	ARG	NH1-CZ-NH2	-6.46	112.29	119.40
7	G	20	ARG	NE-CZ-NH1	-6.46	117.07	120.30
13	6	103	LYS	CB-CA-C	-6.46	97.48	110.40
5	E	22	PHE	CB-CG-CD1	-6.46	116.28	120.80
28	I	365	PHE	CB-CG-CD2	-6.46	116.28	120.80
23	Q	289	CYS	CA-CB-SG	-6.46	102.38	114.00
22	P	65	ARG	NE-CZ-NH1	6.45	123.53	120.30
12	5	172	TYR	CB-CG-CD2	6.45	124.87	121.00
1	A	117	ARG	NE-CZ-NH2	-6.44	117.08	120.30
12	5	77	SER	N-CA-CB	6.44	120.16	110.50
29	K	323	ARG	CD-NE-CZ	-6.43	114.59	123.60
16	V	40	LYS	N-CA-CB	6.43	122.17	110.60
6	F	172	LEU	CB-CG-CD2	6.43	121.93	111.00
22	P	81	ASP	CB-CG-OD1	-6.42	112.53	118.30
21	S	442	VAL	CA-CB-CG1	-6.41	101.29	110.90
30	L	340	ILE	C-N-CA	6.41	137.72	121.70
4	D	36	ARG	NE-CZ-NH2	-6.40	117.10	120.30
1	A	96	TYR	CA-CB-CG	-6.39	101.25	113.40
20	N	22	PHE	CB-CG-CD1	6.39	125.28	120.80
27	H	320	ALA	CB-CA-C	-6.39	100.51	110.10
10	3	55	GLY	N-CA-C	-6.39	97.12	113.10
31	M	241	ARG	NE-CZ-NH2	-6.39	117.11	120.30
11	4	117	TYR	CB-CG-CD2	-6.39	117.17	121.00
23	Q	344	ARG	NE-CZ-NH2	-6.38	117.11	120.30
2	B	24	TYR	CB-CG-CD1	6.38	124.83	121.00
4	D	123	ARG	NE-CZ-NH1	6.38	123.49	120.30
15	W	86	PHE	CZ-CE2-CD2	-6.38	112.45	120.10
19	Z	198	HIS	N-CA-CB	6.38	122.08	110.60
22	P	214	PHE	CB-CG-CD1	6.37	125.26	120.80
31	M	337	ARG	NE-CZ-NH2	-6.37	117.11	120.30
4	D	17	PHE	CB-CG-CD1	-6.37	116.34	120.80
3	C	4	ARG	NE-CZ-NH2	-6.37	117.12	120.30
21	S	463	TYR	CZ-CE2-CD2	6.37	125.53	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	H	118	PHE	CB-CG-CD1	-6.36	116.34	120.80
27	H	375	ARG	NE-CZ-NH1	-6.36	117.12	120.30
4	D	16	LEU	CB-CG-CD1	6.36	121.80	111.00
7	G	175	THR	CA-CB-CG2	-6.36	103.50	112.40
2	B	57	TYR	CA-CB-CG	-6.35	101.33	113.40
19	Z	489	TYR	O-C-N	-6.35	112.54	122.70
15	W	42	ARG	NE-CZ-NH2	-6.35	117.12	120.30
2	B	151	PRO	N-CD-CG	6.34	112.72	103.20
21	S	214	TYR	CB-CG-CD2	6.34	124.81	121.00
3	C	161	ALA	N-CA-CB	6.34	118.98	110.10
24	R	294	TYR	CB-CG-CD2	-6.34	117.19	121.00
7	G	123	TYR	CB-CG-CD2	-6.34	117.20	121.00
5	E	112	VAL	CG1-CB-CG2	6.34	121.04	110.90
14	7	226	ARG	N-CA-CB	6.34	122.01	110.60
11	4	153	ARG	NE-CZ-NH1	-6.34	117.13	120.30
14	7	101	TYR	CB-CG-CD2	-6.33	117.20	121.00
5	E	15	PHE	CB-CG-CD2	-6.33	116.37	120.80
20	N	627	PHE	CB-CG-CD1	6.32	125.23	120.80
20	N	646	PRO	N-CA-CB	6.32	110.89	103.30
21	S	116	PHE	CB-CG-CD1	6.32	125.22	120.80
3	C	226	ARG	NE-CZ-NH2	-6.32	117.14	120.30
7	G	239	TYR	CG-CD2-CE2	-6.32	116.25	121.30
18	Y	68	GLU	OE1-CD-OE2	-6.32	115.72	123.30
13	6	47	PHE	CB-CG-CD2	-6.32	116.38	120.80
15	W	93	ALA	CB-CA-C	-6.31	100.63	110.10
4	D	144	PHE	CB-CG-CD2	6.31	125.22	120.80
6	F	239	ARG	NE-CZ-NH1	6.31	123.45	120.30
20	N	468	ALA	CB-CA-C	6.31	119.56	110.10
20	N	796	LYS	O-C-N	6.31	132.79	122.70
26	O	123	LEU	CB-CG-CD1	6.30	121.72	111.00
8	1	154	VAL	CA-CB-CG2	-6.30	101.45	110.90
24	R	125	ARG	NE-CZ-NH1	6.30	123.45	120.30
26	O	213	PHE	CB-CG-CD2	6.30	125.21	120.80
28	I	348	ASP	CB-CG-OD2	-6.30	112.63	118.30
30	L	372	ASP	CB-CG-OD2	-6.29	112.64	118.30
24	R	289	ALA	N-CA-CB	6.29	118.91	110.10
28	I	119	ASN	N-CA-CB	6.29	121.92	110.60
29	K	338	ARG	NE-CZ-NH1	6.29	123.44	120.30
22	P	75	TYR	CG-CD2-CE2	-6.29	116.27	121.30
27	H	330	ALA	CB-CA-C	-6.28	100.68	110.10
20	N	60	ALA	N-CA-CB	6.28	118.89	110.10
21	S	257	TYR	CB-CG-CD1	6.27	124.76	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O	312	MET	CG-SD-CE	-6.27	90.16	100.20
17	T	292	ARG	NE-CZ-NH2	-6.27	117.16	120.30
31	M	306	ASP	CB-CG-OD2	-6.27	112.66	118.30
9	2	63	ALA	N-CA-CB	6.27	118.88	110.10
32	J	228	ALA	N-CA-CB	6.27	118.88	110.10
24	R	143	TYR	CB-CG-CD1	6.27	124.76	121.00
27	H	383	ALA	CB-CA-C	-6.27	100.70	110.10
10	3	198	ARG	NE-CZ-NH2	-6.26	117.17	120.30
21	S	213	VAL	CA-CB-CG2	6.26	120.30	110.90
28	I	245	ALA	CB-CA-C	6.26	119.50	110.10
14	7	195	ARG	NE-CZ-NH2	-6.26	117.17	120.30
20	N	590	TYR	CB-CG-CD1	-6.26	117.24	121.00
3	C	179	TYR	CG-CD1-CE1	-6.26	116.29	121.30
23	Q	300	ALA	N-CA-CB	6.25	118.86	110.10
4	D	169	ARG	NE-CZ-NH2	-6.25	117.17	120.30
17	T	313	LEU	CB-CG-CD2	6.25	121.63	111.00
26	O	130	ALA	N-CA-CB	6.25	118.85	110.10
24	R	28	LEU	CB-CA-C	6.25	122.08	110.20
26	O	163	TYR	CB-CG-CD1	-6.25	117.25	121.00
26	O	230	ARG	NE-CZ-NH2	-6.25	117.18	120.30
27	H	410	LEU	CB-CG-CD1	6.24	121.61	111.00
8	1	98	PHE	CG-CD1-CE1	6.24	127.66	120.80
13	6	188	VAL	CG1-CB-CG2	-6.24	100.92	110.90
13	6	124	TYR	CA-CB-CG	6.24	125.25	113.40
28	I	295	TYR	CB-CG-CD1	-6.24	117.26	121.00
24	R	342	ARG	NE-CZ-NH2	-6.24	117.18	120.30
31	M	316	LEU	CB-CG-CD1	6.24	121.60	111.00
20	N	601	ARG	NE-CZ-NH1	6.23	123.42	120.30
22	P	94	ARG	NE-CZ-NH2	-6.23	117.19	120.30
14	7	68	ALA	CB-CA-C	6.23	119.44	110.10
16	V	129	THR	CA-CB-CG2	-6.22	103.69	112.40
28	I	80	ARG	NE-CZ-NH2	-6.22	117.19	120.30
2	B	223	PRO	N-CA-CB	6.22	110.77	103.30
11	4	178	PHE	CB-CG-CD2	-6.22	116.45	120.80
19	Z	215	ASP	CB-CA-C	-6.22	97.96	110.40
22	P	329	ARG	NE-CZ-NH2	6.22	123.41	120.30
9	2	51	TYR	CG-CD1-CE1	-6.22	116.33	121.30
5	E	129	ASP	CB-CG-OD2	-6.22	112.70	118.30
21	S	204	ALA	N-CA-CB	6.22	118.80	110.10
21	S	254	TYR	CG-CD2-CE2	6.21	126.27	121.30
10	3	69	PHE	CG-CD2-CE2	-6.21	113.97	120.80
22	P	142	ARG	NE-CZ-NH2	-6.21	117.20	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O	213	PHE	CB-CG-CD1	-6.21	116.45	120.80
18	Y	65	TYR	CB-CG-CD1	6.20	124.72	121.00
21	S	492	PHE	CB-CG-CD2	-6.20	116.46	120.80
24	R	101	ARG	NE-CZ-NH1	6.20	123.40	120.30
12	5	210	GLU	N-CA-CB	6.20	121.75	110.60
19	Z	133	MET	N-CA-CB	6.20	121.75	110.60
21	S	502	GLU	OE1-CD-OE2	6.19	130.73	123.30
30	L	279	ASP	N-CA-CB	6.19	121.75	110.60
14	7	219	VAL	CG1-CB-CG2	-6.19	101.00	110.90
29	K	245	ARG	NE-CZ-NH2	-6.19	117.20	120.30
7	G	224	ARG	NE-CZ-NH1	6.19	123.39	120.30
19	Z	830	LEU	CB-CA-C	-6.19	98.45	110.20
8	1	161	GLY	N-CA-C	-6.18	97.64	113.10
22	P	137	TYR	CB-CG-CD2	-6.18	117.29	121.00
24	R	46	ARG	N-CA-CB	6.18	121.72	110.60
13	6	71	TYR	CZ-CE2-CD2	-6.18	114.24	119.80
22	P	414	ASN	CB-CG-OD1	-6.18	109.25	121.60
24	R	81	LEU	CB-CG-CD2	6.18	121.50	111.00
6	F	26	MET	CG-SD-CE	-6.17	90.32	100.20
9	2	133	TYR	CG-CD2-CE2	-6.17	116.36	121.30
6	F	125	ARG	NE-CZ-NH1	-6.17	117.22	120.30
7	G	224	ARG	NE-CZ-NH2	-6.17	117.21	120.30
26	O	247	ARG	NE-CZ-NH2	-6.17	117.22	120.30
5	E	10	ARG	NE-CZ-NH2	-6.17	117.22	120.30
6	F	239	ARG	NE-CZ-NH2	-6.17	117.22	120.30
19	Z	469	TYR	CA-CB-CG	-6.17	101.68	113.40
32	J	297	ARG	NE-CZ-NH2	6.17	123.38	120.30
28	I	81	ASN	N-CA-CB	6.17	121.70	110.60
28	I	371	ARG	NE-CZ-NH1	-6.17	117.22	120.30
8	1	121	TYR	CD1-CG-CD2	-6.16	111.12	117.90
20	N	929	ALA	N-CA-CB	6.16	118.73	110.10
11	4	28	MET	N-CA-CB	6.16	121.69	110.60
27	H	255	ARG	NE-CZ-NH1	6.16	123.38	120.30
13	6	104	HIS	CA-CB-CG	6.16	124.06	113.60
32	J	221	GLN	N-CA-C	-6.15	94.38	111.00
28	I	349	ARG	NE-CZ-NH1	6.15	123.38	120.30
6	F	100	ASP	CB-CG-OD2	-6.15	112.76	118.30
19	Z	375	SER	N-CA-CB	6.15	119.73	110.50
27	H	79	ASP	CB-CG-OD1	6.15	123.83	118.30
28	I	184	TYR	CB-CG-CD2	-6.15	117.31	121.00
13	6	128	PHE	CB-CG-CD2	-6.14	116.50	120.80
19	Z	794	ALA	N-CA-CB	6.14	118.70	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	403	PHE	CB-CG-CD1	6.14	125.10	120.80
14	7	87	MET	CG-SD-CE	-6.14	90.37	100.20
21	S	29	ALA	CB-CA-C	-6.14	100.89	110.10
22	P	213	PHE	CB-CG-CD1	6.14	125.10	120.80
22	P	215	GLN	N-CA-CB	6.13	121.64	110.60
17	T	121	ARG	NE-CZ-NH2	-6.13	117.23	120.30
25	U	94	TRP	CD1-NE1-CE2	-6.13	103.48	109.00
27	H	343	PHE	N-CA-C	-6.13	94.45	111.00
28	I	78	PHE	CB-CG-CD2	6.13	125.09	120.80
13	6	177	ASP	CB-CG-OD2	-6.13	112.79	118.30
30	L	170	PRO	N-CD-CG	6.13	112.39	103.20
24	R	37	VAL	CG1-CB-CG2	-6.12	101.10	110.90
5	E	77	ALA	N-CA-C	-6.12	94.47	111.00
32	J	85	VAL	CA-CB-CG2	6.12	120.08	110.90
32	J	370	ALA	CB-CA-C	-6.12	100.92	110.10
26	O	73	PRO	N-CA-CB	6.12	110.64	103.30
31	M	162	LEU	CB-CA-C	-6.12	98.57	110.20
6	F	211	SER	N-CA-CB	6.12	119.68	110.50
3	C	62	SER	N-CA-C	-6.11	94.49	111.00
8	1	216	GLY	C-N-CA	6.11	136.98	121.70
31	M	211	HIS	N-CA-CB	6.11	121.60	110.60
17	T	194	LEU	N-CA-CB	6.11	122.62	110.40
14	7	165	PHE	CB-CG-CD1	-6.11	116.52	120.80
21	S	117	PHE	CB-CG-CD2	-6.11	116.52	120.80
11	4	11	ASP	CB-CG-OD2	-6.11	112.81	118.30
24	R	146	ARG	NE-CZ-NH2	-6.11	117.25	120.30
5	E	137	PHE	CB-CG-CD2	-6.10	116.53	120.80
28	I	132	TYR	CB-CG-CD1	-6.10	117.34	121.00
20	N	49	TYR	CB-CG-CD1	6.09	124.66	121.00
25	U	34	ARG	NE-CZ-NH1	6.09	123.35	120.30
9	2	245	TYR	CB-CG-CD2	6.09	124.66	121.00
13	6	60	PHE	C-N-CA	6.09	136.93	121.70
26	O	255	TRP	CB-CG-CD2	-6.09	118.68	126.60
29	K	130	VAL	CA-C-O	-6.09	107.31	120.10
8	1	124	ARG	NE-CZ-NH1	-6.09	117.25	120.30
19	Z	795	GLY	O-C-N	-6.09	112.96	122.70
1	A	21	ARG	NH1-CZ-NH2	-6.09	112.70	119.40
19	Z	98	PHE	CG-CD1-CE1	-6.09	114.10	120.80
23	Q	390	GLU	N-CA-C	-6.08	94.58	111.00
2	B	163	MET	CG-SD-CE	-6.08	90.47	100.20
32	J	232	ARG	NE-CZ-NH1	6.08	123.34	120.30
25	U	79	TYR	CB-CG-CD2	-6.08	117.35	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	S	53	ALA	N-CA-CB	6.07	118.60	110.10
9	2	81	SER	CA-C-O	-6.07	107.36	120.10
24	R	267	ARG	N-CA-CB	6.07	121.52	110.60
20	N	49	TYR	CB-CG-CD2	-6.06	117.36	121.00
20	N	557	TYR	CB-CG-CD1	6.06	124.64	121.00
20	N	586	VAL	CG1-CB-CG2	6.06	120.60	110.90
27	H	256	MET	CG-SD-CE	6.06	109.90	100.20
20	N	176	MET	CA-CB-CG	6.06	123.60	113.30
23	Q	101	ALA	N-CA-CB	6.06	118.58	110.10
12	5	96	ILE	CA-CB-CG1	6.06	122.51	111.00
30	L	55	GLU	O-C-N	-6.06	113.01	122.70
16	V	225	TRP	CG-CD2-CE3	-6.05	128.45	133.90
5	E	156	MET	CG-SD-CE	-6.05	90.52	100.20
25	U	241	SER	C-N-CA	6.05	136.83	121.70
27	H	174	TYR	CB-CG-CD2	6.05	124.63	121.00
21	S	378	PHE	CB-CG-CD2	-6.05	116.57	120.80
13	6	180	VAL	CA-CB-CG2	6.05	119.97	110.90
22	P	137	TYR	CB-CG-CD1	6.05	124.63	121.00
19	Z	434	TYR	N-CA-CB	6.04	121.48	110.60
28	I	348	ASP	CB-CG-OD1	6.04	123.74	118.30
28	I	377	ASP	CB-CG-OD2	-6.04	112.86	118.30
8	1	98	PHE	CB-CG-CD1	6.04	125.03	120.80
22	P	75	TYR	CD1-CE1-CZ	-6.04	114.36	119.80
30	L	209	PHE	CG-CD1-CE1	-6.04	114.15	120.80
15	W	108	ARG	CD-NE-CZ	-6.04	115.14	123.60
3	C	46	ALA	N-CA-CB	6.04	118.55	110.10
20	N	456	ASP	CB-CG-OD1	6.03	123.73	118.30
28	I	132	TYR	CD1-CE1-CZ	-6.03	114.37	119.80
16	V	32	TYR	CB-CG-CD2	6.03	124.62	121.00
26	O	70	ARG	NE-CZ-NH1	-6.03	117.29	120.30
27	H	369	ARG	NE-CZ-NH1	-6.03	117.29	120.30
7	G	123	TYR	CB-CG-CD1	6.03	124.62	121.00
19	Z	675	PHE	CB-CG-CD2	6.03	125.02	120.80
27	H	121	PHE	CB-CG-CD2	-6.02	116.58	120.80
7	G	31	VAL	CA-CB-CG2	-6.02	101.87	110.90
17	T	338	LEU	CB-CG-CD2	-6.02	100.76	111.00
20	N	802	TYR	CG-CD2-CE2	-6.02	116.48	121.30
12	5	73	VAL	N-CA-C	-6.02	94.75	111.00
14	7	237	THR	N-CA-C	-6.01	94.76	111.00
23	Q	303	GLU	CA-CB-CG	6.01	126.63	113.40
31	M	369	MET	CA-CB-CG	6.01	123.52	113.30
20	N	179	TYR	CB-CG-CD1	6.01	124.61	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	172	THR	CA-CB-CG2	-6.01	103.99	112.40
7	G	204	GLU	OE1-CD-OE2	6.01	130.51	123.30
16	V	234	TYR	CB-CG-CD1	-6.01	117.39	121.00
21	S	303	ARG	NE-CZ-NH1	-6.01	117.30	120.30
29	K	362	ASP	CB-CG-OD1	-6.01	112.89	118.30
14	7	114	MET	CA-CB-CG	6.00	123.51	113.30
17	T	170	TYR	CG-CD2-CE2	-6.00	116.50	121.30
19	Z	62	ARG	CA-CB-CG	6.00	126.61	113.40
23	Q	415	TYR	CG-CD1-CE1	-6.00	116.50	121.30
24	R	170	GLU	OE1-CD-OE2	6.00	130.50	123.30
5	E	50	VAL	CA-CB-CG2	-6.00	101.90	110.90
15	W	21	PHE	N-CA-CB	6.00	121.40	110.60
11	4	196	PHE	CB-CG-CD2	-6.00	116.60	120.80
22	P	55	ARG	NE-CZ-NH1	5.99	123.30	120.30
29	K	307	VAL	CA-CB-CG2	-5.99	101.91	110.90
32	J	24	TYR	CB-CG-CD1	5.99	124.60	121.00
19	Z	600	TYR	CB-CG-CD2	-5.99	117.41	121.00
31	M	161	TYR	CB-CG-CD1	-5.99	117.41	121.00
23	Q	235	ALA	N-CA-CB	5.99	118.48	110.10
12	5	204	TYR	CB-CG-CD2	-5.98	117.41	121.00
13	6	110	MET	CG-SD-CE	-5.98	90.63	100.20
24	R	102	ASP	CB-CG-OD2	5.98	123.69	118.30
5	E	63	SER	CB-CA-C	-5.98	98.73	110.10
24	R	366	TYR	CB-CG-CD1	5.98	124.59	121.00
26	O	138	VAL	CA-CB-CG2	5.98	119.87	110.90
12	5	223	THR	CA-CB-CG2	-5.98	104.03	112.40
29	K	60	TYR	CG-CD1-CE1	5.98	126.08	121.30
19	Z	181	ARG	NE-CZ-NH1	5.98	123.29	120.30
11	4	120	TYR	CG-CD1-CE1	-5.98	116.52	121.30
3	C	249	ARG	NE-CZ-NH1	5.97	123.29	120.30
20	N	188	MET	CA-CB-CG	5.97	123.45	113.30
3	C	206	LEU	CB-CG-CD1	5.97	121.15	111.00
30	L	130	ASP	CB-CG-OD1	5.97	123.67	118.30
12	5	225	ARG	NE-CZ-NH1	5.97	123.28	120.30
21	S	344	PHE	CB-CG-CD1	5.97	124.98	120.80
12	5	69	HIS	CA-CB-CG	-5.97	103.46	113.60
27	H	428	ARG	NE-CZ-NH1	5.97	123.28	120.30
16	V	111	TRP	CB-CG-CD1	5.96	134.75	127.00
7	G	239	TYR	CB-CG-CD1	5.96	124.58	121.00
9	2	207	PHE	CB-CG-CD2	-5.96	116.63	120.80
12	5	193	TYR	N-CA-CB	5.96	121.33	110.60
25	U	130	ASP	CB-CG-OD1	5.96	123.67	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	83	ALA	N-CA-CB	5.96	118.44	110.10
20	N	143	ASP	N-CA-CB	5.96	121.33	110.60
1	A	159	TYR	CG-CD2-CE2	-5.96	116.53	121.30
19	Z	828	ARG	NE-CZ-NH2	5.96	123.28	120.30
3	C	31	ALA	CB-CA-C	-5.95	101.17	110.10
10	3	28	PHE	CB-CG-CD2	5.95	124.97	120.80
27	H	428	ARG	NH1-CZ-NH2	-5.95	112.85	119.40
15	W	11	ASP	CB-CG-OD2	-5.95	112.95	118.30
20	N	225	ASP	CA-CB-CG	5.95	126.49	113.40
27	H	261	PHE	CB-CG-CD2	5.95	124.96	120.80
29	K	363	TYR	CB-CG-CD2	-5.94	117.44	121.00
16	V	180	ASN	N-CA-CB	5.94	121.29	110.60
19	Z	18	ALA	CB-CA-C	-5.94	101.19	110.10
19	Z	287	ASP	CB-CG-OD1	-5.94	112.95	118.30
14	7	222	TYR	CA-CB-CG	-5.94	102.12	113.40
29	K	121	ARG	NE-CZ-NH1	-5.94	117.33	120.30
20	N	926	GLU	CA-C-O	-5.93	107.64	120.10
21	S	302	ARG	NE-CZ-NH2	-5.93	117.33	120.30
22	P	79	GLU	OE1-CD-OE2	-5.93	116.18	123.30
14	7	133	HIS	CA-CB-CG	5.93	123.69	113.60
21	S	29	ALA	N-CA-CB	5.93	118.40	110.10
19	Z	765	ALA	N-CA-CB	5.93	118.40	110.10
20	N	97	VAL	CA-CB-CG1	-5.93	102.00	110.90
23	Q	269	ALA	CB-CA-C	-5.93	101.20	110.10
31	M	183	ARG	NH1-CZ-NH2	-5.93	112.88	119.40
25	U	196	HIS	CB-CG-ND1	5.93	138.02	123.20
28	I	222	VAL	N-CA-C	-5.93	94.99	111.00
20	N	644	TYR	CB-CG-CD1	-5.93	117.44	121.00
28	I	259	TYR	CG-CD2-CE2	-5.93	116.56	121.30
10	3	96	TYR	CB-CG-CD1	-5.92	117.44	121.00
17	T	289	GLU	N-CA-CB	5.92	121.25	110.60
2	B	4	ARG	NE-CZ-NH2	-5.92	117.34	120.30
30	L	331	ALA	N-CA-CB	5.91	118.38	110.10
19	Z	280	ASP	CB-CG-OD2	-5.91	112.98	118.30
11	4	196	PHE	CG-CD2-CE2	-5.91	114.30	120.80
16	V	155	VAL	CG1-CB-CG2	-5.91	101.45	110.90
9	2	188	ASP	CB-CG-OD1	-5.90	112.99	118.30
14	7	94	MET	CG-SD-CE	-5.90	90.75	100.20
24	R	63	TRP	CD1-CG-CD2	5.90	111.02	106.30
20	N	619	VAL	CA-CB-CG1	-5.90	102.05	110.90
22	P	123	ARG	NE-CZ-NH1	5.90	123.25	120.30
12	5	149	TYR	CB-CG-CD1	5.90	124.54	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	I	297	SER	CB-CA-C	-5.90	98.89	110.10
4	D	21	TYR	CB-CG-CD2	-5.90	117.46	121.00
4	D	60	ARG	NE-CZ-NH1	5.89	123.25	120.30
32	J	150	MET	CG-SD-CE	-5.89	90.77	100.20
9	2	115	ARG	NE-CZ-NH1	-5.89	117.35	120.30
21	S	208	TYR	CD1-CE1-CZ	-5.89	114.50	119.80
1	A	95	ARG	NE-CZ-NH1	-5.89	117.36	120.30
5	E	20	ARG	NE-CZ-NH2	5.89	123.25	120.30
27	H	292	ASP	CB-CG-OD2	-5.89	113.00	118.30
31	M	229	TYR	CB-CG-CD2	5.89	124.53	121.00
22	P	350	ARG	NE-CZ-NH2	-5.89	117.36	120.30
29	K	182	GLU	CB-CA-C	-5.89	98.63	110.40
32	J	143	VAL	CA-CB-CG1	-5.89	102.07	110.90
30	L	141	PRO	N-CA-CB	5.88	110.36	103.30
2	B	57	TYR	N-CA-CB	5.88	121.19	110.60
9	2	120	VAL	CA-CB-CG2	-5.88	102.08	110.90
22	P	273	TYR	CG-CD2-CE2	-5.88	116.59	121.30
26	O	238	TYR	CB-CG-CD1	5.88	124.53	121.00
31	M	139	VAL	C-N-CA	5.88	136.40	121.70
21	S	113	VAL	CA-CB-CG2	5.88	119.71	110.90
31	M	301	SER	N-CA-CB	5.88	119.31	110.50
3	C	216	LEU	N-CA-C	-5.87	95.14	111.00
5	E	63	SER	N-CA-CB	5.87	119.30	110.50
13	6	28	ARG	NE-CZ-NH1	5.87	123.23	120.30
29	K	267	ILE	C-N-CA	5.87	136.37	121.70
2	B	82	ASP	CB-CG-OD1	-5.87	113.02	118.30
3	C	121	TYR	CB-CG-CD1	5.87	124.52	121.00
27	H	302	LEU	CB-CG-CD1	5.87	120.97	111.00
7	G	130	ARG	NE-CZ-NH2	-5.87	117.37	120.30
19	Z	690	VAL	CA-C-N	5.87	133.52	117.10
29	K	124	LEU	CB-CG-CD1	5.87	120.97	111.00
8	1	181	THR	CA-CB-CG2	-5.86	104.19	112.40
22	P	94	ARG	NE-CZ-NH1	-5.86	117.37	120.30
26	O	198	PHE	CB-CG-CD2	-5.86	116.70	120.80
29	K	57	GLN	N-CA-CB	5.86	121.16	110.60
4	D	3	TYR	CG-CD2-CE2	-5.86	116.61	121.30
16	V	114	SER	N-CA-CB	5.86	119.29	110.50
21	S	237	ARG	CB-CA-C	-5.86	98.68	110.40
9	2	67	MET	CA-CB-CG	5.86	123.26	113.30
25	U	69	PHE	CB-CG-CD1	-5.86	116.70	120.80
4	D	38	ARG	NE-CZ-NH2	5.85	123.23	120.30
27	H	246	VAL	CA-CB-CG2	5.85	119.68	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	97	TYR	CB-CG-CD2	5.85	124.51	121.00
3	C	128	ARG	NE-CZ-NH2	-5.85	117.38	120.30
24	R	213	LEU	CB-CA-C	5.85	121.31	110.20
25	U	82	PHE	CB-CG-CD2	-5.85	116.70	120.80
27	H	111	TYR	CG-CD2-CE2	-5.85	116.62	121.30
32	J	99	VAL	CG1-CB-CG2	5.84	120.25	110.90
16	V	289	ASP	CB-CG-OD2	-5.84	113.04	118.30
19	Z	543	MET	CG-SD-CE	5.84	109.54	100.20
22	P	370	TYR	CD1-CE1-CZ	-5.84	114.54	119.80
4	D	74	ALA	N-CA-CB	5.84	118.27	110.10
14	7	224	ASP	CB-CG-OD1	5.84	123.55	118.30
30	L	124	TYR	CG-CD1-CE1	-5.83	116.63	121.30
17	T	309	ARG	CB-CG-CD	5.83	126.76	111.60
28	I	410	ARG	N-CA-CB	5.83	121.10	110.60
9	2	171	GLY	C-N-CA	5.83	136.27	121.70
20	N	514	LEU	CB-CG-CD2	5.83	120.91	111.00
30	L	133	VAL	CA-CB-CG2	-5.83	102.16	110.90
2	B	149	SER	N-CA-CB	5.83	119.24	110.50
8	1	147	VAL	CA-CB-CG2	-5.83	102.16	110.90
10	3	50	TYR	CG-CD2-CE2	-5.83	116.64	121.30
29	K	77	GLU	CG-CD-OE2	-5.82	106.65	118.30
32	J	292	ILE	CA-CB-CG1	5.82	122.06	111.00
9	2	152	HIS	CA-CB-CG	5.82	123.49	113.60
20	N	361	ARG	CD-NE-CZ	-5.82	115.45	123.60
6	F	94	ASP	CB-CG-OD1	5.82	123.53	118.30
6	F	97	PHE	CB-CG-CD2	-5.82	116.73	120.80
14	7	80	PHE	CB-CG-CD1	5.82	124.87	120.80
2	B	156	PHE	CB-CG-CD1	-5.81	116.73	120.80
16	V	111	TRP	CB-CG-CD2	-5.81	119.05	126.60
21	S	461	ASP	N-CA-CB	5.81	121.06	110.60
29	K	95	ALA	N-CA-CB	5.81	118.23	110.10
4	D	219	ARG	NE-CZ-NH2	-5.81	117.40	120.30
21	S	230	ARG	NE-CZ-NH1	5.81	123.20	120.30
25	U	112	MET	CA-CB-CG	-5.80	103.43	113.30
14	7	140	MET	CG-SD-CE	-5.80	90.92	100.20
29	K	72	PHE	CB-CG-CD1	5.80	124.86	120.80
32	J	16	ALA	N-CA-CB	5.80	118.22	110.10
20	N	488	THR	CA-CB-CG2	-5.80	104.28	112.40
7	G	135	SER	N-CA-C	-5.80	95.35	111.00
16	V	90	VAL	CG1-CB-CG2	-5.80	101.62	110.90
20	N	813	TYR	CB-CG-CD1	-5.80	117.52	121.00
14	7	101	TYR	CB-CG-CD1	5.79	124.48	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O	3	ASP	N-CA-CB	-5.79	100.17	110.60
20	N	484	ALA	CB-CA-C	-5.79	101.41	110.10
23	Q	359	ALA	CB-CA-C	-5.79	101.41	110.10
24	R	268	TYR	CB-CG-CD1	5.79	124.47	121.00
29	K	29	PHE	CB-CG-CD1	-5.79	116.75	120.80
7	G	189	ASP	CB-CG-OD2	-5.79	113.09	118.30
29	K	106	THR	CA-CB-CG2	-5.79	104.30	112.40
22	P	300	PRO	N-CA-CB	5.79	110.24	103.30
14	7	103	ASP	CB-CG-OD2	-5.78	113.09	118.30
20	N	766	PHE	CG-CD1-CE1	5.78	127.16	120.80
27	H	89	SER	N-CA-CB	5.78	119.17	110.50
30	L	295	ARG	NE-CZ-NH2	-5.78	117.41	120.30
27	H	284	ARG	NE-CZ-NH2	5.78	123.19	120.30
27	H	338	ASP	N-CA-CB	5.78	121.00	110.60
1	A	48	ALA	CB-CA-C	-5.78	101.44	110.10
20	N	395	ARG	NE-CZ-NH1	5.77	123.19	120.30
21	S	98	PRO	N-CA-CB	5.77	110.23	103.30
19	Z	751	TYR	CG-CD1-CE1	-5.77	116.69	121.30
13	6	166	GLY	N-CA-C	-5.77	98.68	113.10
13	6	218	ASP	CB-CG-OD2	5.77	123.49	118.30
17	T	190	TYR	CB-CG-CD2	5.77	124.46	121.00
29	K	333	PHE	CB-CA-C	-5.76	98.87	110.40
29	K	340	GLN	CB-CA-C	-5.76	98.88	110.40
31	M	263	PHE	CB-CG-CD1	-5.76	116.77	120.80
14	7	60	PHE	CB-CG-CD1	-5.76	116.77	120.80
2	B	108	ALA	CB-CA-C	-5.75	101.47	110.10
20	N	909	GLY	N-CA-C	-5.75	98.72	113.10
28	I	343	ARG	NE-CZ-NH2	-5.75	117.42	120.30
28	I	353	PHE	CB-CG-CD1	-5.75	116.77	120.80
3	C	43	VAL	CG1-CB-CG2	-5.75	101.70	110.90
20	N	68	PHE	CB-CG-CD1	5.75	124.82	120.80
29	K	398	ASP	CB-CG-OD1	-5.75	113.13	118.30
9	2	75	SER	N-CA-CB	5.75	119.12	110.50
32	J	24	TYR	CB-CG-CD2	-5.75	117.55	121.00
24	R	293	ARG	NE-CZ-NH2	-5.74	117.43	120.30
26	O	309	LEU	O-C-N	-5.74	113.51	122.70
29	K	84	SER	C-N-CA	5.74	136.06	121.70
11	4	134	TYR	CB-CG-CD1	-5.74	117.56	121.00
21	S	126	PHE	CB-CG-CD2	-5.74	116.78	120.80
14	7	223	ARG	NE-CZ-NH2	-5.74	117.43	120.30
21	S	340	ASP	CB-CG-OD2	-5.74	113.14	118.30
11	4	125	ALA	N-CA-CB	5.74	118.13	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	J	102	ASN	O-C-N	5.74	131.88	122.70
1	A	88	ARG	NE-CZ-NH2	-5.74	117.43	120.30
16	V	155	VAL	CB-CA-C	-5.74	100.50	111.40
26	O	108	ASP	N-CA-CB	5.74	120.92	110.60
30	L	22	ALA	N-CA-CB	5.74	118.13	110.10
30	L	227	ARG	NE-CZ-NH2	-5.73	117.43	120.30
20	N	147	TYR	CD1-CE1-CZ	-5.73	114.64	119.80
4	D	135	ILE	CA-CB-CG1	5.73	121.88	111.00
16	V	22	ALA	CB-CA-C	-5.72	101.52	110.10
32	J	283	PHE	CB-CG-CD2	5.72	124.80	120.80
6	F	101	ARG	N-CA-C	-5.72	95.56	111.00
11	4	70	ARG	NE-CZ-NH1	5.72	123.16	120.30
19	Z	822	VAL	CG1-CB-CG2	5.72	120.05	110.90
26	O	113	LEU	CB-CG-CD1	5.72	120.72	111.00
15	W	113	VAL	CG1-CB-CG2	-5.72	101.75	110.90
2	B	51	LYS	CD-CE-NZ	-5.71	98.56	111.70
14	7	129	PRO	N-CD-CG	5.71	111.77	103.20
3	C	156	TYR	CA-CB-CG	5.71	124.25	113.40
5	E	226	PHE	CZ-CE2-CD2	-5.71	113.25	120.10
16	V	112	TYR	CZ-CE2-CD2	5.71	124.94	119.80
16	V	161	ARG	NE-CZ-NH1	5.70	123.15	120.30
4	D	200	ALA	N-CA-CB	-5.70	102.12	110.10
9	2	178	MET	CA-CB-CG	-5.70	103.61	113.30
11	4	73	TYR	CB-CG-CD2	5.70	124.42	121.00
23	Q	133	LEU	CB-CG-CD1	5.70	120.69	111.00
4	D	2	SER	N-CA-CB	5.70	119.05	110.50
13	6	43	ALA	CB-CA-C	-5.70	101.55	110.10
20	N	4	SER	C-N-CA	5.70	135.94	121.70
19	Z	294	MET	CG-SD-CE	-5.70	91.09	100.20
16	V	118	PHE	N-CA-CB	5.69	120.85	110.60
19	Z	311	VAL	CA-CB-CG2	5.69	119.44	110.90
22	P	201	ARG	NE-CZ-NH2	5.69	123.15	120.30
19	Z	496	ASP	CB-CG-OD1	5.69	123.42	118.30
5	E	101	PHE	CB-CG-CD1	5.69	124.78	120.80
16	V	145	VAL	N-CA-C	-5.69	95.64	111.00
21	S	473	HIS	CB-CA-C	-5.69	99.03	110.40
19	Z	728	ALA	N-CA-CB	-5.68	102.14	110.10
20	N	952	ASP	CB-CA-C	-5.68	99.04	110.40
31	M	210	ASN	CA-CB-CG	-5.68	100.90	113.40
21	S	496	SER	N-CA-CB	5.68	119.02	110.50
28	I	71	TYR	CG-CD2-CE2	-5.68	116.76	121.30
31	M	222	PRO	N-CA-CB	5.68	110.11	103.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	136	TRP	CA-CB-CG	5.68	124.49	113.70
13	6	213	ASP	CB-CG-OD2	-5.68	113.19	118.30
9	2	46	ILE	N-CA-C	-5.67	95.68	111.00
22	P	339	ASP	CB-CG-OD1	5.67	123.41	118.30
22	P	417	ARG	NE-CZ-NH1	5.67	123.14	120.30
25	U	228	TYR	CA-CB-CG	5.67	124.18	113.40
19	Z	232	TYR	CB-CG-CD1	5.67	124.40	121.00
2	B	194	THR	CA-CB-CG2	-5.67	104.46	112.40
9	2	72	LYS	O-C-N	5.67	131.77	122.70
31	M	181	ASP	N-CA-C	-5.67	95.69	111.00
3	C	85	VAL	CB-CA-C	5.67	122.17	111.40
13	6	200	ARG	NH1-CZ-NH2	5.67	125.63	119.40
16	V	292	MET	CG-SD-CE	-5.67	91.13	100.20
21	S	114	HIS	CA-CB-CG	-5.67	103.97	113.60
29	K	361	GLU	CG-CD-OE1	5.67	129.63	118.30
19	Z	34	ARG	NE-CZ-NH1	5.67	123.13	120.30
14	7	80	PHE	CB-CG-CD2	-5.66	116.84	120.80
22	P	317	TRP	CA-CB-CG	5.66	124.46	113.70
31	M	367	ARG	NE-CZ-NH1	-5.66	117.47	120.30
21	S	355	PRO	N-CA-CB	5.66	110.09	103.30
29	K	296	MET	CG-SD-CE	-5.66	91.14	100.20
7	G	105	TYR	N-CA-CB	5.66	120.78	110.60
12	5	120	ARG	NE-CZ-NH1	-5.66	117.47	120.30
23	Q	220	ALA	N-CA-CB	5.66	118.02	110.10
14	7	253	TRP	CB-CG-CD2	-5.66	119.25	126.60
2	B	82	ASP	CB-CG-OD2	5.66	123.39	118.30
27	H	154	PRO	N-CA-CB	5.66	110.09	103.30
20	N	926	GLU	CA-C-N	5.65	132.93	117.10
22	P	396	LEU	CB-CG-CD1	5.65	120.61	111.00
8	1	78	ARG	NH1-CZ-NH2	-5.65	113.18	119.40
10	3	66	ARG	NE-CZ-NH1	-5.65	117.47	120.30
30	L	400	TYR	CB-CG-CD1	-5.65	117.61	121.00
11	4	52	ASP	CB-CG-OD1	-5.65	113.22	118.30
31	M	245	ALA	N-CA-CB	-5.65	102.20	110.10
22	P	213	PHE	CB-CG-CD2	-5.64	116.85	120.80
27	H	312	ARG	NH1-CZ-NH2	5.64	125.61	119.40
21	S	76	ARG	NE-CZ-NH1	5.64	123.12	120.30
22	P	412	VAL	CG1-CB-CG2	5.64	119.93	110.90
11	4	191	LEU	CB-CA-C	-5.64	99.49	110.20
25	U	43	TRP	O-C-N	5.64	131.72	122.70
3	C	36	GLY	N-CA-C	-5.64	99.01	113.10
22	P	174	TYR	CB-CG-CD2	-5.64	117.62	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	K	229	ARG	N-CA-C	-5.64	95.78	111.00
11	4	183	ILE	N-CA-C	-5.63	95.79	111.00
17	T	131	PHE	CB-CG-CD2	-5.63	116.86	120.80
19	Z	310	ASP	CB-CG-OD1	-5.63	113.23	118.30
23	Q	316	ASP	CB-CG-OD1	5.63	123.37	118.30
21	S	186	ASP	CB-CG-OD2	5.63	123.37	118.30
17	T	328	PRO	N-CA-CB	5.63	110.06	103.30
6	F	12	VAL	CA-CB-CG2	-5.63	102.46	110.90
1	A	103	TYR	CB-CG-CD1	-5.63	117.62	121.00
20	N	493	VAL	CA-CB-CG1	-5.63	102.46	110.90
25	U	59	ASP	CB-CG-OD2	-5.62	113.24	118.30
25	U	138	TYR	CB-CA-C	-5.62	99.15	110.40
16	V	218	LEU	CB-CA-C	-5.62	99.51	110.20
24	R	183	TYR	CG-CD1-CE1	-5.62	116.80	121.30
26	O	198	PHE	CG-CD1-CE1	-5.62	114.61	120.80
25	U	151	THR	CA-CB-CG2	-5.62	104.53	112.40
2	B	220	ARG	NE-CZ-NH2	-5.62	117.49	120.30
4	D	78	SER	N-CA-CB	5.62	118.93	110.50
13	6	65	ARG	N-CA-CB	5.62	120.71	110.60
17	T	98	TYR	CB-CG-CD1	-5.62	117.63	121.00
14	7	208	GLU	CB-CG-CD	-5.62	99.04	114.20
17	T	169	ARG	NE-CZ-NH1	5.62	123.11	120.30
21	S	235	THR	N-CA-CB	5.62	120.97	110.30
21	S	255	LEU	CB-CG-CD1	5.62	120.55	111.00
22	P	27	ARG	NE-CZ-NH1	-5.62	117.49	120.30
29	K	248	ARG	CB-CA-C	-5.62	99.17	110.40
17	T	169	ARG	NE-CZ-NH2	-5.61	117.49	120.30
20	N	543	LYS	CB-CA-C	-5.61	99.17	110.40
11	4	47	VAL	CA-CB-CG1	-5.61	102.48	110.90
31	M	441	TYR	CA-CB-CG	5.61	124.06	113.40
17	T	190	TYR	CZ-CE2-CD2	5.61	124.85	119.80
19	Z	852	VAL	CA-CB-CG2	-5.61	102.49	110.90
27	H	295	VAL	CG1-CB-CG2	5.61	119.87	110.90
29	K	408	LYS	N-CA-CB	5.61	120.69	110.60
28	I	322	ARG	N-CA-CB	5.61	120.69	110.60
9	2	157	TYR	CZ-CE2-CD2	-5.60	114.76	119.80
22	P	227	TYR	CD1-CE1-CZ	-5.60	114.76	119.80
3	C	132	VAL	CG1-CB-CG2	-5.59	101.95	110.90
20	N	131	GLU	C-N-CA	5.59	134.05	122.30
26	O	35	HIS	CA-CB-CG	5.59	123.11	113.60
26	O	356	TRP	CB-CG-CD1	5.59	134.27	127.00
30	L	67	VAL	CA-CB-CG1	-5.59	102.51	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	304	TYR	CB-CG-CD1	5.59	124.36	121.00
11	4	85	ARG	NE-CZ-NH2	-5.59	117.50	120.30
19	Z	636	ASP	CB-CG-OD1	5.59	123.33	118.30
23	Q	137	TYR	CB-CG-CD1	5.59	124.35	121.00
1	A	125	TYR	CB-CG-CD2	-5.59	117.65	121.00
4	D	145	ASP	CB-CG-OD1	5.59	123.33	118.30
31	M	93	VAL	CA-CB-CG2	-5.59	102.52	110.90
16	V	278	GLN	N-CA-CB	5.59	120.66	110.60
4	D	6	ALA	CB-CA-C	-5.59	101.72	110.10
28	I	259	TYR	CB-CG-CD2	-5.59	117.65	121.00
14	7	139	ALA	O-C-N	-5.58	113.77	122.70
20	N	408	LEU	CB-CG-CD1	5.58	120.49	111.00
20	N	665	ASN	N-CA-CB	5.58	120.65	110.60
21	S	226	PHE	CB-CG-CD1	-5.58	116.89	120.80
32	J	364	THR	CA-CB-CG2	-5.58	104.58	112.40
12	5	146	VAL	CG1-CB-CG2	5.58	119.83	110.90
21	S	163	LEU	CB-CG-CD2	5.58	120.49	111.00
22	P	198	ASP	CB-CG-OD2	-5.58	113.28	118.30
5	E	71	ASP	N-CA-C	-5.57	95.95	111.00
24	R	197	ALA	C-N-CA	5.57	135.63	121.70
4	D	1	MET	CG-SD-CE	-5.57	91.29	100.20
3	C	57	ASP	CB-CG-OD1	-5.57	113.29	118.30
8	1	94	TYR	CB-CG-CD1	5.57	124.34	121.00
13	6	240	ASP	CB-CG-OD2	-5.57	113.29	118.30
30	L	146	TYR	CD1-CE1-CZ	5.57	124.81	119.80
21	S	475	ARG	N-CA-CB	5.57	120.62	110.60
20	N	449	ILE	CA-CB-CG1	5.56	121.57	111.00
27	H	133	ASP	CB-CG-OD1	-5.56	113.29	118.30
30	L	245	PHE	CB-CG-CD1	-5.56	116.91	120.80
31	M	91	TYR	CB-CG-CD2	5.56	124.34	121.00
19	Z	489	TYR	CA-C-N	5.56	129.43	117.20
25	U	162	ILE	N-CA-C	-5.56	95.99	111.00
16	V	107	MET	CG-SD-CE	-5.56	91.31	100.20
25	U	259	VAL	CA-CB-CG2	-5.56	102.56	110.90
32	J	44	ARG	NE-CZ-NH2	-5.56	117.52	120.30
32	J	387	VAL	CA-CB-CG1	5.56	119.24	110.90
5	E	140	ALA	N-CA-CB	5.55	117.88	110.10
25	U	54	PHE	CB-CG-CD2	-5.55	116.91	120.80
29	K	41	TYR	CB-CG-CD2	-5.55	117.67	121.00
30	L	88	THR	CA-CB-CG2	-5.55	104.63	112.40
30	L	92	ARG	NH1-CZ-NH2	-5.55	113.30	119.40
3	C	82	ASP	CB-CG-OD2	-5.55	113.31	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	235	LEU	N-CA-C	-5.55	96.03	111.00
13	6	182	PHE	CB-CG-CD2	5.55	124.68	120.80
20	N	371	ILE	CA-CB-CG1	5.55	121.54	111.00
32	J	223	PHE	CB-CG-CD2	-5.55	116.92	120.80
23	Q	279	TYR	CB-CG-CD1	5.54	124.33	121.00
30	L	255	ARG	NE-CZ-NH2	-5.54	117.53	120.30
6	F	179	PHE	CB-CG-CD1	5.54	124.68	120.80
11	4	103	LEU	N-CA-CB	5.54	121.49	110.40
22	P	377	ARG	NE-CZ-NH2	5.54	123.07	120.30
28	I	365	PHE	CB-CG-CD1	5.54	124.68	120.80
29	K	248	ARG	N-CA-CB	5.54	120.58	110.60
5	E	143	PHE	CB-CG-CD1	5.54	124.68	120.80
13	6	84	PHE	N-CA-CB	5.54	120.56	110.60
32	J	293	MET	CG-SD-CE	-5.54	91.34	100.20
22	P	139	GLU	OE1-CD-OE2	-5.53	116.66	123.30
24	R	219	PHE	CB-CG-CD2	-5.53	116.93	120.80
19	Z	593	THR	CA-CB-CG2	-5.53	104.66	112.40
22	P	308	LEU	CB-CG-CD2	5.53	120.40	111.00
22	P	342	SER	N-CA-C	-5.53	96.08	111.00
23	Q	337	ARG	NE-CZ-NH2	-5.53	117.54	120.30
24	R	287	LEU	CB-CG-CD2	5.53	120.39	111.00
19	Z	838	ARG	NE-CZ-NH1	5.52	123.06	120.30
19	Z	865	PHE	CB-CG-CD2	5.52	124.67	120.80
20	N	240	ASP	O-C-N	-5.52	113.86	122.70
21	S	439	ARG	NE-CZ-NH1	5.52	123.06	120.30
31	M	47	ARG	NH1-CZ-NH2	5.52	125.47	119.40
2	B	49	GLU	N-CA-CB	5.52	120.54	110.60
17	T	272	ASP	CB-CG-OD1	5.52	123.27	118.30
3	C	91	ARG	CB-CA-C	-5.52	99.36	110.40
10	3	157	ASN	N-CA-C	-5.52	96.10	111.00
12	5	62	THR	N-CA-CB	5.52	120.79	110.30
17	T	311	TRP	CD1-NE1-CE2	5.52	113.97	109.00
19	Z	304	PHE	CB-CG-CD2	-5.52	116.94	120.80
24	R	70	LEU	CB-CG-CD2	5.52	120.38	111.00
28	I	327	VAL	CA-CB-CG1	5.52	119.18	110.90
10	3	199	THR	N-CA-CB	5.52	120.78	110.30
20	N	194	ARG	NE-CZ-NH1	-5.52	117.54	120.30
32	J	111	ASN	N-CA-CB	5.52	120.53	110.60
13	6	53	ASP	CB-CG-OD1	5.52	123.26	118.30
16	V	46	ARG	NE-CZ-NH1	-5.52	117.54	120.30
16	V	234	TYR	N-CA-CB	5.52	120.53	110.60
23	Q	116	TRP	CB-CG-CD1	5.52	134.17	127.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	H	401	ARG	CG-CD-NE	-5.51	100.22	111.80
23	Q	120	GLU	OE1-CD-OE2	5.51	129.91	123.30
31	M	234	THR	CA-CB-CG2	-5.51	104.68	112.40
8	1	49	ALA	N-CA-CB	5.51	117.81	110.10
21	S	88	ARG	NE-CZ-NH2	-5.51	117.55	120.30
27	H	122	VAL	CA-CB-CG2	-5.51	102.64	110.90
2	B	2	ALA	N-CA-CB	5.51	117.81	110.10
14	7	130	ARG	NE-CZ-NH2	5.51	123.05	120.30
1	A	70	PHE	CB-CG-CD2	5.51	124.66	120.80
5	E	198	SER	CB-CA-C	-5.51	99.64	110.10
9	2	155	SER	N-CA-CB	5.50	118.75	110.50
20	N	516	LEU	CB-CG-CD2	5.50	120.36	111.00
29	K	79	VAL	C-N-CA	5.50	135.46	121.70
2	B	46	LEU	CB-CA-C	-5.50	99.75	110.20
13	6	84	PHE	CD1-CG-CD2	5.50	125.45	118.30
25	U	209	ARG	NE-CZ-NH2	5.50	123.05	120.30
22	P	250	ILE	CA-CB-CG2	5.50	121.90	110.90
29	K	373	ALA	N-CA-CB	5.50	117.80	110.10
4	D	178	LEU	CB-CG-CD2	5.50	120.35	111.00
10	3	140	GLY	N-CA-C	-5.50	99.35	113.10
14	7	153	THR	N-CA-C	-5.50	96.15	111.00
27	H	208	PRO	N-CA-CB	5.50	109.90	103.30
31	M	383	ASN	N-CA-CB	5.50	120.50	110.60
19	Z	350	LYS	CB-CA-C	-5.50	99.41	110.40
23	Q	334	ASN	N-CA-CB	5.50	120.50	110.60
26	O	246	ASP	O-C-N	-5.50	113.91	122.70
16	V	171	GLY	O-C-N	5.49	131.49	122.70
24	R	46	ARG	NE-CZ-NH1	5.49	123.05	120.30
13	6	172	LEU	CB-CG-CD1	5.49	120.34	111.00
22	P	94	ARG	NH1-CZ-NH2	5.49	125.44	119.40
23	Q	201	TYR	CG-CD1-CE1	-5.49	116.91	121.30
20	N	948	PHE	CB-CG-CD1	5.49	124.64	120.80
28	I	112	LEU	CB-CG-CD2	5.49	120.33	111.00
14	7	54	SER	O-C-N	-5.49	113.92	122.70
20	N	341	PHE	CB-CG-CD2	-5.49	116.96	120.80
29	K	300	ASP	CB-CG-OD1	5.49	123.24	118.30
19	Z	729	MET	CG-SD-CE	-5.48	91.43	100.20
31	M	323	PHE	CB-CG-CD1	5.48	124.64	120.80
4	D	151	TYR	CB-CG-CD2	-5.48	117.71	121.00
29	K	403	TYR	CB-CG-CD1	-5.48	117.71	121.00
21	S	146	ARG	N-CA-CB	-5.48	100.74	110.60
30	L	26	TYR	CB-CG-CD1	-5.48	117.71	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	157	TRP	N-CA-CB	5.48	120.46	110.60
28	I	210	TYR	CB-CG-CD1	-5.48	117.71	121.00
11	4	85	ARG	NE-CZ-NH1	5.47	123.04	120.30
15	W	27	GLN	N-CA-CB	5.47	120.45	110.60
16	V	66	THR	N-CA-CB	5.47	120.70	110.30
26	O	333	MET	N-CA-CB	5.47	120.45	110.60
8	1	152	MET	N-CA-CB	5.47	120.45	110.60
26	O	298	LYS	N-CA-CB	5.47	120.45	110.60
4	D	199	LYS	CB-CA-C	-5.47	99.46	110.40
30	L	237	ARG	CG-CD-NE	-5.47	100.32	111.80
30	L	47	LEU	CB-CG-CD2	5.47	120.30	111.00
8	1	82	ALA	N-CA-CB	5.47	117.75	110.10
16	V	139	ARG	O-C-N	5.47	131.45	122.70
20	N	600	ARG	NE-CZ-NH2	5.47	123.03	120.30
20	N	236	LEU	C-N-CA	5.46	135.36	121.70
27	H	337	LEU	N-CA-CB	5.46	121.32	110.40
30	L	124	TYR	CZ-CE2-CD2	-5.46	114.89	119.80
7	G	159	TYR	CB-CG-CD2	5.46	124.28	121.00
26	O	343	LEU	CB-CG-CD2	5.46	120.28	111.00
22	P	107	GLN	CB-CA-C	-5.46	99.48	110.40
25	U	74	TYR	CG-CD1-CE1	-5.46	116.93	121.30
27	H	323	ARG	NH1-CZ-NH2	-5.46	113.40	119.40
28	I	350	LYS	CB-CA-C	-5.46	99.48	110.40
19	Z	754	LYS	C-N-CA	5.46	135.34	121.70
31	M	154	VAL	O-C-N	5.46	132.47	123.20
24	R	208	PHE	CD1-CG-CD2	5.46	125.39	118.30
27	H	204	LEU	CB-CG-CD2	5.46	120.27	111.00
32	J	211	PHE	CB-CG-CD2	-5.46	116.98	120.80
12	5	133	ILE	N-CA-C	-5.45	96.28	111.00
14	7	212	LEU	CB-CG-CD1	5.45	120.27	111.00
9	2	146	VAL	CB-CA-C	-5.45	101.04	111.40
23	Q	229	TYR	CB-CG-CD1	-5.45	117.73	121.00
23	Q	323	LEU	N-CA-CB	5.45	121.30	110.40
32	J	232	ARG	NH1-CZ-NH2	-5.45	113.41	119.40
10	3	117	PHE	CB-CG-CD1	-5.45	116.99	120.80
31	M	384	TYR	CZ-CE2-CD2	-5.45	114.90	119.80
2	B	134	LEU	CB-CG-CD1	5.45	120.26	111.00
17	T	145	ILE	CA-CB-CG1	5.45	121.35	111.00
19	Z	555	ALA	CB-CA-C	-5.44	101.94	110.10
28	I	322	ARG	NE-CZ-NH1	5.44	123.02	120.30
26	O	163	TYR	N-CA-CB	5.44	120.39	110.60
7	G	145	ASP	CB-CG-OD2	5.44	123.19	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O	148	VAL	CG1-CB-CG2	-5.44	102.20	110.90
20	N	682	TYR	CG-CD1-CE1	-5.44	116.95	121.30
4	D	24	GLU	OE1-CD-OE2	5.43	129.82	123.30
19	Z	363	SER	O-C-N	5.43	131.39	122.70
21	S	276	ALA	N-CA-CB	5.43	117.71	110.10
20	N	273	THR	CA-CB-OG1	5.43	120.41	109.00
12	5	245	ARG	NE-CZ-NH2	5.43	123.02	120.30
19	Z	621	ASP	N-CA-C	-5.43	96.34	111.00
20	N	865	LYS	N-CA-CB	5.43	120.37	110.60
30	L	265	ARG	NE-CZ-NH2	-5.43	117.58	120.30
32	J	249	ASP	CB-CG-OD2	5.43	123.19	118.30
14	7	106	TYR	CG-CD2-CE2	-5.43	116.96	121.30
12	5	143	ALA	CB-CA-C	-5.43	101.96	110.10
20	N	813	TYR	CG-CD1-CE1	-5.43	116.96	121.30
22	P	91	SER	C-N-CA	5.43	135.27	121.70
19	Z	301	HIS	N-CA-CB	5.42	120.36	110.60
20	N	942	PRO	N-CA-CB	5.42	109.81	103.30
21	S	272	PHE	CB-CG-CD2	5.42	124.60	120.80
12	5	212	TYR	CB-CG-CD1	-5.42	117.75	121.00
27	H	174	TYR	CG-CD1-CE1	-5.42	116.96	121.30
17	T	235	LEU	O-C-N	-5.42	114.03	122.70
31	M	88	THR	C-N-CA	5.42	135.25	121.70
13	6	206	PHE	CB-CG-CD1	5.42	124.59	120.80
4	D	6	ALA	N-CA-CB	5.42	117.68	110.10
26	O	54	ASP	CB-CG-OD1	5.42	123.17	118.30
29	K	230	VAL	N-CA-C	-5.42	96.38	111.00
31	M	434	LYS	C-N-CA	5.42	135.24	121.70
19	Z	861	THR	N-CA-C	-5.41	96.38	111.00
4	D	76	VAL	CB-CA-C	-5.41	101.12	111.40
3	C	97	TYR	CZ-CE2-CD2	5.41	124.67	119.80
14	7	90	ASN	N-CA-CB	5.41	120.34	110.60
25	U	95	TYR	CB-CG-CD2	-5.41	117.75	121.00
5	E	162	PHE	CB-CG-CD1	5.41	124.59	120.80
24	R	18	ARG	NE-CZ-NH2	-5.41	117.60	120.30
20	N	628	ARG	CA-CB-CG	5.41	125.29	113.40
25	U	156	GLU	OE1-CD-OE2	5.41	129.78	123.30
31	M	423	TYR	CG-CD1-CE1	5.41	125.62	121.30
28	I	336	THR	CA-CB-CG2	-5.40	104.83	112.40
5	E	88	LEU	CB-CG-CD1	5.40	120.18	111.00
19	Z	421	ASP	CB-CG-OD2	-5.40	113.44	118.30
29	K	166	ASP	N-CA-CB	5.40	120.32	110.60
30	L	52	LYS	N-CA-CB	5.40	120.32	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	K	60	TYR	CD1-CE1-CZ	-5.40	114.94	119.80
14	7	196	GLU	OE1-CD-OE2	5.40	129.78	123.30
29	K	315	ASP	CB-CG-OD1	5.40	123.16	118.30
20	N	384	GLN	CA-CB-CG	5.39	125.26	113.40
32	J	345	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
6	F	123	TYR	CD1-CG-CD2	5.39	123.83	117.90
12	5	201	GLY	N-CA-C	5.39	126.58	113.10
19	Z	457	ASN	CB-CA-C	-5.39	99.62	110.40
9	2	60	ASP	N-CA-CB	5.39	120.30	110.60
20	N	698	GLN	CG-CD-OE1	-5.39	110.82	121.60
1	A	42	VAL	CA-CB-CG2	-5.39	102.82	110.90
19	Z	586	PRO	C-N-CA	5.39	135.17	121.70
20	N	243	LEU	CB-CG-CD2	5.39	120.16	111.00
12	5	193	TYR	CG-CD2-CE2	-5.38	116.99	121.30
25	U	33	LYS	N-CA-CB	5.38	120.29	110.60
28	I	371	ARG	NE-CZ-NH2	5.38	122.99	120.30
30	L	281	PHE	CG-CD2-CE2	-5.38	114.88	120.80
11	4	105	ALA	CB-CA-C	-5.38	102.04	110.10
13	6	153	PRO	N-CA-C	-5.37	98.13	112.10
14	7	54	SER	N-CA-C	-5.37	96.49	111.00
21	S	76	ARG	CD-NE-CZ	-5.37	116.08	123.60
26	O	233	LEU	CB-CG-CD2	5.37	120.13	111.00
31	M	271	VAL	CA-CB-CG1	-5.37	102.84	110.90
3	C	57	ASP	CB-CG-OD2	5.37	123.13	118.30
30	L	257	PHE	CG-CD2-CE2	-5.37	114.89	120.80
9	2	49	VAL	CA-CB-CG1	5.37	118.95	110.90
3	C	156	TYR	CG-CD2-CE2	-5.37	117.01	121.30
13	6	204	ASP	CB-CG-OD2	-5.37	113.47	118.30
31	M	423	TYR	CG-CD2-CE2	-5.37	117.01	121.30
14	7	74	TYR	CD1-CE1-CZ	-5.36	114.97	119.80
7	G	126	TYR	CG-CD1-CE1	-5.36	117.01	121.30
20	N	503	GLN	O-C-N	-5.36	114.12	122.70
21	S	296	LEU	N-CA-CB	5.36	121.12	110.40
14	7	218	ARG	NE-CZ-NH1	-5.36	117.62	120.30
20	N	667	GLU	OE1-CD-OE2	5.36	129.73	123.30
24	R	17	LEU	O-C-N	-5.36	114.12	122.70
1	A	189	TRP	CB-CG-CD2	-5.36	119.63	126.60
14	7	238	GLU	N-CA-CB	5.36	120.24	110.60
21	S	170	PHE	CB-CG-CD1	5.36	124.55	120.80
9	2	241	ARG	NE-CZ-NH1	-5.36	117.62	120.30
29	K	309	MET	CB-CA-C	-5.36	99.69	110.40
32	J	382	ASP	CB-CG-OD2	-5.36	113.48	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	228	TYR	CB-CG-CD1	-5.35	117.79	121.00
4	D	158	THR	N-CA-CB	5.35	120.47	110.30
6	F	153	TYR	CB-CG-CD1	-5.35	117.79	121.00
8	1	83	ALA	CB-CA-C	-5.35	102.07	110.10
15	W	70	ARG	NH1-CZ-NH2	-5.35	113.51	119.40
21	S	220	LEU	CB-CG-CD2	5.35	120.10	111.00
24	R	264	TYR	CB-CG-CD1	5.35	124.21	121.00
31	M	384	TYR	CB-CG-CD2	5.35	124.21	121.00
6	F	107	ARG	NH1-CZ-NH2	-5.35	113.51	119.40
6	F	188	VAL	CG1-CB-CG2	5.35	119.46	110.90
8	1	207	ILE	CG1-CB-CG2	-5.35	99.63	111.40
24	R	246	ILE	CA-CB-CG1	5.35	121.17	111.00
25	U	125	ASP	CB-CG-OD2	-5.35	113.48	118.30
7	G	169	ALA	N-CA-CB	5.35	117.59	110.10
22	P	386	VAL	CA-CB-CG2	5.35	118.92	110.90
7	G	8	TYR	CB-CG-CD2	-5.35	117.79	121.00
19	Z	794	ALA	CB-CA-C	-5.35	102.08	110.10
25	U	261	TYR	CB-CG-CD1	-5.35	117.79	121.00
20	N	392	TRP	CH2-CZ2-CE2	5.35	122.75	117.40
29	K	157	ASP	CB-CG-OD1	5.35	123.11	118.30
19	Z	232	TYR	CB-CG-CD2	-5.34	117.79	121.00
24	R	179	ARG	NE-CZ-NH1	-5.34	117.63	120.30
17	T	339	ALA	CB-CA-C	-5.34	102.08	110.10
1	A	132	ARG	NE-CZ-NH1	5.34	122.97	120.30
7	G	150	TYR	CB-CG-CD1	5.34	124.20	121.00
28	I	327	VAL	CB-CA-C	5.34	121.55	111.40
31	M	72	MET	CG-SD-CE	-5.34	91.66	100.20
32	J	405	TRP	CD1-CG-CD2	5.34	110.57	106.30
3	C	208	ALA	N-CA-CB	5.34	117.57	110.10
21	S	45	SER	N-CA-CB	-5.34	102.50	110.50
22	P	357	ARG	NE-CZ-NH2	-5.34	117.63	120.30
12	5	193	TYR	CB-CG-CD2	5.33	124.20	121.00
24	R	25	LEU	CB-CG-CD2	5.33	120.07	111.00
29	K	182	GLU	N-CA-C	5.33	125.41	111.00
26	O	5	PRO	N-CD-CG	5.33	111.20	103.20
31	M	242	ALA	CB-CA-C	-5.33	102.10	110.10
15	W	185	SER	CB-CA-C	-5.33	99.97	110.10
29	K	53	PHE	CB-CG-CD2	-5.33	117.07	120.80
3	C	147	LEU	CB-CG-CD2	5.33	120.06	111.00
6	F	101	ARG	NE-CZ-NH1	5.33	122.96	120.30
12	5	144	ASN	N-CA-CB	5.33	120.19	110.60
30	L	305	ARG	CA-CB-CG	5.33	125.12	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	104	TYR	C-N-CA	5.33	135.02	121.70
14	7	92	SER	N-CA-CB	5.33	118.49	110.50
13	6	134	TYR	CG-CD2-CE2	5.32	125.56	121.30
16	V	36	LEU	CB-CG-CD1	5.32	120.04	111.00
19	Z	227	SER	N-CA-CB	5.32	118.48	110.50
19	Z	590	PHE	CB-CG-CD1	-5.32	117.08	120.80
21	S	88	ARG	NE-CZ-NH1	5.32	122.96	120.30
25	U	53	SER	N-CA-CB	5.32	118.48	110.50
7	G	119	TYR	CD1-CE1-CZ	-5.32	115.02	119.80
21	S	124	ARG	NE-CZ-NH1	5.32	122.96	120.30
21	S	212	ARG	NE-CZ-NH1	5.32	122.96	120.30
19	Z	776	LEU	CB-CG-CD2	5.31	120.03	111.00
4	D	4	ASP	CB-CG-OD1	-5.31	113.52	118.30
3	C	217	THR	N-CA-C	-5.31	96.66	111.00
19	Z	310	ASP	CB-CG-OD2	5.31	123.08	118.30
20	N	34	PHE	CZ-CE2-CD2	-5.31	113.73	120.10
27	H	77	LEU	N-CA-CB	5.31	121.02	110.40
28	I	414	VAL	CG1-CB-CG2	5.31	119.40	110.90
10	3	142	CYS	C-N-CA	5.31	134.97	121.70
10	3	70	ARG	NE-CZ-NH2	5.31	122.95	120.30
22	P	316	ARG	NE-CZ-NH1	5.31	122.95	120.30
25	U	141	VAL	CA-CB-CG1	-5.31	102.94	110.90
29	K	305	VAL	CA-CB-CG2	-5.31	102.94	110.90
11	4	150	THR	CA-CB-CG2	-5.30	104.97	112.40
19	Z	83	ARG	CG-CD-NE	-5.30	100.66	111.80
28	I	337	LEU	O-C-N	-5.30	114.21	122.70
7	G	239	TYR	CZ-CE2-CD2	5.30	124.57	119.80
23	Q	88	LEU	N-CA-CB	5.30	121.00	110.40
28	I	400	THR	CA-CB-CG2	-5.30	104.98	112.40
9	2	170	MET	CA-CB-CG	5.30	122.31	113.30
19	Z	785	ARG	NH1-CZ-NH2	5.30	125.23	119.40
22	P	230	MET	CG-SD-CE	-5.30	91.72	100.20
10	3	27	ARG	NE-CZ-NH2	-5.30	117.65	120.30
11	4	114	ALA	CB-CA-C	5.30	118.04	110.10
26	O	4	VAL	CA-C-N	5.30	131.93	117.10
6	F	7	ASP	CB-CA-C	-5.29	99.81	110.40
15	W	113	VAL	N-CA-C	-5.29	96.70	111.00
19	Z	800	LEU	CB-CG-CD2	5.29	120.00	111.00
26	O	47	ASP	CA-C-O	-5.29	108.98	120.10
29	K	252	ARG	NE-CZ-NH1	5.29	122.95	120.30
19	Z	278	VAL	CA-CB-CG1	5.29	118.84	110.90
19	Z	296	PHE	CB-CG-CD1	5.29	124.50	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	S	61	ARG	NE-CZ-NH2	-5.29	117.66	120.30
31	M	106	ASP	CB-CG-OD2	-5.29	113.54	118.30
12	5	166	ARG	C-N-CA	5.29	133.41	122.30
30	L	124	TYR	CD1-CG-CD2	5.29	123.72	117.90
12	5	127	LEU	CB-CG-CD2	5.29	119.99	111.00
22	P	236	HIS	N-CA-CB	5.29	120.11	110.60
32	J	273	MET	CA-CB-CG	5.29	122.29	113.30
24	R	348	ASP	N-CA-C	-5.28	96.74	111.00
3	C	31	ALA	C-N-CA	5.28	133.39	122.30
24	R	213	LEU	CB-CG-CD2	5.28	119.98	111.00
4	D	10	PHE	CB-CG-CD2	-5.28	117.10	120.80
22	P	370	TYR	CB-CG-CD1	-5.28	117.83	121.00
15	W	57	ASP	C-N-CA	5.28	134.89	121.70
19	Z	51	GLN	CG-CD-OE1	-5.28	111.04	121.60
14	7	188	TYR	CB-CG-CD1	-5.28	117.83	121.00
15	W	164	ASP	CB-CG-OD2	-5.28	113.55	118.30
16	V	78	SER	N-CA-CB	5.28	118.41	110.50
24	R	48	ASN	C-N-CA	5.28	134.89	121.70
28	I	59	ARG	NE-CZ-NH1	5.28	122.94	120.30
28	I	428	TYR	CB-CG-CD2	5.28	124.17	121.00
3	C	222	LYS	O-C-N	5.27	131.14	122.70
3	C	233	VAL	CA-CB-CG1	-5.27	102.99	110.90
16	V	74	ALA	C-N-CA	5.27	134.88	121.70
20	N	136	LYS	CB-CA-C	-5.27	99.86	110.40
14	7	222	TYR	CB-CG-CD2	5.27	124.16	121.00
17	T	336	THR	CA-CB-CG2	-5.27	105.03	112.40
17	T	209	ALA	CB-CA-C	-5.27	102.20	110.10
28	I	91	LYS	CA-C-O	-5.27	109.04	120.10
28	I	103	ARG	CA-CB-CG	5.26	124.98	113.40
31	M	384	TYR	CB-CG-CD1	-5.26	117.84	121.00
4	D	210	LYS	N-CA-CB	5.26	120.07	110.60
25	U	127	LYS	CA-C-N	5.26	131.84	117.10
6	F	89	ARG	N-CA-CB	5.26	120.07	110.60
8	1	219	ARG	NE-CZ-NH2	-5.26	117.67	120.30
16	V	73	PHE	N-CA-C	-5.26	96.80	111.00
20	N	481	LEU	CB-CG-CD1	5.26	119.94	111.00
28	I	337	LEU	CB-CG-CD1	5.26	119.94	111.00
1	A	8	GLY	N-CA-C	-5.26	99.95	113.10
4	D	213	GLU	N-CA-C	-5.26	96.80	111.00
17	T	190	TYR	CA-CB-CG	-5.26	103.41	113.40
21	S	110	TYR	CB-CG-CD1	-5.26	117.84	121.00
19	Z	615	ILE	O-C-N	-5.26	114.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	N	771	PHE	CB-CG-CD2	-5.26	117.12	120.80
29	K	374	ASP	CB-CG-OD2	-5.26	113.57	118.30
20	N	48	LEU	CB-CG-CD2	-5.25	102.07	111.00
3	C	13	SER	CA-C-N	5.25	131.81	117.10
20	N	927	PRO	C-N-CA	5.25	134.83	121.70
23	Q	412	ASP	CB-CG-OD1	5.25	123.03	118.30
27	H	397	ILE	N-CA-CB	5.25	122.88	110.80
24	R	150	PHE	O-C-N	5.25	131.10	122.70
27	H	171	ASP	CB-CG-OD2	-5.25	113.58	118.30
9	2	71	ASP	CB-CG-OD2	-5.25	113.58	118.30
11	4	119	ASP	CB-CA-C	-5.25	99.91	110.40
31	M	171	TYR	CB-CG-CD2	5.25	124.15	121.00
31	M	332	ILE	N-CA-C	-5.25	96.84	111.00
19	Z	681	TYR	CB-CG-CD1	-5.25	117.85	121.00
30	L	256	ARG	NE-CZ-NH2	-5.25	117.68	120.30
21	S	472	PHE	CB-CG-CD2	5.24	124.47	120.80
28	I	164	MET	CG-SD-CE	-5.24	91.81	100.20
26	O	351	ASP	CB-CG-OD2	-5.24	113.58	118.30
22	P	427	ASP	CB-CG-OD1	5.23	123.01	118.30
31	M	30	ASP	CB-CG-OD2	5.23	123.01	118.30
32	J	310	ARG	NE-CZ-NH1	5.23	122.92	120.30
11	4	3	TYR	CG-CD2-CE2	-5.23	117.11	121.30
20	N	490	ARG	NE-CZ-NH2	-5.23	117.68	120.30
21	S	351	ARG	NH1-CZ-NH2	-5.23	113.64	119.40
32	J	69	GLN	O-C-N	-5.23	114.31	123.20
4	D	172	LYS	CB-CG-CD	5.23	125.20	111.60
20	N	775	LEU	CB-CG-CD2	5.23	119.89	111.00
19	Z	369	ARG	NE-CZ-NH1	5.23	122.92	120.30
19	Z	597	VAL	CA-CB-CG2	-5.23	103.06	110.90
10	3	73	LEU	O-C-N	-5.23	114.34	122.70
17	T	237	GLN	N-CA-CB	5.23	120.01	110.60
20	N	51	ASP	CB-CG-OD2	5.23	123.00	118.30
3	C	179	TYR	CB-CG-CD2	-5.22	117.87	121.00
8	1	169	TYR	CB-CG-CD2	5.22	124.13	121.00
1	A	240	VAL	CA-CB-CG1	-5.22	103.07	110.90
5	E	50	VAL	CG1-CB-CG2	5.22	119.25	110.90
15	W	91	ARG	CD-NE-CZ	5.22	130.91	123.60
29	K	136	SER	N-CA-CB	5.22	118.33	110.50
31	M	314	LEU	CB-CG-CD1	5.22	119.87	111.00
7	G	71	ASP	CB-CA-C	5.22	120.83	110.40
12	5	132	ARG	NE-CZ-NH2	-5.22	117.69	120.30
14	7	144	ARG	NH1-CZ-NH2	-5.22	113.66	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	175	ASP	CB-CG-OD2	5.22	122.99	118.30
27	H	265	ARG	NH1-CZ-NH2	-5.22	113.66	119.40
30	L	342	TYR	CG-CD2-CE2	5.22	125.47	121.30
32	J	229	ARG	NE-CZ-NH2	-5.22	117.69	120.30
2	B	87	VAL	CA-CB-CG2	-5.21	103.08	110.90
10	3	164	PHE	CB-CG-CD2	-5.21	117.15	120.80
11	4	120	TYR	CB-CG-CD1	-5.21	117.87	121.00
15	W	57	ASP	CB-CG-OD1	-5.21	113.61	118.30
27	H	331	LEU	CB-CG-CD2	5.21	119.87	111.00
9	2	156	ILE	CA-CB-CG1	5.21	120.90	111.00
17	T	296	PHE	CB-CG-CD2	5.21	124.45	120.80
21	S	166	LEU	CB-CG-CD1	5.21	119.86	111.00
31	M	120	ARG	N-CA-CB	5.21	119.98	110.60
11	4	183	ILE	CA-CB-CG2	-5.21	100.48	110.90
23	Q	145	GLU	OE1-CD-OE2	5.21	129.55	123.30
24	R	137	ARG	NE-CZ-NH2	-5.21	117.70	120.30
20	N	456	ASP	CB-CG-OD2	-5.21	113.61	118.30
24	R	67	MET	CG-SD-CE	-5.21	91.87	100.20
24	R	170	GLU	N-CA-CB	5.21	119.97	110.60
20	N	770	TRP	CH2-CZ2-CE2	5.21	122.61	117.40
30	L	62	LYS	CB-CG-CD	5.20	125.13	111.60
28	I	398	ILE	O-C-N	5.20	131.02	122.70
10	3	110	ALA	CB-CA-C	5.20	117.90	110.10
22	P	185	PHE	CG-CD2-CE2	-5.20	115.08	120.80
22	P	324	TYR	CB-CG-CD1	5.20	124.12	121.00
25	U	255	ASP	CB-CG-OD1	-5.20	113.62	118.30
27	H	334	PRO	CA-C-N	5.20	126.59	116.20
19	Z	209	MET	CA-CB-CG	5.20	122.13	113.30
21	S	347	PRO	C-N-CA	5.20	134.69	121.70
30	L	274	LEU	CB-CG-CD1	5.20	119.83	111.00
8	1	196	ALA	CB-CA-C	-5.19	102.31	110.10
6	F	198	THR	CA-CB-OG1	5.19	119.90	109.00
13	6	162	PHE	CG-CD2-CE2	-5.19	115.09	120.80
30	L	358	ARG	NE-CZ-NH1	5.19	122.90	120.30
31	M	392	ASP	CB-CG-OD1	5.19	122.97	118.30
3	C	49	ARG	NE-CZ-NH1	-5.19	117.70	120.30
4	D	162	TRP	CE3-CZ3-CH2	5.19	126.91	121.20
19	Z	215	ASP	CB-CG-OD2	5.19	122.97	118.30
21	S	497	TYR	CG-CD1-CE1	-5.19	117.15	121.30
23	Q	34	ASP	CB-CG-OD1	5.19	122.97	118.30
32	J	140	VAL	CA-CB-CG1	-5.19	103.11	110.90
4	D	41	VAL	CA-CB-CG2	-5.19	103.12	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	157	TRP	CG-CD2-CE3	-5.19	129.23	133.90
22	P	392	PHE	CB-CG-CD2	5.19	124.43	120.80
23	Q	161	ASP	CB-CG-OD2	5.19	122.97	118.30
23	Q	276	ALA	N-CA-CB	5.19	117.36	110.10
32	J	147	THR	CA-CB-CG2	-5.19	105.14	112.40
20	N	900	TYR	CD1-CG-CD2	5.19	123.60	117.90
32	J	43	ARG	NH1-CZ-NH2	5.19	125.10	119.40
13	6	126	ARG	NE-CZ-NH1	5.18	122.89	120.30
31	M	30	ASP	CB-CA-C	-5.18	100.03	110.40
29	K	275	PHE	CB-CG-CD1	-5.18	117.17	120.80
2	B	8	PHE	CB-CG-CD2	-5.18	117.17	120.80
17	T	218	LEU	N-CA-C	5.18	124.98	111.00
14	7	204	LEU	CA-CB-CG	5.18	127.21	115.30
31	M	171	TYR	CG-CD1-CE1	-5.18	117.16	121.30
4	D	70	CYS	CA-CB-SG	5.18	123.32	114.00
17	T	228	TYR	CB-CG-CD2	-5.18	117.89	121.00
19	Z	846	VAL	N-CA-C	-5.18	97.02	111.00
22	P	110	THR	N-CA-CB	5.18	120.13	110.30
19	Z	304	PHE	N-CA-CB	5.17	119.92	110.60
5	E	173	ALA	N-CA-CB	5.17	117.34	110.10
17	T	161	CYS	N-CA-CB	5.17	119.91	110.60
1	A	62	ASP	N-CA-C	-5.17	97.05	111.00
32	J	286	THR	CA-CB-CG2	-5.17	105.17	112.40
3	C	26	GLU	OE1-CD-OE2	5.17	129.50	123.30
21	S	404	ARG	NE-CZ-NH1	-5.17	117.72	120.30
3	C	73	ALA	N-CA-CB	5.16	117.33	110.10
19	Z	690	VAL	CA-CB-CG1	-5.16	103.16	110.90
19	Z	835	GLU	CB-CG-CD	-5.16	100.26	114.20
8	1	94	TYR	CZ-CE2-CD2	-5.16	115.16	119.80
6	F	160	SER	CB-CA-C	-5.16	100.29	110.10
9	2	172	SER	N-CA-CB	5.16	118.24	110.50
22	P	365	ILE	N-CA-CB	5.16	122.67	110.80
32	J	230	MET	CA-CB-CG	5.16	122.07	113.30
1	A	93	ARG	NE-CZ-NH2	-5.16	117.72	120.30
20	N	918	SER	N-CA-C	-5.16	97.07	111.00
28	I	201	VAL	CA-CB-CG1	-5.16	103.16	110.90
32	J	184	LYS	N-CA-C	-5.16	97.07	111.00
2	B	36	VAL	CG1-CB-CG2	5.16	119.15	110.90
3	C	108	GLU	N-CA-CB	5.16	119.88	110.60
29	K	264	ILE	O-C-N	5.16	130.95	122.70
30	L	35	GLU	OE1-CD-OE2	5.16	129.49	123.30
1	A	103	TYR	CD1-CG-CD2	5.15	123.57	117.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	74	ALA	CB-CA-C	-5.15	102.37	110.10
26	O	172	TYR	CZ-CE2-CD2	5.15	124.44	119.80
13	6	212	ARG	NE-CZ-NH1	5.15	122.88	120.30
21	S	257	TYR	CB-CG-CD2	-5.15	117.91	121.00
27	H	254	ALA	N-CA-CB	5.15	117.31	110.10
9	2	50	VAL	C-N-CA	5.15	134.57	121.70
27	H	347	ASP	N-CA-CB	5.15	119.87	110.60
31	M	52	ASP	CB-CG-OD2	5.15	122.94	118.30
22	P	127	THR	N-CA-CB	5.15	120.08	110.30
23	Q	240	ASP	CB-CG-OD1	-5.15	113.67	118.30
3	C	132	VAL	CA-CB-CG1	5.14	118.62	110.90
10	3	69	PHE	CB-CG-CD1	-5.14	117.20	120.80
6	F	128	TYR	CZ-CE2-CD2	-5.14	115.17	119.80
6	F	229	VAL	CA-CB-CG2	-5.14	103.19	110.90
17	T	142	GLN	CG-CD-OE1	-5.14	111.31	121.60
19	Z	369	ARG	N-CA-CB	5.14	119.86	110.60
9	2	116	LEU	CB-CG-CD1	5.14	119.74	111.00
11	4	23	SER	N-CA-C	-5.14	97.12	111.00
13	6	75	ASP	CB-CG-OD1	-5.14	113.67	118.30
2	B	98	TYR	CB-CG-CD2	5.14	124.08	121.00
26	O	276	CYS	CA-CB-SG	-5.14	104.75	114.00
28	I	132	TYR	CZ-CE2-CD2	-5.14	115.17	119.80
29	K	204	MET	CG-SD-CE	-5.14	91.98	100.20
2	B	160	ALA	CB-CA-C	-5.14	102.39	110.10
13	6	34	PHE	CB-CG-CD2	-5.14	117.20	120.80
24	R	311	TYR	CB-CG-CD1	-5.14	117.92	121.00
28	I	73	LEU	CB-CG-CD1	5.14	119.73	111.00
29	K	140	VAL	CA-CB-CG1	-5.14	103.20	110.90
10	3	14	MET	N-CA-C	-5.13	97.14	111.00
10	3	33	GLN	N-CA-CB	5.13	119.84	110.60
21	S	287	TYR	CB-CG-CD2	-5.13	117.92	121.00
30	L	145	SER	O-C-N	5.13	130.91	122.70
13	6	203	LYS	CB-CA-C	-5.13	100.14	110.40
16	V	36	LEU	CB-CG-CD2	-5.13	102.28	111.00
19	Z	703	ARG	N-CA-CB	5.13	119.84	110.60
19	Z	803	PHE	N-CA-C	-5.13	97.14	111.00
20	N	770	TRP	CD2-CE2-CZ2	-5.13	116.14	122.30
32	J	340	ARG	NE-CZ-NH2	-5.13	117.73	120.30
2	B	155	TYR	CB-CG-CD2	-5.13	117.92	121.00
24	R	61	LEU	N-CA-CB	5.13	120.66	110.40
1	A	150	GLN	CG-CD-OE1	-5.13	111.34	121.60
6	F	139	ASP	CB-CA-C	-5.13	100.14	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Z	664	GLU	CB-CA-C	-5.13	100.14	110.40
19	Z	734	SER	N-CA-CB	5.13	118.19	110.50
20	N	490	ARG	NE-CZ-NH1	5.13	122.86	120.30
22	P	55	ARG	N-CA-CB	-5.13	101.37	110.60
30	L	92	ARG	N-CA-CB	5.13	119.83	110.60
31	M	105	ASN	CA-CB-CG	-5.13	102.12	113.40
3	C	141	LYS	CB-CA-C	-5.13	100.14	110.40
11	4	90	ASP	CB-CG-OD1	-5.13	113.69	118.30
15	W	10	VAL	CA-CB-CG1	-5.13	103.21	110.90
22	P	89	LEU	CB-CG-CD2	5.13	119.72	111.00
32	J	4	ASP	CB-CG-OD1	5.13	122.91	118.30
23	Q	259	ILE	N-CA-CB	5.12	122.59	110.80
2	B	8	PHE	CB-CG-CD1	5.12	124.39	120.80
22	P	198	ASP	CB-CG-OD1	5.12	122.91	118.30
9	2	203	ALA	N-CA-CB	5.12	117.27	110.10
11	4	5	ILE	CA-CB-CG1	5.12	120.73	111.00
19	Z	349	TYR	CB-CG-CD1	-5.12	117.93	121.00
22	P	145	LEU	C-N-CA	5.12	134.50	121.70
19	Z	804	LEU	O-C-N	-5.12	114.51	122.70
26	O	222	LEU	CB-CA-C	-5.12	100.47	110.20
27	H	237	PHE	CB-CG-CD2	-5.12	117.22	120.80
1	A	115	CYS	CA-CB-SG	5.12	123.21	114.00
8	1	53	THR	N-CA-C	-5.12	97.18	111.00
16	V	78	SER	CB-CA-C	-5.12	100.38	110.10
20	N	176	MET	CG-SD-CE	-5.12	92.01	100.20
19	Z	91	SER	N-CA-CB	5.12	118.17	110.50
22	P	276	LEU	CB-CG-CD1	5.12	119.70	111.00
29	K	112	TYR	CB-CG-CD2	-5.12	117.93	121.00
17	T	338	LEU	CB-CG-CD1	5.12	119.69	111.00
30	L	201	VAL	CA-CB-CG2	5.12	118.57	110.90
21	S	185	ASP	CB-CG-OD1	5.11	122.90	118.30
27	H	141	GLY	N-CA-C	-5.11	100.32	113.10
10	3	77	LYS	CB-CG-CD	5.11	124.89	111.60
21	S	286	TYR	CB-CG-CD2	5.11	124.07	121.00
25	U	228	TYR	N-CA-CB	5.11	119.80	110.60
26	O	59	LEU	CB-CG-CD1	-5.11	102.31	111.00
12	5	113	PHE	CB-CG-CD2	-5.11	117.22	120.80
19	Z	335	ARG	NE-CZ-NH1	5.11	122.85	120.30
22	P	449	GLU	CA-C-O	5.11	130.83	120.10
24	R	124	PHE	CB-CG-CD2	-5.11	117.22	120.80
25	U	256	GLN	CA-CB-CG	5.11	124.64	113.40
28	I	325	VAL	CG1-CB-CG2	5.11	119.07	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	168	VAL	CA-CB-CG2	5.11	118.56	110.90
18	Y	52	PHE	CD1-CG-CD2	-5.11	111.66	118.30
22	P	80	TRP	CG-CD2-CE3	-5.11	129.31	133.90
32	J	147	THR	C-N-CA	5.11	134.47	121.70
3	C	60	PHE	N-CA-C	-5.10	97.22	111.00
6	F	153	TYR	CB-CG-CD2	5.10	124.06	121.00
30	L	212	VAL	CB-CA-C	-5.10	101.71	111.40
29	K	391	ARG	NH1-CZ-NH2	5.10	125.01	119.40
29	K	405	THR	CA-CB-CG2	-5.10	105.26	112.40
30	L	173	PHE	CG-CD2-CE2	5.10	126.41	120.80
7	G	8	TYR	O-C-N	5.10	130.86	122.70
15	W	67	ASP	CB-CG-OD2	-5.10	113.71	118.30
27	H	163	MET	CG-SD-CE	-5.10	92.04	100.20
28	I	338	ASP	CB-CG-OD2	-5.10	113.71	118.30
29	K	335	LEU	CA-C-N	5.10	131.37	117.10
10	3	191	GLU	OE1-CD-OE2	5.10	129.41	123.30
14	7	111	LEU	CB-CG-CD2	5.10	119.66	111.00
9	2	96	ASP	CB-CG-OD2	5.09	122.89	118.30
19	Z	351	THR	O-C-N	-5.09	114.55	122.70
21	S	263	ALA	CB-CA-C	-5.09	102.46	110.10
29	K	285	VAL	CG1-CB-CG2	-5.09	102.75	110.90
17	T	347	ARG	NE-CZ-NH2	-5.09	117.75	120.30
21	S	371	PHE	CB-CG-CD2	5.09	124.36	120.80
27	H	95	VAL	CA-CB-CG2	5.09	118.54	110.90
31	M	395	ASN	C-N-CA	5.09	132.99	122.30
3	C	133	SER	N-CA-C	-5.09	97.26	111.00
11	4	27	GLN	O-C-N	-5.09	114.56	122.70
20	N	188	MET	O-C-N	-5.09	114.56	122.70
31	M	67	HIS	CA-CB-CG	-5.09	104.95	113.60
19	Z	63	LEU	CB-CG-CD2	5.09	119.65	111.00
8	1	127	LEU	CB-CG-CD1	5.09	119.64	111.00
12	5	258	TYR	CG-CD1-CE1	5.09	125.37	121.30
19	Z	830	LEU	CB-CG-CD2	5.09	119.65	111.00
23	Q	302	PHE	CB-CG-CD1	-5.08	117.24	120.80
29	K	417	TYR	CD1-CE1-CZ	-5.08	115.22	119.80
19	Z	824	ALA	CB-CA-C	-5.08	102.48	110.10
20	N	392	TRP	CD2-CE2-CZ2	-5.08	116.20	122.30
7	G	39	GLY	O-C-N	5.08	130.83	122.70
20	N	502	TYR	CD1-CE1-CZ	-5.08	115.23	119.80
19	Z	423	ASP	CB-CG-OD2	-5.08	113.73	118.30
19	Z	509	LYS	N-CA-CB	5.08	119.74	110.60
22	P	12	ARG	NE-CZ-NH2	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	U	68	TRP	CB-CG-CD2	-5.08	120.00	126.60
30	L	373	HIS	N-CA-C	-5.08	97.30	111.00
20	N	802	TYR	N-CA-CB	5.07	119.73	110.60
28	I	390	LEU	C-N-CA	5.07	134.38	121.70
16	V	200	TYR	CB-CG-CD1	-5.07	117.96	121.00
28	I	316	LEU	O-C-N	-5.07	114.59	122.70
8	1	50	ASP	CB-CG-OD1	-5.07	113.74	118.30
27	H	161	VAL	N-CA-CB	-5.07	100.35	111.50
3	C	25	MET	CG-SD-CE	-5.07	92.09	100.20
1	A	189	TRP	CB-CG-CD1	5.07	133.58	127.00
2	B	155	TYR	CB-CG-CD1	5.07	124.04	121.00
4	D	65	LEU	C-N-CA	5.07	134.36	121.70
10	3	147	TYR	CD1-CE1-CZ	5.07	124.36	119.80
19	Z	434	TYR	CG-CD2-CE2	-5.07	117.25	121.30
22	P	96	GLN	N-CA-CB	5.07	119.72	110.60
22	P	116	THR	OG1-CB-CG2	-5.07	98.35	110.00
30	L	39	ARG	NE-CZ-NH2	5.07	122.83	120.30
28	I	307	ARG	NH1-CZ-NH2	5.06	124.97	119.40
16	V	36	LEU	N-CA-CB	5.06	120.52	110.40
23	Q	261	LEU	C-N-CA	5.06	134.35	121.70
23	Q	395	LYS	CA-C-N	5.06	128.33	117.20
31	M	160	SER	N-CA-C	-5.06	97.34	111.00
21	S	249	LEU	O-C-N	5.06	130.79	122.70
23	Q	25	ASP	CB-CG-OD2	-5.06	113.75	118.30
8	1	208	ARG	NH1-CZ-NH2	5.06	124.96	119.40
24	R	297	ARG	NE-CZ-NH1	5.06	122.83	120.30
29	K	128	ALA	CB-CA-C	-5.06	102.52	110.10
11	4	98	TYR	CB-CG-CD2	-5.05	117.97	121.00
25	U	68	TRP	CD1-CG-CD2	5.05	110.34	106.30
27	H	62	LEU	CB-CG-CD2	5.05	119.59	111.00
28	I	239	VAL	CA-CB-CG1	-5.05	103.32	110.90
3	C	50	ARG	NE-CZ-NH1	5.05	122.83	120.30
15	W	17	ARG	NE-CZ-NH2	-5.05	117.78	120.30
23	Q	415	TYR	CB-CG-CD1	5.05	124.03	121.00
20	N	19	LEU	CB-CA-C	-5.05	100.60	110.20
26	O	300	ALA	CB-CA-C	-5.05	102.53	110.10
29	K	387	VAL	CA-CB-CG1	5.05	118.47	110.90
19	Z	266	LEU	CB-CG-CD2	5.05	119.58	111.00
24	R	125	ARG	CA-CB-CG	5.05	124.50	113.40
29	K	234	GLU	CG-CD-OE2	5.05	128.39	118.30
21	S	152	SER	N-CA-CB	5.04	118.06	110.50
21	S	414	SER	N-CA-CB	5.04	118.06	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Q	74	ARG	CA-C-N	5.04	131.22	117.10
12	5	110	ASP	CB-CG-OD1	5.04	122.84	118.30
19	Z	137	ARG	NH1-CZ-NH2	5.04	124.95	119.40
29	K	208	PRO	N-CA-CB	5.04	109.35	103.30
8	1	121	TYR	CG-CD2-CE2	5.04	125.33	121.30
10	3	194	LYS	CB-CG-CD	5.04	124.70	111.60
32	J	302	ASP	CB-CA-C	-5.04	100.33	110.40
10	3	74	TYR	CA-CB-CG	-5.04	103.83	113.40
18	Y	52	PHE	CG-CD2-CE2	5.03	126.33	120.80
22	P	314	LEU	N-CA-CB	5.03	120.46	110.40
6	F	158	ALA	N-CA-CB	5.03	117.14	110.10
19	Z	128	VAL	CB-CA-C	-5.03	101.84	111.40
21	S	425	ASP	CB-CG-OD2	5.03	122.83	118.30
29	K	310	ALA	CB-CA-C	5.03	117.65	110.10
21	S	502	GLU	CG-CD-OE1	-5.03	108.24	118.30
30	L	196	LEU	CB-CG-CD2	-5.03	102.45	111.00
26	O	163	TYR	CA-CB-CG	-5.03	103.85	113.40
6	F	137	TYR	CB-CG-CD1	-5.02	117.98	121.00
12	5	196	GLY	N-CA-C	5.02	125.65	113.10
17	T	258	SER	N-CA-C	-5.02	97.44	111.00
21	S	38	GLU	CG-CD-OE2	5.02	128.35	118.30
23	Q	342	PHE	CB-CA-C	-5.02	100.36	110.40
28	I	133	VAL	CA-CB-CG2	5.02	118.43	110.90
11	4	99	HIS	C-N-CA	5.02	134.25	121.70
6	F	204	ASP	CB-CG-OD1	5.02	122.82	118.30
10	3	133	THR	CA-CB-OG1	5.02	119.54	109.00
20	N	206	MET	CG-SD-CE	-5.02	92.17	100.20
25	U	182	THR	O-C-N	5.02	130.73	122.70
27	H	362	MET	CG-SD-CE	-5.02	92.17	100.20
2	B	71	HIS	CA-CB-CG	5.02	122.13	113.60
4	D	33	VAL	CA-CB-CG2	-5.02	103.37	110.90
19	Z	466	LEU	CB-CG-CD2	-5.02	102.47	111.00
20	N	118	LEU	CA-C-O	-5.02	109.56	120.10
24	R	261	PHE	CB-CG-CD2	-5.02	117.29	120.80
28	I	326	LYS	N-CA-CB	5.02	119.63	110.60
31	M	154	VAL	CA-CB-CG2	-5.02	103.38	110.90
32	J	377	HIS	CA-CB-CG	5.02	122.13	113.60
6	F	13	TRP	CD1-NE1-CE2	5.01	113.51	109.00
7	G	209	ALA	N-CA-C	-5.01	97.46	111.00
32	J	113	ARG	NE-CZ-NH2	-5.01	117.79	120.30
29	K	365	ALA	CB-CA-C	-5.01	102.58	110.10
19	Z	28	SER	N-CA-CB	5.01	118.02	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	S	177	TYR	CD1-CE1-CZ	-5.01	115.29	119.80
25	U	60	GLU	N-CA-C	-5.01	97.47	111.00
29	K	303	VAL	CA-CB-CG2	5.01	118.42	110.90
5	E	33	LEU	CB-CG-CD1	5.01	119.52	111.00
8	1	193	LEU	O-C-N	-5.01	114.68	122.70
14	7	104	PHE	CB-CA-C	5.01	120.42	110.40
28	I	274	ALA	O-C-N	-5.01	114.68	122.70
30	L	235	TYR	CB-CG-CD2	-5.01	118.00	121.00
19	Z	723	TYR	CZ-CE2-CD2	-5.01	115.29	119.80
6	F	67	ASP	CB-CG-OD2	-5.00	113.80	118.30
12	5	152	MET	O-C-N	-5.00	114.69	123.20
23	Q	182	ASN	CB-CG-OD1	-5.00	111.59	121.60
16	V	112	TYR	CD1-CE1-CZ	-5.00	115.30	119.80
22	P	144	ARG	NH1-CZ-NH2	-5.00	113.90	119.40
24	R	268	TYR	CB-CG-CD2	-5.00	118.00	121.00

All (1) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
9	2	231	PRO	CA

All (282) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	105	GLU	Peptide
8	1	145	TYR	Sidechain
8	1	167	TYR	Sidechain
8	1	169	TYR	Sidechain
8	1	52	ARG	Sidechain
8	1	58	TYR	Sidechain
9	2	115	ARG	Sidechain
9	2	124	ARG	Sidechain
9	2	132	ARG	Sidechain
9	2	141	LEU	Mainchain
9	2	186	ARG	Sidechain
9	2	85	TYR	Sidechain
10	3	74	TYR	Sidechain
11	4	127	ALA	Mainchain
11	4	134	TYR	Sidechain
11	4	147	TYR	Sidechain
11	4	153	ARG	Sidechain
11	4	171	PHE	Sidechain

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Mol	Chain	Res	Type	Group
11	4	19	ARG	Sidechain
11	4	30	ASP	Mainchain
11	4	67	TYR	Sidechain
11	4	85	ARG	Sidechain
11	4	95	ARG	Sidechain
12	5	147	TYR	Sidechain
12	5	171	TYR	Sidechain
12	5	172	TYR	Sidechain
12	5	202	TYR	Sidechain
12	5	228	TYR	Sidechain
12	5	62	THR	Mainchain,Peptide
12	5	69	HIS	Sidechain
12	5	78	ARG	Sidechain
12	5	84	TYR	Sidechain
12	5	99	TYR	Sidechain
13	6	151	PHE	Sidechain
13	6	159	ARG	Sidechain
13	6	215	TYR	Sidechain
13	6	65	ARG	Sidechain
13	6	71	TYR	Sidechain
14	7	101	TYR	Sidechain
14	7	127	TYR	Sidechain
14	7	167	GLY	Peptide
14	7	168	TYR	Sidechain
14	7	176	TYR	Sidechain
14	7	222	TYR	Sidechain
14	7	228	TYR	Sidechain
14	7	230	ARG	Sidechain
14	7	74	TYR	Sidechain
1	A	105	TYR	Sidechain
1	A	107	TYR	Sidechain
1	A	159	TYR	Sidechain
1	A	227	PHE	Mainchain
1	A	245	ARG	Sidechain
1	A	9	PHE	Sidechain
1	A	93	ARG	Sidechain
1	A	95	ARG	Sidechain
2	B	101	TYR	Sidechain
2	B	121	TYR	Sidechain
2	B	155	TYR	Sidechain
2	B	167	TYR	Sidechain
2	B	229	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	57	TYR	Sidechain
2	B	6	TYR	Sidechain
2	B	97	TYR	Sidechain
2	B	98	TYR	Sidechain
3	C	148	TYR	Sidechain
3	C	156	TYR	Sidechain
3	C	17	ARG	Sidechain
3	C	179	TYR	Sidechain
4	D	112	TYR	Sidechain
4	D	116	TYR	Sidechain
4	D	123	ARG	Sidechain
4	D	169	ARG	Sidechain
4	D	182	TYR	Sidechain
4	D	21	TYR	Sidechain
4	D	234	TYR	Sidechain
4	D	73	PHE	Sidechain
4	D	87	ARG	Sidechain
5	E	10	ARG	Sidechain
5	E	123	PHE	Sidechain
5	E	15	PHE	Sidechain
5	E	20	ARG	Sidechain
5	E	93	ARG	Sidechain
6	F	126	ARG	Sidechain
6	F	171	TYR	Sidechain
6	F	232	PHE	Sidechain
6	F	6	TYR	Sidechain
6	F	65	HIS	Sidechain
6	F	87	PHE	Sidechain
6	F	89	ARG	Sidechain
7	G	150	TYR	Sidechain
7	G	159	TYR	Sidechain
7	G	188	ARG	Sidechain
7	G	210	PHE	Sidechain
7	G	239	TYR	Sidechain
7	G	8	TYR	Sidechain
7	G	86	ARG	Sidechain
27	H	188	ARG	Sidechain
27	H	227	ARG	Sidechain
27	H	232	ARG	Sidechain
27	H	237	PHE	Sidechain
27	H	265	ARG	Sidechain
27	H	360	ARG	Sidechain

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Mol	Chain	Res	Type	Group
27	H	398	ARG	Sidechain
27	H	41	TYR	Sidechain
27	H	97	ARG	Sidechain
28	I	189	GLY	Peptide
28	I	346	ARG	Sidechain
28	I	349	ARG	Sidechain
28	I	411	ARG	Sidechain
28	I	439	TYR	Sidechain
28	I	71	TYR	Sidechain
32	J	117	ARG	Sidechain
32	J	12	GLU	Peptide
32	J	189	TYR	Sidechain
32	J	23	TYR	Sidechain
32	J	271	ARG	Sidechain
32	J	297	ARG	Sidechain
32	J	313	ARG	Sidechain
32	J	340	ARG	Sidechain
32	J	372	ARG	Sidechain
32	J	43	ARG	Sidechain
32	J	72	TYR	Sidechain
29	K	111	TYR	Sidechain
29	K	133	HIS	Sidechain
29	K	164	TYR	Sidechain
29	K	283	ARG	Sidechain
29	K	299	PHE	Sidechain
29	K	323	ARG	Sidechain
29	K	366	ARG	Sidechain
29	K	399	PHE	Sidechain
29	K	92	PHE	Sidechain
30	L	111	ARG	Sidechain
30	L	134	TYR	Sidechain
30	L	138	HIS	Sidechain
30	L	146	TYR	Sidechain
30	L	157	ARG	Sidechain
30	L	173	PHE	Sidechain
30	L	221	TYR	Sidechain
30	L	235	TYR	Sidechain
30	L	27	ARG	Sidechain
30	L	280	GLY	Peptide
30	L	286	ARG	Sidechain
30	L	305	ARG	Sidechain
30	L	342	TYR	Sidechain

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Mol	Chain	Res	Type	Group
30	L	370	ARG	Sidechain
30	L	381	PHE	Sidechain
30	L	386	ARG	Sidechain
30	L	400	TYR	Sidechain
31	M	229	TYR	Sidechain
31	M	241	ARG	Sidechain
31	M	324	GLN	Peptide
31	M	384	TYR	Sidechain
31	M	49	ARG	Sidechain
20	N	140	ARG	Sidechain
20	N	194	ARG	Sidechain
20	N	253	TYR	Sidechain
20	N	34	PHE	Sidechain
20	N	361	ARG	Sidechain
20	N	375	PHE	Sidechain
20	N	450	HIS	Sidechain
20	N	494	TYR	Sidechain
20	N	572	ARG	Sidechain
20	N	579	ARG	Sidechain
20	N	584	TYR	Sidechain
20	N	604	HIS	Sidechain
20	N	684	ARG	Sidechain
20	N	710	ARG	Sidechain
20	N	713	TYR	Sidechain
20	N	802	TYR	Sidechain
26	O	155	PHE	Sidechain
26	O	238	TYR	Sidechain
26	O	247	ARG	Sidechain
26	O	282	PHE	Sidechain
26	O	284	ARG	Sidechain
26	O	289	ARG	Sidechain
26	O	330	ARG	Sidechain
26	O	339	ARG	Sidechain
26	O	352	ARG	Sidechain
26	O	60	TYR	Sidechain
26	O	69	HIS	Sidechain
26	O	7	PHE	Sidechain
26	O	82	HIS	Sidechain
22	P	182	ARG	Sidechain
22	P	20	TYR	Sidechain
22	P	227	TYR	Sidechain
22	P	247	TYR	Sidechain

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Mol	Chain	Res	Type	Group
22	P	302	TYR	Sidechain
22	P	350	ARG	Sidechain
22	P	357	ARG	Sidechain
22	P	364	ARG	Sidechain
22	P	370	TYR	Sidechain
22	P	94	ARG	Sidechain
23	Q	132	ARG	Sidechain
23	Q	229	TYR	Sidechain
23	Q	233	TYR	Sidechain
23	Q	253	TYR	Sidechain
23	Q	279	TYR	Sidechain
23	Q	363	ARG	Sidechain
23	Q	72	TYR	Sidechain
23	Q	96	PHE	Sidechain
24	R	128	TYR	Sidechain
24	R	137	ARG	Sidechain
24	R	142	PHE	Sidechain
24	R	146	ARG	Sidechain
24	R	177	ARG	Sidechain
24	R	192	ARG	Sidechain
24	R	233	ARG	Sidechain
24	R	251	HIS	Sidechain
24	R	261	PHE	Sidechain
24	R	264	TYR	Sidechain
24	R	272	PHE	Sidechain
24	R	293	ARG	Sidechain
24	R	304	TYR	Sidechain
24	R	311	TYR	Sidechain
21	S	162	TYR	Sidechain
21	S	208	TYR	Sidechain
21	S	254	TYR	Sidechain
21	S	257	TYR	Sidechain
21	S	260	TYR	Sidechain
21	S	283	ARG	Sidechain
21	S	284	TYR	Sidechain
21	S	286	TYR	Sidechain
21	S	302	ARG	Sidechain
21	S	310	ARG	Sidechain
21	S	345	ARG	Sidechain
21	S	364	ARG	Sidechain
21	S	410	TYR	Sidechain
21	S	478	PHE	Sidechain

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Mol	Chain	Res	Type	Group
21	S	491	ARG	Sidechain
21	S	76	ARG	Sidechain
21	S	95	ARG	Sidechain
17	T	107	ARG	Sidechain
17	T	148	ARG	Sidechain
17	T	169	ARG	Sidechain
17	T	178	TYR	Sidechain
17	T	180	ASP	Peptide
17	T	217	ARG	Sidechain
17	T	228	TYR	Sidechain
17	T	262	PHE	Sidechain
17	T	282	TYR	Sidechain
17	T	318	TYR	Sidechain
17	T	319	TYR	Sidechain
17	T	340	ARG	Sidechain
25	U	211	TYR	Sidechain
25	U	228	TYR	Sidechain
25	U	25	ARG	Sidechain
25	U	250	TYR	Sidechain
25	U	261	TYR	Sidechain
25	U	79	TYR	Sidechain
16	V	112	TYR	Sidechain
16	V	139	ARG	Sidechain
16	V	255	TYR	Sidechain
16	V	282	ARG	Sidechain
16	V	309	PHE	Sidechain
16	V	46	ARG	Sidechain
16	V	68	ARG	Sidechain
15	W	108	ARG	Sidechain
15	W	21	PHE	Sidechain
15	W	99	HIS	Sidechain
18	Y	57	ARG	Sidechain
19	Z	143	ARG	Sidechain
19	Z	160	ARG	Sidechain
19	Z	217	LEU	Peptide
19	Z	226	TYR	Sidechain
19	Z	239	TYR	Sidechain
19	Z	323	ASN	Peptide
19	Z	34	ARG	Sidechain
19	Z	371	ASN	Peptide
19	Z	376	PHE	Sidechain
19	Z	456	ARG	Sidechain

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Mol	Chain	Res	Type	Group
19	Z	459	CYS	Peptide
19	Z	485	LEU	Mainchain
19	Z	489	TYR	Sidechain
19	Z	556	ARG	Sidechain
19	Z	746	ARG	Sidechain
19	Z	755	ASP	Peptide
19	Z	781	TYR	Sidechain
19	Z	816	TYR	Sidechain
19	Z	865	PHE	Sidechain
19	Z	887	PHE	Sidechain
19	Z	98	PHE	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	A	1920	0	1927	0	0
2	B	1828	0	1823	0	0
3	C	1960	0	1983	0	0
4	D	1926	0	1955	0	0
5	E	1778	0	1756	0	0
6	F	1871	0	1856	0	0
7	G	1912	0	1907	0	0
8	1	1516	0	1485	0	0
9	2	1651	0	1674	0	0
10	3	1600	0	1621	0	0
11	4	1572	0	1575	0	0
12	5	1560	0	1519	0	0
13	6	1659	0	1654	0	0
14	7	1686	0	1662	0	0
15	W	1480	0	1522	0	0
16	V	2272	0	2288	0	0
17	T	2149	0	2170	0	0
18	Y	199	0	180	0	0
19	Z	6913	0	6910	0	0
20	N	7082	0	7121	0	0
21	S	3844	0	3888	0	0
22	P	3706	0	3817	0	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
23	Q	3335	0	3435	0	0
24	R	3204	0	3204	0	0
25	U	2299	0	2334	0	0
26	O	3011	0	3042	0	0
27	H	3113	0	3162	0	0
28	I	3042	0	3098	0	0
29	K	3125	0	3151	0	0
30	L	3098	0	3171	0	0
31	M	3252	0	3321	0	0
32	J	3194	0	3311	0	0
All	All	82757	0	83522	0	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). Clashscore could not be calculated for this entry.

There are no clashes within the asymmetric unit.

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	A	244/246 (99%)	234 (96%)	6 (2%)	4 (2%)	9 44
2	B	232/234 (99%)	209 (90%)	17 (7%)	6 (3%)	5 31
3	C	247/261 (95%)	236 (96%)	8 (3%)	3 (1%)	13 50
4	D	244/254 (96%)	223 (91%)	13 (5%)	8 (3%)	4 26
5	E	231/241 (96%)	215 (93%)	13 (6%)	3 (1%)	12 48
6	F	236/263 (90%)	219 (93%)	16 (7%)	1 (0%)	34 72
7	G	243/255 (95%)	222 (91%)	17 (7%)	4 (2%)	9 44
8	1	200/238 (84%)	168 (84%)	19 (10%)	13 (6%)	1 16
9	2	217/277 (78%)	179 (82%)	22 (10%)	16 (7%)	1 14

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	3	203/205 (99%)	165 (81%)	21 (10%)	17 (8%)	1	12
11	4	194/201 (96%)	173 (89%)	14 (7%)	7 (4%)	3	25
12	5	199/263 (76%)	168 (84%)	21 (11%)	10 (5%)	2	20
13	6	211/240 (88%)	173 (82%)	21 (10%)	17 (8%)	1	12
14	7	214/263 (81%)	195 (91%)	12 (6%)	7 (3%)	4	26
15	W	193/377 (51%)	175 (91%)	14 (7%)	4 (2%)	7	36
16	V	287/310 (93%)	266 (93%)	15 (5%)	6 (2%)	7	36
17	T	261/353 (74%)	224 (86%)	24 (9%)	13 (5%)	2	20
18	Y	22/70 (31%)	21 (96%)	1 (4%)	0	100	100
19	Z	894/908 (98%)	792 (89%)	68 (8%)	34 (4%)	3	24
20	N	901/953 (94%)	822 (91%)	55 (6%)	24 (3%)	5	31
21	S	474/530 (89%)	427 (90%)	34 (7%)	13 (3%)	5	31
22	P	454/456 (100%)	429 (94%)	17 (4%)	8 (2%)	8	40
23	Q	420/422 (100%)	395 (94%)	19 (4%)	6 (1%)	11	46
24	R	387/389 (100%)	363 (94%)	16 (4%)	8 (2%)	7	36
25	U	286/320 (89%)	268 (94%)	11 (4%)	7 (2%)	6	33
26	O	374/376 (100%)	354 (95%)	15 (4%)	5 (1%)	12	48
27	H	394/433 (91%)	362 (92%)	24 (6%)	8 (2%)	7	38
28	I	383/440 (87%)	347 (91%)	24 (6%)	12 (3%)	4	27
29	K	389/418 (93%)	354 (91%)	26 (7%)	9 (2%)	6	34
30	L	387/403 (96%)	349 (90%)	33 (8%)	5 (1%)	12	48
31	M	413/442 (93%)	370 (90%)	30 (7%)	13 (3%)	4	27
32	J	404/406 (100%)	368 (91%)	29 (7%)	7 (2%)	9	42
All	All	10438/11447 (91%)	9465 (91%)	675 (6%)	298 (3%)	7	29

All (298) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	16	PHE
2	B	63	HIS
2	B	205	GLU
4	D	74	ALA
4	D	75	VAL
4	D	77	ALA

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Mol	Chain	Res	Type
4	D	82	LEU
8	1	53	THR
8	1	105	GLU
8	1	152	MET
8	1	217	VAL
9	2	53	ASP
9	2	63	ALA
9	2	81	SER
9	2	91	THR
9	2	172	SER
9	2	231	PRO
10	3	57	ALA
11	4	50	ALA
11	4	114	ALA
11	4	149	PRO
13	6	57	SER
13	6	62	ILE
13	6	85	HIS
13	6	157	TYR
13	6	158	GLN
13	6	168	ALA
13	6	193	LEU
14	7	65	VAL
16	V	25	VAL
17	T	94	ALA
19	Z	66	LYS
19	Z	134	SER
19	Z	147	SER
19	Z	460	ASP
19	Z	755	ASP
20	N	435	SER
20	N	574	LYS
20	N	798	PRO
20	N	855	GLU
20	N	923	GLU
20	N	926	GLU
20	N	928	VAL
21	S	138	GLU
21	S	238	HIS
21	S	314	GLN
21	S	461	ASP
22	P	452	ILE

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Mol	Chain	Res	Type
24	R	51	ALA
25	U	5	ALA
25	U	238	PRO
25	U	242	LEU
26	O	3	ASP
28	I	119	ASN
28	I	216	ILE
28	I	391	SER
28	I	439	TYR
29	K	335	LEU
29	K	415	GLU
30	L	140	ASP
31	M	132	ARG
31	M	325	PRO
31	M	338	VAL
31	M	340	ILE
31	M	379	SER
31	M	435	LYS
1	A	186	LYS
4	D	47	LYS
4	D	80	SER
7	G	9	ASP
7	G	209	ALA
8	1	163	SER
8	1	232	ILE
9	2	84	ILE
9	2	136	TYR
9	2	256	THR
10	3	32	ALA
10	3	107	PRO
10	3	186	ILE
10	3	204	MET
11	4	13	VAL
11	4	22	ALA
12	5	62	THR
12	5	79	ALA
12	5	101	LEU
12	5	179	ARG
13	6	32	TYR
13	6	61	SER
14	7	164	SER
14	7	175	ALA

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Mol	Chain	Res	Type
16	V	275	VAL
17	T	258	SER
17	T	332	THR
19	Z	174	ASP
19	Z	237	VAL
19	Z	293	GLN
19	Z	490	ALA
19	Z	851	ASP
20	N	432	SER
20	N	899	ARG
20	N	929	ALA
21	S	132	GLU
21	S	178	LYS
21	S	276	ALA
21	S	296	LEU
22	P	9	ALA
22	P	410	ALA
23	Q	201	TYR
23	Q	271	VAL
23	Q	355	LYS
23	Q	393	VAL
24	R	132	VAL
24	R	192	ARG
27	H	157	ILE
27	H	181	LYS
28	I	118	ASP
28	I	377	ASP
29	K	118	THR
29	K	137	ASN
29	K	156	SER
30	L	178	ILE
30	L	279	ASP
31	M	181	ASP
32	J	152	GLY
2	B	16	SER
5	E	55	THR
5	E	122	GLN
5	E	127	ASP
7	G	3	SER
8	1	43	GLY
8	1	72	ASP
8	1	216	GLY

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Mol	Chain	Res	Type
9	2	55	ILE
9	2	82	PRO
9	2	117	PRO
9	2	189	MET
10	3	3	VAL
10	3	105	THR
10	3	182	GLY
12	5	168	PRO
12	5	230	GLY
12	5	233	VAL
13	6	39	VAL
13	6	109	ALA
15	W	45	PRO
17	T	116	GLY
17	T	119	LEU
17	T	132	LEU
17	T	186	PRO
17	T	219	PRO
17	T	335	SER
19	Z	30	GLY
19	Z	87	THR
19	Z	306	GLU
19	Z	309	GLU
19	Z	357	ARG
19	Z	426	LEU
19	Z	491	GLY
19	Z	509	LYS
19	Z	738	ASN
19	Z	756	PRO
19	Z	839	PRO
19	Z	864	GLY
20	N	560	MET
21	S	272	PHE
22	P	7	GLU
22	P	341	PHE
24	R	359	PRO
25	U	27	GLY
25	U	44	GLN
26	O	101	ARG
27	H	72	LEU
27	H	281	GLY
28	I	86	LYS

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Mol	Chain	Res	Type
28	I	179	ALA
28	I	372	MET
29	K	200	ARG
29	K	390	ASN
32	J	262	GLY
32	J	263	SER
2	B	6	TYR
2	B	61	SER
3	C	204	SER
8	1	44	GLY
10	3	10	ALA
10	3	19	CYS
10	3	20	VAL
10	3	156	PRO
11	4	188	ILE
13	6	37	GLY
13	6	60	PHE
13	6	132	TYR
13	6	220	LEU
14	7	101	TYR
15	W	58	CYS
15	W	135	LYS
16	V	189	ILE
17	T	97	MET
19	Z	310	ASP
19	Z	385	PHE
19	Z	428	GLN
19	Z	437	GLU
19	Z	453	SER
19	Z	492	SER
19	Z	765	ALA
19	Z	842	VAL
19	Z	889	PRO
20	N	429	LYS
20	N	433	PRO
20	N	486	MET
20	N	754	HIS
20	N	819	VAL
20	N	849	LYS
21	S	239	ASP
21	S	348	SER
22	P	2	ALA

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Mol	Chain	Res	Type
22	P	136	ILE
22	P	336	PRO
24	R	95	LEU
25	U	243	GLN
26	O	69	HIS
26	O	375	LEU
27	H	285	PHE
28	I	321	SER
28	I	410	ARG
29	K	148	ASP
31	M	187	GLN
31	M	282	ALA
31	M	326	ASN
32	J	120	SER
32	J	142	LYS
1	A	57	PRO
1	A	73	THR
3	C	205	LYS
6	F	103	LEU
8	1	158	PHE
8	1	207	ILE
9	2	137	ILE
10	3	33	GLN
10	3	43	PHE
10	3	119	PRO
10	3	137	VAL
11	4	26	VAL
12	5	81	ALA
14	7	191	GLN
14	7	232	GLN
14	7	256	ALA
17	T	133	PRO
17	T	182	LYS
19	Z	508	SER
19	Z	703	ARG
19	Z	715	HIS
20	N	591	CYS
20	N	854	MET
21	S	152	SER
23	Q	202	CYS
24	R	47	GLU
24	R	290	PRO

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Mol	Chain	Res	Type
25	U	219	LYS
26	O	32	LYS
27	H	427	PRO
29	K	408	LYS
30	L	280	GLY
31	M	107	GLN
31	M	380	PRO
2	B	7	SER
3	C	7	SER
4	D	78	SER
7	G	205	VAL
10	3	49	LEU
12	5	192	VAL
16	V	106	GLU
20	N	170	SER
20	N	398	ASN
20	N	887	ALA
23	Q	374	PHE
24	R	251	HIS
28	I	89	GLU
31	M	102	VAL
13	6	129	PHE
16	V	187	PRO
20	N	933	PRO
21	S	442	VAL
30	L	340	ILE
32	J	91	PRO
9	2	158	PRO
16	V	105	PRO
17	T	328	PRO
20	N	856	VAL
27	H	170	PRO
4	D	222	PRO
9	2	187	PRO
27	H	280	ILE
32	J	224	ILE
12	5	83	PRO
13	6	68	PRO
15	W	2	VAL
8	1	148	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
1	A	210/210 (100%)	199 (95%)	11 (5%)	23 48
2	B	191/191 (100%)	170 (89%)	21 (11%)	6 22
3	C	209/221 (95%)	192 (92%)	17 (8%)	11 35
4	D	208/215 (97%)	198 (95%)	10 (5%)	25 51
5	E	195/203 (96%)	185 (95%)	10 (5%)	24 48
6	F	204/224 (91%)	194 (95%)	10 (5%)	25 50
7	G	202/212 (95%)	192 (95%)	10 (5%)	24 49
8	1	160/185 (86%)	149 (93%)	11 (7%)	15 40
9	2	180/227 (79%)	166 (92%)	14 (8%)	12 36
10	3	175/175 (100%)	150 (86%)	25 (14%)	3 16
11	4	167/172 (97%)	151 (90%)	16 (10%)	8 27
12	5	158/205 (77%)	136 (86%)	22 (14%)	3 17
13	6	179/200 (90%)	159 (89%)	20 (11%)	6 22
14	7	178/215 (83%)	158 (89%)	20 (11%)	6 22
15	W	168/312 (54%)	160 (95%)	8 (5%)	25 51
16	V	253/268 (94%)	245 (97%)	8 (3%)	39 61
17	T	233/298 (78%)	220 (94%)	13 (6%)	21 46
18	Y	22/63 (35%)	22 (100%)	0	100 100
19	Z	753/765 (98%)	709 (94%)	44 (6%)	20 45
20	N	776/814 (95%)	718 (92%)	58 (8%)	13 38
21	S	414/458 (90%)	397 (96%)	17 (4%)	30 55
22	P	419/419 (100%)	396 (94%)	23 (6%)	21 47
23	Q	362/362 (100%)	336 (93%)	26 (7%)	14 39
24	R	345/345 (100%)	317 (92%)	28 (8%)	11 35
25	U	259/289 (90%)	247 (95%)	12 (5%)	27 52
26	O	334/334 (100%)	307 (92%)	27 (8%)	11 35

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
27	H	341/372 (92%)	329 (96%)	12 (4%)	36 59
28	I	341/385 (89%)	326 (96%)	15 (4%)	28 53
29	K	343/367 (94%)	324 (94%)	19 (6%)	21 47
30	L	341/353 (97%)	329 (96%)	12 (4%)	36 59
31	M	357/382 (94%)	329 (92%)	28 (8%)	12 36
32	J	352/352 (100%)	336 (96%)	16 (4%)	27 52
All	All	9029/9793 (92%)	8446 (94%)	583 (6%)	21 42

All (583) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	50	ILE
1	A	60	LEU
1	A	81	THR
1	A	101	TRP
1	A	107	TYR
1	A	113	MET
1	A	161	CYS
1	A	166	THR
1	A	210	PHE
1	A	229	ILE
1	A	239	LEU
2	B	1	MET
2	B	59	GLU
2	B	62	VAL
2	B	75	VAL
2	B	84	ARG
2	B	85	VAL
2	B	97	TYR
2	B	107	THR
2	B	119	GLN
2	B	127	VAL
2	B	133	SER
2	B	136	ILE
2	B	143	ARG
2	B	147	PHE
2	B	167	TYR
2	B	177	ARG
2	B	200	GLU
2	B	202	GLN

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Mol	Chain	Res	Type
2	B	208	ILE
2	B	219	ARG
2	B	222	THR
3	C	1	MET
3	C	35	LEU
3	C	38	LEU
3	C	43	VAL
3	C	44	LEU
3	C	60	PHE
3	C	72	MET
3	C	81	SER
3	C	98	LEU
3	C	101	TYR
3	C	114	LEU
3	C	137	ILE
3	C	147	LEU
3	C	156	TYR
3	C	194	VAL
3	C	211	VAL
3	C	240	HIS
4	D	10	PHE
4	D	27	LYS
4	D	43	LEU
4	D	68	ASN
4	D	104	VAL
4	D	135	ILE
4	D	151	TYR
4	D	152	GLN
4	D	192	LEU
4	D	243	GLU
5	E	14	THR
5	E	42	THR
5	E	100	TRP
5	E	129	ASP
5	E	133	MET
5	E	135	ARG
5	E	181	LEU
5	E	210	LEU
5	E	215	ILE
5	E	219	THR
6	F	10	VAL
6	F	13	TRP

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Mol	Chain	Res	Type
6	F	39	LYS
6	F	96	ARG
6	F	138	ASP
6	F	139	ASP
6	F	140	MET
6	F	180	MET
6	F	222	THR
6	F	236	LEU
7	G	15	PHE
7	G	42	CYS
7	G	61	GLU
7	G	67	LEU
7	G	84	ASP
7	G	111	HIS
7	G	162	TRP
7	G	166	ILE
7	G	182	MET
7	G	230	LYS
8	1	59	ILE
8	1	62	ARG
8	1	94	TYR
8	1	115	LEU
8	1	118	GLU
8	1	131	ILE
8	1	143	GLN
8	1	144	VAL
8	1	197	MET
8	1	212	ILE
8	1	213	GLN
9	2	57	LEU
9	2	77	ILE
9	2	79	PHE
9	2	80	ILE
9	2	100	GLN
9	2	156	ILE
9	2	157	TYR
9	2	175	LEU
9	2	195	LYS
9	2	207	PHE
9	2	218	LEU
9	2	230	ARG
9	2	249	LYS

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Mol	Chain	Res	Type
9	2	259	VAL
10	3	3	VAL
10	3	11	VAL
10	3	12	MET
10	3	22	ILE
10	3	25	ASP
10	3	26	ARG
10	3	28	PHE
10	3	37	THR
10	3	45	MET
10	3	71	LEU
10	3	74	TYR
10	3	91	VAL
10	3	102	PRO
10	3	109	ILE
10	3	121	ILE
10	3	124	LEU
10	3	141	THR
10	3	142	CYS
10	3	154	TRP
10	3	161	GLU
10	3	163	LEU
10	3	164	PHE
10	3	169	GLN
10	3	172	LEU
10	3	201	LYS
11	4	5	ILE
11	4	7	ILE
11	4	19	ARG
11	4	28	MET
11	4	42	ILE
11	4	43	LEU
11	4	55	GLN
11	4	62	LYS
11	4	84	THR
11	4	100	VAL
11	4	102	LEU
11	4	137	PHE
11	4	138	LEU
11	4	148	THR
11	4	150	THR
11	4	185	LYS

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Mol	Chain	Res	Type
12	5	62	THR
12	5	63	LEU
12	5	67	PHE
12	5	93	VAL
12	5	96	ILE
12	5	98	PRO
12	5	117	LEU
12	5	118	LEU
12	5	121	GLN
12	5	127	LEU
12	5	135	VAL
12	5	142	LEU
12	5	163	TRP
12	5	164	ASP
12	5	173	VAL
12	5	180	ILE
12	5	183	THR
12	5	204	TYR
12	5	220	TYR
12	5	249	ASP
12	5	253	ASP
12	5	257	LYS
13	6	47	PHE
13	6	50	VAL
13	6	55	ARG
13	6	64	THR
13	6	65	ARG
13	6	72	LYS
13	6	77	THR
13	6	84	PHE
13	6	101	MET
13	6	119	LEU
13	6	124	TYR
13	6	133	VAL
13	6	134	TYR
13	6	137	ILE
13	6	148	VAL
13	6	159	ARG
13	6	162	PHE
13	6	180	VAL
13	6	216	THR
13	6	231	ARG

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Mol	Chain	Res	Type
14	7	56	LEU
14	7	66	ILE
14	7	70	MET
14	7	74	TYR
14	7	80	PHE
14	7	92	SER
14	7	136	LEU
14	7	146	LYS
14	7	148	ASN
14	7	155	VAL
14	7	171	MET
14	7	172	LEU
14	7	183	THR
14	7	189	LEU
14	7	194	LEU
14	7	204	LEU
14	7	231	PHE
14	7	241	VAL
14	7	243	ILE
14	7	250	GLN
15	W	34	ASN
15	W	62	THR
15	W	68	THR
15	W	72	LEU
15	W	85	THR
15	W	107	MET
15	W	153	LEU
15	W	168	SER
16	V	46	ARG
16	V	125	VAL
16	V	152	LYS
16	V	178	THR
16	V	181	LEU
16	V	190	GLN
16	V	264	LYS
16	V	284	LEU
17	T	119	LEU
17	T	132	LEU
17	T	133	PRO
17	T	164	ILE
17	T	179	PHE
17	T	191	MET

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Mol	Chain	Res	Type
17	T	208	VAL
17	T	219	PRO
17	T	240	MET
17	T	251	LYS
17	T	266	LEU
17	T	282	TYR
17	T	330	ASP
19	Z	2	GLU
19	Z	27	LYS
19	Z	56	LEU
19	Z	81	GLN
19	Z	91	SER
19	Z	96	LEU
19	Z	185	LEU
19	Z	191	ILE
19	Z	199	ASN
19	Z	281	ILE
19	Z	293	GLN
19	Z	298	LEU
19	Z	307	LEU
19	Z	316	ASP
19	Z	335	ARG
19	Z	344	VAL
19	Z	357	ARG
19	Z	366	ASP
19	Z	378	ASN
19	Z	399	LEU
19	Z	420	TRP
19	Z	426	LEU
19	Z	428	GLN
19	Z	460	ASP
19	Z	465	LEU
19	Z	466	LEU
19	Z	487	LEU
19	Z	507	ASP
19	Z	525	ILE
19	Z	562	LEU
19	Z	605	ASN
19	Z	608	LYS
19	Z	619	HIS
19	Z	628	ASP
19	Z	631	LYS

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Mol	Chain	Res	Type
19	Z	660	ILE
19	Z	678	LEU
19	Z	704	LEU
19	Z	777	THR
19	Z	799	VAL
19	Z	800	LEU
19	Z	810	ILE
19	Z	822	VAL
19	Z	868	HIS
20	N	15	GLU
20	N	41	SER
20	N	82	LEU
20	N	87	LEU
20	N	93	ASN
20	N	100	ILE
20	N	128	GLN
20	N	141	CYS
20	N	146	LYS
20	N	147	TYR
20	N	163	PHE
20	N	166	THR
20	N	167	ILE
20	N	173	VAL
20	N	176	MET
20	N	183	LEU
20	N	213	PHE
20	N	220	LEU
20	N	236	LEU
20	N	248	ILE
20	N	251	ASP
20	N	252	LEU
20	N	258	GLN
20	N	332	GLU
20	N	333	MET
20	N	361	ARG
20	N	423	MET
20	N	427	LEU
20	N	444	TYR
20	N	446	LEU
20	N	479	LEU
20	N	481	LEU
20	N	496	LEU

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Mol	Chain	Res	Type
20	N	508	THR
20	N	527	GLN
20	N	543	LYS
20	N	548	LEU
20	N	574	LYS
20	N	609	ASP
20	N	625	ILE
20	N	627	PHE
20	N	708	GLN
20	N	751	ARG
20	N	767	THR
20	N	769	PHE
20	N	779	LEU
20	N	786	THR
20	N	797	MET
20	N	849	LYS
20	N	861	LYS
20	N	863	GLU
20	N	865	LYS
20	N	869	LYS
20	N	899	ARG
20	N	905	PRO
20	N	911	ILE
20	N	924	LEU
20	N	937	GLU
21	S	169	ILE
21	S	196	ARG
21	S	226	PHE
21	S	230	ARG
21	S	249	LEU
21	S	267	VAL
21	S	285	LEU
21	S	298	TYR
21	S	302	ARG
21	S	327	LEU
21	S	329	ILE
21	S	338	ILE
21	S	390	LEU
21	S	393	ARG
21	S	413	ILE
21	S	447	ILE
21	S	481	ASP

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Mol	Chain	Res	Type
22	P	7	GLU
22	P	33	LYS
22	P	34	LEU
22	P	78	LYS
22	P	90	LEU
22	P	131	VAL
22	P	169	LEU
22	P	189	GLN
22	P	217	GLU
22	P	243	ILE
22	P	247	TYR
22	P	253	THR
22	P	269	SER
22	P	276	LEU
22	P	305	LEU
22	P	308	LEU
22	P	329	ARG
22	P	344	THR
22	P	354	LEU
22	P	373	ILE
22	P	402	ILE
22	P	416	GLN
22	P	440	ASN
23	Q	13	GLN
23	Q	45	VAL
23	Q	51	LEU
23	Q	59	LYS
23	Q	90	ARG
23	Q	93	LEU
23	Q	132	ARG
23	Q	137	TYR
23	Q	169	VAL
23	Q	180	LEU
23	Q	181	SER
23	Q	198	ASN
23	Q	200	ILE
23	Q	206	LEU
23	Q	213	GLN
23	Q	302	PHE
23	Q	306	LEU
23	Q	310	ARG
23	Q	337	ARG

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Mol	Chain	Res	Type
23	Q	340	GLU
23	Q	348	GLU
23	Q	353	LEU
23	Q	371	ASP
23	Q	377	ILE
23	Q	386	ILE
23	Q	387	ILE
24	R	7	GLU
24	R	16	ASP
24	R	23	ARG
24	R	25	LEU
24	R	37	VAL
24	R	46	ARG
24	R	69	LEU
24	R	78	GLU
24	R	100	ILE
24	R	121	LEU
24	R	145	LEU
24	R	169	GLU
24	R	175	ASP
24	R	204	THR
24	R	209	THR
24	R	225	TYR
24	R	228	MET
24	R	233	ARG
24	R	246	ILE
24	R	247	LEU
24	R	257	ARG
24	R	260	LEU
24	R	287	LEU
24	R	292	TYR
24	R	293	ARG
24	R	353	ILE
24	R	375	LEU
24	R	382	LYS
25	U	1	MET
25	U	79	TYR
25	U	95	TYR
25	U	118	ASN
25	U	127	LYS
25	U	196	HIS
25	U	198	LEU

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Mol	Chain	Res	Type
25	U	199	LYS
25	U	210	THR
25	U	230	LEU
25	U	244	GLU
25	U	253	THR
26	O	22	TRP
26	O	28	LEU
26	O	35	HIS
26	O	47	ASP
26	O	56	LEU
26	O	58	LYS
26	O	63	PHE
26	O	70	ARG
26	O	84	VAL
26	O	124	ASN
26	O	125	ILE
26	O	135	ILE
26	O	145	LEU
26	O	155	PHE
26	O	156	TYR
26	O	158	LEU
26	O	184	ASP
26	O	236	THR
26	O	240	PHE
26	O	241	ASN
26	O	261	LEU
26	O	268	LEU
26	O	320	VAL
26	O	333	MET
26	O	341	LEU
26	O	347	LYS
26	O	372	GLN
27	H	50	ASP
27	H	60	ASN
27	H	97	ARG
27	H	102	ILE
27	H	138	MET
27	H	158	ASP
27	H	275	ASP
27	H	338	ASP
27	H	345	LEU
27	H	364	VAL

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Mol	Chain	Res	Type
27	H	376	LEU
27	H	405	THR
28	I	79	ILE
28	I	85	MET
28	I	107	MET
28	I	115	ILE
28	I	117	ASP
28	I	135	ILE
28	I	222	VAL
28	I	250	VAL
28	I	256	ILE
28	I	332	ASN
28	I	366	GLN
28	I	376	ASP
28	I	387	LYS
28	I	398	ILE
28	I	414	VAL
29	K	41	TYR
29	K	79	VAL
29	K	93	LEU
29	K	98	GLN
29	K	153	MET
29	K	154	LEU
29	K	155	THR
29	K	172	ILE
29	K	190	LEU
29	K	191	TYR
29	K	196	ILE
29	K	214	MET
29	K	229	ARG
29	K	231	VAL
29	K	250	VAL
29	K	292	LEU
29	K	356	GLU
29	K	360	LEU
29	K	391	ARG
30	L	92	ARG
30	L	98	ARG
30	L	103	LYS
30	L	110	THR
30	L	127	ARG
30	L	227	ARG

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Mol	Chain	Res	Type
30	L	229	ILE
30	L	266	GLU
30	L	303	LEU
30	L	308	ARG
30	L	350	ASP
30	L	360	VAL
31	M	44	ILE
31	M	50	LEU
31	M	72	MET
31	M	106	ASP
31	M	118	SER
31	M	137	LEU
31	M	164	LEU
31	M	175	VAL
31	M	191	ILE
31	M	207	LEU
31	M	218	LEU
31	M	223	PRO
31	M	238	LEU
31	M	250	THR
31	M	262	MET
31	M	285	ILE
31	M	298	ARG
31	M	316	LEU
31	M	325	PRO
31	M	330	LYS
31	M	332	ILE
31	M	346	LEU
31	M	350	ARG
31	M	360	PRO
31	M	373	SER
31	M	422	ASP
31	M	440	TYR
31	M	441	TYR
32	J	3	LEU
32	J	28	ILE
32	J	49	ARG
32	J	71	SER
32	J	85	VAL
32	J	143	VAL
32	J	147	THR
32	J	164	VAL

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Mol	Chain	Res	Type
32	J	187	LEU
32	J	194	THR
32	J	271	ARG
32	J	280	LEU
32	J	286	THR
32	J	314	LYS
32	J	326	LEU
32	J	343	ASN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. There are no such sidechains identified.

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

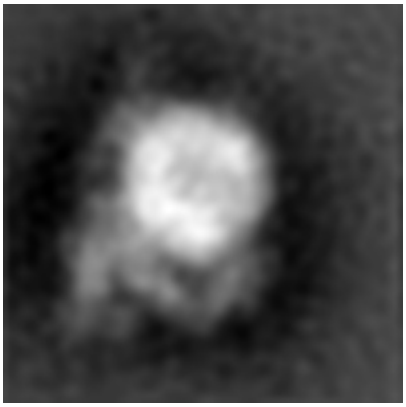
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3914. These allow visual inspection of the internal detail of the map and identification of artifacts.

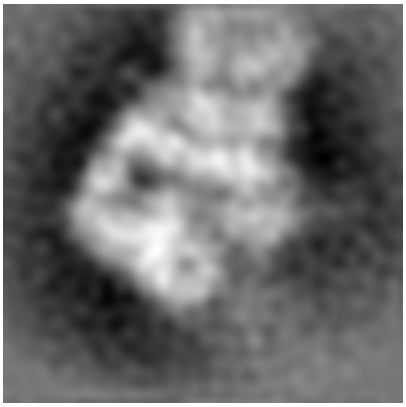
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

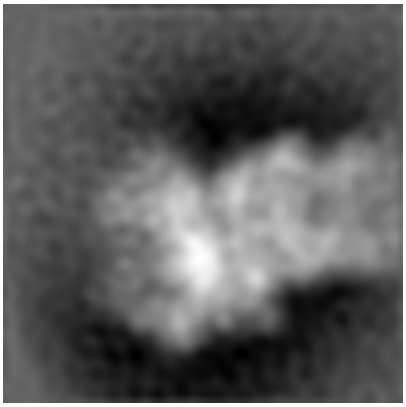
6.1.1 Primary map



X



Y



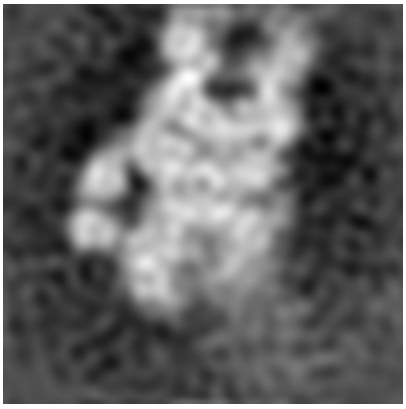
Z

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

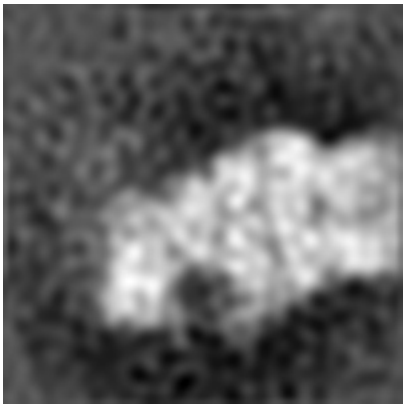
6.2 Central slices

6.2.1 Primary map

X Index: 45



Y Index: 45

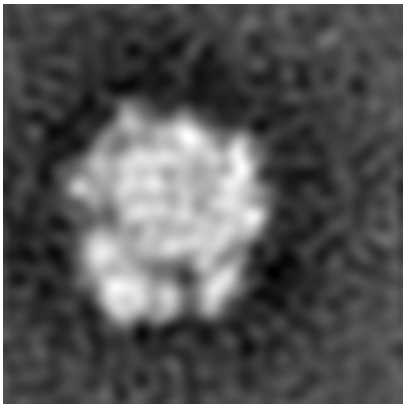


Z Index: 45

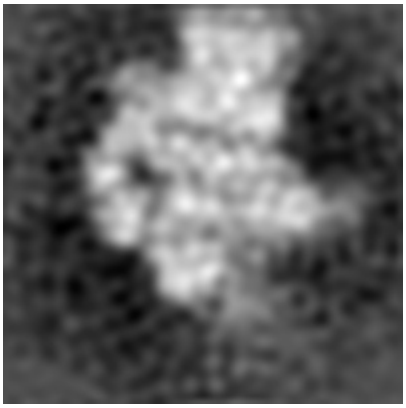
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

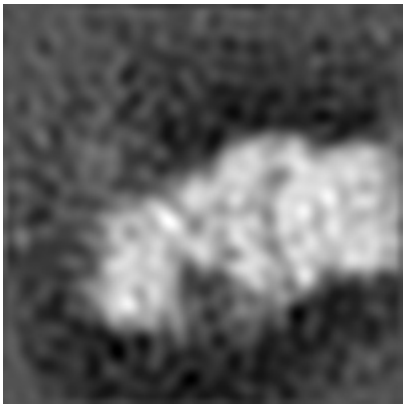
6.3.1 Primary map



X Index: 55



Y Index: 34

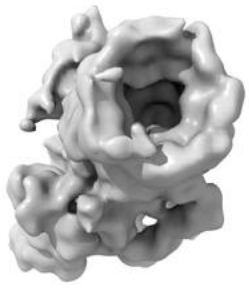


Z Index: 43

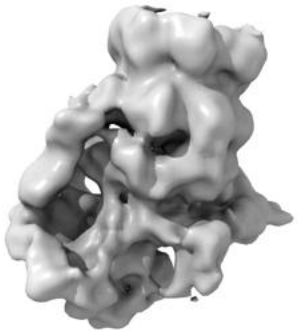
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

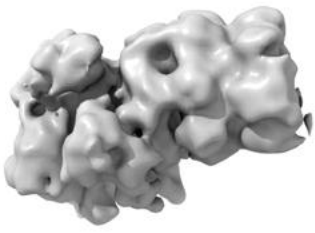
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

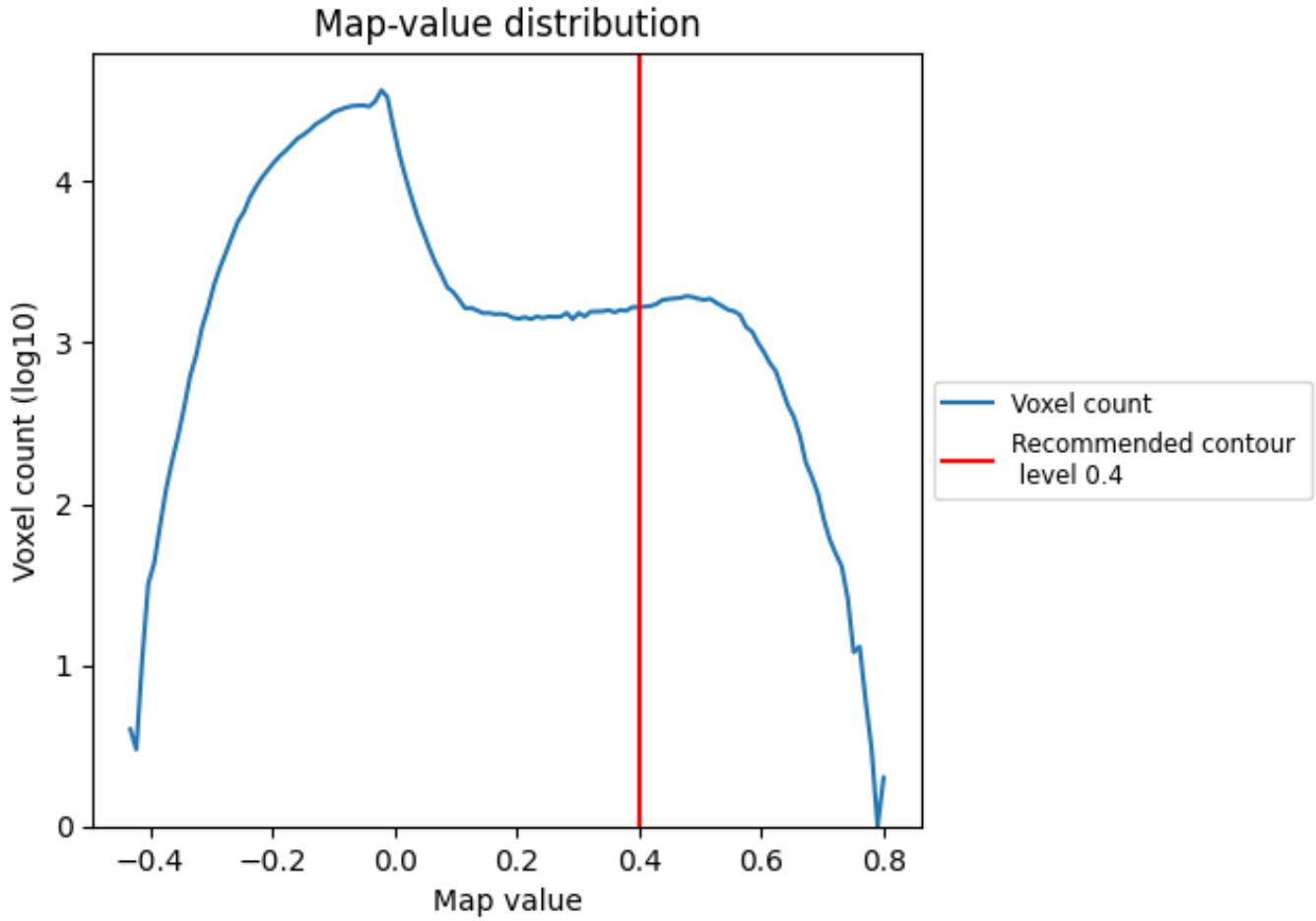
6.5 Mask visualisation (i)

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

7 Map analysis

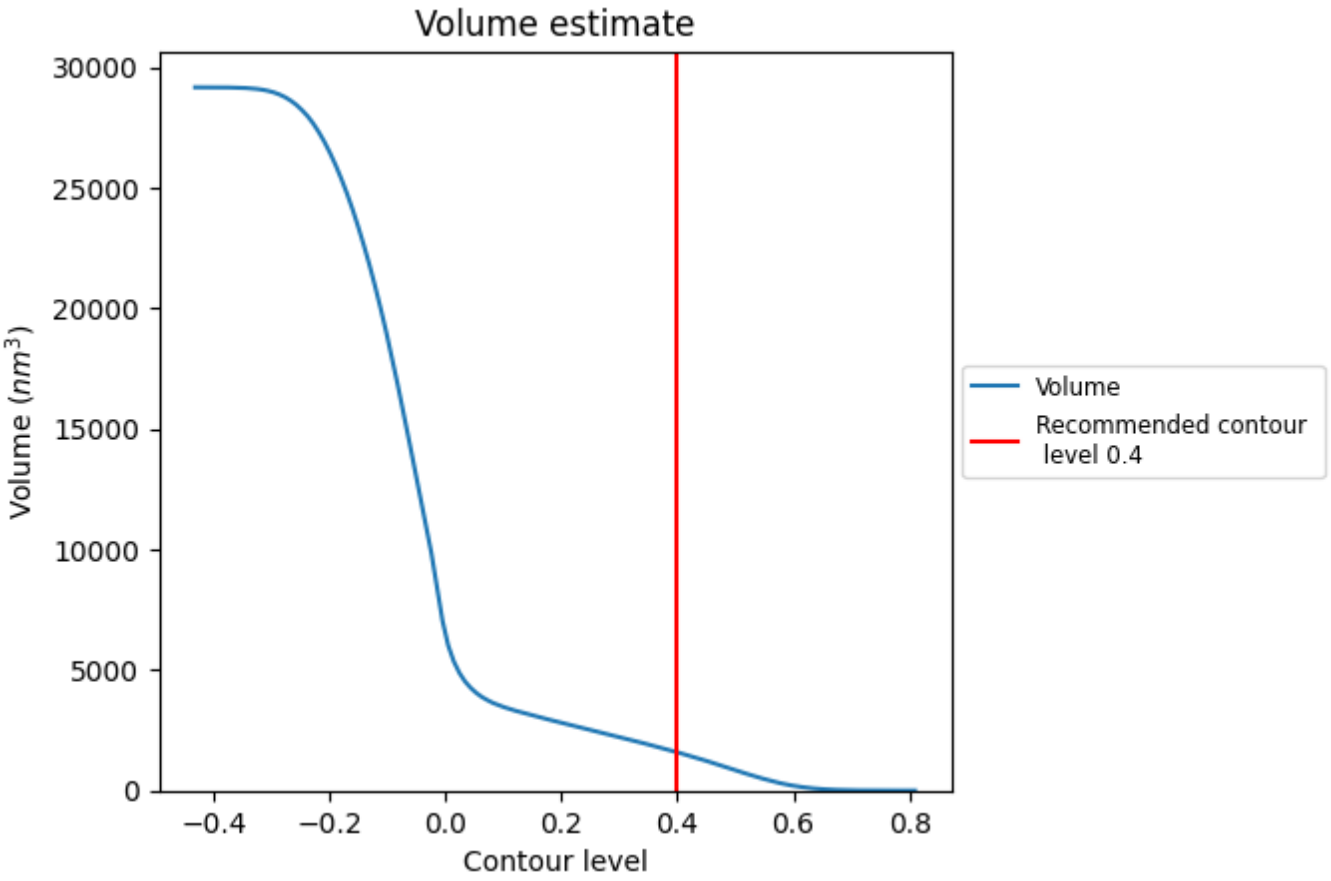
This section contains the results of statistical analysis of the map.

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.

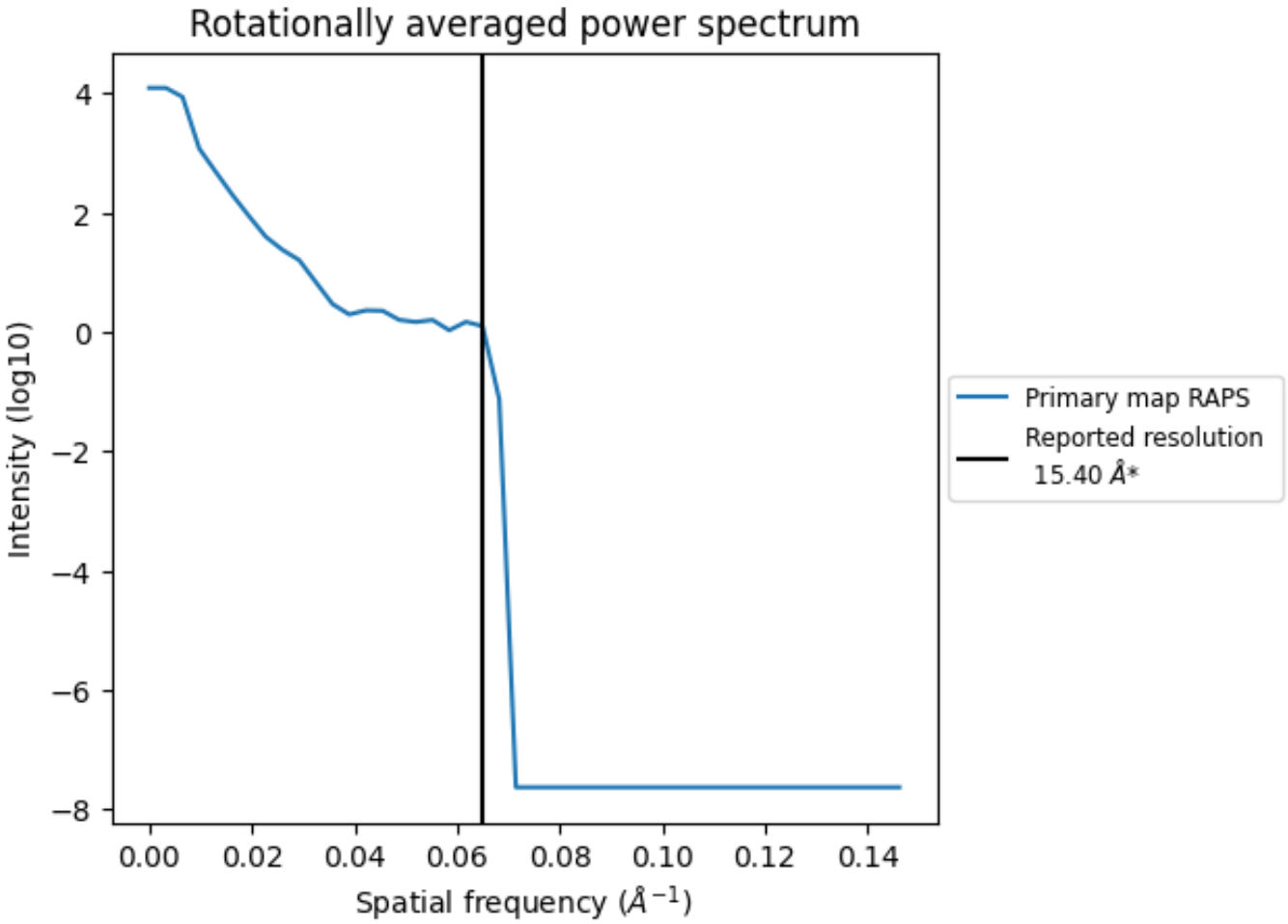
7.2 Volume estimate



The volume at the recommended contour level is 1585 nm^3; this corresponds to an approximate mass of 1431 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 0.065 Å^{-1}

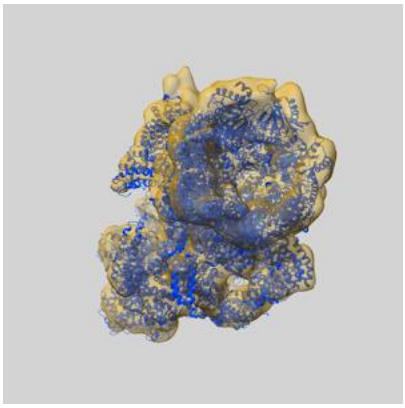
8 Fourier-Shell correlation (i)

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

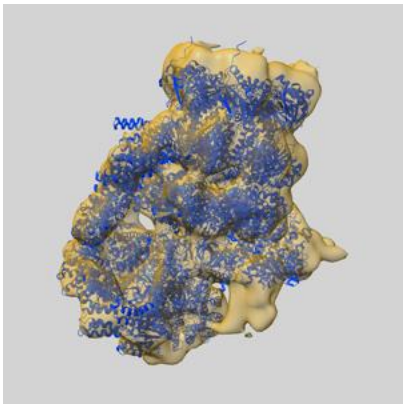
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3914 and PDB model 6EPD. Per-residue inclusion information can be found in section 3 on page 9.

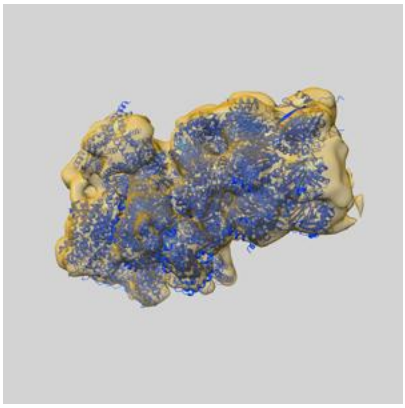
9.1 Map-model overlay



X



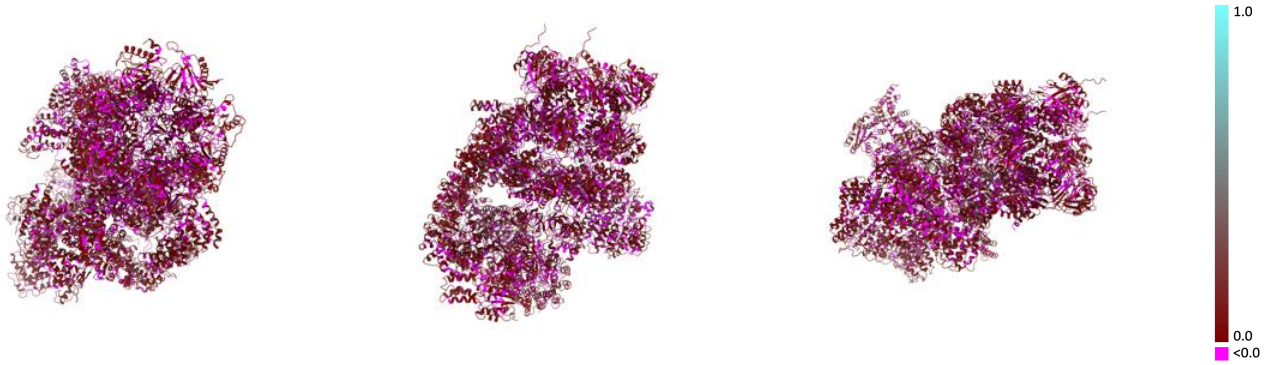
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.4 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.

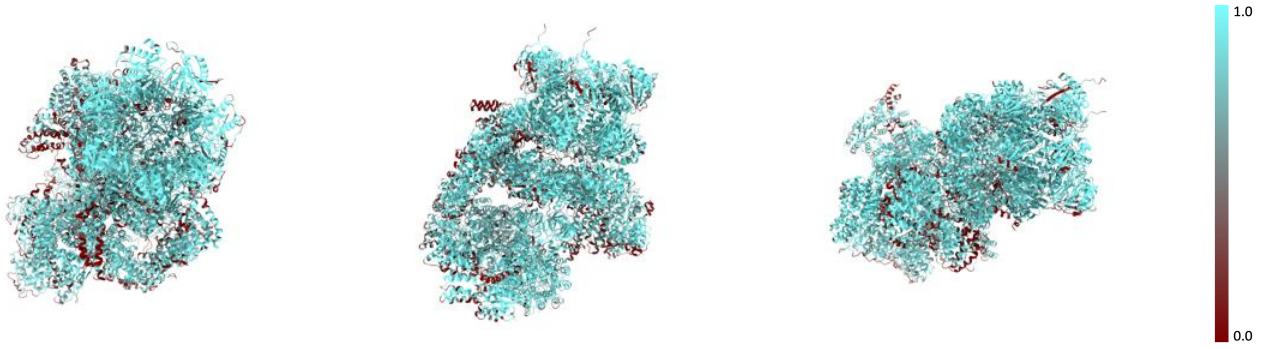
9.2 Q-score mapped to coordinate model



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.

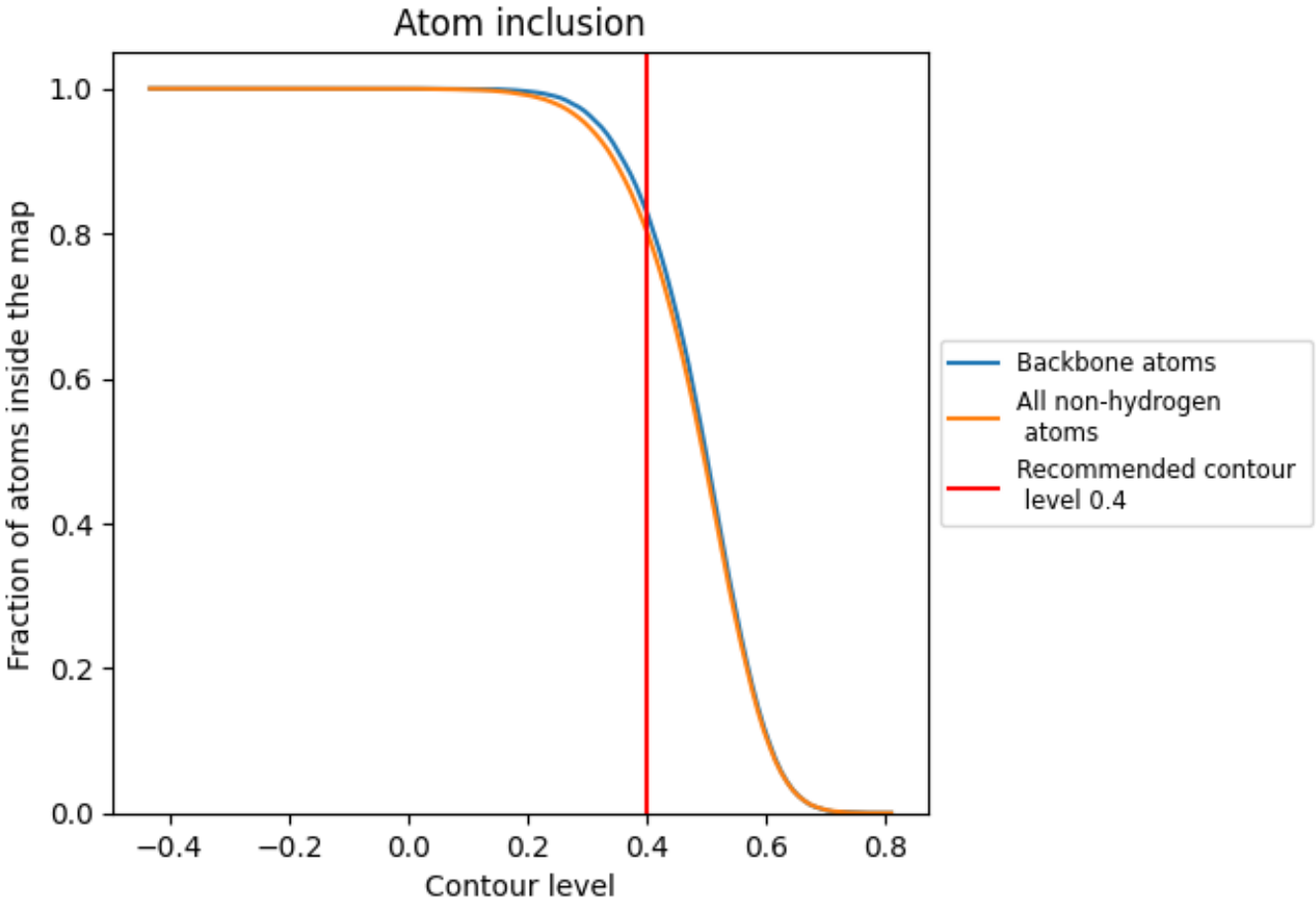
9.3 Atom inclusion mapped to coordinate model



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 (0.4).

9.4 Atom inclusion (i)



At the recommended contour level, 83% of all backbone atoms, 80% 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 (0.4) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8040	0.0500
1	0.8452	0.0460
2	0.7614	0.0440
3	0.8230	0.0390
4	0.8300	0.0470
5	0.8830	0.0610
6	0.7807	0.0290
7	0.8354	0.0480
A	0.8293	0.0490
B	0.8809	0.0310
C	0.8632	0.0550
D	0.8585	0.0430
E	0.9041	0.0310
F	0.9595	0.0560
G	0.8707	0.0350
H	0.8537	0.0400
I	0.8311	0.0470
J	0.8033	0.0500
K	0.7939	0.0470
L	0.8074	0.0540
M	0.8705	0.0350
N	0.8239	0.0520
O	0.7037	0.0780
P	0.7247	0.0700
Q	0.6993	0.0530
R	0.7562	0.0570
S	0.8171	0.0610
T	0.7345	0.0770
U	0.8169	0.0470
V	0.9157	0.0480
W	0.7936	0.0580
Y	0.5867	0.0630
Z	0.6881	0.0370