Full wwPDB EM Validation Report (i)

Nov 19, 2022 – 09:06 pm GMT

PDB ID	:	6EPC
EMDB ID	:	EMD-3913
Title	:	Ground state 26S proteasome (GS2)
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-Busnadiego, R.
Deposited on	:	2017-10-11
Resolution	:	12.30 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 (i) 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 (i)) were used in the production of this report:

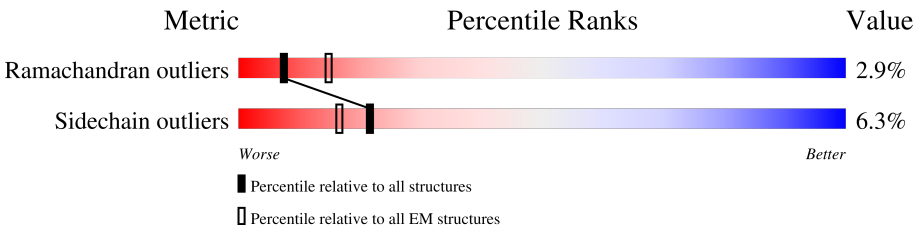
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.2

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 12.30 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	10% 74% 25% ••
2	B	234	14% 73% 23% •
3	C	261	18% 74% 18% • 5%
4	D	254	12% 74% 17% 5% • •
5	E	241	7% 78% 17% • •
6	F	263	5% 65% 24% • 10%
7	G	255	5% 72% 22% • •
8	1	238	17% 59% 18% 7% • 15%
9	2	277	21% 55% 19% • • 21%

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Mol	Chain	Length	Quality of chain
10	3	205	21% 65% 31% •
11	4	201	24% 64% 27% 6% •
12	5	263	15% 53% 18% • • 24%
13	6	240	23% 59% 23% 6% • 11%
14	7	263	17% 51% 22% 9% 18%
15	W	377	12% 40% 10% • 48%
16	V	310	5% 71% 19% • 7%
17	T	353	21% 55% 16% • 25%
18	Y	70	14% 24% 9% • 66%
19	Z	908	14% 75% 20% • •
20	N	953	15% 73% 18% • 5%
21	S	530	15% 64% 22% • 10%
22	P	456	22% 73% 22% •
23	Q	422	16% 76% 22% •
24	R	389	22% 75% 22% • •
25	U	320	20% 65% 22% • 10%
26	O	376	34% 79% 18% •
27	H	433	• 70% 18% • 9%
28	I	440	14% 67% 17% • 12%
29	K	418	10% 71% 19% • 6%
30	L	403	14% 70% 22% • •
31	M	442	16% 71% 19% • 6%
32	J	406	18% 76% 22% •

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
			Total	C	N	O	S		
7	G	245	1912	1212	326	362	12	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

- Molecule 18 is a protein called RCG28037.

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

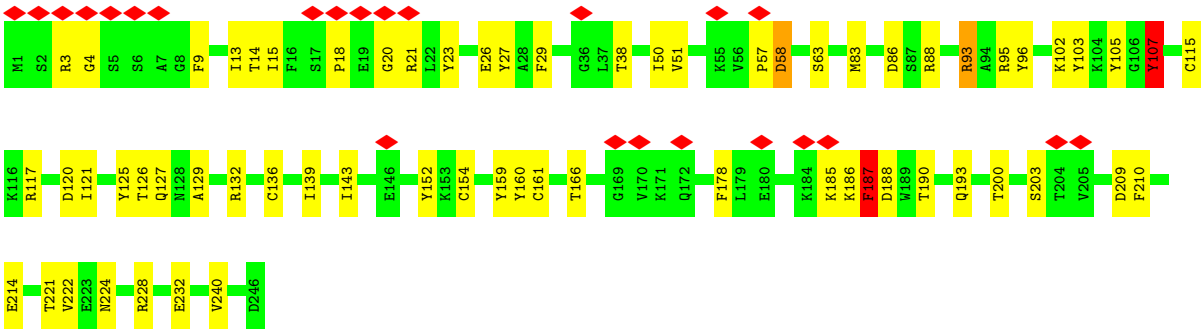
Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
32	J	406	3194	2006	569	599	20	0	0

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.

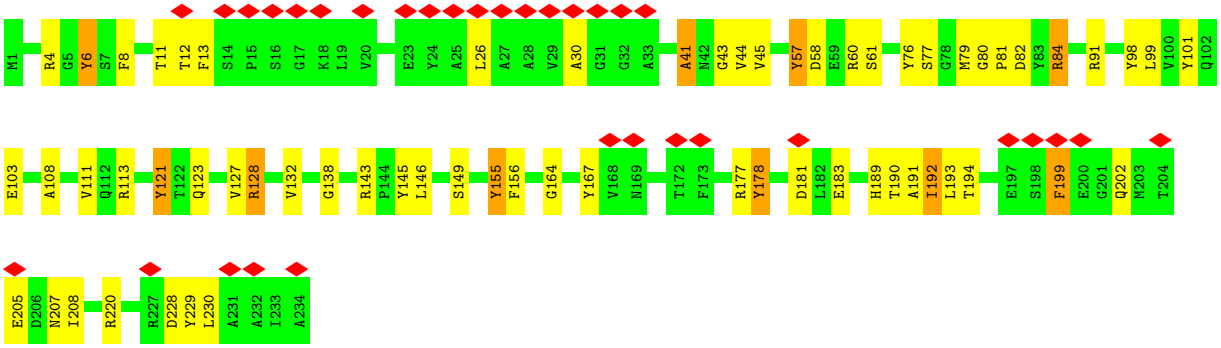
• Molecule 1: Proteasome subunit alpha type-6

Chain A:



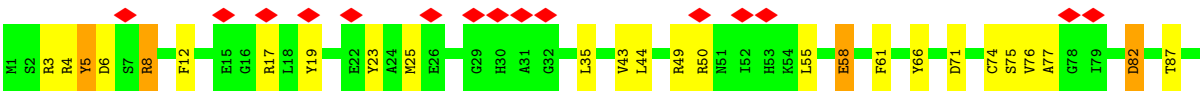
• Molecule 2: Proteasome subunit alpha type-2

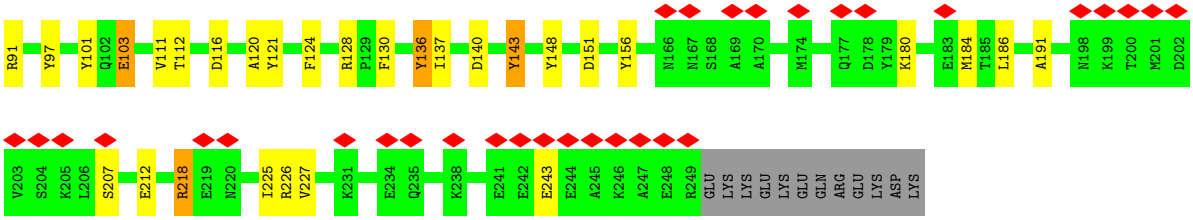
Chain B:



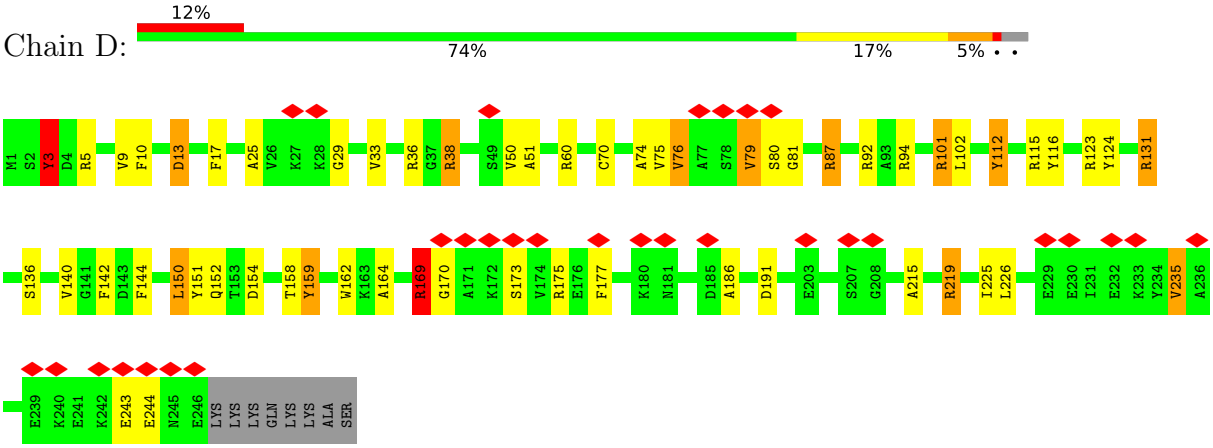
• Molecule 3: Proteasome subunit alpha type-4

Chain C:

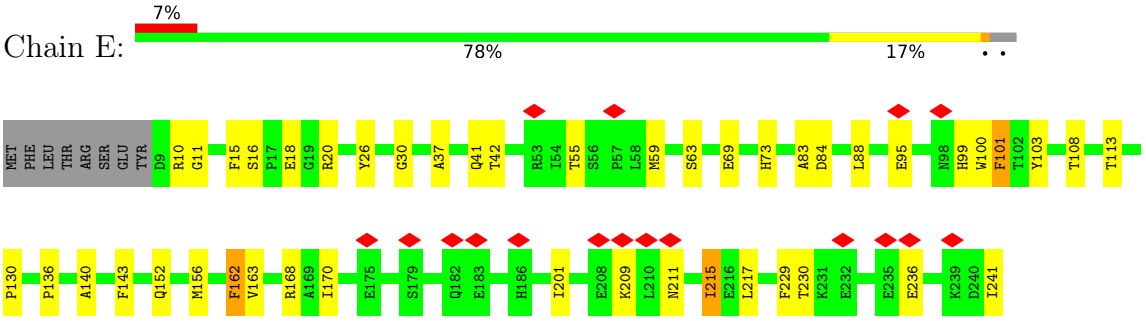




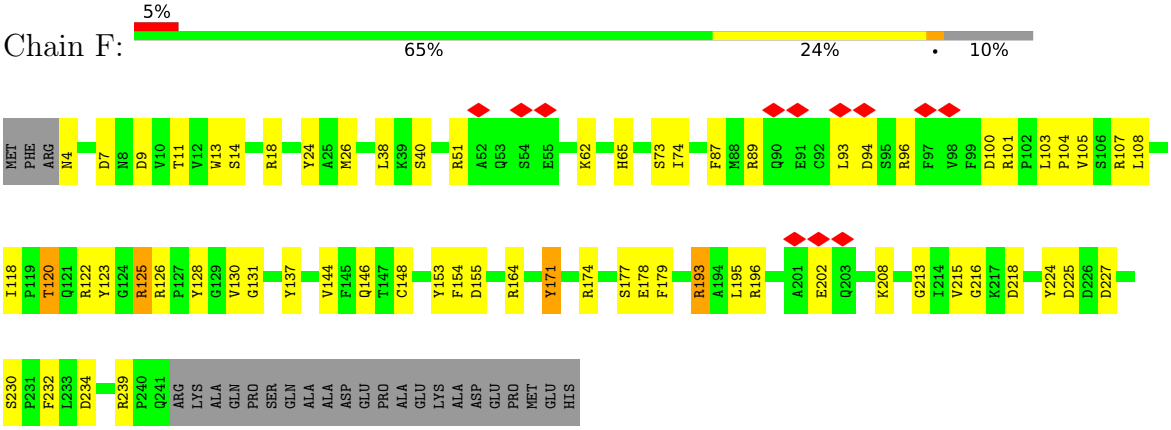
• Molecule 4: Proteasome subunit alpha type-7



• Molecule 5: Proteasome subunit alpha type-5

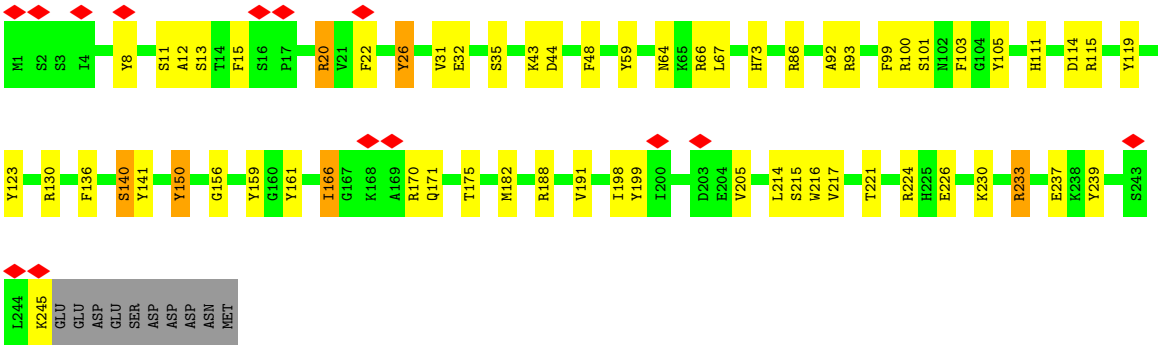


• Molecule 6: Proteasome subunit alpha type-1



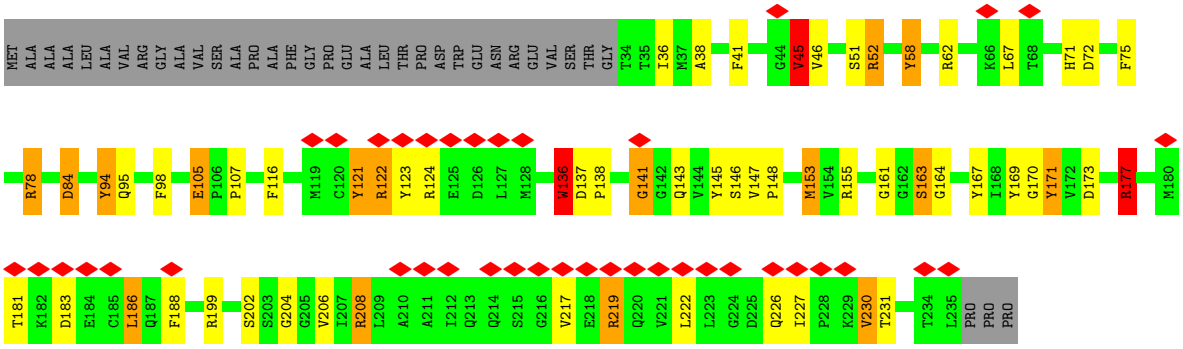
• Molecule 7: Proteasome subunit alpha type-3

Chain G:



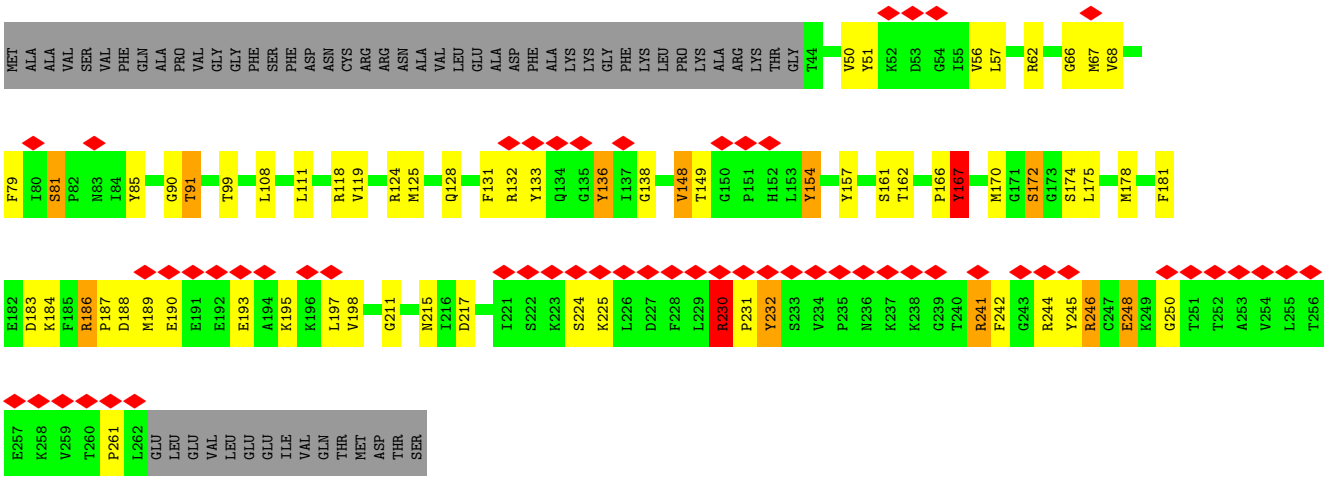
- Molecule 8: Proteasome subunit beta type-6

Chain 1:



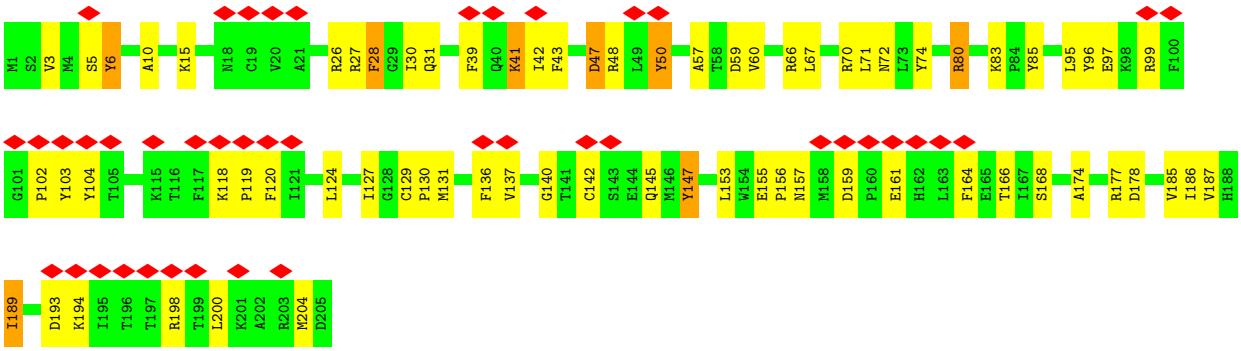
- Molecule 9: Proteasome subunit beta type-7

Chain 2:



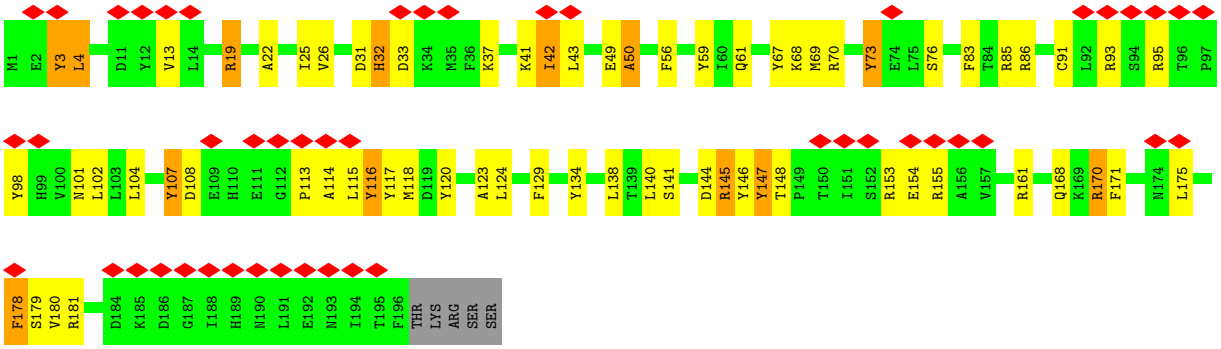
- Molecule 10: Proteasome subunit beta type-3

Chain 3:



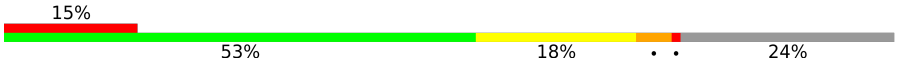
- Molecule 11: Proteasome subunit beta type-2

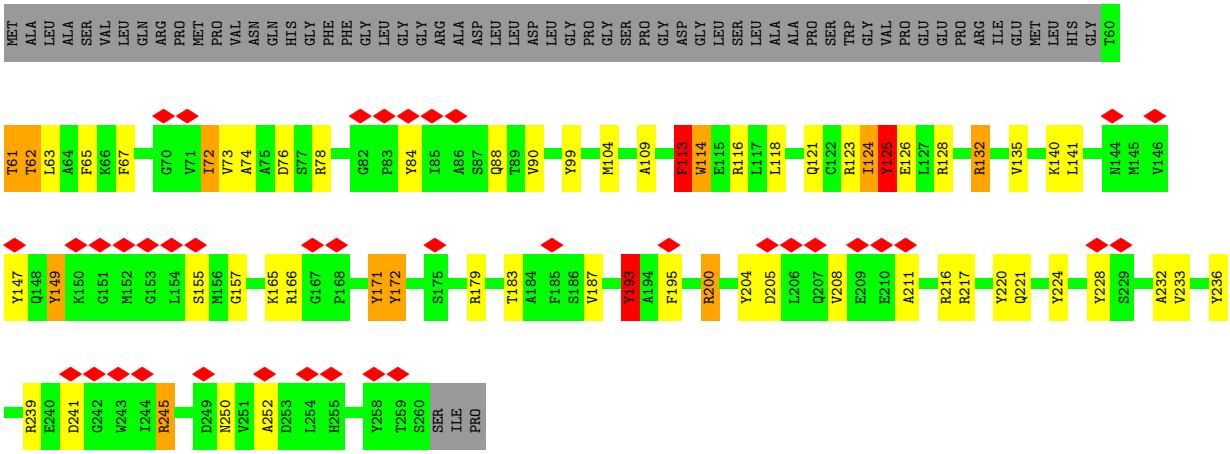
Chain 4:



- Molecule 12: Proteasome subunit beta type-5

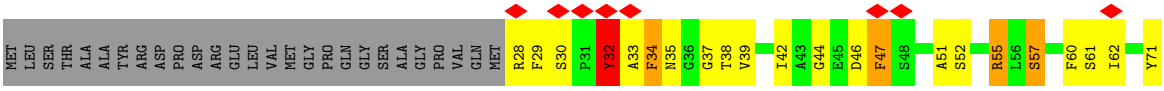
Chain 5:

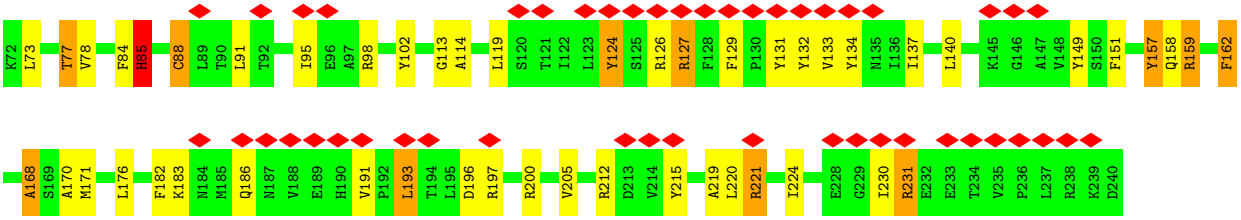




- Molecule 13: Proteasome subunit beta type-1

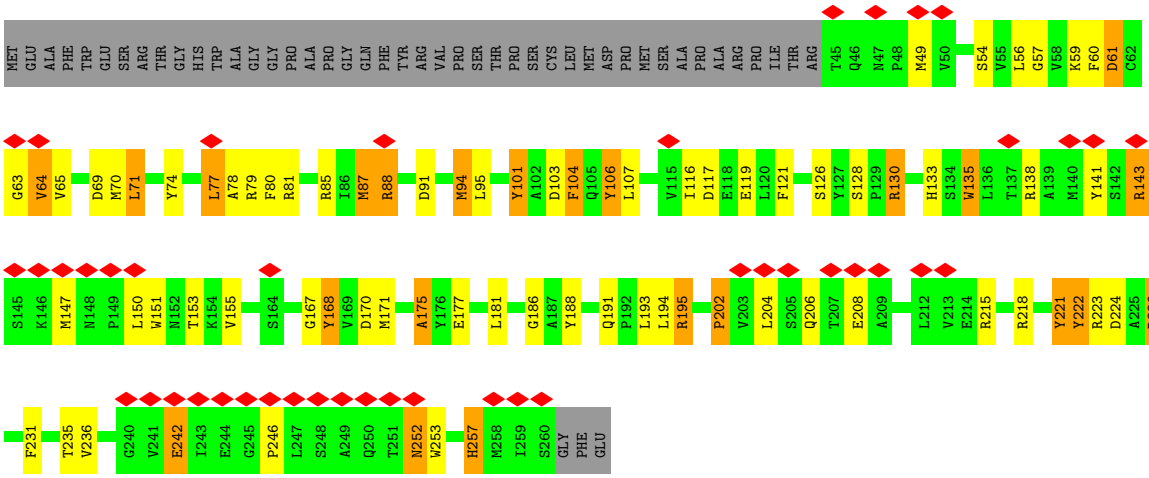
Chain 6:





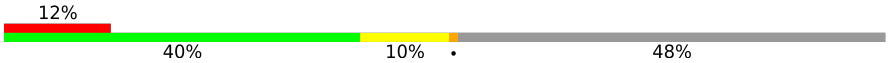
• Molecule 14: Proteasome subunit beta type-4

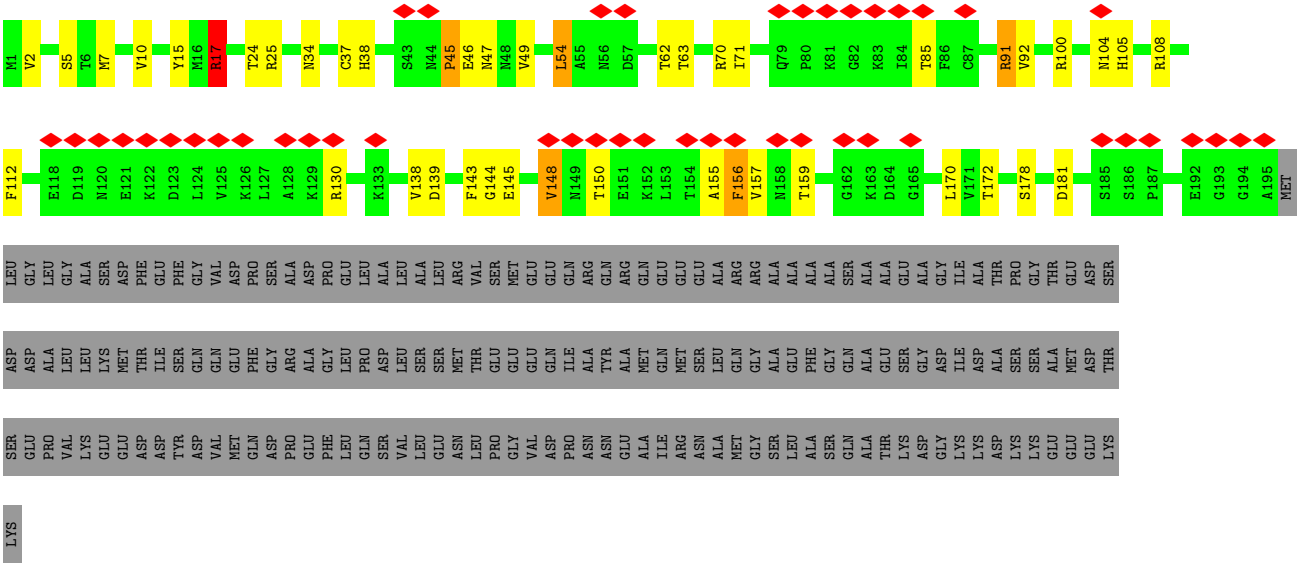
Chain 7:



• Molecule 15: 26S proteasome subunit S5a

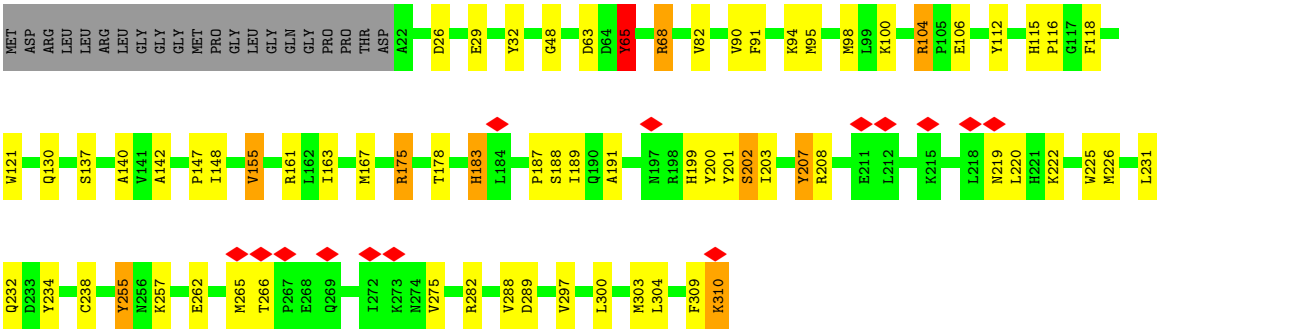
Chain W:





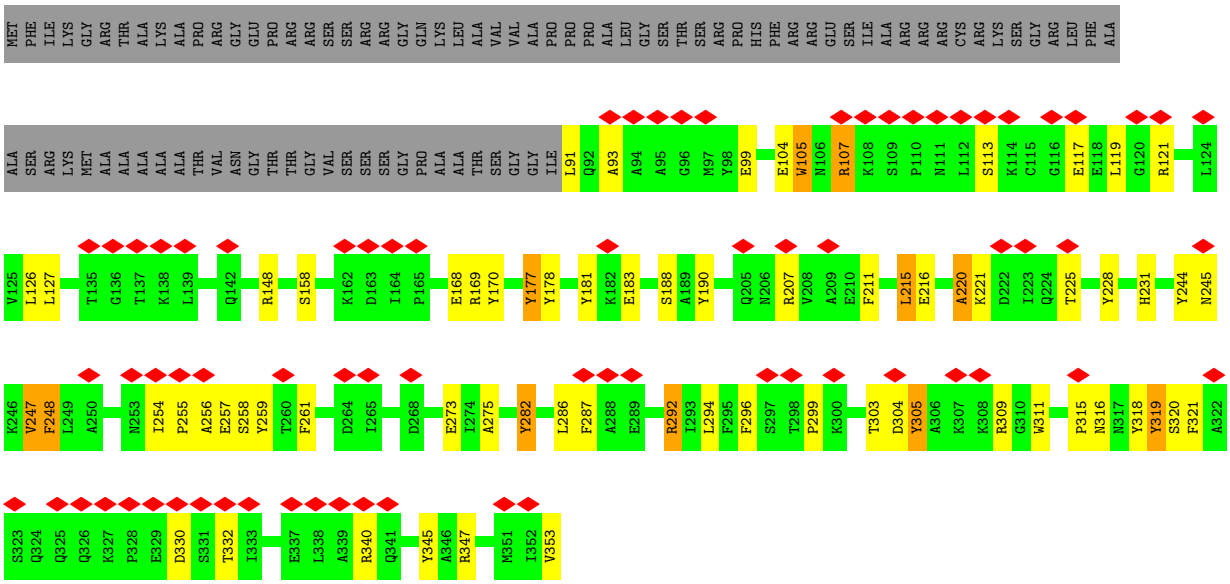
• Molecule 16: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 14

Chain V:



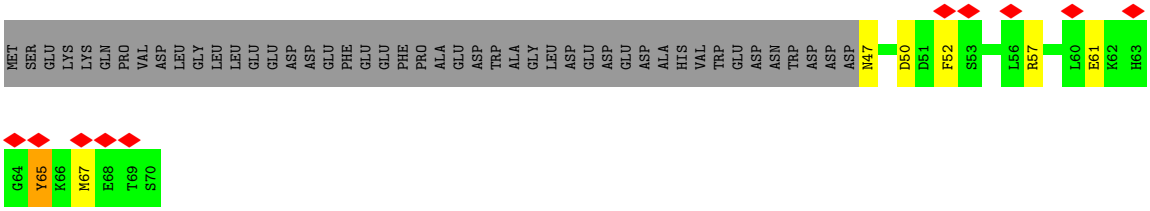
- Molecule 17: Proteasome 26S subunit, non-ATPase 8

Chain T:



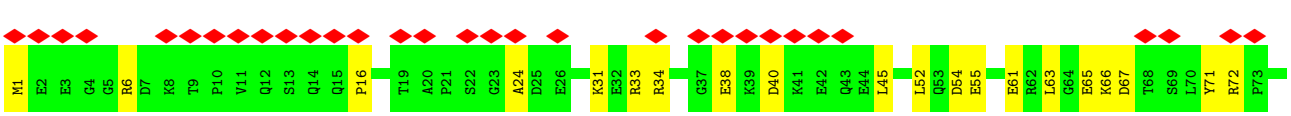
- Molecule 18: RCG28037

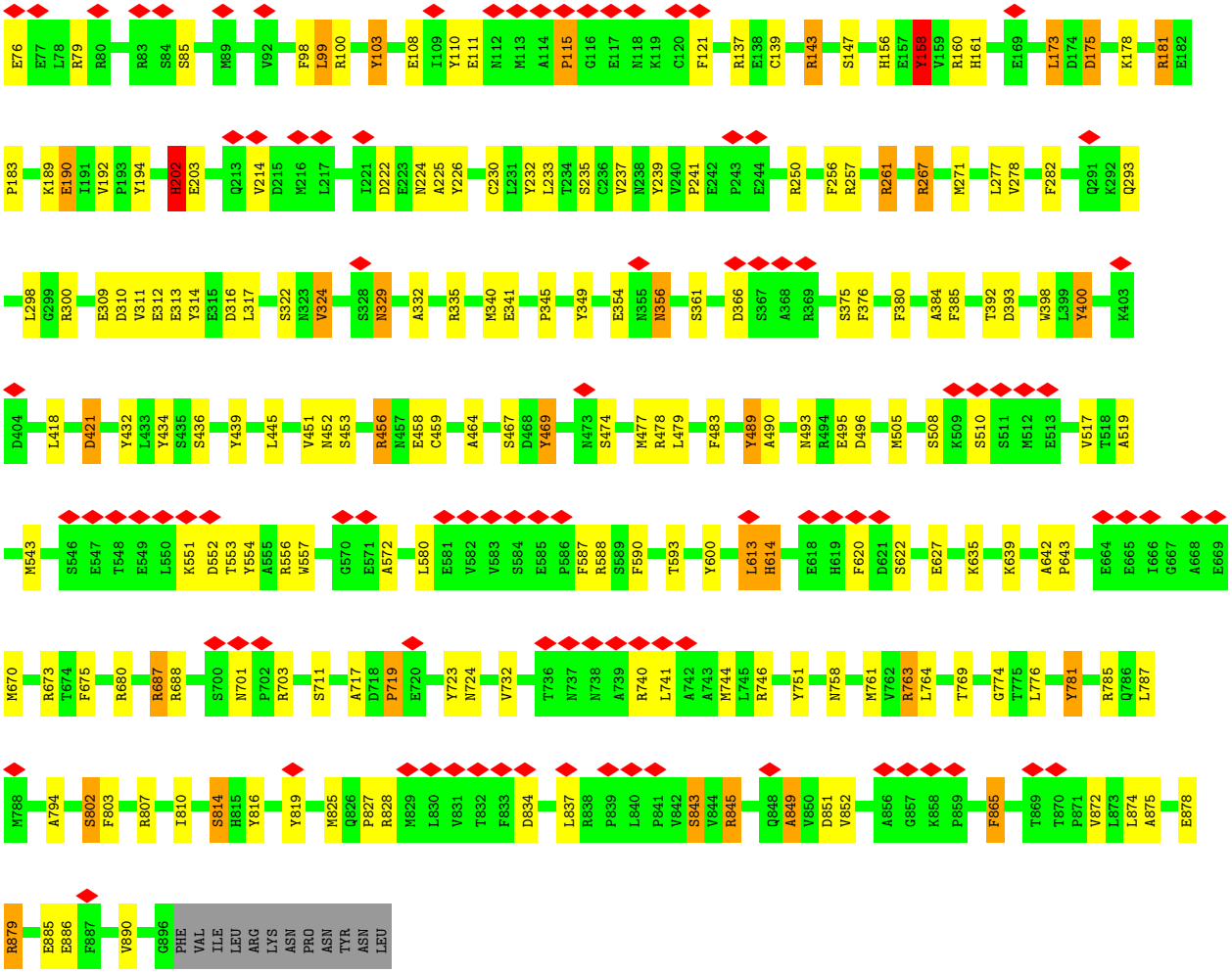
Chain Y:



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

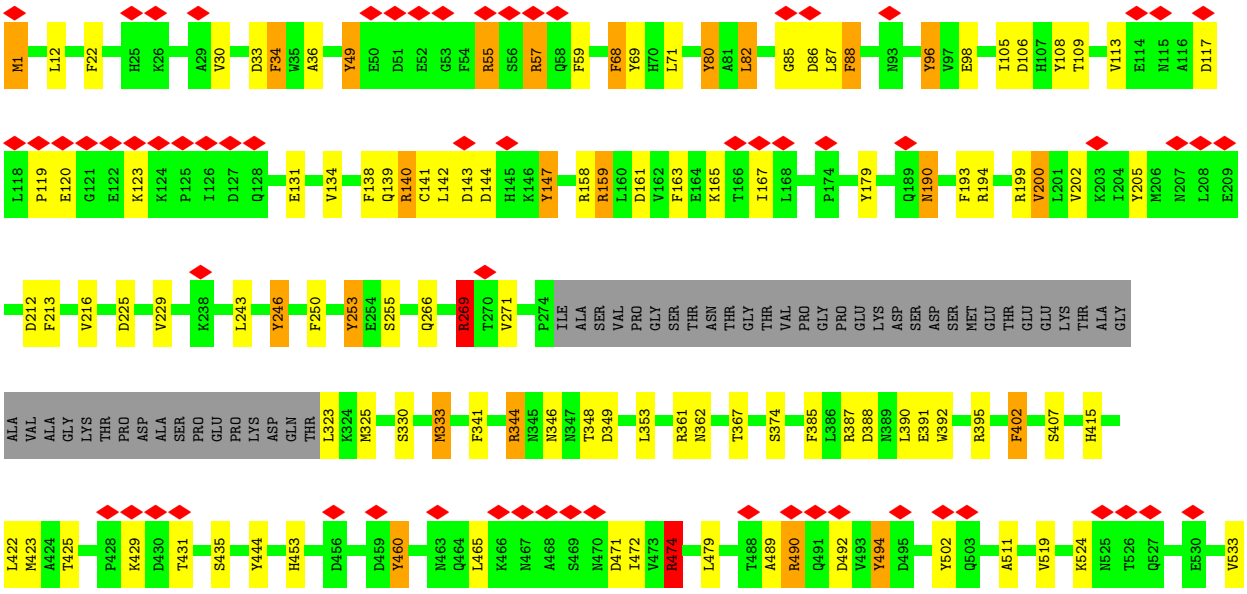
Chain Z:

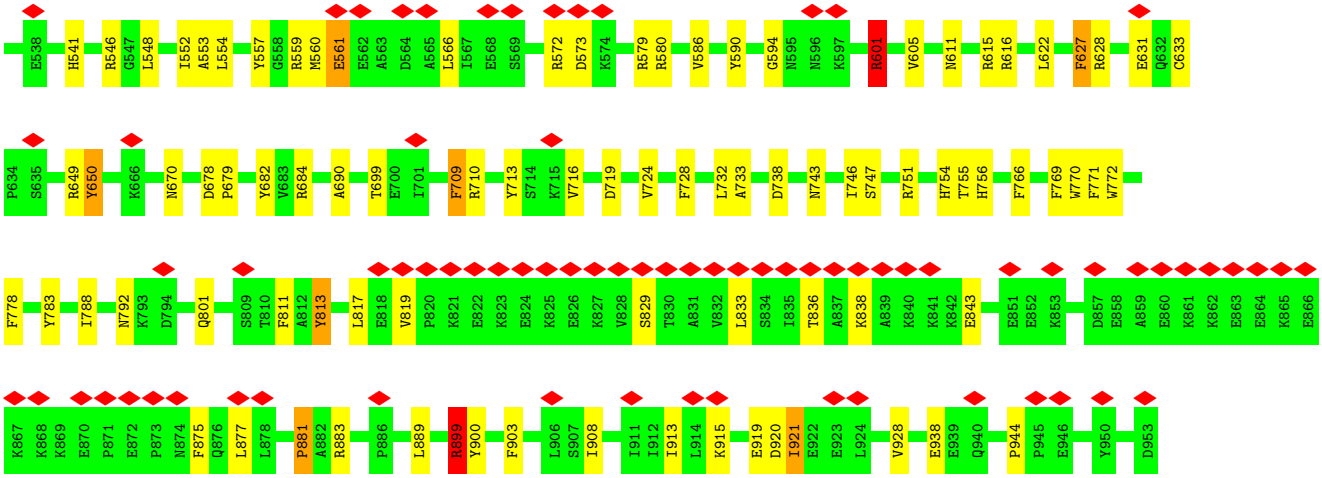




- Molecule 20: 26S proteasome non-ATPase regulatory subunit 1

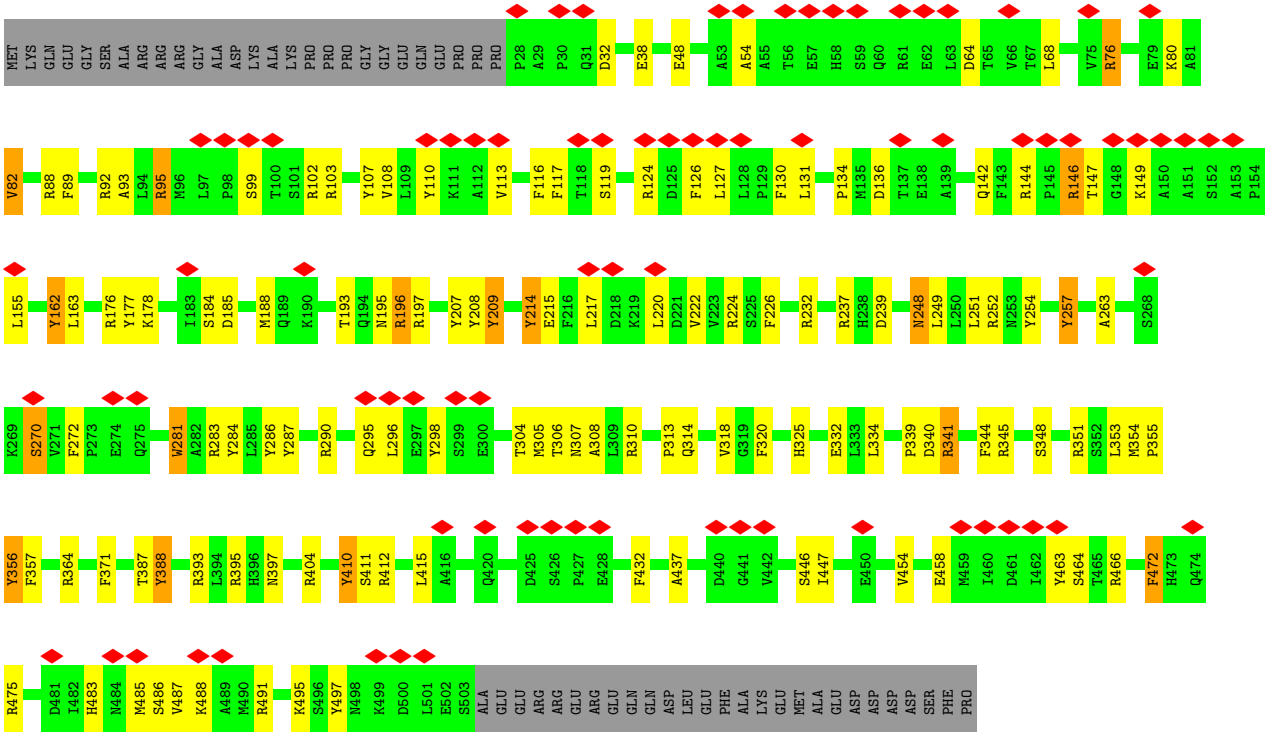
Chain N:





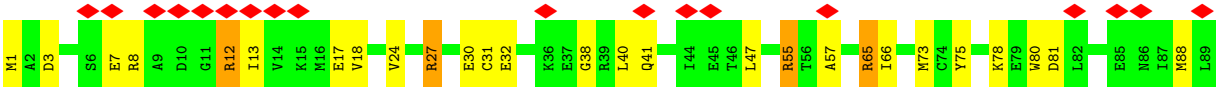
• Molecule 21: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 3

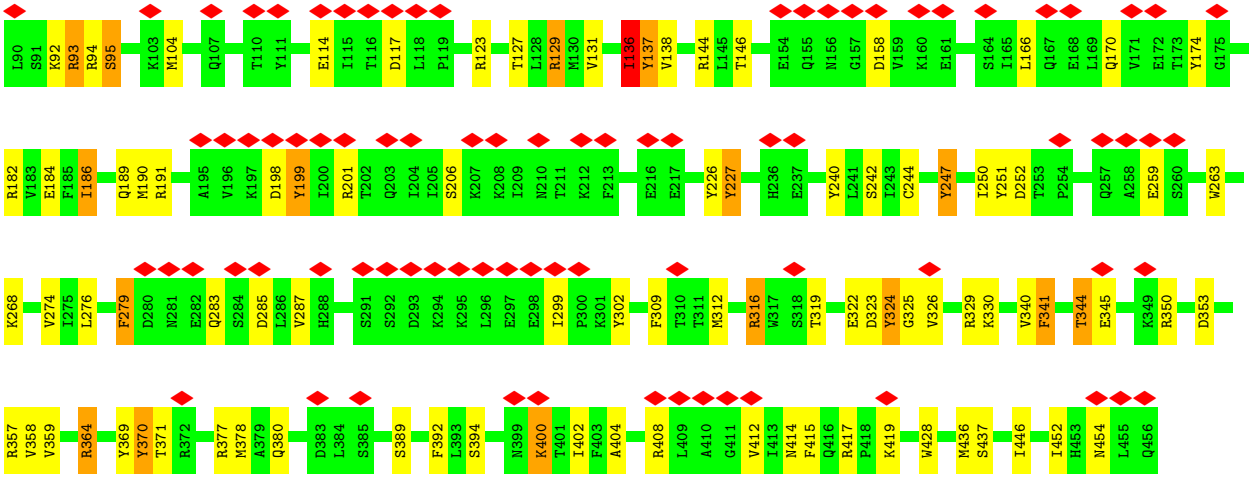
Chain S:



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

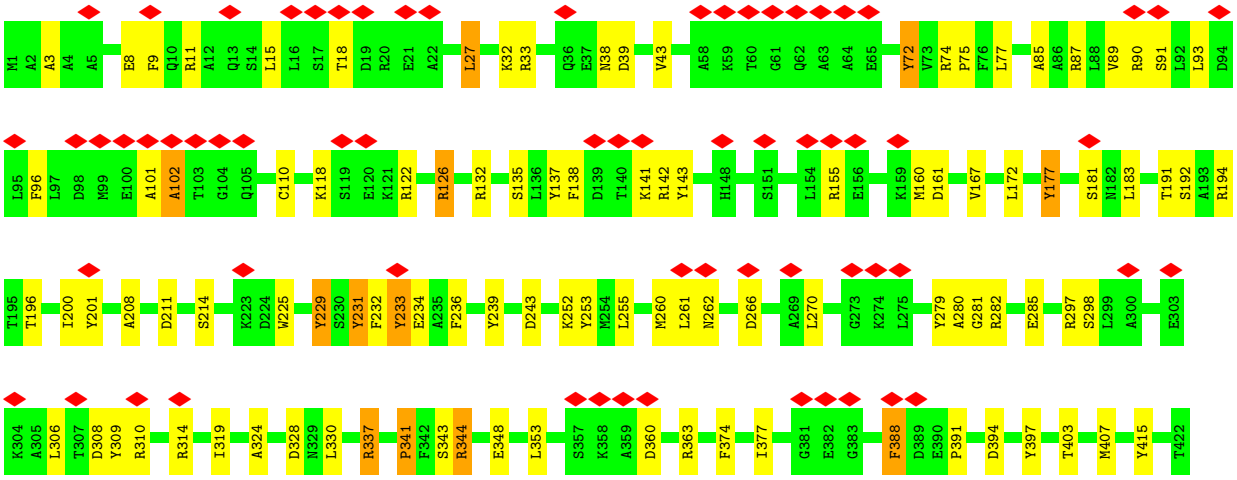
Chain P:





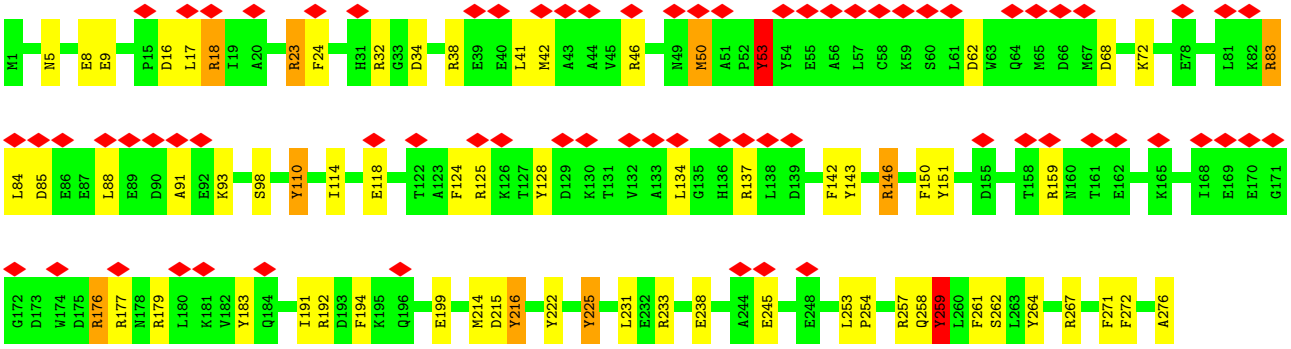
- Molecule 23: 26S proteasome non-ATPase regulatory subunit 11

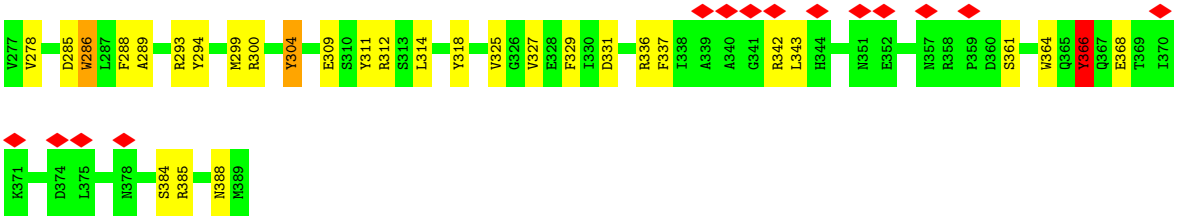
Chain Q:



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

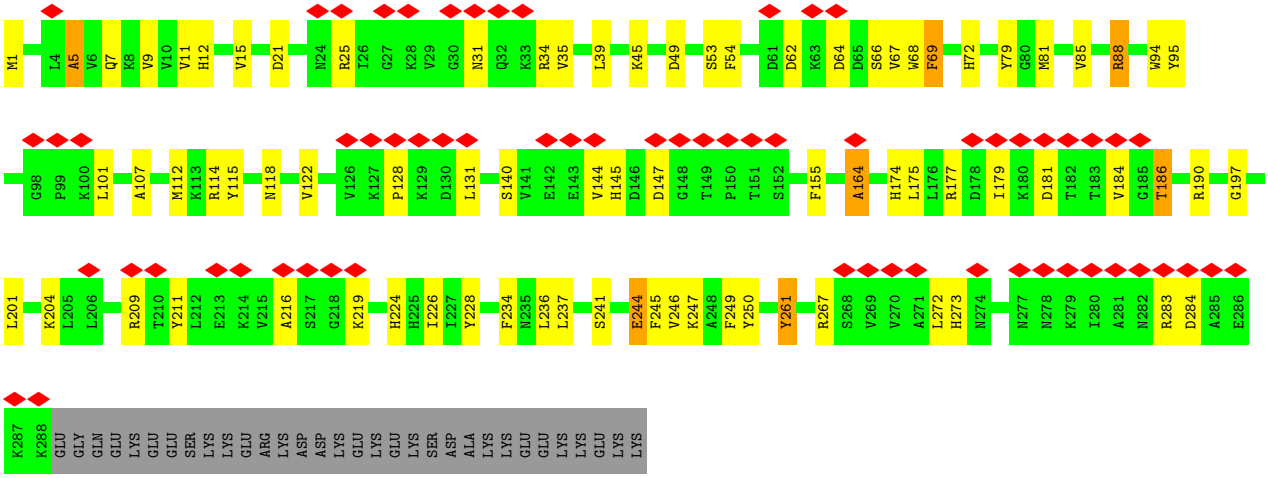
Chain R:





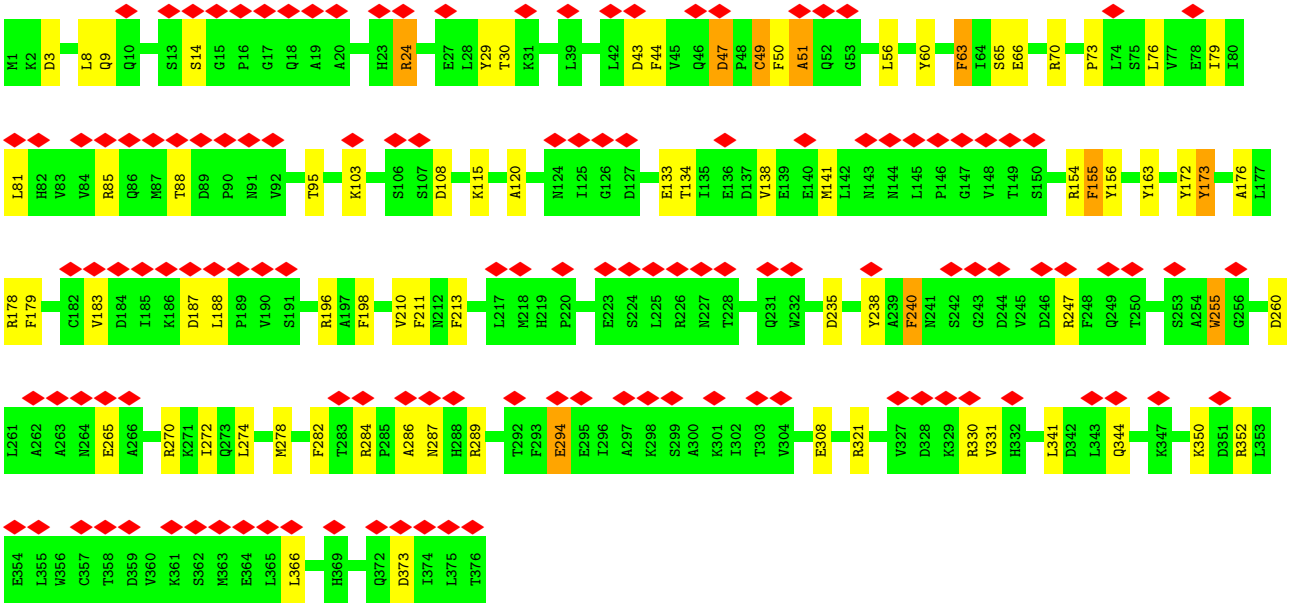
• Molecule 25: Proteasome (Prosome, macropain) 26S subunit, non-ATPase, 7 (Predicted)

Chain U:



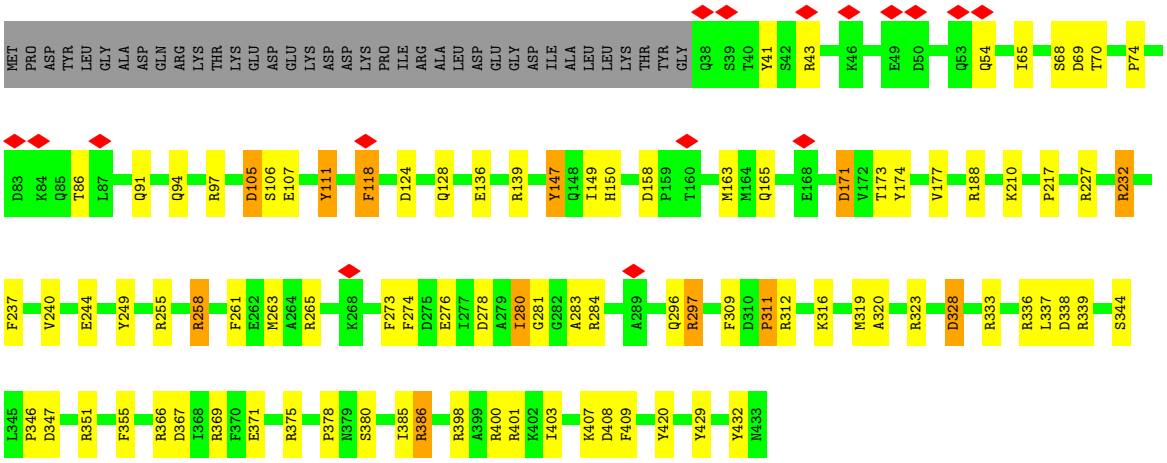
• Molecule 26: 26S proteasome non-ATPase regulatory subunit 13

Chain O:



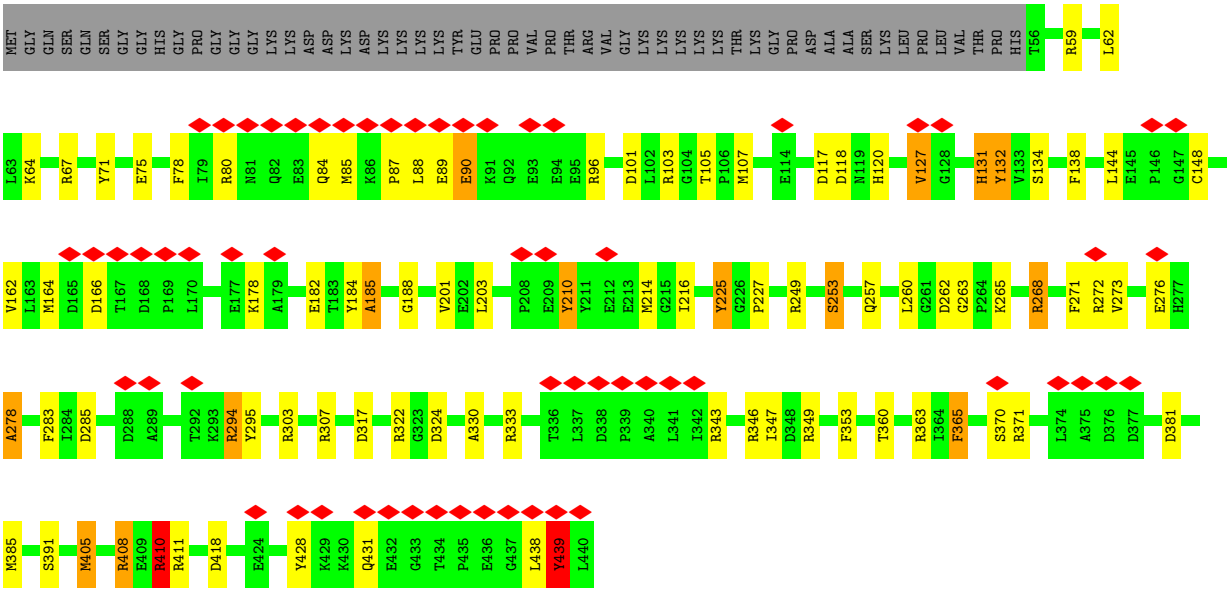
• Molecule 27: 26S proteasome regulatory subunit 7

Chain H:



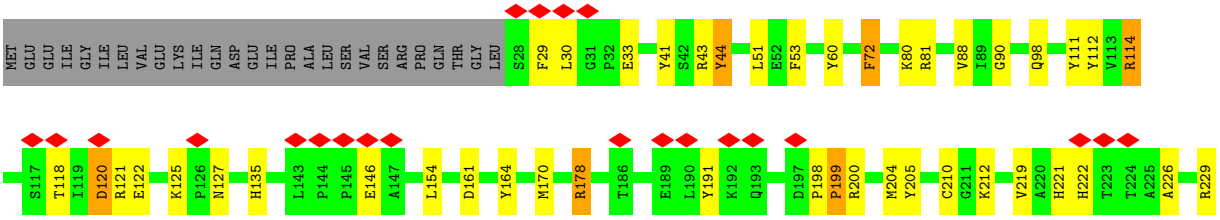
- Molecule 28: 26S proteasome regulatory subunit 4

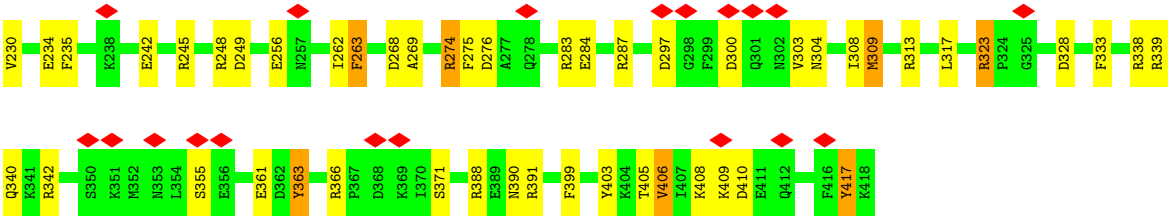
Chain I:



- Molecule 29: 26S proteasome regulatory subunit 6B

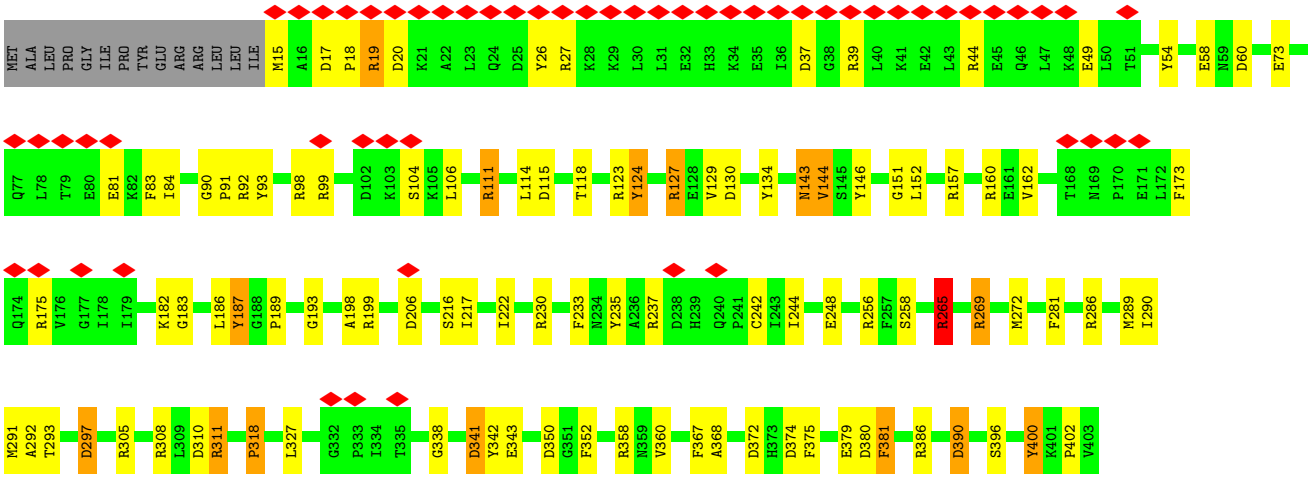
Chain K:





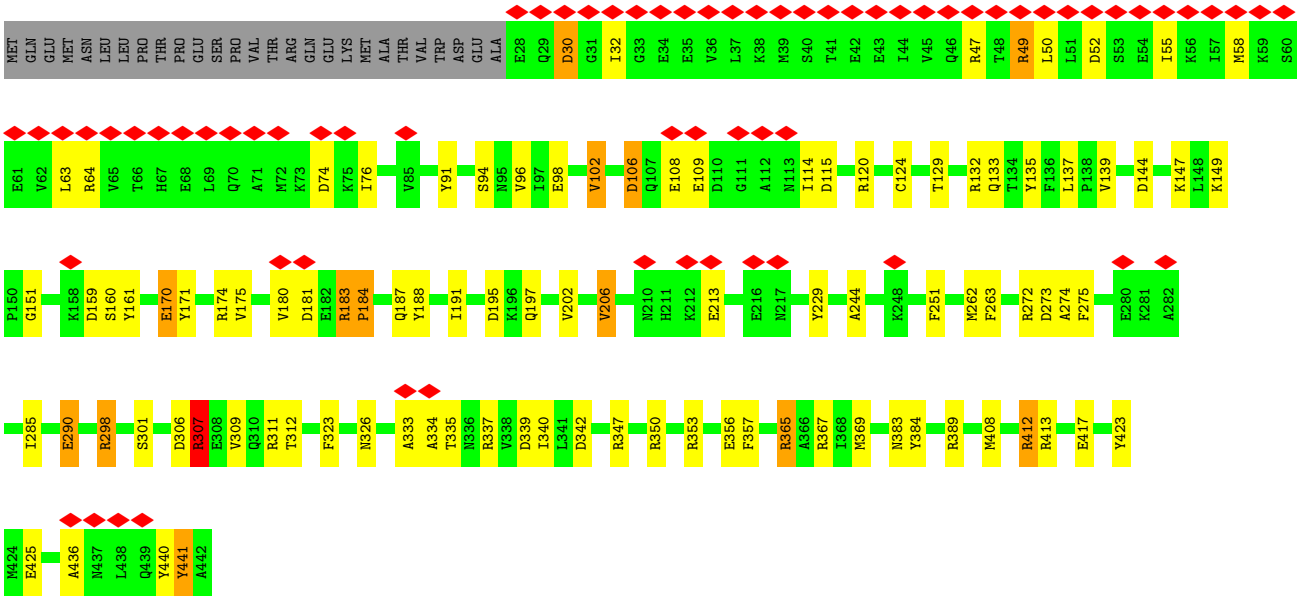
• Molecule 30: Proteasome 26S subunit, ATPase 6

Chain L:



• Molecule 31: 26S proteasome regulatory subunit 6A

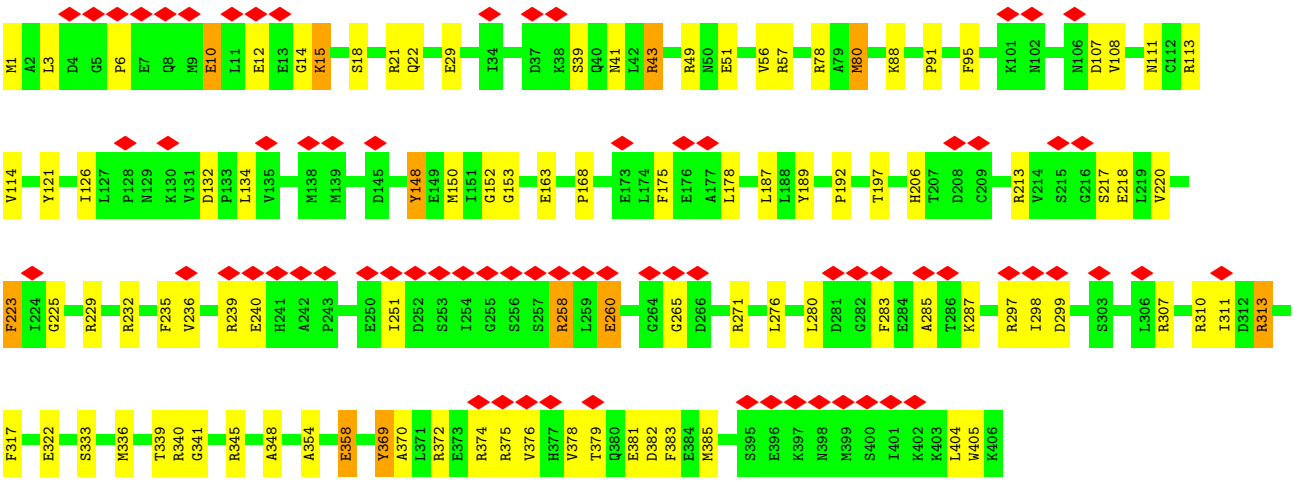
Chain M:



• Molecule 32: 26S proteasome regulatory subunit 8

Chain J:

18%
76%
22%


M1 A2 L3 D4 G5 P6 E7 Q8 M9 E10 L11 E12 E13 G14 K15 S18 R21 Q22 E29 I34 D37 K38 S39 Q40 N41 L42 R43 R49 N50 E51 V56 R57 R78 A79 M80 K88 P91 F95 K101 N102 N106 D107 V108 N111 C112 R113
V114 Y121 I126 L127 P128 N129 K130 V131 D132 P133 L134 V135 M138 M139 D145 Y148 E149 M150 I151 G152 G153 E163 P168 E173 L174 F175 E176 A177 L178 L187 L188 Y189 P192 T197 H206 T207 D208 C209 R213 V214 S215 G216 S217 E218 L219 V220
F223 I224 G225 R229 R232 F235 V236 R239 E240 H241 A242 P243 E250 I251 D252 S253 I254 G255 S256 S257 R258 L259 E260 G264 G265 D266 R271 L276 L280 D281 G282 F283 E284 A285 T286 K287 R297 I298 D299 S303 L306 R307 R310 I311 D312 R313
F317 E322 S333 M336 T339 R340 G341 R345 A348 A354 E358 Y369 A370 L371 R372 E373 R374 R375 V376 H377 V378 T379 Q380 E381 D382 F383 E384 M385 S395 E396 K397 N398 M399 S400 I401 K402 K403 L404 W405 K406

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SUBTOMOGRAM AVERAGING	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of subtomograms used	2070	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	0.747	Depositor
Minimum map value	-0.400	Depositor
Average map value	-0.037	Depositor
Map value standard deviation	0.167	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 (i)

5.1 Standard geometry (i)

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
1	A	1.79	19/1954 (1.0%)	2.04	59/2638 (2.2%)
2	B	1.79	26/1867 (1.4%)	1.94	39/2527 (1.5%)
3	C	1.76	19/1990 (1.0%)	2.01	53/2680 (2.0%)
4	D	1.75	11/1953 (0.6%)	2.04	55/2637 (2.1%)
5	E	1.66	11/1806 (0.6%)	1.84	31/2439 (1.3%)
6	F	1.72	20/1906 (1.0%)	1.99	56/2577 (2.2%)
7	G	2.28	20/1947 (1.0%)	2.27	55/2620 (2.1%)
8	1	1.78	15/1542 (1.0%)	2.16	46/2089 (2.2%)
9	2	1.76	15/1679 (0.9%)	2.06	42/2271 (1.8%)
10	3	1.73	13/1629 (0.8%)	1.96	49/2195 (2.2%)
11	4	1.76	18/1604 (1.1%)	2.06	51/2170 (2.4%)
12	5	1.82	22/1592 (1.4%)	2.11	56/2152 (2.6%)
13	6	1.79	17/1690 (1.0%)	2.15	53/2278 (2.3%)
14	7	2.89	26/1720 (1.5%)	2.09	66/2327 (2.8%)
15	W	1.62	10/1500 (0.7%)	1.91	35/2030 (1.7%)
16	V	1.63	14/2315 (0.6%)	1.92	51/3129 (1.6%)
17	T	1.73	24/2195 (1.1%)	1.99	65/2964 (2.2%)
18	Y	1.81	3/201 (1.5%)	1.87	7/266 (2.6%)
19	Z	1.73	69/7026 (1.0%)	1.90	154/9495 (1.6%)
20	N	1.67	49/7206 (0.7%)	1.90	158/9738 (1.6%)
21	S	1.74	40/3918 (1.0%)	2.00	115/5287 (2.2%)
22	P	1.68	28/3754 (0.7%)	1.94	101/5049 (2.0%)
23	Q	1.69	29/3381 (0.9%)	1.93	86/4558 (1.9%)
24	R	1.72	34/3263 (1.0%)	2.01	88/4393 (2.0%)
25	U	1.70	18/2344 (0.8%)	1.94	61/3178 (1.9%)
26	O	1.69	24/3066 (0.8%)	1.93	66/4148 (1.6%)
27	H	1.72	25/3166 (0.8%)	1.91	61/4275 (1.4%)
28	I	1.74	27/3085 (0.9%)	1.94	78/4158 (1.9%)
29	K	1.71	19/3178 (0.6%)	1.96	79/4290 (1.8%)
30	L	1.78	42/3146 (1.3%)	2.02	74/4233 (1.7%)
31	M	1.70	29/3293 (0.9%)	1.99	86/4436 (1.9%)
32	J	1.74	33/3236 (1.0%)	1.92	66/4347 (1.5%)
All	All	1.77	769/84152 (0.9%)	1.98	2142/113574 (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	4
2	B	0	7
3	C	0	6
4	D	0	11
5	E	0	2
6	F	0	6
7	G	0	6
8	1	0	6
9	2	0	6
10	3	0	7
11	4	0	10
12	5	0	8
13	6	0	8
14	7	0	12
15	W	0	5
16	V	0	5
17	T	0	6
18	Y	0	1
19	Z	0	16
20	N	0	27
21	S	0	14
22	P	0	13
23	Q	0	7
24	R	0	10
25	U	0	6
26	O	0	4
27	H	0	7
28	I	0	7
29	K	0	10
30	L	0	9
31	M	0	9
32	J	0	5
All	All	0	260

All (769) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	G	224	ARG	CZ-NH1	64.53	2.17	1.33
14	7	121	PHE	CG-CD2	50.92	2.15	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	121	PHE	CG-CD1	42.89	2.03	1.38
14	7	121	PHE	CE1-CZ	35.55	2.04	1.37
14	7	121	PHE	CE2-CZ	33.59	2.01	1.37
14	7	121	PHE	CD2-CE2	32.35	2.04	1.39
14	7	121	PHE	CD1-CE1	30.53	2.00	1.39
15	W	108	ARG	NE-CZ	10.62	1.46	1.33
24	R	312	ARG	CZ-NH2	9.40	1.45	1.33
3	C	74	CYS	CB-SG	9.26	1.98	1.82
28	I	408	ARG	CD-NE	9.04	1.61	1.46
3	C	218	ARG	NE-CZ	8.84	1.44	1.33
13	6	157	TYR	CE2-CZ	8.80	1.50	1.38
27	H	336	ARG	CZ-NH2	8.61	1.44	1.33
1	A	160	TYR	CZ-OH	8.57	1.52	1.37
31	M	132	ARG	CZ-NH1	8.56	1.44	1.33
27	H	344	SER	CA-CB	8.52	1.65	1.52
7	G	215	SER	CA-CB	8.50	1.65	1.52
26	O	70	ARG	CZ-NH1	8.46	1.44	1.33
7	G	26	TYR	CE2-CZ	8.44	1.49	1.38
32	J	51	GLU	CD-OE2	-8.33	1.16	1.25
31	M	307	ARG	CZ-NH2	8.31	1.43	1.33
21	S	89	PHE	CG-CD2	8.31	1.51	1.38
23	Q	8	GLU	CD-OE1	8.24	1.34	1.25
19	Z	478	ARG	CD-NE	8.17	1.60	1.46
23	Q	253	TYR	CE1-CZ	8.14	1.49	1.38
10	3	97	GLU	CD-OE1	8.13	1.34	1.25
13	6	124	TYR	CZ-OH	8.13	1.51	1.37
6	F	216	GLY	CA-C	-8.12	1.38	1.51
26	O	238	TYR	CE2-CZ	8.12	1.49	1.38
3	C	121	TYR	CG-CD1	7.83	1.49	1.39
8	1	204	GLY	CA-C	-7.79	1.39	1.51
22	P	182	ARG	NE-CZ	7.77	1.43	1.33
22	P	31	CYS	CB-SG	7.74	1.95	1.82
30	L	90	GLY	N-CA	-7.73	1.34	1.46
16	V	137	SER	CA-CB	7.70	1.64	1.52
30	L	248	GLU	CG-CD	7.69	1.63	1.51
2	B	113	ARG	NE-CZ	7.68	1.43	1.33
24	R	128	TYR	CB-CG	-7.68	1.40	1.51
27	H	401	ARG	NE-CZ	7.68	1.43	1.33
1	A	203	SER	CA-CB	7.66	1.64	1.52
17	T	168	GLU	CG-CD	7.66	1.63	1.51
8	1	124	ARG	CD-NE	7.61	1.59	1.46
32	J	258	ARG	CZ-NH2	7.58	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	K	417	TYR	CG-CD1	7.57	1.49	1.39
26	O	247	ARG	NE-CZ	7.52	1.42	1.33
22	P	17	GLU	CG-CD	7.50	1.63	1.51
9	2	241	ARG	CZ-NH2	7.50	1.42	1.33
27	H	255	ARG	NE-CZ	7.49	1.42	1.33
20	N	679	PRO	N-CA	-7.49	1.34	1.47
29	K	274	ARG	CZ-NH2	7.42	1.42	1.33
30	L	19	ARG	CD-NE	7.41	1.59	1.46
21	S	124	ARG	NE-CZ	7.41	1.42	1.33
17	T	178	TYR	CG-CD1	7.39	1.48	1.39
19	Z	203	GLU	CB-CG	7.38	1.66	1.52
8	1	62	ARG	NE-CZ	7.37	1.42	1.33
27	H	297	ARG	CZ-NH2	7.35	1.42	1.33
5	E	236	GLU	CD-OE1	7.32	1.33	1.25
2	B	178	TYR	CE2-CZ	7.30	1.48	1.38
19	Z	495	GLU	CG-CD	7.28	1.62	1.51
24	R	267	ARG	NE-CZ	7.28	1.42	1.33
31	M	183	ARG	NE-CZ	7.27	1.42	1.33
11	4	155	ARG	CD-NE	7.26	1.58	1.46
24	R	23	ARG	CZ-NH2	7.26	1.42	1.33
9	2	157	TYR	CZ-OH	7.24	1.50	1.37
9	2	241	ARG	CZ-NH1	7.24	1.42	1.33
9	2	62	ARG	NE-CZ	7.23	1.42	1.33
7	G	188	ARG	NE-CZ	7.21	1.42	1.33
6	F	177	SER	CA-CB	7.16	1.63	1.52
28	I	227	PRO	N-CD	-7.16	1.37	1.47
8	1	202	SER	CA-CB	7.14	1.63	1.52
19	Z	879	ARG	CZ-NH2	7.10	1.42	1.33
21	S	404	ARG	CD-NE	7.08	1.58	1.46
4	D	115	ARG	CZ-NH2	7.08	1.42	1.33
21	S	270	SER	CA-CB	7.08	1.63	1.52
27	H	400	ARG	NE-CZ	7.07	1.42	1.33
3	C	75	SER	CA-CB	7.04	1.63	1.52
2	B	61	SER	CA-CB	7.04	1.63	1.52
28	I	333	ARG	CZ-NH2	7.03	1.42	1.33
2	B	60	ARG	NE-CZ	7.02	1.42	1.33
14	7	128	SER	CA-CB	7.00	1.63	1.52
31	M	353	ARG	NE-CZ	6.98	1.42	1.33
2	B	81	PRO	N-CD	6.96	1.57	1.47
20	N	559	ARG	CD-NE	6.93	1.58	1.46
21	S	475	ARG	CD-NE	6.92	1.58	1.46
26	O	155	PHE	CB-CG	6.92	1.63	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Q	229	TYR	CZ-OH	6.90	1.49	1.37
20	N	460	TYR	CE1-CZ	6.90	1.47	1.38
2	B	149	SER	CA-CB	6.90	1.63	1.52
12	5	123	ARG	NE-CZ	6.85	1.42	1.33
25	U	250	TYR	CG-CD2	6.84	1.48	1.39
3	C	58	GLU	CD-OE1	-6.79	1.18	1.25
24	R	337	PHE	CG-CD1	6.78	1.49	1.38
20	N	490	ARG	CZ-NH2	6.77	1.41	1.33
30	L	98	ARG	NE-CZ	6.75	1.41	1.33
27	H	139	ARG	CD-NE	6.75	1.57	1.46
29	K	245	ARG	CZ-NH2	6.74	1.41	1.33
6	F	51	ARG	CD-NE	6.74	1.57	1.46
12	5	239	ARG	CD-NE	6.74	1.57	1.46
23	Q	388	PHE	CG-CD2	6.70	1.48	1.38
23	Q	314	ARG	CD-NE	6.70	1.57	1.46
28	I	343	ARG	CZ-NH1	6.70	1.41	1.33
1	A	232	GLU	CG-CD	6.70	1.61	1.51
19	Z	335	ARG	CZ-NH2	6.70	1.41	1.33
3	C	156	TYR	CG-CD1	6.69	1.47	1.39
2	B	183	GLU	CD-OE2	6.68	1.32	1.25
28	I	90	GLU	CG-CD	6.68	1.61	1.51
19	Z	627	GLU	CD-OE1	6.67	1.32	1.25
19	Z	72	ARG	NE-CZ	6.66	1.41	1.33
8	1	62	ARG	CD-NE	6.66	1.57	1.46
23	Q	314	ARG	NE-CZ	6.65	1.41	1.33
22	P	437	SER	CA-CB	6.64	1.62	1.52
31	M	49	ARG	NE-CZ	6.64	1.41	1.33
27	H	97	ARG	NE-CZ	6.64	1.41	1.33
7	G	233	ARG	CD-NE	6.64	1.57	1.46
1	A	95	ARG	NE-CZ	6.62	1.41	1.33
1	A	63	SER	CA-CB	6.62	1.62	1.52
20	N	601	ARG	CZ-NH2	6.60	1.41	1.33
1	A	93	ARG	NE-CZ	6.60	1.41	1.33
23	Q	225	TRP	CD2-CE2	6.58	1.49	1.41
24	R	98	SER	CA-CB	6.56	1.62	1.52
22	P	316	ARG	NE-CZ	6.56	1.41	1.33
14	7	74	TYR	CE2-CZ	6.56	1.47	1.38
22	P	129	ARG	CZ-NH2	6.55	1.41	1.33
19	Z	79	ARG	CZ-NH2	6.55	1.41	1.33
23	Q	281	GLY	CA-C	-6.54	1.41	1.51
6	F	174	ARG	CD-NE	6.54	1.57	1.46
22	P	55	ARG	CZ-NH2	6.53	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	4	76	SER	CA-CB	6.53	1.62	1.52
19	Z	65	GLU	CG-CD	6.52	1.61	1.51
19	Z	774	GLY	CA-C	-6.52	1.41	1.51
20	N	710	ARG	CZ-NH1	6.52	1.41	1.33
1	A	96	TYR	CE1-CZ	6.52	1.47	1.38
3	C	3	ARG	CA-CB	6.52	1.68	1.53
21	S	162	TYR	CE1-CZ	6.51	1.47	1.38
19	Z	16	PRO	CA-C	-6.51	1.39	1.52
7	G	130	ARG	CD-NE	6.51	1.57	1.46
1	A	95	ARG	CZ-NH2	6.50	1.41	1.33
30	L	92	ARG	NE-CZ	6.50	1.41	1.33
13	6	170	ALA	CA-CB	6.50	1.66	1.52
25	U	209	ARG	CZ-NH1	6.49	1.41	1.33
24	R	53	TYR	CZ-OH	6.48	1.48	1.37
12	5	166	ARG	NE-CZ	6.48	1.41	1.33
16	V	188	SER	CA-CB	6.48	1.62	1.52
17	T	121	ARG	NE-CZ	6.46	1.41	1.33
17	T	257	GLU	CG-CD	6.45	1.61	1.51
32	J	14	GLY	N-CA	-6.44	1.36	1.46
4	D	81	GLY	CA-C	6.44	1.62	1.51
30	L	134	TYR	CB-CG	6.44	1.61	1.51
22	P	8	ARG	CZ-NH2	6.42	1.41	1.33
21	S	102	ARG	NE-CZ	6.41	1.41	1.33
14	7	253	TRP	CG-CD1	6.40	1.45	1.36
16	V	255	TYR	CE2-CZ	6.40	1.46	1.38
14	7	218	ARG	NE-CZ	6.40	1.41	1.33
2	B	57	TYR	CG-CD2	6.39	1.47	1.39
30	L	235	TYR	CG-CD2	6.39	1.47	1.39
19	Z	298	LEU	C-N	6.38	1.44	1.33
6	F	213	GLY	CA-C	-6.38	1.41	1.51
25	U	34	ARG	CZ-NH2	6.38	1.41	1.33
23	Q	214	SER	CA-CB	6.38	1.62	1.52
12	5	200	ARG	NE-CZ	6.37	1.41	1.33
19	Z	322	SER	CA-CB	6.37	1.62	1.52
30	L	49	GLU	CG-CD	6.36	1.61	1.51
31	M	171	TYR	CE1-CZ	6.35	1.46	1.38
7	G	140	SER	CA-CB	6.35	1.62	1.52
12	5	84	TYR	CB-CG	-6.35	1.42	1.51
2	B	101	TYR	CG-CD2	6.35	1.47	1.39
27	H	111	TYR	CE1-CZ	6.34	1.46	1.38
9	2	193	GLU	CD-OE1	6.34	1.32	1.25
19	Z	878	GLU	CG-CD	6.34	1.61	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	115	CYS	CB-SG	-6.34	1.71	1.82
20	N	444	TYR	CD2-CE2	-6.33	1.29	1.39
24	R	38	ARG	CD-NE	6.33	1.57	1.46
22	P	417	ARG	NE-CZ	6.32	1.41	1.33
29	K	391	ARG	NE-CZ	6.32	1.41	1.33
14	7	130	ARG	NE-CZ	6.32	1.41	1.33
22	P	324	TYR	CZ-OH	6.32	1.48	1.37
27	H	432	TYR	CZ-OH	6.32	1.48	1.37
29	K	338	ARG	CZ-NH1	6.31	1.41	1.33
13	6	113	GLY	CA-C	-6.30	1.41	1.51
17	T	99	GLU	CG-CD	6.30	1.61	1.51
24	R	304	TYR	CZ-OH	6.30	1.48	1.37
19	Z	828	ARG	CD-NE	6.30	1.57	1.46
14	7	223	ARG	NE-CZ	6.29	1.41	1.33
29	K	366	ARG	NE-CZ	6.29	1.41	1.33
19	Z	746	ARG	CD-NE	6.29	1.57	1.46
32	J	113	ARG	CZ-NH2	6.26	1.41	1.33
4	D	136	SER	CA-CB	6.26	1.62	1.52
20	N	751	ARG	CD-NE	6.26	1.57	1.46
19	Z	85	SER	CA-CB	6.26	1.62	1.52
15	W	70	ARG	CZ-NH2	6.26	1.41	1.33
24	R	146	ARG	CZ-NH2	6.24	1.41	1.33
24	R	384	SER	CA-CB	6.22	1.62	1.52
23	Q	87	ARG	NE-CZ	6.22	1.41	1.33
18	Y	52	PHE	CG-CD2	6.21	1.48	1.38
19	Z	723	TYR	CE2-CZ	6.21	1.46	1.38
24	R	336	ARG	CZ-NH1	6.19	1.41	1.33
21	S	344	PHE	CG-CD1	6.19	1.48	1.38
23	Q	132	ARG	CZ-NH2	6.18	1.41	1.33
30	L	73	GLU	CB-CG	6.18	1.63	1.52
3	C	226	ARG	CZ-NH2	6.17	1.41	1.33
17	T	117	GLU	CB-CG	6.15	1.63	1.52
20	N	159	ARG	CZ-NH2	6.15	1.41	1.33
29	K	388	ARG	NE-CZ	6.15	1.41	1.33
28	I	184	TYR	CG-CD2	6.14	1.47	1.39
30	L	134	TYR	CE2-CZ	6.14	1.46	1.38
32	J	265	GLY	CA-C	-6.14	1.42	1.51
19	Z	261	ARG	CZ-NH2	6.13	1.41	1.33
32	J	163	GLU	CD-OE1	6.13	1.32	1.25
21	S	281	TRP	CD2-CE3	6.12	1.49	1.40
19	Z	807	ARG	CZ-NH1	6.11	1.41	1.33
2	B	4	ARG	CZ-NH2	6.11	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	18	ARG	CD-NE	6.10	1.56	1.46
20	N	650	TYR	C-N	6.10	1.44	1.33
19	Z	467	SER	CA-CB	-6.10	1.43	1.52
24	R	177	ARG	NE-CZ	6.09	1.41	1.33
21	S	88	ARG	CD-NE	6.09	1.56	1.46
20	N	829	SER	CA-CB	6.08	1.62	1.52
22	P	199	TYR	CG-CD1	6.08	1.47	1.39
13	6	132	TYR	CE2-CZ	6.07	1.46	1.38
12	5	245	ARG	CZ-NH1	6.07	1.41	1.33
26	O	196	ARG	NE-CZ	6.07	1.41	1.33
20	N	194	ARG	NE-CZ	6.06	1.41	1.33
6	F	14	SER	CA-CB	6.06	1.62	1.52
12	5	193	TYR	CZ-OH	6.05	1.48	1.37
28	I	80	ARG	CZ-NH2	6.05	1.41	1.33
14	7	147	MET	CA-CB	6.05	1.67	1.53
12	5	217	ARG	CZ-NH1	6.05	1.41	1.33
7	G	20	ARG	CZ-NH2	6.04	1.41	1.33
5	E	10	ARG	CZ-NH2	6.04	1.41	1.33
7	G	101	SER	CA-CB	6.04	1.62	1.52
31	M	356	GLU	CB-CG	6.04	1.63	1.52
27	H	265	ARG	CZ-NH1	6.04	1.40	1.33
32	J	178	LEU	C-N	6.03	1.44	1.33
26	O	178	ARG	NE-CZ	6.03	1.40	1.33
28	I	59	ARG	CZ-NH1	6.03	1.40	1.33
29	K	339	ARG	NE-CZ	6.03	1.40	1.33
21	S	95	ARG	CZ-NH2	6.02	1.40	1.33
27	H	244	GLU	CG-CD	6.01	1.60	1.51
3	C	91	ARG	NE-CZ	6.00	1.40	1.33
30	L	386	ARG	CZ-NH2	6.00	1.40	1.33
16	V	112	TYR	CG-CD1	6.00	1.47	1.39
32	J	148	TYR	CE2-CZ	6.00	1.46	1.38
32	J	240	GLU	CD-OE2	5.99	1.32	1.25
12	5	125	TYR	CE1-CZ	5.99	1.46	1.38
1	A	21	ARG	CD-NE	5.98	1.56	1.46
20	N	751	ARG	CZ-NH2	5.98	1.40	1.33
19	Z	556	ARG	CZ-NH2	5.97	1.40	1.33
22	P	412	VAL	CB-CG1	5.97	1.65	1.52
21	S	144	ARG	CD-NE	5.97	1.56	1.46
31	M	47	ARG	CZ-NH2	5.96	1.40	1.33
29	K	222	HIS	CB-CG	5.96	1.60	1.50
23	Q	135	SER	CA-CB	5.96	1.61	1.52
13	6	44	GLY	CA-C	-5.96	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	S	176	ARG	CZ-NH1	5.96	1.40	1.33
6	F	239	ARG	CZ-NH1	5.95	1.40	1.33
19	Z	232	TYR	CE1-CZ	5.95	1.46	1.38
11	4	178	PHE	CE1-CZ	5.95	1.48	1.37
19	Z	226	TYR	CG-CD2	5.94	1.46	1.39
24	R	361	SER	CA-CB	5.93	1.61	1.52
24	R	294	TYR	CE1-CZ	5.93	1.46	1.38
28	I	333	ARG	CD-NE	5.92	1.56	1.46
9	2	90	GLY	N-CA	-5.92	1.37	1.46
12	5	128	ARG	CZ-NH2	5.91	1.40	1.33
10	3	99	ARG	CD-NE	5.91	1.56	1.46
21	S	146	ARG	CD-NE	5.91	1.56	1.46
27	H	97	ARG	CD-NE	5.91	1.56	1.46
30	L	175	ARG	CZ-NH2	5.91	1.40	1.33
20	N	113	VAL	CB-CG1	5.91	1.65	1.52
25	U	88	ARG	CZ-NH2	5.90	1.40	1.33
32	J	1	MET	CG-SD	5.90	1.96	1.81
8	1	78	ARG	CZ-NH1	5.90	1.40	1.33
18	Y	65	TYR	CE2-CZ	-5.90	1.30	1.38
17	T	107	ARG	CD-NE	5.89	1.56	1.46
6	F	171	TYR	CE2-CZ	5.89	1.46	1.38
28	I	363	ARG	NE-CZ	5.89	1.40	1.33
24	R	309	GLU	CB-CG	5.88	1.63	1.52
29	K	44	TYR	CB-CG	5.88	1.60	1.51
19	Z	314	TYR	CE2-CZ	5.88	1.46	1.38
20	N	435	SER	CA-CB	5.88	1.61	1.52
25	U	25	ARG	CZ-NH2	5.88	1.40	1.33
2	B	121	TYR	CG-CD2	5.87	1.46	1.39
28	I	271	PHE	CG-CD2	5.87	1.47	1.38
14	7	218	ARG	CD-NE	5.87	1.56	1.46
17	T	158	SER	CA-CB	5.87	1.61	1.52
24	R	8	GLU	CD-OE1	5.85	1.32	1.25
10	3	198	ARG	CD-NE	5.85	1.56	1.46
20	N	344	ARG	CZ-NH2	5.85	1.40	1.33
27	H	398	ARG	CZ-NH1	5.85	1.40	1.33
12	5	125	TYR	CG-CD2	5.84	1.46	1.39
28	I	272	ARG	NE-CZ	5.84	1.40	1.33
16	V	68	ARG	CZ-NH1	5.83	1.40	1.33
31	M	323	PHE	CG-CD2	5.83	1.47	1.38
17	T	320	SER	CA-CB	5.83	1.61	1.52
2	B	229	TYR	CB-CG	-5.82	1.43	1.51
11	4	155	ARG	NE-CZ	5.82	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	199	GLU	CB-CG	5.82	1.63	1.52
5	E	30	GLY	CA-C	-5.81	1.42	1.51
31	M	290	GLU	CG-CD	5.81	1.60	1.51
20	N	158	ARG	NE-CZ	5.80	1.40	1.33
31	M	108	GLU	CG-CD	5.80	1.60	1.51
9	2	85	TYR	CD2-CE2	5.80	1.48	1.39
9	2	132	ARG	NE-CZ	5.80	1.40	1.33
22	P	94	ARG	CZ-NH1	5.80	1.40	1.33
11	4	95	ARG	NE-CZ	5.80	1.40	1.33
26	O	308	GLU	CG-CD	5.80	1.60	1.51
23	Q	282	ARG	CZ-NH1	5.79	1.40	1.33
8	1	171	TYR	CD2-CE2	5.79	1.48	1.39
27	H	249	TYR	CE2-CZ	5.79	1.46	1.38
8	1	169	TYR	CE1-CZ	5.78	1.46	1.38
10	3	66	ARG	CD-NE	5.78	1.56	1.46
14	7	116	ILE	C-N	5.78	1.47	1.34
3	C	17	ARG	CD-NE	5.78	1.56	1.46
21	S	437	ALA	CA-CB	5.78	1.64	1.52
13	6	52	SER	CA-CB	5.77	1.61	1.52
30	L	175	ARG	CD-NE	5.77	1.56	1.46
19	Z	111	GLU	CG-CD	-5.77	1.43	1.51
9	2	167	TYR	CB-CG	-5.76	1.43	1.51
10	3	85	TYR	CB-CG	-5.76	1.43	1.51
16	V	222	LYS	CA-CB	5.76	1.66	1.53
20	N	883	ARG	NE-CZ	5.75	1.40	1.33
27	H	111	TYR	CG-CD2	5.74	1.46	1.39
1	A	154	CYS	CB-SG	5.74	1.92	1.82
3	C	116	ASP	CA-CB	5.74	1.66	1.53
20	N	684	ARG	CZ-NH2	5.74	1.40	1.33
20	N	616	ARG	CZ-NH2	5.74	1.40	1.33
20	N	395	ARG	CZ-NH1	5.73	1.40	1.33
23	Q	236	PHE	CG-CD2	5.73	1.47	1.38
23	Q	298	SER	CA-CB	5.73	1.61	1.52
30	L	104	SER	CA-CB	5.73	1.61	1.52
30	L	342	TYR	CD1-CE1	5.73	1.48	1.39
19	Z	439	TYR	CG-CD2	5.73	1.46	1.39
21	S	487	VAL	CB-CG2	5.73	1.64	1.52
31	M	272	ARG	CZ-NH2	5.72	1.40	1.33
26	O	85	ARG	CZ-NH1	5.72	1.40	1.33
26	O	172	TYR	CZ-OH	5.72	1.47	1.37
6	F	7	ASP	CB-CG	5.72	1.63	1.51
11	4	19	ARG	CZ-NH1	5.72	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	N	713	TYR	CE1-CZ	5.72	1.46	1.38
31	M	94	SER	CA-CB	5.71	1.61	1.52
19	Z	400	TYR	CG-CD2	5.71	1.46	1.39
32	J	218	GLU	CD-OE1	5.71	1.31	1.25
20	N	843	GLU	CG-CD	5.71	1.60	1.51
23	Q	155	ARG	CZ-NH2	5.71	1.40	1.33
21	S	412	ARG	NE-CZ	5.71	1.40	1.33
8	1	146	SER	CA-CB	5.70	1.61	1.52
1	A	21	ARG	NE-CZ	5.69	1.40	1.33
19	Z	250	ARG	CD-NE	5.69	1.56	1.46
25	U	114	ARG	CZ-NH2	5.69	1.40	1.33
30	L	379	GLU	CG-CD	5.69	1.60	1.51
14	7	143	ARG	CZ-NH2	5.69	1.40	1.33
17	T	121	ARG	CZ-NH2	5.69	1.40	1.33
29	K	114	ARG	NE-CZ	5.69	1.40	1.33
23	Q	194	ARG	CZ-NH1	5.68	1.40	1.33
30	L	281	PHE	CG-CD1	5.68	1.47	1.38
23	Q	348	GLU	CD-OE1	5.68	1.31	1.25
11	4	73	TYR	CG-CD1	5.68	1.46	1.39
31	M	98	GLU	CD-OE1	5.68	1.31	1.25
21	S	144	ARG	NE-CZ	5.67	1.40	1.33
24	R	233	ARG	CD-NE	5.67	1.56	1.46
19	Z	72	ARG	CZ-NH2	5.67	1.40	1.33
26	O	173	TYR	CD2-CE2	5.67	1.47	1.39
32	J	297	ARG	CD-NE	5.67	1.56	1.46
30	L	39	ARG	CD-NE	5.67	1.56	1.46
31	M	425	GLU	CG-CD	5.67	1.60	1.51
4	D	244	GLU	CB-CG	5.67	1.62	1.52
20	N	682	TYR	CE1-CZ	5.67	1.46	1.38
2	B	80	GLY	N-CA	-5.66	1.37	1.46
14	7	88	ARG	CZ-NH2	5.66	1.40	1.33
7	G	20	ARG	NE-CZ	5.65	1.40	1.33
12	5	99	TYR	CE1-CZ	5.65	1.45	1.38
29	K	221	HIS	CB-CG	-5.65	1.39	1.50
12	5	204	TYR	CG-CD1	5.64	1.46	1.39
7	G	156	GLY	CA-C	-5.64	1.42	1.51
9	2	167	TYR	CA-CB	5.64	1.66	1.53
3	C	50	ARG	NE-CZ	5.64	1.40	1.33
16	V	121	TRP	CZ2-CH2	5.64	1.48	1.37
15	W	108	ARG	CZ-NH2	5.64	1.40	1.33
19	Z	588	ARG	CZ-NH1	5.64	1.40	1.33
27	H	284	ARG	CZ-NH1	5.63	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
19	Z	890	VAL	CB-CG1	5.63	1.64	1.52
2	B	138	GLY	N-CA	-5.63	1.37	1.46
15	W	45	PRO	N-CA	-5.63	1.37	1.47
17	T	340	ARG	NE-CZ	5.62	1.40	1.33
31	M	120	ARG	CD-NE	5.62	1.56	1.46
20	N	716	VAL	CB-CG2	5.62	1.64	1.52
27	H	54	GLN	CA-CB	5.62	1.66	1.53
6	F	40	SER	CA-CB	5.62	1.61	1.52
19	Z	100	ARG	NE-CZ	5.62	1.40	1.33
6	F	153	TYR	CZ-OH	5.61	1.47	1.37
27	H	369	ARG	CD-NE	5.61	1.55	1.46
17	T	299	PRO	N-CD	5.61	1.55	1.47
20	N	255	SER	CA-CB	5.61	1.61	1.52
2	B	177	ARG	CZ-NH1	5.61	1.40	1.33
20	N	374	SER	CA-CB	5.60	1.61	1.52
14	7	168	TYR	CG-CD1	5.60	1.46	1.39
26	O	65	SER	CA-CB	5.59	1.61	1.52
19	Z	519	ALA	CA-CB	5.58	1.64	1.52
8	1	105	GLU	N-CA	-5.57	1.35	1.46
19	Z	572	ALA	C-N	5.57	1.46	1.34
7	G	15	PHE	CG-CD2	5.57	1.47	1.38
20	N	98	GLU	CD-OE1	-5.57	1.19	1.25
21	S	332	GLU	CD-OE1	5.57	1.31	1.25
4	D	5	ARG	CZ-NH1	5.57	1.40	1.33
20	N	474	ARG	CZ-NH2	5.57	1.40	1.33
20	N	801	GLN	CG-CD	5.57	1.63	1.51
11	4	70	ARG	NE-CZ	5.57	1.40	1.33
13	6	132	TYR	CG-CD1	5.57	1.46	1.39
19	Z	329	ASN	CB-CG	5.56	1.63	1.51
31	M	350	ARG	CD-NE	5.56	1.55	1.46
1	A	214	GLU	CD-OE2	5.56	1.31	1.25
11	4	32	HIS	CB-CG	5.56	1.60	1.50
27	H	432	TYR	CE1-CZ	5.56	1.45	1.38
31	M	197	GLN	CA-CB	5.56	1.66	1.53
32	J	150	MET	N-CA	-5.56	1.35	1.46
16	V	106	GLU	CD-OE2	5.55	1.31	1.25
20	N	57	ARG	CZ-NH2	5.55	1.40	1.33
30	L	381	PHE	CA-CB	5.55	1.66	1.53
10	3	66	ARG	CZ-NH1	5.55	1.40	1.33
30	L	305	ARG	NE-CZ	5.55	1.40	1.33
28	I	303	ARG	CZ-NH1	5.55	1.40	1.33
12	5	113	PHE	CB-CG	5.54	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	S	466	ARG	CD-NE	5.54	1.55	1.46
25	U	241	SER	CA-CB	5.54	1.61	1.52
30	L	39	ARG	NE-CZ	5.54	1.40	1.33
13	6	131	TYR	CE1-CZ	5.53	1.45	1.38
19	Z	361	SER	CA-CB	5.53	1.61	1.52
10	3	39	PHE	CE2-CZ	5.53	1.47	1.37
32	J	372	ARG	CZ-NH1	5.53	1.40	1.33
17	T	340	ARG	CZ-NH1	5.53	1.40	1.33
27	H	386	ARG	CD-NE	5.53	1.55	1.46
8	1	177	ARG	CZ-NH2	5.52	1.40	1.33
22	P	184	GLU	CB-CG	5.52	1.62	1.52
20	N	747	SER	CA-CB	-5.52	1.44	1.52
15	W	15	TYR	CE1-CZ	5.52	1.45	1.38
8	1	141	GLY	C-N	5.51	1.43	1.33
15	W	37	CYS	CB-SG	5.51	1.91	1.82
28	I	268	ARG	CG-CD	5.51	1.65	1.51
19	Z	98	PHE	CG-CD2	5.51	1.47	1.38
21	S	117	PHE	CG-CD1	5.50	1.47	1.38
29	K	199	PRO	N-CD	-5.50	1.40	1.47
10	3	70	ARG	NE-CZ	5.50	1.40	1.33
23	Q	126	ARG	CZ-NH1	5.49	1.40	1.33
12	5	61	THR	C-N	5.49	1.46	1.34
32	J	51	GLU	CD-OE1	5.49	1.31	1.25
6	F	73	SER	CA-CB	5.49	1.61	1.52
16	V	238	CYS	CB-SG	5.49	1.91	1.82
23	Q	91	SER	CA-CB	5.49	1.61	1.52
13	6	102	TYR	CD2-CE2	5.48	1.47	1.39
8	1	58	TYR	CE2-CZ	5.48	1.45	1.38
23	Q	285	GLU	CD-OE1	5.48	1.31	1.25
20	N	546	ARG	NE-CZ	5.47	1.40	1.33
24	R	114	ILE	C-N	5.47	1.42	1.33
11	4	85	ARG	CZ-NH2	5.46	1.40	1.33
29	K	403	TYR	CZ-OH	5.46	1.47	1.37
7	G	224	ARG	CD-NE	5.46	1.55	1.46
21	S	252	ARG	CZ-NH1	5.46	1.40	1.33
8	1	219	ARG	NE-CZ	5.46	1.40	1.33
6	F	105	VAL	CB-CG2	5.45	1.64	1.52
13	6	98	ARG	CD-NE	5.45	1.55	1.46
26	O	235	ASP	N-CA	-5.45	1.35	1.46
19	Z	34	ARG	NE-CZ	5.45	1.40	1.33
6	F	178	GLU	CD-OE1	5.45	1.31	1.25
15	W	17	ARG	CZ-NH2	5.44	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	L	27	ARG	NE-CZ	5.44	1.40	1.33
22	P	240	TYR	CG-CD1	5.44	1.46	1.39
21	S	483	HIS	CB-CG	5.44	1.59	1.50
30	L	44	ARG	CZ-NH1	5.43	1.40	1.33
22	P	325	GLY	N-CA	5.43	1.54	1.46
19	Z	885	GLU	CD-OE2	5.43	1.31	1.25
19	Z	143	ARG	NE-CZ	5.43	1.40	1.33
3	C	4	ARG	CZ-NH1	5.42	1.40	1.33
28	I	59	ARG	NE-CZ	5.42	1.40	1.33
6	F	171	TYR	CG-CD2	5.42	1.46	1.39
31	M	365	ARG	NE-CZ	5.42	1.40	1.33
31	M	440	TYR	CE2-CZ	5.42	1.45	1.38
12	5	228	TYR	CZ-OH	5.42	1.47	1.37
21	S	215	GLU	CG-CD	-5.42	1.43	1.51
9	2	245	TYR	CG-CD1	5.42	1.46	1.39
15	W	155	ALA	N-CA	-5.42	1.35	1.46
17	T	259	TYR	CE2-CZ	5.42	1.45	1.38
26	O	154	ARG	CZ-NH2	5.42	1.40	1.33
8	1	170	GLY	CA-C	-5.42	1.43	1.51
29	K	122	GLU	CD-OE1	5.42	1.31	1.25
32	J	6	PRO	N-CD	-5.42	1.40	1.47
21	S	272	PHE	CG-CD2	5.41	1.46	1.38
28	I	272	ARG	CZ-NH1	5.41	1.40	1.33
17	T	178	TYR	CE1-CZ	5.41	1.45	1.38
19	Z	398	TRP	NE1-CE2	-5.41	1.30	1.37
20	N	546	ARG	CD-NE	5.41	1.55	1.46
22	P	144	ARG	NE-CZ	5.41	1.40	1.33
21	S	48	GLU	CD-OE1	5.41	1.31	1.25
24	R	267	ARG	CD-NE	5.41	1.55	1.46
25	U	25	ARG	NE-CZ	5.41	1.40	1.33
31	M	171	TYR	CZ-OH	5.41	1.47	1.37
19	Z	250	ARG	CZ-NH2	5.40	1.40	1.33
2	B	123	GLN	CA-CB	5.40	1.65	1.53
19	Z	300	ARG	CZ-NH1	5.40	1.40	1.33
20	N	361	ARG	NE-CZ	5.40	1.40	1.33
30	L	402	PRO	N-CD	-5.40	1.40	1.47
5	E	11	GLY	N-CA	-5.39	1.38	1.46
26	O	66	GLU	CG-CD	5.39	1.60	1.51
24	R	262	SER	CB-OG	-5.39	1.35	1.42
32	J	121	TYR	CG-CD2	5.39	1.46	1.39
21	S	95	ARG	CZ-NH1	5.38	1.40	1.33
22	P	330	LYS	C-N	5.38	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	148	ARG	NE-CZ	5.38	1.40	1.33
24	R	216	TYR	CE2-CZ	5.38	1.45	1.38
7	G	159	TYR	CE2-CZ	-5.37	1.31	1.38
14	7	74	TYR	CB-CG	5.37	1.59	1.51
4	D	3	TYR	CG-CD1	5.37	1.46	1.39
5	E	143	PHE	CB-CG	-5.37	1.42	1.51
13	6	95	ILE	C-N	5.37	1.46	1.34
4	D	219	ARG	CZ-NH2	5.36	1.40	1.33
9	2	186	ARG	CD-NE	5.36	1.55	1.46
24	R	137	ARG	NE-CZ	5.36	1.40	1.33
19	Z	751	TYR	CG-CD1	5.36	1.46	1.39
22	P	242	SER	CA-CB	5.36	1.60	1.52
1	A	125	TYR	CG-CD1	5.35	1.46	1.39
20	N	580	ARG	CZ-NH1	5.35	1.40	1.33
30	L	199	ARG	CZ-NH1	5.35	1.40	1.33
26	O	196	ARG	CZ-NH1	5.35	1.40	1.33
28	I	410	ARG	CD-NE	5.35	1.55	1.46
32	J	333	SER	CA-CB	5.35	1.60	1.52
25	U	147	ASP	CB-CG	5.35	1.62	1.51
2	B	43	GLY	CA-C	-5.34	1.43	1.51
31	M	175	VAL	CB-CG1	5.34	1.64	1.52
20	N	920	ASP	CA-CB	5.34	1.65	1.53
5	E	241	ILE	CA-CB	-5.34	1.42	1.54
28	I	131	HIS	CA-CB	5.34	1.65	1.53
16	V	48	GLY	N-CA	-5.34	1.38	1.46
20	N	341	PHE	CG-CD2	5.34	1.46	1.38
28	I	263	GLY	N-CA	5.34	1.54	1.46
26	O	282	PHE	CA-CB	5.33	1.65	1.53
32	J	148	TYR	CG-CD1	5.33	1.46	1.39
11	4	59	TYR	CE1-CZ	5.33	1.45	1.38
32	J	341	GLY	CA-C	-5.33	1.43	1.51
32	J	29	GLU	CD-OE2	5.33	1.31	1.25
32	J	381	GLU	CD-OE2	5.33	1.31	1.25
9	2	181	PHE	CG-CD2	5.32	1.46	1.38
20	N	561	GLU	CD-OE2	5.32	1.31	1.25
19	Z	746	ARG	NE-CZ	5.32	1.40	1.33
28	I	295	TYR	CE1-CZ	5.32	1.45	1.38
22	P	170	GLN	C-N	5.32	1.46	1.34
11	4	161	ARG	CD-NE	5.32	1.55	1.46
14	7	106	TYR	CE2-CZ	5.32	1.45	1.38
30	L	311	ARG	NE-CZ	5.32	1.40	1.33
32	J	225	GLY	N-CA	-5.32	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	J	340	ARG	NE-CZ	5.32	1.40	1.33
21	S	232	ARG	CZ-NH2	5.31	1.40	1.33
26	O	163	TYR	CG-CD2	5.31	1.46	1.39
2	B	84	ARG	CZ-NH2	5.31	1.40	1.33
3	C	243	GLU	CD-OE1	5.31	1.31	1.25
11	4	56	PHE	CG-CD2	5.31	1.46	1.38
17	T	318	TYR	CE2-CZ	5.31	1.45	1.38
30	L	189	PRO	N-CD	-5.31	1.40	1.47
30	L	173	PHE	CB-CG	-5.29	1.42	1.51
10	3	48	ARG	NE-CZ	5.29	1.40	1.33
19	Z	495	GLU	CB-CG	5.29	1.62	1.52
20	N	633	CYS	CA-CB	5.28	1.65	1.53
28	I	268	ARG	NE-CZ	5.28	1.40	1.33
30	L	256	ARG	NE-CZ	5.28	1.40	1.33
20	N	1	MET	CA-CB	5.28	1.65	1.53
19	Z	61	GLU	CD-OE1	5.28	1.31	1.25
19	Z	458	GLU	CG-CD	5.28	1.59	1.51
16	V	32	TYR	CZ-OH	5.28	1.46	1.37
30	L	26	TYR	CG-CD1	5.28	1.46	1.39
21	S	92	ARG	CD-NE	5.27	1.55	1.46
15	W	144	GLY	N-CA	-5.27	1.38	1.46
24	R	233	ARG	CZ-NH1	5.27	1.40	1.33
3	C	23	TYR	CD2-CE2	5.27	1.47	1.39
25	U	1	MET	CA-CB	5.27	1.65	1.53
31	M	188	TYR	CZ-OH	5.26	1.46	1.37
17	T	320	SER	N-CA	-5.26	1.35	1.46
21	S	298	TYR	N-CA	-5.26	1.35	1.46
7	G	100	ARG	NE-CZ	5.26	1.39	1.33
26	O	60	TYR	CE1-CZ	5.25	1.45	1.38
26	O	284	ARG	CZ-NH1	5.25	1.39	1.33
13	6	159	ARG	NE-CZ	5.25	1.39	1.33
28	I	307	ARG	NE-CZ	5.24	1.39	1.33
32	J	18	SER	CB-OG	5.24	1.49	1.42
24	R	257	ARG	CZ-NH1	5.23	1.39	1.33
17	T	315	PRO	N-CD	-5.23	1.40	1.47
14	7	81	ARG	NE-CZ	5.23	1.39	1.33
23	Q	211	ASP	CA-C	-5.23	1.39	1.52
30	L	198	ALA	CA-CB	5.23	1.63	1.52
32	J	322	GLU	CD-OE2	5.23	1.31	1.25
23	Q	126	ARG	CZ-NH2	5.23	1.39	1.33
17	T	119	LEU	C-N	5.22	1.42	1.33
26	O	321	ARG	CZ-NH2	5.22	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	16	SER	CA-CB	5.22	1.60	1.52
22	P	191	ARG	CD-NE	5.22	1.55	1.46
4	D	140	VAL	CA-C	-5.22	1.39	1.52
5	E	168	ARG	CZ-NH1	5.22	1.39	1.33
22	P	350	ARG	N-CA	-5.22	1.35	1.46
30	L	230	ARG	CD-NE	5.22	1.55	1.46
5	E	162	PHE	CB-CG	5.21	1.60	1.51
14	7	144	ARG	CZ-NH2	5.21	1.39	1.33
21	S	486	SER	CA-CB	5.21	1.60	1.52
12	5	195	PHE	N-CA	-5.21	1.35	1.46
1	A	224	ASN	N-CA	-5.20	1.35	1.46
19	Z	375	SER	CA-CB	5.20	1.60	1.52
21	S	82	VAL	CA-CB	-5.20	1.43	1.54
9	2	138	GLY	CA-C	-5.20	1.43	1.51
13	6	57	SER	CA-CB	5.20	1.60	1.52
22	P	408	ARG	CZ-NH2	5.20	1.39	1.33
29	K	366	ARG	CZ-NH2	5.20	1.39	1.33
21	S	393	ARG	NE-CZ	5.20	1.39	1.33
24	R	238	GLU	CG-CD	5.20	1.59	1.51
13	6	221	ARG	NE-CZ	5.20	1.39	1.33
24	R	18	ARG	CZ-NH2	5.20	1.39	1.33
2	B	6	TYR	CE1-CZ	5.19	1.45	1.38
1	A	38	THR	C-N	5.19	1.46	1.34
22	P	247	TYR	CE1-CZ	5.19	1.45	1.38
3	C	207	SER	CB-OG	5.19	1.49	1.42
17	T	275	ALA	C-N	5.19	1.42	1.33
19	Z	474	SER	CB-OG	5.19	1.49	1.42
24	R	364	TRP	CE3-CZ3	-5.19	1.29	1.38
30	L	83	PHE	CG-CD1	5.19	1.46	1.38
32	J	235	PHE	CG-CD2	5.19	1.46	1.38
19	Z	226	TYR	CZ-OH	5.18	1.46	1.37
23	Q	341	PRO	N-CD	5.18	1.55	1.47
16	V	91	PHE	CG-CD2	5.18	1.46	1.38
1	A	228	ARG	CZ-NH1	5.18	1.39	1.33
6	F	148	CYS	CA-CB	5.17	1.65	1.53
20	N	33	ASP	CA-CB	5.17	1.65	1.53
20	N	615	ARG	CD-NE	5.17	1.55	1.46
22	P	32	GLU	CG-CD	-5.17	1.44	1.51
29	K	146	GLU	CD-OE2	-5.17	1.20	1.25
1	A	63	SER	CA-C	-5.17	1.39	1.52
26	O	265	GLU	CG-CD	5.17	1.59	1.51
2	B	30	ALA	C-N	5.17	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	S	144	ARG	CZ-NH2	5.17	1.39	1.33
17	T	248	PHE	CG-CD2	5.17	1.46	1.38
19	Z	680	ARG	CD-NE	5.17	1.55	1.46
31	M	389	ARG	CZ-NH2	5.17	1.39	1.33
11	4	93	ARG	CZ-NH1	5.16	1.39	1.33
31	M	64	ARG	CZ-NH1	5.16	1.39	1.33
19	Z	879	ARG	CZ-NH1	5.16	1.39	1.33
25	U	283	ARG	CZ-NH2	5.16	1.39	1.33
27	H	124	ASP	CA-CB	5.16	1.65	1.53
28	I	330	ALA	CA-C	-5.16	1.39	1.52
31	M	151	GLY	CA-C	-5.16	1.43	1.51
1	A	26	GLU	CA-CB	5.16	1.65	1.53
16	V	112	TYR	CB-CG	5.16	1.59	1.51
24	R	9	GLU	CD-OE2	-5.15	1.20	1.25
3	C	4	ARG	CD-NE	5.15	1.55	1.46
6	F	125	ARG	CZ-NH2	5.15	1.39	1.33
25	U	68	TRP	CE2-CZ2	5.15	1.48	1.39
20	N	631	GLU	CB-CG	5.15	1.61	1.52
27	H	174	TYR	CE1-CZ	5.15	1.45	1.38
2	B	108	ALA	CA-CB	5.14	1.63	1.52
3	C	8	ARG	CD-NE	5.14	1.55	1.46
20	N	385	PHE	CG-CD2	5.14	1.46	1.38
23	Q	181	SER	CA-CB	5.14	1.60	1.52
24	R	192	ARG	CZ-NH2	5.14	1.39	1.33
14	7	61	ASP	CB-CG	5.14	1.62	1.51
19	Z	600	TYR	CE1-CZ	5.14	1.45	1.38
19	Z	785	ARG	NE-CZ	5.14	1.39	1.33
32	J	91	PRO	N-CA	-5.14	1.38	1.47
2	B	167	TYR	CA-CB	5.13	1.65	1.53
32	J	168	PRO	CA-C	-5.13	1.42	1.52
30	L	19	ARG	N-CA	-5.13	1.36	1.46
21	S	214	TYR	CZ-OH	5.13	1.46	1.37
28	I	349	ARG	CD-NE	5.13	1.55	1.46
21	S	318	VAL	CB-CG2	5.12	1.63	1.52
4	D	124	TYR	CG-CD1	5.12	1.45	1.39
24	R	245	GLU	CB-CG	5.12	1.61	1.52
28	I	188	GLY	CA-C	-5.12	1.43	1.51
11	4	141	SER	CB-OG	5.12	1.49	1.42
25	U	79	TYR	CZ-OH	5.12	1.46	1.37
19	Z	688	ARG	CZ-NH2	5.11	1.39	1.33
20	N	131	GLU	CA-CB	-5.11	1.42	1.53
23	Q	234	GLU	CD-OE1	5.11	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	5	228	TYR	CG-CD1	5.11	1.45	1.39
29	K	229	ARG	NE-CZ	5.10	1.39	1.33
19	Z	827	PRO	N-CD	-5.10	1.40	1.47
21	S	404	ARG	NE-CZ	5.10	1.39	1.33
32	J	22	GLN	CA-C	5.10	1.66	1.52
6	F	125	ARG	NE-CZ	5.10	1.39	1.33
17	T	347	ARG	CD-NE	5.10	1.55	1.46
22	P	93	ARG	NE-CZ	5.09	1.39	1.33
32	J	345	ARG	NE-CZ	5.09	1.39	1.33
7	G	13	SER	CA-CB	5.09	1.60	1.52
7	G	32	GLU	CB-CG	5.09	1.61	1.52
11	4	179	SER	CA-CB	5.09	1.60	1.52
28	I	271	PHE	CB-CG	-5.09	1.42	1.51
12	5	245	ARG	NE-CZ	5.09	1.39	1.33
21	S	207	TYR	CE1-CZ	5.09	1.45	1.38
10	3	27	ARG	NE-CZ	5.09	1.39	1.33
30	L	187	TYR	CZ-OH	5.08	1.46	1.37
12	5	140	LYS	CA-C	-5.08	1.39	1.52
25	U	250	TYR	CB-CG	5.08	1.59	1.51
11	4	181	ARG	CD-NE	5.08	1.55	1.46
12	5	149	TYR	CG-CD2	5.08	1.45	1.39
13	6	51	ALA	CA-CB	5.08	1.63	1.52
5	E	113	THR	CA-C	-5.08	1.39	1.52
19	Z	724	ASN	N-CA	-5.08	1.36	1.46
20	N	190	ASN	CB-CG	5.08	1.62	1.51
23	Q	33	ARG	CG-CD	5.08	1.64	1.51
27	H	237	PHE	CE2-CZ	5.08	1.47	1.37
30	L	157	ARG	CZ-NH2	5.08	1.39	1.33
14	7	208	GLU	CG-CD	5.07	1.59	1.51
28	I	96	ARG	CD-NE	5.07	1.55	1.46
14	7	143	ARG	CD-NE	5.07	1.55	1.46
19	Z	161	HIS	CB-CG	5.07	1.59	1.50
20	N	199	ARG	CD-NE	5.07	1.55	1.46
25	U	140	SER	CA-CB	5.07	1.60	1.52
30	L	216	SER	CA-CB	5.07	1.60	1.52
2	B	192	ILE	C-N	5.07	1.45	1.34
30	L	396	SER	CA-CB	5.07	1.60	1.52
10	3	103	TYR	CG-CD2	5.07	1.45	1.39
11	4	59	TYR	CA-CB	5.07	1.65	1.53
25	U	197	GLY	CA-C	-5.07	1.43	1.51
31	M	412	ARG	NE-CZ	5.07	1.39	1.33
19	Z	76	GLU	CG-CD	5.06	1.59	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	S	130	PHE	CE1-CZ	5.06	1.47	1.37
23	Q	397	TYR	CZ-OH	5.06	1.46	1.37
7	G	150	TYR	CG-CD1	5.06	1.45	1.39
30	L	381	PHE	CD2-CE2	5.06	1.49	1.39
2	B	84	ARG	CD-NE	5.06	1.55	1.46
26	O	198	PHE	CG-CD2	5.06	1.46	1.38
29	K	72	PHE	CE1-CZ	5.06	1.47	1.37
31	M	229	TYR	CA-CB	5.06	1.65	1.53
22	P	357	ARG	CZ-NH2	5.06	1.39	1.33
31	M	350	ARG	CZ-NH2	5.06	1.39	1.33
13	6	32	TYR	CG-CD2	5.05	1.45	1.39
17	T	282	TYR	CD1-CE1	5.05	1.47	1.39
19	Z	587	PHE	CG-CD1	5.05	1.46	1.38
24	R	325	VAL	C-N	5.05	1.42	1.33
25	U	12	HIS	C-N	-5.05	1.24	1.34
19	Z	160	ARG	NE-CZ	5.05	1.39	1.33
25	U	261	TYR	CG-CD2	5.05	1.45	1.39
7	G	237	GLU	CD-OE1	5.05	1.31	1.25
10	3	103	TYR	CE2-CZ	5.05	1.45	1.38
19	Z	354	GLU	CD-OE1	5.05	1.31	1.25
22	P	65	ARG	CZ-NH1	5.04	1.39	1.33
2	B	77	SER	CA-CB	5.04	1.60	1.52
9	2	167	TYR	CD1-CE1	5.04	1.47	1.39
26	O	289	ARG	CZ-NH1	5.04	1.39	1.33
19	Z	703	ARG	CZ-NH1	5.04	1.39	1.33
19	Z	349	TYR	CG-CD1	5.03	1.45	1.39
19	Z	781	TYR	CE1-CZ	5.03	1.45	1.38
20	N	30	VAL	CB-CG1	5.03	1.63	1.52
14	7	126	SER	CA-CB	5.03	1.60	1.52
27	H	284	ARG	CD-NE	5.03	1.54	1.46
3	C	212	GLU	CD-OE2	5.03	1.31	1.25
7	G	170	ARG	CZ-NH2	5.02	1.39	1.33
19	Z	230	CYS	CB-SG	5.02	1.90	1.82
4	D	60	ARG	CD-NE	5.02	1.54	1.46
4	D	50	VAL	N-CA	-5.02	1.36	1.46
12	5	78	ARG	CZ-NH1	5.02	1.39	1.33
32	J	175	PHE	CE1-CZ	5.02	1.46	1.37
32	J	223	PHE	CG-CD2	5.02	1.46	1.38
2	B	164	GLY	N-CA	-5.02	1.38	1.46
30	L	157	ARG	NE-CZ	5.02	1.39	1.33
6	F	202	GLU	CA-CB	5.01	1.65	1.53
19	Z	493	ASN	CG-ND2	5.01	1.45	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
23	Q	231	TYR	CG-CD2	5.01	1.45	1.39
16	V	29	GLU	CB-CG	5.01	1.61	1.52
21	S	395	ARG	CZ-NH2	5.01	1.39	1.33
26	O	294	GLU	C-N	5.01	1.45	1.34
30	L	151	GLY	N-CA	-5.01	1.38	1.46
5	E	152	GLN	CG-CD	5.01	1.62	1.51
18	Y	47	ASN	N-CA	5.01	1.56	1.46
15	W	145	GLU	CB-CG	5.01	1.61	1.52
6	F	18	ARG	CZ-NH2	5.00	1.39	1.33
30	L	379	GLU	CD-OE1	5.00	1.31	1.25
10	3	194	LYS	N-CA	-5.00	1.36	1.46

All (2142) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	G	224	ARG	NE-CZ-NH2	-41.07	99.77	120.30
8	1	121	TYR	CB-CG-CD1	-25.21	105.87	121.00
23	Q	132	ARG	NE-CZ-NH2	-19.96	110.32	120.30
19	Z	335	ARG	NE-CZ-NH1	19.67	130.13	120.30
21	S	357	PHE	CB-CG-CD2	-19.00	107.50	120.80
7	G	224	ARG	NE-CZ-NH1	17.67	129.14	120.30
4	D	5	ARG	NE-CZ-NH1	17.00	128.80	120.30
1	A	103	TYR	CB-CG-CD2	-16.70	110.98	121.00
7	G	123	TYR	CB-CG-CD1	16.33	130.80	121.00
23	Q	132	ARG	NE-CZ-NH1	15.89	128.25	120.30
23	Q	177	TYR	CB-CG-CD2	-15.81	111.51	121.00
17	T	190	TYR	CB-CG-CD2	-15.63	111.62	121.00
15	W	108	ARG	NE-CZ-NH2	-15.58	112.51	120.30
30	L	26	TYR	CB-CG-CD1	15.47	130.28	121.00
20	N	615	ARG	NE-CZ-NH1	15.46	128.03	120.30
22	P	174	TYR	CB-CG-CD2	-15.44	111.74	121.00
26	O	60	TYR	CB-CG-CD2	-15.37	111.78	121.00
9	2	232	TYR	CB-CG-CD1	-15.35	111.79	121.00
30	L	311	ARG	NE-CZ-NH2	-15.29	112.66	120.30
20	N	627	PHE	CB-CG-CD2	-15.23	110.14	120.80
8	1	116	PHE	CB-CG-CD2	-15.16	110.19	120.80
30	L	146	TYR	CB-CG-CD1	15.16	130.10	121.00
21	S	475	ARG	NE-CZ-NH2	-15.10	112.75	120.30
1	A	107	TYR	CB-CG-CD1	14.76	129.86	121.00
8	1	121	TYR	CB-CG-CD2	14.74	129.85	121.00
12	5	224	TYR	CB-CG-CD2	-14.70	112.18	121.00
30	L	146	TYR	CB-CG-CD2	-14.49	112.30	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	1	122	ARG	NE-CZ-NH2	-14.37	113.11	120.30
30	L	342	TYR	CB-CG-CD1	14.33	129.60	121.00
28	I	411	ARG	NE-CZ-NH1	14.32	127.46	120.30
7	G	170	ARG	NE-CZ-NH1	14.31	127.45	120.30
20	N	875	PHE	CB-CG-CD2	14.00	130.60	120.80
32	J	78	ARG	NE-CZ-NH1	13.95	127.27	120.30
21	S	257	TYR	CB-CG-CD1	13.91	129.35	121.00
13	6	149	TYR	CB-CG-CD1	-13.89	112.67	121.00
22	P	174	TYR	CB-CG-CD1	13.81	129.29	121.00
26	O	50	PHE	CB-CG-CD2	13.80	130.46	120.80
13	6	127	ARG	NE-CZ-NH1	13.79	127.19	120.30
22	P	377	ARG	NE-CZ-NH1	13.79	127.19	120.30
8	1	98	PHE	CB-CG-CD1	-13.78	111.16	120.80
24	R	259	TYR	CB-CG-CD2	-13.65	112.81	121.00
30	L	54	TYR	CB-CG-CD1	-13.61	112.83	121.00
19	Z	380	PHE	CB-CG-CD2	-13.61	111.27	120.80
3	C	128	ARG	NE-CZ-NH2	-13.54	113.53	120.30
31	M	229	TYR	CB-CG-CD2	-13.52	112.89	121.00
1	A	3	ARG	NE-CZ-NH1	13.49	127.05	120.30
3	C	136	TYR	CB-CG-CD2	-13.41	112.96	121.00
21	S	357	PHE	CB-CG-CD1	13.41	130.19	120.80
9	2	232	TYR	CB-CG-CD2	13.38	129.03	121.00
9	2	132	ARG	NE-CZ-NH1	13.37	126.98	120.30
26	O	154	ARG	NE-CZ-NH2	-13.33	113.63	120.30
11	4	19	ARG	NE-CZ-NH1	13.33	126.97	120.30
24	R	159	ARG	NE-CZ-NH2	13.26	126.93	120.30
23	Q	177	TYR	CB-CG-CD1	13.19	128.91	121.00
12	5	62	THR	N-CA-CB	13.17	135.32	110.30
31	M	311	ARG	NE-CZ-NH2	-13.14	113.73	120.30
4	D	3	TYR	CB-CG-CD1	13.00	128.80	121.00
20	N	179	TYR	CB-CG-CD1	12.91	128.75	121.00
20	N	194	ARG	NE-CZ-NH2	-12.82	113.89	120.30
19	Z	232	TYR	CB-CG-CD1	-12.79	113.32	121.00
15	W	17	ARG	NE-CZ-NH1	12.79	126.69	120.30
29	K	164	TYR	CB-CG-CD2	12.75	128.65	121.00
30	L	26	TYR	CB-CG-CD2	-12.75	113.35	121.00
14	7	85	ARG	NE-CZ-NH1	12.72	126.66	120.30
7	G	103	PHE	CB-CG-CD1	12.71	129.69	120.80
26	O	284	ARG	NE-CZ-NH1	-12.69	113.95	120.30
5	E	26	TYR	CB-CG-CD1	12.67	128.60	121.00
3	C	23	TYR	CB-CG-CD2	-12.66	113.40	121.00
24	R	151	TYR	CB-CG-CD2	12.65	128.59	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	4	147	TYR	CB-CG-CD2	-12.60	113.44	121.00
21	S	209	TYR	CB-CG-CD1	12.60	128.56	121.00
23	Q	297	ARG	NE-CZ-NH1	12.55	126.58	120.30
5	E	10	ARG	NE-CZ-NH1	12.54	126.57	120.30
14	7	143	ARG	NE-CZ-NH2	-12.53	114.03	120.30
17	T	169	ARG	NE-CZ-NH2	-12.53	114.03	120.30
24	R	259	TYR	CB-CG-CD1	12.53	128.52	121.00
14	7	130	ARG	NE-CZ-NH2	-12.50	114.05	120.30
28	I	349	ARG	NE-CZ-NH1	12.48	126.54	120.30
22	P	316	ARG	NE-CZ-NH1	12.43	126.52	120.30
4	D	36	ARG	NE-CZ-NH2	-12.43	114.09	120.30
28	I	80	ARG	NE-CZ-NH1	12.42	126.51	120.30
22	P	93	ARG	NE-CZ-NH1	12.40	126.50	120.30
30	L	99	ARG	NE-CZ-NH2	-12.34	114.13	120.30
31	M	353	ARG	NE-CZ-NH2	-12.34	114.13	120.30
11	4	50	ALA	N-CA-CB	12.33	127.37	110.10
3	C	4	ARG	NE-CZ-NH1	12.27	126.43	120.30
2	B	178	TYR	CB-CG-CD1	-12.26	113.64	121.00
24	R	336	ARG	NE-CZ-NH2	12.22	126.41	120.30
6	F	196	ARG	NE-CZ-NH2	-12.21	114.20	120.30
26	O	178	ARG	NE-CZ-NH1	12.17	126.39	120.30
24	R	342	ARG	NE-CZ-NH2	-12.03	114.28	120.30
23	Q	72	TYR	CB-CG-CD2	-12.03	113.78	121.00
25	U	115	TYR	CB-CG-CD2	-12.02	113.79	121.00
7	G	161	TYR	CB-CG-CD2	11.99	128.19	121.00
15	W	17	ARG	NE-CZ-NH2	-11.94	114.33	120.30
22	P	93	ARG	NE-CZ-NH2	-11.91	114.35	120.30
31	M	49	ARG	NE-CZ-NH2	-11.90	114.35	120.30
7	G	59	TYR	CB-CG-CD2	-11.88	113.87	121.00
29	K	44	TYR	CB-CG-CD2	11.88	128.13	121.00
24	R	150	PHE	CB-CG-CD1	11.85	129.09	120.80
21	S	207	TYR	CB-CG-CD2	-11.81	113.91	121.00
21	S	284	TYR	CB-CG-CD2	-11.77	113.94	121.00
30	L	54	TYR	CB-CG-CD2	11.73	128.04	121.00
24	R	46	ARG	NE-CZ-NH2	-11.68	114.46	120.30
10	3	104	TYR	CB-CG-CD1	-11.66	114.00	121.00
25	U	261	TYR	CG-CD1-CE1	-11.59	112.03	121.30
20	N	875	PHE	CB-CG-CD1	-11.56	112.71	120.80
19	Z	746	ARG	NE-CZ-NH2	-11.55	114.52	120.30
24	R	300	ARG	NE-CZ-NH1	11.54	126.07	120.30
20	N	615	ARG	NE-CZ-NH2	-11.53	114.54	120.30
31	M	49	ARG	NE-CZ-NH1	11.51	126.05	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	91	ARG	NE-CZ-NH1	11.46	126.03	120.30
20	N	402	PHE	CB-CG-CD1	11.46	128.82	120.80
21	S	76	ARG	NE-CZ-NH2	-11.45	114.58	120.30
1	A	9	PHE	CB-CG-CD2	11.44	128.81	120.80
6	F	232	PHE	CB-CG-CD2	-11.38	112.83	120.80
21	S	124	ARG	NE-CZ-NH1	-11.37	114.62	120.30
22	P	377	ARG	NE-CZ-NH2	-11.37	114.62	120.30
19	Z	556	ARG	NE-CZ-NH2	-11.33	114.64	120.30
28	I	410	ARG	NE-CZ-NH1	11.27	125.94	120.30
4	D	115	ARG	NE-CZ-NH1	11.23	125.92	120.30
17	T	319	TYR	CB-CG-CD1	11.22	127.73	121.00
29	K	44	TYR	CB-CG-CD1	-11.22	114.27	121.00
11	4	161	ARG	NE-CZ-NH2	11.21	125.91	120.30
19	Z	335	ARG	NE-CZ-NH2	-11.21	114.70	120.30
21	S	410	TYR	CB-CG-CD2	-11.20	114.28	121.00
6	F	193	ARG	NE-CZ-NH2	-11.19	114.70	120.30
4	D	36	ARG	NE-CZ-NH1	11.16	125.88	120.30
29	K	300	ASP	CB-CG-OD1	-11.13	108.28	118.30
24	R	257	ARG	NE-CZ-NH2	-11.12	114.74	120.30
7	G	161	TYR	CB-CG-CD1	-11.12	114.33	121.00
26	O	156	TYR	CB-CG-CD2	-11.12	114.33	121.00
29	K	60	TYR	CB-CG-CD2	-11.10	114.34	121.00
31	M	229	TYR	CB-CG-CD1	11.06	127.63	121.00
13	6	34	PHE	CB-CG-CD2	-11.05	113.06	120.80
20	N	163	PHE	CB-CG-CD1	10.97	128.48	120.80
1	A	9	PHE	CB-CG-CD1	-10.95	113.14	120.80
12	5	128	ARG	NE-CZ-NH1	10.95	125.77	120.30
16	V	65	TYR	CB-CG-CD1	10.92	127.55	121.00
19	Z	380	PHE	CB-CG-CD1	10.92	128.44	120.80
13	6	200	ARG	NE-CZ-NH1	10.83	125.72	120.30
25	U	261	TYR	CD1-CE1-CZ	10.82	129.54	119.80
3	C	97	TYR	CB-CG-CD2	10.82	127.49	121.00
1	A	93	ARG	NE-CZ-NH1	10.80	125.70	120.30
20	N	57	ARG	NE-CZ-NH1	10.77	125.69	120.30
7	G	86	ARG	NE-CZ-NH2	-10.75	114.92	120.30
30	L	157	ARG	NE-CZ-NH2	-10.75	114.92	120.30
16	V	200	TYR	CB-CG-CD2	-10.74	114.55	121.00
32	J	78	ARG	NE-CZ-NH2	-10.73	114.93	120.30
13	6	98	ARG	NE-CZ-NH2	-10.73	114.93	120.30
20	N	783	TYR	CB-CG-CD1	-10.73	114.56	121.00
17	T	309	ARG	NE-CZ-NH1	10.70	125.65	120.30
20	N	627	PHE	CB-CG-CD1	10.70	128.29	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	J	271	ARG	NE-CZ-NH1	-10.68	114.96	120.30
29	K	72	PHE	CB-CG-CD1	-10.66	113.34	120.80
10	3	85	TYR	CB-CG-CD2	10.66	127.40	121.00
16	V	121	TRP	CG-CD2-CE3	-10.65	124.31	133.90
3	C	143	TYR	CB-CG-CD1	10.63	127.38	121.00
22	P	88	MET	CG-SD-CE	-10.63	83.19	100.20
7	G	224	ARG	NH1-CZ-NH2	10.62	131.09	119.40
7	G	103	PHE	CB-CG-CD2	-10.61	113.37	120.80
13	6	134	TYR	CB-CG-CD1	10.61	127.36	121.00
29	K	342	ARG	NE-CZ-NH2	-10.61	115.00	120.30
21	S	410	TYR	CB-CG-CD1	10.60	127.36	121.00
13	6	134	TYR	CB-CG-CD2	-10.58	114.65	121.00
17	T	319	TYR	CB-CG-CD2	-10.57	114.66	121.00
10	3	28	PHE	CB-CG-CD1	10.53	128.17	120.80
6	F	122	ARG	NE-CZ-NH2	10.52	125.56	120.30
13	6	55	ARG	NE-CZ-NH2	-10.48	115.06	120.30
23	Q	201	TYR	CB-CG-CD2	-10.47	114.72	121.00
6	F	179	PHE	CB-CG-CD1	10.45	128.12	120.80
3	C	128	ARG	NE-CZ-NH1	10.44	125.52	120.30
13	6	55	ARG	NE-CZ-NH1	10.43	125.52	120.30
27	H	232	ARG	NE-CZ-NH2	-10.41	115.10	120.30
32	J	43	ARG	NE-CZ-NH2	-10.40	115.10	120.30
17	T	304	ASP	CB-CG-OD1	-10.38	108.95	118.30
3	C	226	ARG	NE-CZ-NH1	10.38	125.49	120.30
17	T	220	ALA	N-CA-CB	10.36	124.61	110.10
30	L	175	ARG	NE-CZ-NH1	10.36	125.48	120.30
16	V	65	TYR	CB-CG-CD2	-10.35	114.79	121.00
30	L	311	ARG	NE-CZ-NH1	10.33	125.47	120.30
21	S	176	ARG	NE-CZ-NH1	10.32	125.46	120.30
24	R	271	PHE	CB-CG-CD2	10.31	128.02	120.80
21	S	76	ARG	NE-CZ-NH1	10.31	125.45	120.30
19	Z	232	TYR	CB-CG-CD2	10.30	127.18	121.00
27	H	375	ARG	NE-CZ-NH1	10.30	125.45	120.30
4	D	101	ARG	NE-CZ-NH2	10.30	125.45	120.30
22	P	350	ARG	NE-CZ-NH1	10.27	125.44	120.30
31	M	413	ARG	NE-CZ-NH2	-10.27	115.17	120.30
32	J	21	ARG	NE-CZ-NH2	-10.26	115.17	120.30
3	C	101	TYR	CB-CG-CD1	-10.25	114.85	121.00
21	S	272	PHE	CB-CG-CD1	-10.23	113.64	120.80
13	6	215	TYR	CB-CG-CD1	-10.22	114.87	121.00
20	N	899	ARG	NE-CZ-NH2	-10.21	115.20	120.30
13	6	200	ARG	NE-CZ-NH2	-10.18	115.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	C	226	ARG	NE-CZ-NH2	-10.17	115.21	120.30
6	F	155	ASP	CB-CG-OD2	-10.17	109.15	118.30
15	W	70	ARG	NE-CZ-NH2	-10.14	115.23	120.30
11	4	67	TYR	CG-CD1-CE1	10.13	129.41	121.30
3	C	23	TYR	CB-CG-CD1	10.12	127.08	121.00
14	7	222	TYR	CB-CG-CD2	-10.12	114.93	121.00
9	2	242	PHE	CB-CG-CD2	-10.11	113.73	120.80
19	Z	496	ASP	CB-CG-OD2	-10.10	109.21	118.30
29	K	366	ARG	NE-CZ-NH1	10.07	125.33	120.30
11	4	70	ARG	NE-CZ-NH1	10.06	125.33	120.30
29	K	164	TYR	CB-CG-CD1	-10.01	114.99	121.00
8	1	98	PHE	CB-CG-CD2	10.01	127.81	120.80
7	G	20	ARG	NE-CZ-NH2	-10.01	115.30	120.30
19	Z	71	TYR	CB-CG-CD1	-10.00	115.00	121.00
24	R	125	ARG	NE-CZ-NH2	-9.99	115.30	120.30
24	R	318	TYR	CB-CG-CD1	9.99	127.00	121.00
12	5	236	TYR	CB-CG-CD2	-9.99	115.00	121.00
21	S	117	PHE	CB-CG-CD2	9.98	127.79	120.80
32	J	229	ARG	NE-CZ-NH1	9.94	125.27	120.30
19	Z	816	TYR	CB-CG-CD2	9.94	126.96	121.00
27	H	398	ARG	NE-CZ-NH2	9.88	125.24	120.30
22	P	226	TYR	CB-CG-CD1	9.88	126.93	121.00
14	7	143	ARG	NE-CZ-NH1	9.87	125.23	120.30
27	H	309	PHE	CB-CG-CD1	9.86	127.70	120.80
20	N	253	TYR	CB-CG-CD2	-9.86	115.08	121.00
24	R	150	PHE	CB-CG-CD2	-9.86	113.90	120.80
11	4	116	TYR	CB-CG-CD2	-9.85	115.09	121.00
16	V	282	ARG	NE-CZ-NH2	-9.85	115.38	120.30
6	F	18	ARG	NE-CZ-NH1	9.84	125.22	120.30
16	V	234	TYR	CB-CG-CD2	-9.84	115.10	121.00
25	U	267	ARG	NE-CZ-NH2	-9.80	115.40	120.30
4	D	124	TYR	CB-CG-CD2	-9.79	115.13	121.00
16	V	112	TYR	CB-CG-CD1	-9.78	115.13	121.00
16	V	161	ARG	NE-CZ-NH2	-9.78	115.41	120.30
13	6	149	TYR	CB-CG-CD2	9.76	126.85	121.00
27	H	111	TYR	CB-CG-CD1	-9.72	115.17	121.00
26	O	178	ARG	NE-CZ-NH2	-9.71	115.44	120.30
27	H	351	ARG	NE-CZ-NH2	-9.67	115.47	120.30
19	Z	376	PHE	CB-CG-CD1	-9.66	114.03	120.80
30	L	115	ASP	CB-CG-OD1	9.66	127.00	118.30
13	6	84	PHE	CB-CG-CD2	9.66	127.56	120.80
28	I	428	TYR	CB-CG-CD1	9.65	126.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	4	147	TYR	CB-CG-CD1	9.64	126.78	121.00
23	Q	155	ARG	NE-CZ-NH1	9.59	125.10	120.30
20	N	883	ARG	NE-CZ-NH1	9.58	125.09	120.30
23	Q	337	ARG	NE-CZ-NH2	-9.53	115.53	120.30
7	G	20	ARG	NE-CZ-NH1	9.53	125.06	120.30
26	O	211	PHE	CB-CG-CD1	9.52	127.46	120.80
29	K	338	ARG	NE-CZ-NH1	9.52	125.06	120.30
31	M	337	ARG	NE-CZ-NH2	9.49	125.05	120.30
27	H	309	PHE	CB-CG-CD2	-9.46	114.17	120.80
24	R	271	PHE	CB-CG-CD1	-9.45	114.19	120.80
30	L	44	ARG	NE-CZ-NH2	9.45	125.03	120.30
28	I	363	ARG	NE-CZ-NH2	-9.45	115.58	120.30
24	R	288	PHE	CB-CG-CD1	-9.44	114.19	120.80
1	A	125	TYR	CB-CG-CD2	-9.43	115.34	121.00
16	V	309	PHE	CB-CG-CD1	-9.41	114.21	120.80
26	O	85	ARG	NE-CZ-NH2	-9.40	115.60	120.30
28	I	303	ARG	NE-CZ-NH1	-9.40	115.60	120.30
11	4	3	TYR	CB-CG-CD1	9.37	126.62	121.00
9	2	241	ARG	NE-CZ-NH1	9.35	124.97	120.30
31	M	206	VAL	CA-CB-CG1	-9.34	96.89	110.90
22	P	129	ARG	NE-CZ-NH1	9.33	124.96	120.30
23	Q	11	ARG	NE-CZ-NH2	-9.33	115.64	120.30
25	U	34	ARG	NE-CZ-NH1	-9.32	115.64	120.30
19	Z	590	PHE	CB-CG-CD2	-9.30	114.29	120.80
21	S	209	TYR	CB-CG-CD2	-9.29	115.43	121.00
7	G	105	TYR	CB-CG-CD2	-9.28	115.43	121.00
26	O	50	PHE	CB-CG-CD1	-9.28	114.31	120.80
2	B	101	TYR	CB-CG-CD1	9.26	126.56	121.00
6	F	179	PHE	CB-CG-CD2	-9.22	114.35	120.80
1	A	93	ARG	NE-CZ-NH2	-9.21	115.70	120.30
20	N	557	TYR	CB-CG-CD1	-9.21	115.48	121.00
24	R	32	ARG	NE-CZ-NH2	-9.20	115.70	120.30
22	P	369	TYR	CB-CG-CD1	9.19	126.52	121.00
30	L	233	PHE	CB-CG-CD1	-9.19	114.37	120.80
20	N	616	ARG	NE-CZ-NH1	9.18	124.89	120.30
12	5	216	ARG	NE-CZ-NH2	-9.17	115.71	120.30
30	L	127	ARG	NE-CZ-NH2	-9.17	115.72	120.30
1	A	27	TYR	CB-CG-CD1	-9.14	115.52	121.00
26	O	155	PHE	CB-CG-CD1	-9.13	114.41	120.80
21	S	310	ARG	NE-CZ-NH1	9.12	124.86	120.30
4	D	87	ARG	NE-CZ-NH2	-9.12	115.74	120.30
27	H	429	TYR	CB-CG-CD2	-9.12	115.53	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O	154	ARG	NE-CZ-NH1	9.08	124.84	120.30
4	D	87	ARG	NE-CZ-NH1	9.08	124.84	120.30
4	D	101	ARG	NE-CZ-NH1	-9.08	115.76	120.30
15	W	91	ARG	NE-CZ-NH2	9.07	124.83	120.30
27	H	420	TYR	CB-CG-CD2	-9.07	115.56	121.00
4	D	123	ARG	NE-CZ-NH2	-9.05	115.77	120.30
30	L	123	ARG	NE-CZ-NH2	-9.05	115.77	120.30
29	K	200	ARG	NE-CZ-NH2	-9.05	115.77	120.30
25	U	34	ARG	NE-CZ-NH2	9.04	124.82	120.30
4	D	5	ARG	NH1-CZ-NH2	-9.03	109.47	119.40
29	K	263	PHE	CB-CG-CD1	-9.01	114.50	120.80
21	S	272	PHE	CB-CG-CD2	8.99	127.09	120.80
15	W	100	ARG	NE-CZ-NH2	8.97	124.78	120.30
29	K	72	PHE	CB-CG-CD2	8.97	127.08	120.80
30	L	115	ASP	CB-CG-OD2	-8.96	110.23	118.30
7	G	93	ARG	NE-CZ-NH2	-8.96	115.82	120.30
17	T	207	ARG	NE-CZ-NH2	-8.94	115.83	120.30
27	H	41	TYR	CB-CG-CD1	8.93	126.36	121.00
26	O	270	ARG	NE-CZ-NH2	-8.92	115.84	120.30
29	K	274	ARG	NE-CZ-NH1	8.91	124.75	120.30
12	5	193	TYR	N-CA-CB	8.87	126.57	110.60
27	H	97	ARG	NE-CZ-NH1	8.87	124.73	120.30
27	H	336	ARG	NE-CZ-NH1	8.87	124.73	120.30
13	6	159	ARG	NE-CZ-NH2	-8.86	115.87	120.30
22	P	1	MET	CG-SD-CE	-8.86	86.03	100.20
8	1	72	ASP	CB-CG-OD1	8.85	126.26	118.30
8	1	124	ARG	NE-CZ-NH1	-8.85	115.88	120.30
1	A	29	PHE	CB-CG-CD1	8.83	126.98	120.80
19	Z	763	ARG	NE-CZ-NH1	8.83	124.72	120.30
28	I	381	ASP	CB-CG-OD2	8.81	126.23	118.30
31	M	272	ARG	NE-CZ-NH2	-8.81	115.89	120.30
21	S	254	TYR	CB-CG-CD2	-8.81	115.72	121.00
8	1	84	ASP	CB-CG-OD2	8.78	126.20	118.30
28	I	283	PHE	CB-CG-CD1	8.78	126.94	120.80
20	N	713	TYR	CB-CG-CD1	8.77	126.26	121.00
23	Q	266	ASP	CB-CG-OD2	8.77	126.19	118.30
7	G	141	TYR	CB-CG-CD2	-8.76	115.74	121.00
17	T	304	ASP	CB-CG-OD2	8.76	126.18	118.30
16	V	200	TYR	CB-CG-CD1	8.75	126.25	121.00
22	P	369	TYR	CB-CG-CD2	-8.74	115.75	121.00
11	4	108	ASP	CB-CG-OD1	-8.73	110.44	118.30
1	A	58	ASP	CB-CG-OD2	8.73	126.16	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	I	71	TYR	CB-CG-CD2	8.73	126.24	121.00
9	2	124	ARG	NE-CZ-NH1	8.72	124.66	120.30
31	M	275	PHE	CB-CG-CD2	-8.72	114.69	120.80
4	D	3	TYR	CB-CG-CD2	-8.71	115.77	121.00
22	P	95	SER	N-CA-CB	8.71	123.57	110.50
29	K	112	TYR	CB-CG-CD1	8.71	126.23	121.00
2	B	60	ARG	NE-CZ-NH1	-8.70	115.95	120.30
5	E	26	TYR	CB-CG-CD2	-8.69	115.78	121.00
21	S	364	ARG	NE-CZ-NH2	-8.69	115.95	120.30
30	L	310	ASP	CB-CG-OD1	-8.69	110.48	118.30
3	C	97	TYR	CB-CG-CD1	-8.69	115.79	121.00
4	D	115	ARG	NE-CZ-NH2	-8.68	115.96	120.30
12	5	179	ARG	NE-CZ-NH2	8.68	124.64	120.30
14	7	222	TYR	CG-CD1-CE1	-8.68	114.36	121.30
4	D	116	TYR	CB-CG-CD2	-8.66	115.81	121.00
30	L	157	ARG	NE-CZ-NH1	8.65	124.63	120.30
11	4	73	TYR	CB-CG-CD2	8.65	126.19	121.00
25	U	95	TYR	CB-CG-CD2	-8.64	115.81	121.00
20	N	163	PHE	CB-CG-CD2	-8.64	114.75	120.80
32	J	95	PHE	CB-CA-C	-8.64	93.13	110.40
20	N	402	PHE	CB-CG-CD2	-8.63	114.76	120.80
19	Z	72	ARG	NE-CZ-NH2	-8.62	115.99	120.30
15	W	108	ARG	NE-CZ-NH1	8.61	124.60	120.30
22	P	263	TRP	N-CA-CB	8.61	126.09	110.60
5	E	103	TYR	CB-CG-CD2	-8.60	115.84	121.00
20	N	253	TYR	CG-CD1-CE1	-8.59	114.43	121.30
31	M	357	PHE	CB-CG-CD2	-8.59	114.79	120.80
2	B	6	TYR	CB-CG-CD1	8.58	126.15	121.00
29	K	204	MET	CG-SD-CE	-8.58	86.47	100.20
4	D	131	ARG	NE-CZ-NH2	-8.58	116.01	120.30
30	L	269	ARG	NE-CZ-NH2	-8.58	116.01	120.30
3	C	148	TYR	CB-CG-CD1	-8.58	115.85	121.00
22	P	247	TYR	CB-CG-CD1	-8.57	115.86	121.00
23	Q	310	ARG	NE-CZ-NH2	-8.56	116.02	120.30
9	2	186	ARG	NE-CZ-NH2	-8.56	116.02	120.30
19	Z	489	TYR	CB-CG-CD2	-8.56	115.87	121.00
19	Z	816	TYR	CB-CG-CD1	-8.55	115.87	121.00
21	S	371	PHE	CB-CG-CD1	8.55	126.79	120.80
19	Z	256	PHE	CB-CG-CD1	8.55	126.79	120.80
1	A	132	ARG	NE-CZ-NH2	-8.54	116.03	120.30
8	1	167	TYR	CB-CG-CD1	-8.53	115.88	121.00
18	Y	50	ASP	CB-CG-OD2	8.52	125.97	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	N	108	TYR	CB-CG-CD1	-8.52	115.89	121.00
3	C	101	TYR	CB-CG-CD2	8.51	126.11	121.00
13	6	159	ARG	NE-CZ-NH1	8.49	124.55	120.30
9	2	242	PHE	CB-CG-CD1	8.49	126.74	120.80
25	U	88	ARG	NE-CZ-NH2	-8.49	116.05	120.30
32	J	375	ARG	NE-CZ-NH1	-8.49	116.05	120.30
6	F	51	ARG	NE-CZ-NH2	8.48	124.54	120.30
10	3	67	LEU	CB-CG-CD2	8.48	125.41	111.00
9	2	230	ARG	NE-CZ-NH2	-8.47	116.06	120.30
21	S	232	ARG	NE-CZ-NH2	8.46	124.53	120.30
8	1	136	TRP	N-CA-CB	8.46	125.82	110.60
19	Z	103	TYR	CB-CG-CD2	-8.45	115.93	121.00
11	4	171	PHE	CB-CG-CD2	-8.45	114.89	120.80
14	7	87	MET	CG-SD-CE	-8.44	86.69	100.20
21	S	126	PHE	CB-CG-CD2	-8.44	114.89	120.80
22	P	316	ARG	NE-CZ-NH2	-8.44	116.08	120.30
17	T	228	TYR	CB-CG-CD1	8.44	126.06	121.00
28	I	80	ARG	NE-CZ-NH2	-8.42	116.09	120.30
10	3	103	TYR	CB-CG-CD1	-8.41	115.95	121.00
27	H	336	ARG	NE-CZ-NH2	-8.40	116.10	120.30
3	C	5	TYR	CB-CG-CD2	-8.39	115.97	121.00
24	R	146	ARG	NE-CZ-NH1	8.39	124.50	120.30
19	Z	257	ARG	NE-CZ-NH2	-8.38	116.11	120.30
29	K	235	PHE	CB-CG-CD2	-8.37	114.94	120.80
26	O	211	PHE	CB-CG-CD2	-8.36	114.95	120.80
21	S	252	ARG	NE-CZ-NH2	-8.35	116.12	120.30
1	A	23	TYR	CG-CD2-CE2	8.35	127.98	121.30
7	G	48	PHE	CB-CG-CD1	-8.35	114.96	120.80
24	R	159	ARG	NH1-CZ-NH2	-8.35	110.22	119.40
21	S	341	ARG	NE-CZ-NH1	8.30	124.45	120.30
3	C	124	PHE	CB-CG-CD1	8.30	126.61	120.80
14	7	79	ARG	NE-CZ-NH1	8.29	124.45	120.30
21	S	351	ARG	NE-CZ-NH2	8.29	124.44	120.30
4	D	142	PHE	CB-CG-CD1	-8.28	115.00	120.80
17	T	259	TYR	CB-CG-CD1	-8.28	116.03	121.00
21	S	92	ARG	NE-CZ-NH2	-8.27	116.17	120.30
24	R	216	TYR	CB-CG-CD2	-8.26	116.04	121.00
24	R	222	TYR	CB-CG-CD2	-8.25	116.05	121.00
19	Z	33	ARG	NE-CZ-NH1	8.25	124.43	120.30
6	F	164	ARG	NE-CZ-NH2	-8.24	116.18	120.30
22	P	417	ARG	NE-CZ-NH1	-8.24	116.18	120.30
15	W	70	ARG	NE-CZ-NH1	8.24	124.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	I	272	ARG	NE-CZ-NH2	-8.23	116.19	120.30
6	F	196	ARG	NE-CZ-NH1	8.22	124.41	120.30
27	H	333	ARG	NE-CZ-NH2	8.20	124.40	120.30
32	J	271	ARG	NE-CZ-NH2	8.19	124.40	120.30
11	4	145	ARG	NE-CZ-NH2	-8.19	116.20	120.30
22	P	81	ASP	CB-CG-OD1	-8.19	110.93	118.30
23	Q	9	PHE	CB-CG-CD1	-8.19	115.07	120.80
28	I	78	PHE	CB-CG-CD2	-8.18	115.07	120.80
23	Q	160	MET	CG-SD-CE	-8.17	87.12	100.20
30	L	342	TYR	CB-CG-CD2	-8.17	116.10	121.00
1	A	210	PHE	CB-CG-CD2	-8.16	115.08	120.80
20	N	69	TYR	CB-CG-CD1	8.16	125.90	121.00
4	D	175	ARG	NE-CZ-NH2	-8.16	116.22	120.30
6	F	128	TYR	CB-CG-CD1	-8.16	116.11	121.00
12	5	195	PHE	CB-CG-CD1	-8.16	115.09	120.80
1	A	21	ARG	NE-CZ-NH1	8.15	124.38	120.30
24	R	128	TYR	CB-CG-CD2	-8.13	116.12	121.00
27	H	265	ARG	CD-NE-CZ	-8.13	112.22	123.60
28	I	103	ARG	NE-CZ-NH2	-8.13	116.24	120.30
17	T	256	ALA	N-CA-CB	8.12	121.47	110.10
17	T	190	TYR	CG-CD1-CE1	-8.11	114.81	121.30
17	T	282	TYR	CB-CG-CD1	-8.11	116.13	121.00
17	T	244	TYR	CB-CG-CD2	-8.10	116.14	121.00
1	A	152	TYR	CG-CD1-CE1	-8.10	114.82	121.30
14	7	147	MET	CG-SD-CE	-8.10	87.24	100.20
28	I	307	ARG	NE-CZ-NH2	-8.10	116.25	120.30
27	H	429	TYR	CB-CG-CD1	8.10	125.86	121.00
22	P	182	ARG	NE-CZ-NH2	8.08	124.34	120.30
24	R	293	ARG	NE-CZ-NH2	-8.05	116.27	120.30
5	E	101	PHE	CB-CG-CD1	8.05	126.44	120.80
7	G	48	PHE	CB-CG-CD2	8.05	126.44	120.80
27	H	351	ARG	NE-CZ-NH1	8.04	124.32	120.30
7	G	123	TYR	CB-CG-CD2	-8.04	116.18	121.00
19	Z	1	MET	CG-SD-CE	-8.03	87.35	100.20
23	Q	137	TYR	CB-CG-CD1	8.02	125.81	121.00
9	2	246	ARG	NE-CZ-NH2	-8.02	116.29	120.30
24	R	304	TYR	CB-CG-CD2	8.01	125.81	121.00
9	2	186	ARG	NE-CZ-NH1	7.99	124.30	120.30
27	H	177	VAL	CA-CB-CG1	-7.99	98.91	110.90
3	C	61	PHE	CB-CG-CD1	-7.99	115.21	120.80
32	J	283	PHE	CB-CG-CD2	7.99	126.39	120.80
25	U	267	ARG	NE-CZ-NH1	7.99	124.29	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	M	307	ARG	NE-CZ-NH2	-7.98	116.31	120.30
1	A	125	TYR	CZ-CE2-CD2	7.98	126.98	119.80
31	M	183	ARG	NE-CZ-NH2	-7.97	116.31	120.30
14	7	74	TYR	CB-CG-CD1	7.97	125.78	121.00
19	Z	620	PHE	CB-CG-CD2	-7.97	115.22	120.80
25	U	184	VAL	CA-CB-CG1	7.97	122.85	110.90
21	S	284	TYR	CB-CG-CD1	7.96	125.78	121.00
11	4	70	ARG	NE-CZ-NH2	-7.96	116.32	120.30
23	Q	143	TYR	CB-CG-CD1	-7.95	116.23	121.00
26	O	156	TYR	CB-CG-CD1	7.95	125.77	121.00
26	O	3	ASP	CB-CG-OD1	7.94	125.45	118.30
20	N	751	ARG	NE-CZ-NH2	-7.93	116.33	120.30
17	T	261	PHE	CB-CG-CD1	-7.92	115.25	120.80
29	K	60	TYR	CG-CD2-CE2	-7.92	114.97	121.30
20	N	728	PHE	CB-CG-CD2	-7.91	115.26	120.80
19	Z	34	ARG	NE-CZ-NH1	7.91	124.25	120.30
19	Z	225	ALA	CB-CA-C	-7.90	98.25	110.10
22	P	370	TYR	CB-CG-CD1	7.89	125.73	121.00
7	G	115	ARG	NE-CZ-NH1	7.89	124.25	120.30
14	7	107	LEU	CB-CG-CD1	7.89	124.41	111.00
26	O	260	ASP	CB-CG-OD2	-7.89	111.20	118.30
10	3	178	ASP	CB-CG-OD1	7.87	125.38	118.30
17	T	282	TYR	CB-CG-CD2	7.87	125.72	121.00
27	H	41	TYR	CB-CG-CD2	-7.87	116.28	121.00
6	F	123	TYR	CG-CD2-CE2	7.86	127.59	121.30
19	Z	434	TYR	CB-CG-CD2	-7.86	116.28	121.00
24	R	272	PHE	CB-CG-CD1	7.85	126.30	120.80
20	N	205	TYR	CB-CG-CD2	-7.85	116.29	121.00
20	N	719	ASP	CB-CG-OD1	-7.85	111.24	118.30
26	O	255	TRP	CA-CB-CG	7.84	128.60	113.70
22	P	378	MET	CG-SD-CE	-7.84	87.66	100.20
13	6	98	ARG	NE-CZ-NH1	7.83	124.22	120.30
19	Z	314	TYR	CB-CG-CD1	-7.81	116.31	121.00
24	R	311	TYR	CB-CG-CD1	7.81	125.69	121.00
14	7	130	ARG	NE-CZ-NH1	7.80	124.20	120.30
24	R	329	PHE	CB-CG-CD2	-7.80	115.34	120.80
29	K	403	TYR	CG-CD2-CE2	-7.80	115.06	121.30
21	S	95	ARG	NE-CZ-NH1	7.80	124.20	120.30
14	7	228	TYR	CB-CG-CD1	7.80	125.68	121.00
7	G	170	ARG	NE-CZ-NH2	-7.79	116.40	120.30
31	M	171	TYR	CB-CG-CD1	-7.79	116.33	121.00
21	S	196	ARG	NE-CZ-NH2	7.78	124.19	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O	60	TYR	CB-CG-CD1	7.77	125.66	121.00
24	R	385	ARG	NE-CZ-NH2	-7.77	116.42	120.30
22	P	73	MET	CG-SD-CE	-7.76	87.78	100.20
28	I	385	MET	CG-SD-CE	-7.76	87.78	100.20
23	Q	232	PHE	CB-CG-CD2	-7.75	115.38	120.80
4	D	140	VAL	CA-CB-CG1	7.74	122.52	110.90
3	C	77	ALA	N-CA-CB	7.74	120.94	110.10
6	F	9	ASP	CB-CG-OD2	-7.74	111.33	118.30
22	P	65	ARG	NE-CZ-NH1	7.74	124.17	120.30
7	G	224	ARG	CD-NE-CZ	7.74	134.43	123.60
12	5	67	PHE	CB-CG-CD2	7.74	126.22	120.80
29	K	210	CYS	CA-CB-SG	-7.73	100.08	114.00
9	2	181	PHE	CB-CG-CD1	7.72	126.21	120.80
23	Q	253	TYR	CB-CG-CD1	7.72	125.63	121.00
19	Z	469	TYR	CB-CG-CD2	-7.71	116.37	121.00
4	D	112	TYR	CB-CG-CD1	-7.70	116.38	121.00
16	V	226	MET	CG-SD-CE	-7.70	87.88	100.20
19	Z	489	TYR	CG-CD2-CE2	-7.70	115.14	121.30
27	H	420	TYR	CB-CG-CD1	7.68	125.61	121.00
6	F	18	ARG	NE-CZ-NH2	-7.68	116.46	120.30
1	A	107	TYR	CB-CG-CD2	-7.67	116.40	121.00
25	U	177	ARG	NE-CZ-NH1	7.67	124.14	120.30
29	K	29	PHE	CB-CG-CD1	-7.67	115.43	120.80
24	R	293	ARG	NE-CZ-NH1	7.67	124.13	120.30
13	6	73	LEU	CB-CG-CD2	7.66	124.03	111.00
16	V	104	ARG	NE-CZ-NH1	7.65	124.12	120.30
19	Z	763	ARG	NE-CZ-NH2	-7.65	116.47	120.30
32	J	313	ARG	NE-CZ-NH2	-7.65	116.48	120.30
2	B	8	PHE	CB-CG-CD1	-7.65	115.45	120.80
17	T	113	SER	N-CA-CB	7.64	121.96	110.50
8	1	52	ARG	NE-CZ-NH1	7.64	124.12	120.30
24	R	142	PHE	CB-CG-CD2	-7.63	115.46	120.80
16	V	91	PHE	CB-CG-CD1	7.63	126.14	120.80
24	R	294	TYR	CB-CG-CD2	-7.62	116.43	121.00
20	N	579	ARG	NE-CZ-NH2	-7.62	116.49	120.30
23	Q	9	PHE	CB-CG-CD2	7.62	126.13	120.80
19	Z	620	PHE	CB-CG-CD1	7.61	126.13	120.80
23	Q	74	ARG	NE-CZ-NH2	-7.61	116.50	120.30
17	T	248	PHE	CB-CG-CD1	-7.60	115.48	120.80
8	1	62	ARG	NE-CZ-NH2	7.60	124.10	120.30
20	N	502	TYR	CB-CG-CD1	7.60	125.56	121.00
29	K	245	ARG	NE-CZ-NH1	7.59	124.09	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	K	249	ASP	CB-CG-OD2	-7.59	111.47	118.30
7	G	26	TYR	CB-CG-CD1	-7.58	116.45	121.00
19	Z	489	TYR	CG-CD1-CE1	-7.58	115.24	121.30
26	O	88	THR	CA-CB-CG2	-7.58	101.79	112.40
21	S	254	TYR	CB-CG-CD1	7.58	125.55	121.00
27	H	258	ARG	NE-CZ-NH1	-7.58	116.51	120.30
31	M	441	TYR	CG-CD2-CE2	-7.58	115.24	121.30
20	N	494	TYR	CB-CG-CD1	7.58	125.55	121.00
1	A	88	ARG	NE-CZ-NH2	-7.56	116.52	120.30
19	Z	316	ASP	CB-CG-OD2	-7.56	111.50	118.30
19	Z	814	SER	N-CA-CB	7.56	121.84	110.50
25	U	228	TYR	CB-CG-CD2	-7.55	116.47	121.00
32	J	340	ARG	NE-CZ-NH2	-7.55	116.53	120.30
22	P	189	GLN	N-CA-CB	7.55	124.18	110.60
9	2	244	ARG	NE-CZ-NH1	7.54	124.07	120.30
27	H	328	ASP	CB-CG-OD1	-7.54	111.52	118.30
21	S	110	TYR	CB-CG-CD2	7.54	125.52	121.00
19	Z	173	LEU	CB-CG-CD1	7.53	123.81	111.00
31	M	367	ARG	NE-CZ-NH1	7.53	124.06	120.30
29	K	333	PHE	CB-CG-CD2	-7.53	115.53	120.80
22	P	27	ARG	NE-CZ-NH1	7.52	124.06	120.30
21	S	410	TYR	CD1-CE1-CZ	7.52	126.57	119.80
22	P	287	VAL	CA-CB-CG1	7.52	122.17	110.90
22	P	341	PHE	CB-CG-CD2	7.51	126.06	120.80
22	P	408	ARG	NE-CZ-NH2	-7.50	116.55	120.30
6	F	96	ARG	NE-CZ-NH1	7.50	124.05	120.30
23	Q	282	ARG	NE-CZ-NH2	-7.50	116.55	120.30
27	H	284	ARG	NE-CZ-NH1	-7.50	116.55	120.30
32	J	197	THR	CA-CB-CG2	-7.50	101.90	112.40
11	4	134	TYR	CB-CG-CD1	-7.49	116.50	121.00
21	S	356	TYR	CZ-CE2-CD2	-7.47	113.07	119.80
24	R	179	ARG	NE-CZ-NH1	7.47	124.04	120.30
14	7	253	TRP	CD1-CG-CD2	-7.47	100.32	106.30
20	N	34	PHE	CB-CG-CD2	-7.47	115.57	120.80
17	T	305	TYR	CG-CD1-CE1	-7.46	115.33	121.30
17	T	169	ARG	NE-CZ-NH1	7.46	124.03	120.30
21	S	176	ARG	NE-CZ-NH2	-7.45	116.58	120.30
29	K	363	TYR	CB-CG-CD2	7.44	125.46	121.00
32	J	113	ARG	NE-CZ-NH1	-7.44	116.58	120.30
6	F	100	ASP	CB-CG-OD2	-7.44	111.61	118.30
20	N	346	ASN	CB-CG-OD1	-7.43	106.73	121.60
31	M	365	ARG	NE-CZ-NH1	-7.43	116.59	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Z	314	TYR	CB-CG-CD2	7.42	125.45	121.00
16	V	262	GLU	N-CA-CB	7.41	123.93	110.60
25	U	234	PHE	CB-CG-CD2	7.41	125.98	120.80
19	Z	100	ARG	NE-CZ-NH2	7.40	124.00	120.30
20	N	813	TYR	CB-CG-CD2	-7.40	116.56	121.00
17	T	340	ARG	NE-CZ-NH1	-7.39	116.60	120.30
25	U	283	ARG	NE-CZ-NH1	7.39	123.99	120.30
10	3	6	TYR	CB-CG-CD1	7.39	125.43	121.00
3	C	91	ARG	NE-CZ-NH2	-7.38	116.61	120.30
24	R	18	ARG	NE-CZ-NH2	-7.38	116.61	120.30
19	Z	277	LEU	CB-CG-CD2	7.38	123.55	111.00
16	V	282	ARG	NE-CZ-NH1	7.38	123.99	120.30
23	Q	137	TYR	CB-CG-CD2	-7.37	116.58	121.00
31	M	350	ARG	NE-CZ-NH2	-7.37	116.62	120.30
21	S	220	LEU	CB-CG-CD2	7.36	123.51	111.00
20	N	769	PHE	CB-CG-CD2	7.36	125.95	120.80
28	I	273	VAL	CA-CB-CG1	7.36	121.94	110.90
28	I	317	ASP	CB-CG-OD1	-7.35	111.69	118.30
31	M	311	ARG	NE-CZ-NH1	7.35	123.97	120.30
22	P	166	LEU	CB-CG-CD1	7.35	123.49	111.00
6	F	232	PHE	CB-CG-CD1	7.34	125.94	120.80
20	N	80	TYR	CB-CG-CD2	-7.34	116.60	121.00
17	T	207	ARG	NE-CZ-NH1	7.34	123.97	120.30
18	Y	52	PHE	CB-CG-CD1	-7.33	115.67	120.80
32	J	297	ARG	NE-CZ-NH1	7.33	123.97	120.30
3	C	227	VAL	CG1-CB-CG2	7.33	122.63	110.90
30	L	83	PHE	CB-CG-CD2	-7.33	115.67	120.80
19	Z	143	ARG	NE-CZ-NH2	-7.32	116.64	120.30
16	V	207	TYR	CB-CG-CD1	-7.32	116.61	121.00
30	L	111	ARG	NE-CZ-NH2	-7.31	116.64	120.30
23	Q	279	TYR	CB-CG-CD2	-7.30	116.62	121.00
11	4	129	PHE	CB-CG-CD2	-7.29	115.69	120.80
27	H	274	PHE	CB-CG-CD1	-7.29	115.70	120.80
17	T	215	LEU	CB-CG-CD2	7.29	123.39	111.00
20	N	502	TYR	CB-CG-CD2	-7.29	116.63	121.00
29	K	297	ASP	CB-CG-OD2	-7.27	111.76	118.30
32	J	307	ARG	NE-CZ-NH2	7.25	123.93	120.30
1	A	210	PHE	CB-CG-CD1	7.25	125.88	120.80
14	7	60	PHE	CB-CG-CD2	-7.25	115.72	120.80
7	G	239	TYR	CB-CG-CD1	-7.25	116.65	121.00
19	Z	121	PHE	CB-CG-CD2	-7.24	115.73	120.80
1	A	95	ARG	NE-CZ-NH2	-7.24	116.68	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	278	VAL	CA-CB-CG2	-7.24	100.04	110.90
22	P	73	MET	CA-CB-CG	-7.24	101.00	113.30
25	U	245	PHE	CB-CG-CD2	-7.24	115.73	120.80
23	Q	344	ARG	NE-CZ-NH1	7.23	123.92	120.30
25	U	88	ARG	NE-CZ-NH1	-7.23	116.69	120.30
26	O	51	ALA	N-CA-CB	7.23	120.22	110.10
1	A	83	MET	CG-SD-CE	-7.23	88.64	100.20
22	P	350	ARG	NE-CZ-NH2	-7.23	116.69	120.30
28	I	322	ARG	NE-CZ-NH1	7.22	123.91	120.30
1	A	120	ASP	CB-CA-C	-7.21	95.97	110.40
12	5	149	TYR	CB-CG-CD2	7.21	125.33	121.00
30	L	367	PHE	CB-CG-CD1	-7.21	115.76	120.80
17	T	170	TYR	CB-CG-CD2	-7.20	116.68	121.00
8	1	116	PHE	CB-CG-CD1	7.20	125.84	120.80
20	N	616	ARG	NE-CZ-NH2	-7.20	116.70	120.30
25	U	115	TYR	CB-CG-CD1	7.20	125.32	121.00
13	6	131	TYR	CG-CD2-CE2	-7.20	115.54	121.30
30	L	358	ARG	NE-CZ-NH1	7.20	123.90	120.30
2	B	128	ARG	NE-CZ-NH1	7.19	123.89	120.30
28	I	346	ARG	NE-CZ-NH1	-7.19	116.71	120.30
7	G	100	ARG	NE-CZ-NH1	-7.18	116.71	120.30
24	R	53	TYR	CB-CG-CD2	-7.18	116.69	121.00
19	Z	349	TYR	CB-CG-CD1	7.17	125.30	121.00
26	O	289	ARG	NE-CZ-NH1	7.17	123.88	120.30
20	N	387	ARG	NE-CZ-NH1	7.17	123.88	120.30
30	L	20	ASP	CB-CG-OD2	-7.17	111.85	118.30
17	T	332	THR	CA-CB-CG2	-7.16	102.38	112.40
28	I	59	ARG	NE-CZ-NH1	-7.16	116.72	120.30
17	T	345	TYR	CG-CD2-CE2	-7.15	115.58	121.30
4	D	94	ARG	NE-CZ-NH2	-7.14	116.73	120.30
30	L	91	PRO	N-CA-CB	7.14	111.87	103.30
27	H	408	ASP	CB-CG-OD1	7.13	124.72	118.30
20	N	813	TYR	CB-CG-CD1	7.13	125.28	121.00
15	W	91	ARG	NE-CZ-NH1	-7.13	116.74	120.30
27	H	278	ASP	CB-CG-OD2	7.13	124.71	118.30
30	L	350	ASP	CB-CG-OD2	-7.13	111.89	118.30
23	Q	394	ASP	CB-CG-OD1	-7.12	111.89	118.30
7	G	31	VAL	CA-CB-CG2	7.12	121.57	110.90
25	U	112	MET	CG-SD-CE	-7.11	88.82	100.20
21	S	356	TYR	CD1-CE1-CZ	-7.11	113.40	119.80
31	M	188	TYR	CB-CG-CD2	-7.11	116.73	121.00
5	E	229	PHE	CB-CG-CD1	7.10	125.77	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	R	179	ARG	NE-CZ-NH2	-7.10	116.75	120.30
10	3	85	TYR	CG-CD2-CE2	7.10	126.98	121.30
12	5	147	TYR	CB-CG-CD2	-7.08	116.75	121.00
28	I	303	ARG	NE-CZ-NH2	7.08	123.84	120.30
23	Q	360	ASP	CB-CG-OD1	-7.08	111.93	118.30
20	N	158	ARG	NE-CZ-NH1	-7.08	116.76	120.30
28	I	278	ALA	CB-CA-C	7.08	120.72	110.10
14	7	54	SER	N-CA-C	-7.07	91.90	111.00
26	O	274	LEU	CB-CG-CD2	7.06	123.00	111.00
6	F	87	PHE	CB-CG-CD2	7.06	125.74	120.80
21	S	178	LYS	N-CA-CB	7.06	123.30	110.60
29	K	333	PHE	CB-CG-CD1	7.06	125.74	120.80
8	1	94	TYR	CB-CG-CD1	7.05	125.23	121.00
13	6	196	ASP	CB-CG-OD1	7.05	124.64	118.30
19	Z	505	MET	CG-SD-CE	7.05	111.48	100.20
1	A	23	TYR	CZ-CE2-CD2	-7.05	113.46	119.80
19	Z	453	SER	C-N-CA	7.05	137.10	122.30
21	S	130	PHE	CB-CG-CD1	-7.05	115.87	120.80
31	M	202	VAL	CA-CB-CG2	-7.04	100.34	110.90
21	S	224	ARG	NE-CZ-NH2	-7.04	116.78	120.30
20	N	733	ALA	CB-CA-C	-7.03	99.55	110.10
32	J	239	ARG	NE-CZ-NH1	7.03	123.82	120.30
21	S	239	ASP	CB-CG-OD1	-7.03	111.97	118.30
28	I	90	GLU	OE1-CD-OE2	7.03	131.74	123.30
29	K	43	ARG	NE-CZ-NH2	-7.03	116.78	120.30
12	5	149	TYR	CB-CG-CD1	-7.03	116.78	121.00
31	M	275	PHE	CB-CG-CD1	7.03	125.72	120.80
27	H	43	ARG	NE-CZ-NH2	-7.02	116.79	120.30
20	N	330	SER	N-CA-CB	7.00	121.00	110.50
28	I	132	TYR	CG-CD1-CE1	-7.00	115.70	121.30
29	K	287	ARG	NE-CZ-NH1	7.00	123.80	120.30
14	7	61	ASP	CB-CG-OD2	-7.00	112.00	118.30
19	Z	332	ALA	N-CA-CB	7.00	119.90	110.10
26	O	213	PHE	CB-CG-CD2	7.00	125.70	120.80
31	M	367	ARG	NE-CZ-NH2	-7.00	116.80	120.30
2	B	228	ASP	CB-CG-OD2	-6.99	112.01	118.30
23	Q	161	ASP	CB-CG-OD2	6.99	124.59	118.30
19	Z	802	SER	CB-CA-C	-6.99	96.82	110.10
31	M	120	ARG	NE-CZ-NH2	-6.98	116.81	120.30
18	Y	52	PHE	CB-CG-CD2	6.98	125.69	120.80
24	R	192	ARG	NE-CZ-NH1	6.98	123.79	120.30
21	S	472	PHE	CB-CG-CD2	-6.98	115.92	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	392	PHE	CB-CG-CD1	6.98	125.69	120.80
7	G	216	TRP	CB-CG-CD2	-6.97	117.54	126.60
19	Z	54	ASP	CB-CG-OD1	6.96	124.57	118.30
15	W	100	ARG	NE-CZ-NH1	-6.96	116.82	120.30
1	A	178	PHE	CB-CG-CD1	-6.95	115.94	120.80
14	7	175	ALA	N-CA-CB	6.94	119.82	110.10
23	Q	266	ASP	CB-CG-OD1	-6.94	112.05	118.30
32	J	372	ARG	NE-CZ-NH1	6.94	123.77	120.30
29	K	405	THR	CA-CB-CG2	-6.94	102.68	112.40
27	H	263	MET	CG-SD-CE	-6.94	89.10	100.20
8	1	163	SER	N-CA-CB	6.94	120.91	110.50
20	N	57	ARG	NE-CZ-NH2	-6.94	116.83	120.30
16	V	309	PHE	CB-CG-CD2	6.94	125.66	120.80
29	K	111	TYR	CG-CD2-CE2	6.93	126.84	121.30
24	R	388	ASN	N-CA-CB	6.92	123.06	110.60
28	I	96	ARG	NE-CZ-NH2	-6.92	116.84	120.30
24	R	46	ARG	NE-CZ-NH1	6.92	123.76	120.30
25	U	236	LEU	C-N-CA	6.92	139.00	121.70
9	2	133	TYR	CG-CD1-CE1	6.91	126.83	121.30
1	A	103	TYR	CB-CG-CD1	6.91	125.14	121.00
12	5	109	ALA	N-CA-CB	6.91	119.77	110.10
30	L	269	ARG	NE-CZ-NH1	6.90	123.75	120.30
6	F	239	ARG	NE-CZ-NH1	-6.90	116.85	120.30
25	U	155	PHE	CB-CG-CD1	6.90	125.63	120.80
22	P	227	TYR	CG-CD2-CE2	6.90	126.82	121.30
17	T	190	TYR	CD1-CG-CD2	6.89	125.48	117.90
28	I	253	SER	N-CA-CB	6.89	120.84	110.50
28	I	295	TYR	CZ-CE2-CD2	6.89	126.00	119.80
20	N	362	ASN	N-CA-CB	6.89	123.00	110.60
3	C	130	PHE	CB-CG-CD2	-6.88	115.98	120.80
5	E	215	ILE	CA-CB-CG1	6.88	124.07	111.00
14	7	78	ALA	N-CA-CB	6.88	119.72	110.10
12	5	236	TYR	CB-CA-C	-6.87	96.66	110.40
20	N	622	LEU	CB-CA-C	-6.87	97.16	110.20
2	B	13	PHE	CB-CG-CD2	-6.86	116.00	120.80
10	3	136	PHE	CB-CG-CD1	-6.86	116.00	120.80
12	5	224	TYR	CG-CD2-CE2	-6.86	115.81	121.30
31	M	337	ARG	NE-CZ-NH1	-6.86	116.87	120.30
14	7	94	MET	CG-SD-CE	-6.86	89.23	100.20
4	D	235	VAL	N-CA-CB	6.85	126.57	111.50
23	Q	142	ARG	NE-CZ-NH2	-6.85	116.88	120.30
32	J	310	ARG	NE-CZ-NH2	-6.85	116.88	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	H	366	ARG	NE-CZ-NH1	6.85	123.72	120.30
24	R	267	ARG	NE-CZ-NH2	-6.84	116.88	120.30
26	O	49	CYS	N-CA-CB	6.84	122.91	110.60
13	6	47	PHE	CB-CG-CD1	6.83	125.58	120.80
25	U	9	VAL	CA-CB-CG2	-6.83	100.65	110.90
28	I	210	TYR	CB-CG-CD2	-6.83	116.90	121.00
30	L	44	ARG	NE-CZ-NH1	-6.83	116.89	120.30
7	G	233	ARG	NE-CZ-NH1	6.83	123.71	120.30
10	3	164	PHE	CB-CG-CD1	6.83	125.58	120.80
20	N	628	ARG	NE-CZ-NH2	6.83	123.71	120.30
11	4	95	ARG	NE-CZ-NH2	-6.82	116.89	120.30
31	M	413	ARG	NE-CZ-NH1	6.82	123.71	120.30
20	N	783	TYR	CB-CG-CD2	6.82	125.09	121.00
30	L	233	PHE	CB-CG-CD2	6.81	125.57	120.80
17	T	148	ARG	NE-CZ-NH2	-6.81	116.90	120.30
31	M	132	ARG	NE-CZ-NH1	-6.80	116.90	120.30
21	S	437	ALA	C-N-CA	6.80	138.70	121.70
26	O	63	PHE	CB-CG-CD2	-6.80	116.04	120.80
17	T	211	PHE	CB-CG-CD2	6.79	125.56	120.80
16	V	161	ARG	NE-CZ-NH1	6.79	123.70	120.30
31	M	273	ASP	CB-CG-OD2	-6.79	112.19	118.30
29	K	339	ARG	NE-CZ-NH2	-6.79	116.91	120.30
20	N	385	PHE	CB-CG-CD1	6.78	125.54	120.80
23	Q	89	VAL	CA-CB-CG1	6.77	121.06	110.90
14	7	119	GLU	N-CA-CB	6.77	122.79	110.60
4	D	3	TYR	CA-CB-CG	6.77	126.26	113.40
8	1	186	LEU	CB-CG-CD1	6.77	122.50	111.00
29	K	112	TYR	CB-CG-CD2	-6.76	116.94	121.00
19	Z	137	ARG	NE-CZ-NH2	-6.76	116.92	120.30
10	3	47	ASP	CB-CG-OD1	6.76	124.38	118.30
13	6	84	PHE	CB-CG-CD1	-6.75	116.07	120.80
27	H	323	ARG	NE-CZ-NH1	-6.75	116.92	120.30
32	J	405	TRP	CE3-CZ3-CH2	6.75	128.63	121.20
25	U	79	TYR	CA-CB-CG	6.75	126.22	113.40
24	R	72	LYS	N-CA-CB	6.75	122.74	110.60
22	P	123	ARG	NE-CZ-NH1	6.74	123.67	120.30
14	7	74	TYR	CG-CD1-CE1	6.74	126.69	121.30
19	Z	825	MET	CG-SD-CE	-6.74	89.42	100.20
28	I	271	PHE	CB-CG-CD2	6.73	125.51	120.80
19	Z	261	ARG	NE-CZ-NH2	-6.73	116.93	120.30
32	J	148	TYR	CB-CG-CD2	-6.72	116.97	121.00
24	R	151	TYR	CB-CG-CD1	-6.72	116.97	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	370	TYR	CB-CG-CD2	-6.72	116.97	121.00
11	4	107	TYR	N-CA-CB	6.72	122.69	110.60
17	T	318	TYR	CB-CG-CD1	-6.71	116.97	121.00
28	I	166	ASP	CB-CG-OD2	6.71	124.34	118.30
24	R	311	TYR	CG-CD1-CE1	6.71	126.67	121.30
1	A	125	TYR	CB-CG-CD1	6.70	125.02	121.00
23	Q	308	ASP	CB-CG-OD2	-6.70	112.27	118.30
31	M	263	PHE	CB-CG-CD2	6.70	125.49	120.80
32	J	310	ARG	NE-CZ-NH1	6.70	123.65	120.30
27	H	232	ARG	NE-CZ-NH1	6.70	123.65	120.30
23	Q	102	ALA	N-CA-CB	6.69	119.47	110.10
23	Q	324	ALA	CB-CA-C	-6.69	100.06	110.10
26	O	30	THR	CA-CB-OG1	6.69	123.05	109.00
4	D	33	VAL	CA-CB-CG1	6.69	120.93	110.90
27	H	158	ASP	CB-CG-OD2	-6.69	112.28	118.30
28	I	295	TYR	CD1-CE1-CZ	6.68	125.81	119.80
31	M	251	PHE	CB-CG-CD1	6.68	125.48	120.80
24	R	194	PHE	CB-CG-CD2	-6.68	116.12	120.80
26	O	270	ARG	NE-CZ-NH1	6.68	123.64	120.30
12	5	220	TYR	CG-CD2-CE2	6.68	126.64	121.30
14	7	91	ASP	CB-CG-OD2	-6.68	112.29	118.30
31	M	181	ASP	CB-CG-OD1	6.67	124.31	118.30
21	S	110	TYR	CB-CG-CD1	-6.67	117.00	121.00
29	K	323	ARG	NE-CZ-NH2	-6.67	116.96	120.30
31	M	367	ARG	CD-NE-CZ	6.67	132.94	123.60
19	Z	489	TYR	CB-CA-C	6.67	123.74	110.40
30	L	286	ARG	NE-CZ-NH2	-6.67	116.97	120.30
3	C	111	VAL	CA-CB-CG1	-6.67	100.90	110.90
3	C	71	ASP	CB-CG-OD2	-6.67	112.30	118.30
25	U	122	VAL	CA-CB-CG1	-6.67	100.90	110.90
13	6	168	ALA	N-CA-CB	6.66	119.42	110.10
10	3	168	SER	N-CA-CB	6.66	120.49	110.50
20	N	385	PHE	CB-CG-CD2	-6.66	116.14	120.80
30	L	230	ARG	NE-CZ-NH2	6.65	123.63	120.30
12	5	241	ASP	CB-CG-OD2	6.65	124.29	118.30
20	N	344	ARG	NE-CZ-NH1	-6.65	116.97	120.30
12	5	99	TYR	CB-CG-CD1	-6.65	117.01	121.00
15	W	54	LEU	CB-CG-CD1	6.65	122.31	111.00
26	O	188	LEU	CB-CG-CD1	6.65	122.31	111.00
20	N	811	PHE	CB-CG-CD1	6.65	125.45	120.80
21	S	306	THR	N-CA-CB	6.64	122.92	110.30
8	1	75	PHE	CB-CG-CD1	6.64	125.45	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	U	250	TYR	CB-CG-CD2	-6.63	117.02	121.00
26	O	85	ARG	NE-CZ-NH1	6.63	123.61	120.30
25	U	95	TYR	CB-CG-CD1	6.63	124.98	121.00
13	6	71	TYR	CB-CG-CD2	-6.62	117.03	121.00
19	Z	590	PHE	CB-CG-CD1	6.62	125.43	120.80
22	P	240	TYR	CG-CD1-CE1	-6.61	116.01	121.30
32	J	385	MET	CG-SD-CE	-6.61	89.63	100.20
25	U	53	SER	N-CA-CB	6.61	120.41	110.50
17	T	318	TYR	N-CA-C	-6.60	93.17	111.00
21	S	446	SER	N-CA-CB	6.60	120.40	110.50
2	B	113	ARG	CG-CD-NE	-6.60	97.95	111.80
24	R	124	PHE	CB-CG-CD1	6.59	125.42	120.80
19	Z	483	PHE	CB-CG-CD2	-6.59	116.19	120.80
19	Z	483	PHE	CB-CG-CD1	6.59	125.41	120.80
22	P	309	PHE	CB-CG-CD2	-6.59	116.19	120.80
20	N	179	TYR	CG-CD1-CE1	6.58	126.57	121.30
8	1	121	TYR	CG-CD2-CE2	-6.58	116.03	121.30
19	Z	464	ALA	CB-CA-C	-6.58	100.22	110.10
25	U	115	TYR	CG-CD2-CE2	-6.58	116.04	121.30
21	S	126	PHE	CB-CG-CD1	6.58	125.40	120.80
28	I	405	MET	CG-SD-CE	-6.57	89.68	100.20
23	Q	282	ARG	NE-CZ-NH1	6.57	123.59	120.30
19	Z	496	ASP	CB-CG-OD1	6.57	124.21	118.30
22	P	136	ILE	CA-CB-CG1	6.57	123.48	111.00
6	F	146	GLN	CG-CD-OE1	-6.56	108.48	121.60
6	F	87	PHE	CB-CG-CD1	-6.56	116.21	120.80
21	S	248	ASN	CB-CA-C	-6.56	97.28	110.40
30	L	308	ARG	NE-CZ-NH2	-6.56	117.02	120.30
31	M	159	ASP	CB-CG-OD2	-6.56	112.40	118.30
22	P	428	TRP	CG-CD2-CE3	-6.55	128.00	133.90
8	1	136	TRP	CE3-CZ3-CH2	-6.55	114.00	121.20
10	3	155	GLU	CA-C-O	-6.55	106.35	120.10
19	Z	235	SER	N-CA-CB	6.55	120.32	110.50
26	O	108	ASP	CB-CG-OD2	-6.55	112.41	118.30
17	T	330	ASP	CB-CG-OD2	6.54	124.19	118.30
19	Z	400	TYR	CG-CD1-CE1	-6.54	116.07	121.30
19	Z	803	PHE	CB-CG-CD1	6.54	125.38	120.80
28	I	408	ARG	CB-CA-C	-6.54	97.32	110.40
2	B	6	TYR	CB-CG-CD2	-6.53	117.08	121.00
32	J	80	MET	CG-SD-CE	-6.53	89.75	100.20
10	3	6	TYR	CB-CG-CD2	-6.53	117.08	121.00
6	F	171	TYR	CG-CD2-CE2	-6.53	116.08	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	B	132	VAL	CA-CB-CG1	6.52	120.69	110.90
9	2	57	LEU	N-CA-C	-6.52	93.39	111.00
17	T	296	PHE	CB-CG-CD1	6.52	125.36	120.80
23	Q	211	ASP	CB-CG-OD1	6.52	124.17	118.30
32	J	213	ARG	NE-CZ-NH2	-6.52	117.04	120.30
7	G	175	THR	CA-CB-CG2	-6.52	103.27	112.40
21	S	251	LEU	CB-CA-C	-6.52	97.82	110.20
20	N	269	ARG	NE-CZ-NH2	-6.51	117.04	120.30
20	N	713	TYR	CB-CG-CD2	-6.51	117.09	121.00
19	Z	256	PHE	CB-CG-CD2	-6.51	116.24	120.80
29	K	219	VAL	CA-CB-CG2	6.51	120.66	110.90
27	H	249	TYR	CB-CG-CD1	-6.51	117.10	121.00
22	P	404	ALA	N-CA-CB	6.50	119.21	110.10
8	1	208	ARG	NE-CZ-NH1	6.50	123.55	120.30
23	Q	310	ARG	NE-CZ-NH1	6.50	123.55	120.30
22	P	263	TRP	CD1-CG-CD2	-6.50	101.10	106.30
19	Z	670	MET	CG-SD-CE	-6.49	89.81	100.20
3	C	3	ARG	NE-CZ-NH2	6.49	123.55	120.30
10	3	26	ARG	NE-CZ-NH1	6.49	123.54	120.30
15	W	157	VAL	CG1-CB-CG2	6.49	121.28	110.90
26	O	330	ARG	CB-CA-C	-6.48	97.44	110.40
4	D	112	TYR	CZ-CE2-CD2	6.48	125.63	119.80
27	H	409	PHE	CB-CG-CD2	6.48	125.33	120.80
16	V	225	TRP	CA-CB-CG	6.47	126.00	113.70
24	R	312	ARG	NE-CZ-NH2	-6.47	117.06	120.30
22	P	369	TYR	CA-CB-CG	-6.46	101.12	113.40
11	4	3	TYR	CB-CG-CD2	-6.46	117.12	121.00
28	I	439	TYR	CB-CG-CD2	6.46	124.88	121.00
9	2	136	TYR	CG-CD2-CE2	6.46	126.47	121.30
21	S	371	PHE	CB-CG-CD2	-6.46	116.28	120.80
3	C	148	TYR	CB-CG-CD2	6.45	124.87	121.00
26	O	352	ARG	NE-CZ-NH2	-6.45	117.07	120.30
4	D	144	PHE	CB-CG-CD2	6.45	125.31	120.80
26	O	3	ASP	CB-CG-OD2	-6.45	112.49	118.30
28	I	276	GLU	N-CA-CB	-6.45	98.99	110.60
4	D	173	SER	CA-C-O	6.45	133.64	120.10
20	N	158	ARG	NE-CZ-NH2	6.45	123.52	120.30
21	S	263	ALA	N-CA-CB	6.45	119.12	110.10
24	R	91	ALA	N-CA-CB	6.45	119.12	110.10
25	U	69	PHE	CB-CG-CD2	6.45	125.31	120.80
22	P	415	PHE	CB-CG-CD2	-6.44	116.29	120.80
20	N	444	TYR	CG-CD1-CE1	-6.44	116.15	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	177	TYR	CB-CG-CD2	-6.43	117.14	121.00
31	M	195	ASP	CB-CG-OD2	-6.43	112.51	118.30
12	5	65	PHE	CB-CG-CD1	6.43	125.30	120.80
14	7	77	LEU	N-CA-C	-6.43	93.64	111.00
28	I	295	TYR	CB-CG-CD1	6.43	124.86	121.00
20	N	546	ARG	NE-CZ-NH2	-6.43	117.09	120.30
1	A	29	PHE	CB-CG-CD2	-6.43	116.30	120.80
22	P	370	TYR	CD1-CE1-CZ	-6.42	114.02	119.80
31	M	251	PHE	CB-CG-CD2	-6.42	116.30	120.80
30	L	17	ASP	CB-CG-OD2	-6.42	112.52	118.30
14	7	193	LEU	CB-CG-CD1	6.42	121.91	111.00
11	4	146	TYR	CA-CB-CG	-6.42	101.21	113.40
15	W	47	ASN	N-CA-CB	6.41	122.14	110.60
17	T	292	ARG	NE-CZ-NH2	-6.41	117.10	120.30
22	P	190	MET	CG-SD-CE	-6.41	89.95	100.20
23	Q	297	ARG	NE-CZ-NH2	-6.40	117.10	120.30
23	Q	101	ALA	CB-CA-C	-6.40	100.50	110.10
17	T	259	TYR	CB-CG-CD2	6.40	124.84	121.00
25	U	88	ARG	NH1-CZ-NH2	6.39	126.43	119.40
19	Z	852	VAL	CG1-CB-CG2	6.39	121.13	110.90
23	Q	255	LEU	N-CA-CB	6.39	123.18	110.40
26	O	179	PHE	CB-CG-CD1	-6.39	116.33	120.80
20	N	109	THR	N-CA-CB	6.39	122.44	110.30
3	C	87	THR	CA-CB-CG2	-6.38	103.46	112.40
22	P	247	TYR	CG-CD1-CE1	-6.38	116.19	121.30
19	Z	67	ASP	CB-CA-C	-6.38	97.64	110.40
28	I	353	PHE	CB-CG-CD2	-6.38	116.33	120.80
32	J	57	ARG	NE-CZ-NH1	6.38	123.49	120.30
9	2	178	MET	CG-SD-CE	-6.38	90.00	100.20
19	Z	158	TYR	CZ-CE2-CD2	6.38	125.54	119.80
30	L	27	ARG	NE-CZ-NH1	6.38	123.49	120.30
20	N	12	LEU	CB-CG-CD2	6.38	121.84	111.00
8	1	167	TYR	CB-CG-CD2	6.37	124.82	121.00
11	4	155	ARG	NE-CZ-NH2	-6.37	117.11	120.30
31	M	298	ARG	NE-CZ-NH2	-6.37	117.11	120.30
12	5	128	ARG	NE-CZ-NH2	-6.37	117.12	120.30
17	T	345	TYR	CB-CG-CD2	-6.37	117.18	121.00
1	A	127	GLN	CA-CB-CG	6.37	127.41	113.40
20	N	557	TYR	CG-CD1-CE1	-6.37	116.21	121.30
20	N	678	ASP	CB-CG-OD1	6.36	124.03	118.30
1	A	159	TYR	CB-CG-CD2	6.36	124.82	121.00
1	A	188	ASP	N-CA-CB	6.36	122.04	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	H	158	ASP	CB-CG-OD1	6.36	124.02	118.30
31	M	161	TYR	CB-CG-CD2	-6.34	117.19	121.00
12	5	132	ARG	NE-CZ-NH1	-6.34	117.13	120.30
15	W	148	VAL	CA-CB-CG2	6.34	120.41	110.90
23	Q	90	ARG	NE-CZ-NH2	-6.34	117.13	120.30
20	N	200	VAL	CA-CB-CG2	-6.33	101.41	110.90
19	Z	366	ASP	CB-CG-OD2	-6.33	112.61	118.30
20	N	333	MET	CG-SD-CE	-6.33	90.08	100.20
23	Q	38	ASN	N-CA-CB	6.32	121.98	110.60
20	N	710	ARG	NE-CZ-NH1	-6.32	117.14	120.30
31	M	333	ALA	N-CA-CB	6.32	118.95	110.10
11	4	171	PHE	CB-CG-CD1	6.32	125.22	120.80
12	5	228	TYR	CG-CD1-CE1	-6.32	116.25	121.30
3	C	124	PHE	CB-CG-CD2	-6.31	116.38	120.80
28	I	263	GLY	CA-C-O	-6.31	109.24	120.60
24	R	327	VAL	CG1-CB-CG2	6.31	121.00	110.90
26	O	240	PHE	CB-CG-CD1	-6.31	116.39	120.80
7	G	11	SER	N-CA-CB	6.30	119.96	110.50
29	K	328	ASP	CB-CG-OD2	-6.30	112.63	118.30
23	Q	239	TYR	CB-CG-CD1	-6.30	117.22	121.00
16	V	289	ASP	CB-CG-OD1	-6.30	112.63	118.30
6	F	107	ARG	N-CA-CB	6.29	121.93	110.60
10	3	104	TYR	CG-CD1-CE1	-6.29	116.27	121.30
20	N	68	PHE	CB-CG-CD1	-6.29	116.39	120.80
21	S	355	PRO	O-C-N	6.29	132.76	122.70
22	P	80	TRP	CE3-CZ3-CH2	6.29	128.11	121.20
30	L	400	TYR	CD1-CE1-CZ	-6.29	114.14	119.80
20	N	519	VAL	CG1-CB-CG2	6.28	120.95	110.90
21	S	64	ASP	CB-CG-OD1	6.28	123.95	118.30
23	Q	18	THR	CA-CB-CG2	-6.28	103.61	112.40
10	3	39	PHE	CB-CG-CD1	6.28	125.20	120.80
31	M	129	THR	CA-CB-CG2	-6.28	103.61	112.40
5	E	230	THR	CA-CB-CG2	-6.27	103.62	112.40
14	7	167	GLY	N-CA-C	-6.27	97.41	113.10
11	4	98	TYR	CD1-CE1-CZ	6.27	125.44	119.80
19	Z	761	MET	CG-SD-CE	-6.27	90.17	100.20
28	I	225	TYR	CB-CG-CD2	6.27	124.76	121.00
29	K	120	ASP	CB-CG-OD1	6.27	123.94	118.30
4	D	169	ARG	N-CA-CB	6.26	121.88	110.60
19	Z	845	ARG	NE-CZ-NH2	-6.26	117.17	120.30
11	4	91	CYS	N-CA-CB	6.26	121.87	110.60
17	T	148	ARG	NE-CZ-NH1	-6.26	117.17	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	5	73	VAL	CA-CB-CG1	6.26	120.28	110.90
14	7	221	TYR	CB-CG-CD1	-6.26	117.25	121.00
32	J	114	VAL	CB-CA-C	-6.26	99.51	111.40
5	E	101	PHE	CB-CG-CD2	-6.25	116.42	120.80
8	1	136	TRP	CB-CG-CD2	6.25	134.73	126.60
31	M	301	SER	N-CA-CB	6.25	119.88	110.50
9	2	181	PHE	CB-CG-CD2	-6.25	116.43	120.80
20	N	59	PHE	CB-CG-CD1	-6.25	116.43	120.80
32	J	348	ALA	N-CA-CB	6.25	118.84	110.10
19	Z	432	TYR	CB-CG-CD1	-6.24	117.26	121.00
31	M	272	ARG	NE-CZ-NH1	6.24	123.42	120.30
6	F	164	ARG	NE-CZ-NH1	6.24	123.42	120.30
22	P	27	ARG	CD-NE-CZ	-6.24	114.87	123.60
31	M	307	ARG	NE-CZ-NH1	6.24	123.42	120.30
13	6	57	SER	N-CA-CB	6.23	119.85	110.50
25	U	49	ASP	CB-CG-OD2	-6.23	112.69	118.30
21	S	93	ALA	N-CA-CB	6.23	118.83	110.10
16	V	175	ARG	NE-CZ-NH1	6.22	123.41	120.30
19	Z	38	GLU	OE1-CD-OE2	-6.22	115.84	123.30
23	Q	72	TYR	CG-CD2-CE2	-6.21	116.33	121.30
7	G	66	ARG	NE-CZ-NH1	6.21	123.41	120.30
28	I	322	ARG	NE-CZ-NH2	-6.21	117.20	120.30
12	5	211	ALA	N-CA-CB	6.21	118.79	110.10
9	2	51	TYR	CB-CG-CD2	6.20	124.72	121.00
10	3	177	ARG	NE-CZ-NH2	-6.20	117.20	120.30
14	7	153	THR	N-CA-CB	6.20	122.09	110.30
19	Z	282	PHE	CB-CG-CD1	-6.20	116.46	120.80
32	J	383	PHE	CB-CG-CD2	6.20	125.14	120.80
15	W	10	VAL	CA-CB-CG1	-6.20	101.60	110.90
19	Z	556	ARG	NH1-CZ-NH2	6.20	126.22	119.40
26	O	47	ASP	CA-C-N	6.20	134.45	117.10
2	B	155	TYR	N-CA-CB	6.19	121.74	110.60
22	P	201	ARG	CB-CA-C	-6.19	98.02	110.40
9	2	79	PHE	CB-CG-CD1	-6.19	116.47	120.80
20	N	460	TYR	CZ-CE2-CD2	6.19	125.37	119.80
32	J	107	ASP	CB-CG-OD2	-6.19	112.73	118.30
29	K	248	ARG	NE-CZ-NH1	-6.19	117.21	120.30
14	7	63	GLY	C-N-CA	6.18	137.16	121.70
16	V	94	LYS	N-CA-CB	6.18	121.73	110.60
23	Q	344	ARG	NE-CZ-NH2	-6.18	117.21	120.30
21	S	99	SER	N-CA-CB	6.18	119.76	110.50
28	I	333	ARG	NE-CZ-NH1	-6.18	117.21	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	M	91	TYR	CB-CG-CD2	-6.18	117.29	121.00
8	1	188	PHE	CB-CG-CD2	-6.17	116.48	120.80
11	4	67	TYR	CD1-CE1-CZ	-6.17	114.24	119.80
22	P	344	THR	CA-CB-CG2	-6.17	103.76	112.40
4	D	215	ALA	N-CA-CB	6.17	118.74	110.10
29	K	323	ARG	CG-CD-NE	-6.17	98.84	111.80
31	M	350	ARG	NE-CZ-NH1	6.17	123.39	120.30
28	I	371	ARG	NE-CZ-NH2	-6.16	117.22	120.30
5	E	136	PRO	O-C-N	6.16	132.56	122.70
3	C	66	TYR	CZ-CE2-CD2	-6.16	114.25	119.80
21	S	290	ARG	NE-CZ-NH1	-6.16	117.22	120.30
9	2	154	TYR	CB-CG-CD1	-6.16	117.31	121.00
23	Q	122	ARG	NE-CZ-NH1	6.16	123.38	120.30
32	J	43	ARG	NE-CZ-NH1	6.15	123.38	120.30
4	D	164	ALA	N-CA-CB	6.15	118.71	110.10
28	I	262	ASP	CB-CG-OD2	6.15	123.84	118.30
6	F	131	GLY	N-CA-C	-6.15	97.72	113.10
14	7	70	MET	CG-SD-CE	6.15	110.03	100.20
19	Z	349	TYR	CD1-CE1-CZ	-6.15	114.27	119.80
32	J	3	LEU	CB-CG-CD1	6.15	121.45	111.00
13	6	157	TYR	CB-CG-CD2	-6.14	117.31	121.00
19	Z	593	THR	CA-CB-CG2	-6.14	103.80	112.40
23	Q	233	TYR	CD1-CE1-CZ	-6.14	114.27	119.80
8	1	62	ARG	NE-CZ-NH1	-6.14	117.23	120.30
14	7	231	PHE	CB-CG-CD1	-6.14	116.50	120.80
25	U	107	ALA	CB-CA-C	-6.14	100.89	110.10
10	3	104	TYR	CG-CD2-CE2	-6.13	116.39	121.30
6	F	144	VAL	CG1-CB-CG2	6.13	120.71	110.90
23	Q	309	TYR	CB-CG-CD2	-6.13	117.32	121.00
7	G	59	TYR	CG-CD1-CE1	-6.13	116.40	121.30
32	J	313	ARG	NE-CZ-NH1	6.13	123.36	120.30
4	D	25	ALA	CB-CA-C	-6.13	100.91	110.10
14	7	64	VAL	CG1-CB-CG2	6.13	120.70	110.90
17	T	248	PHE	CB-CG-CD2	6.13	125.09	120.80
21	S	103	ARG	NE-CZ-NH1	6.12	123.36	120.30
21	S	310	ARG	NE-CZ-NH2	-6.12	117.24	120.30
24	R	288	PHE	CB-CG-CD2	6.12	125.08	120.80
19	Z	687	ARG	NE-CZ-NH2	-6.12	117.24	120.30
30	L	327	LEU	CB-CG-CD1	6.12	121.40	111.00
22	P	377	ARG	CD-NE-CZ	-6.12	115.04	123.60
25	U	62	ASP	CB-CG-OD1	-6.12	112.80	118.30
10	3	59	ASP	CB-CG-OD2	-6.11	112.80	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	N	594	GLY	N-CA-C	-6.11	97.81	113.10
30	L	380	ASP	CB-CA-C	-6.11	98.18	110.40
15	W	2	VAL	CG1-CB-CG2	6.11	120.68	110.90
22	P	371	THR	N-CA-CB	6.11	121.91	110.30
8	1	143	GLN	CB-CA-C	-6.11	98.19	110.40
21	S	89	PHE	CB-CG-CD1	6.11	125.07	120.80
19	Z	580	LEU	CB-CG-CD2	6.10	121.38	111.00
3	C	12	PHE	CB-CG-CD1	6.10	125.07	120.80
20	N	139	GLN	N-CA-CB	6.10	121.58	110.60
16	V	191	ALA	N-CA-CB	6.10	118.64	110.10
27	H	163	MET	CG-SD-CE	-6.10	90.44	100.20
29	K	328	ASP	CB-CG-OD1	6.10	123.79	118.30
2	B	156	PHE	CB-CG-CD1	6.09	125.06	120.80
21	S	287	TYR	CB-CG-CD1	6.09	124.65	121.00
11	4	67	TYR	CB-CG-CD1	6.08	124.65	121.00
19	Z	40	ASP	CB-CG-OD2	6.08	123.78	118.30
2	B	98	TYR	CB-CG-CD2	-6.08	117.35	121.00
23	Q	33	ARG	NE-CZ-NH2	-6.08	117.26	120.30
24	R	110	TYR	CB-CG-CD1	-6.07	117.36	121.00
7	G	99	PHE	CB-CG-CD1	-6.07	116.55	120.80
14	7	155	VAL	CG1-CB-CG2	6.07	120.61	110.90
27	H	69	ASP	CB-CG-OD1	-6.07	112.84	118.30
24	R	285	ASP	CB-CG-OD1	6.06	123.76	118.30
8	1	95	GLN	CB-CA-C	-6.06	98.28	110.40
32	J	148	TYR	CB-CG-CD1	6.06	124.64	121.00
12	5	171	TYR	CB-CG-CD1	-6.06	117.37	121.00
1	A	107	TYR	CG-CD2-CE2	6.05	126.14	121.30
21	S	107	TYR	CB-CG-CD2	6.05	124.63	121.00
21	S	249	LEU	CB-CA-C	-6.05	98.70	110.20
29	K	164	TYR	CZ-CE2-CD2	-6.05	114.36	119.80
2	B	191	ALA	N-CA-CB	6.05	118.57	110.10
14	7	101	TYR	CG-CD1-CE1	-6.05	116.46	121.30
9	2	136	TYR	CG-CD1-CE1	-6.04	116.47	121.30
19	Z	300	ARG	NE-CZ-NH1	-6.04	117.28	120.30
14	7	186	GLY	O-C-N	6.04	132.36	122.70
23	Q	298	SER	N-CA-CB	6.04	119.55	110.50
4	D	191	ASP	CB-CG-OD1	6.03	123.73	118.30
30	L	297	ASP	CB-CG-OD2	-6.03	112.87	118.30
1	A	20	GLY	O-C-N	6.03	132.35	122.70
21	S	207	TYR	CB-CG-CD1	6.03	124.62	121.00
25	U	147	ASP	CB-CG-OD2	-6.03	112.88	118.30
20	N	271	VAL	CA-CB-CG2	6.03	119.94	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	225	THR	N-CA-CB	6.02	121.75	110.30
19	Z	434	TYR	CB-CG-CD1	6.02	124.61	121.00
20	N	142	LEU	CB-CG-CD1	6.02	121.23	111.00
20	N	649	ARG	NE-CZ-NH1	6.02	123.31	120.30
22	P	81	ASP	CB-CG-OD2	6.02	123.72	118.30
1	A	152	TYR	CB-CG-CD2	-6.01	117.39	121.00
24	R	151	TYR	CG-CD2-CE2	6.01	126.11	121.30
9	2	132	ARG	NE-CZ-NH2	-6.01	117.29	120.30
3	C	25	MET	CG-SD-CE	-6.01	90.59	100.20
23	Q	161	ASP	CB-CG-OD1	-6.01	112.89	118.30
27	H	74	PRO	CA-C-N	6.01	133.92	117.10
30	L	124	TYR	CB-CG-CD1	6.01	124.60	121.00
27	H	188	ARG	NE-CZ-NH1	-6.00	117.30	120.30
26	O	373	ASP	CB-CG-OD1	-6.00	112.90	118.30
19	Z	489	TYR	CA-CB-CG	-6.00	102.01	113.40
24	R	176	ARG	NE-CZ-NH1	-6.00	117.30	120.30
21	S	410	TYR	CG-CD1-CE1	-5.99	116.51	121.30
25	U	244	GLU	OE1-CD-OE2	5.99	130.49	123.30
8	1	107	PRO	N-CD-CG	5.99	112.19	103.20
14	7	231	PHE	CB-CG-CD2	5.99	124.99	120.80
25	U	246	VAL	CA-CB-CG1	-5.99	101.91	110.90
9	2	62	ARG	NE-CZ-NH2	-5.99	117.31	120.30
9	2	198	VAL	CA-CB-CG2	5.99	119.88	110.90
13	6	193	LEU	CB-CG-CD2	5.99	121.18	111.00
21	S	207	TYR	CZ-CE2-CD2	5.99	125.19	119.80
31	M	244	ALA	CB-CA-C	-5.99	101.12	110.10
19	Z	588	ARG	NE-CZ-NH2	5.99	123.29	120.30
11	4	102	LEU	CB-CG-CD2	5.98	121.17	111.00
19	Z	464	ALA	N-CA-CB	5.98	118.47	110.10
25	U	54	PHE	CB-CG-CD1	-5.98	116.61	120.80
14	7	60	PHE	CB-CG-CD1	5.98	124.98	120.80
7	G	26	TYR	CZ-CE2-CD2	-5.98	114.42	119.80
13	6	34	PHE	CB-CG-CD1	5.98	124.98	120.80
6	F	122	ARG	NH1-CZ-NH2	-5.97	112.83	119.40
20	N	429	LYS	N-CA-CB	5.97	121.35	110.60
19	Z	787	LEU	CB-CG-CD1	5.97	121.15	111.00
20	N	71	LEU	CB-CG-CD1	5.97	121.15	111.00
19	Z	194	TYR	CB-CG-CD2	-5.96	117.42	121.00
30	L	20	ASP	CB-CG-OD1	5.96	123.67	118.30
7	G	93	ARG	NE-CZ-NH1	5.96	123.28	120.30
26	O	366	LEU	CB-CG-CD1	5.95	121.12	111.00
13	6	114	ALA	CB-CA-C	-5.95	101.17	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	P	326	VAL	CA-CB-CG2	-5.95	101.97	110.90
32	J	307	ARG	NH1-CZ-NH2	-5.95	112.85	119.40
19	Z	517	VAL	CA-CB-CG2	-5.95	101.98	110.90
11	4	116	TYR	CB-CG-CD1	5.95	124.57	121.00
13	6	219	ALA	C-N-CA	5.95	136.57	121.70
20	N	212	ASP	CB-CG-OD1	5.95	123.65	118.30
8	1	123	TYR	CD1-CE1-CZ	-5.95	114.45	119.80
25	U	21	ASP	CB-CG-OD1	-5.94	112.95	118.30
8	1	171	TYR	CA-CB-CG	5.94	124.69	113.40
10	3	83	LYS	N-CA-CB	-5.94	99.91	110.60
11	4	49	GLU	O-C-N	5.94	132.20	122.70
29	K	297	ASP	CB-CG-OD1	5.94	123.65	118.30
19	Z	613	LEU	C-N-CA	5.94	136.54	121.70
24	R	327	VAL	CA-CB-CG1	-5.94	101.99	110.90
27	H	261	PHE	CB-CG-CD2	-5.94	116.64	120.80
21	S	195	ASN	N-CA-CB	5.93	121.28	110.60
3	C	111	VAL	CA-CB-CG2	5.93	119.80	110.90
5	E	15	PHE	CB-CG-CD2	5.93	124.95	120.80
19	Z	845	ARG	NE-CZ-NH1	5.93	123.27	120.30
12	5	172	TYR	O-C-N	5.93	132.18	122.70
29	K	118	THR	CA-CB-CG2	-5.93	104.10	112.40
31	M	412	ARG	NE-CZ-NH2	-5.93	117.34	120.30
11	4	170	ARG	CD-NE-CZ	5.92	131.89	123.60
2	B	111	VAL	CB-CA-C	-5.92	100.15	111.40
20	N	771	PHE	CB-CG-CD2	-5.92	116.66	120.80
25	U	5	ALA	CB-CA-C	-5.92	101.22	110.10
16	V	90	VAL	CA-CB-CG2	-5.92	102.02	110.90
19	Z	72	ARG	NE-CZ-NH1	5.92	123.26	120.30
27	H	171	ASP	CB-CG-OD2	5.92	123.63	118.30
16	V	207	TYR	CB-CG-CD2	5.92	124.55	121.00
31	M	174	ARG	NE-CZ-NH1	-5.91	117.34	120.30
11	4	19	ARG	NE-CZ-NH2	-5.91	117.34	120.30
20	N	511	ALA	CB-CA-C	-5.90	101.24	110.10
24	R	258	GLN	CA-CB-CG	5.90	126.39	113.40
28	I	201	VAL	CA-CB-CG2	5.90	119.76	110.90
1	A	23	TYR	CB-CG-CD1	5.90	124.54	121.00
28	I	96	ARG	NE-CZ-NH1	5.90	123.25	120.30
20	N	915	LYS	N-CA-CB	5.90	121.22	110.60
6	F	218	ASP	CB-CG-OD2	5.90	123.61	118.30
12	5	155	SER	N-CA-CB	5.89	119.34	110.50
20	N	140	ARG	NE-CZ-NH1	5.89	123.25	120.30
32	J	374	ARG	NE-CZ-NH2	5.89	123.25	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	Q	233	TYR	CZ-CE2-CD2	-5.89	114.50	119.80
9	2	183	ASP	CB-CG-OD1	-5.88	113.00	118.30
21	S	214	TYR	CB-CA-C	-5.88	98.63	110.40
21	S	226	PHE	CB-CG-CD1	5.88	124.92	120.80
24	R	259	TYR	CA-CB-CG	5.88	124.58	113.40
22	P	394	SER	N-CA-CB	-5.88	101.67	110.50
14	7	218	ARG	NE-CZ-NH2	5.88	123.24	120.30
19	Z	239	TYR	CG-CD2-CE2	5.88	126.00	121.30
27	H	283	ALA	CB-CA-C	-5.88	101.28	110.10
25	U	128	PRO	O-C-N	5.88	132.10	122.70
24	R	285	ASP	CB-CG-OD2	-5.88	113.01	118.30
20	N	117	ASP	CB-CG-OD1	-5.88	113.01	118.30
29	K	371	SER	N-CA-CB	5.88	119.31	110.50
23	Q	74	ARG	NE-CZ-NH1	5.87	123.24	120.30
28	I	84	GLN	C-N-CA	5.87	136.36	121.70
21	S	475	ARG	NH1-CZ-NH2	5.86	125.85	119.40
22	P	227	TYR	CZ-CE2-CD2	-5.86	114.53	119.80
20	N	134	VAL	CA-CB-CG2	-5.86	102.11	110.90
6	F	94	ASP	CB-CG-OD2	-5.86	113.03	118.30
11	4	33	ASP	CB-CG-OD1	-5.85	113.03	118.30
24	R	318	TYR	CB-CG-CD2	-5.85	117.49	121.00
17	T	169	ARG	N-CA-CB	5.85	121.13	110.60
25	U	64	ASP	CB-CG-OD1	5.85	123.56	118.30
5	E	88	LEU	CB-CG-CD1	5.85	120.94	111.00
9	2	81	SER	CB-CA-C	5.85	121.21	110.10
19	Z	781	TYR	CB-CG-CD1	-5.85	117.49	121.00
13	6	158	GLN	N-CA-CB	5.85	121.12	110.60
13	6	126	ARG	NE-CZ-NH1	5.84	123.22	120.30
3	C	76	VAL	CA-CB-CG1	-5.84	102.14	110.90
5	E	37	ALA	N-CA-CB	5.84	118.28	110.10
3	C	191	ALA	CB-CA-C	-5.84	101.34	110.10
22	P	414	ASN	CA-CB-CG	-5.84	100.56	113.40
1	A	129	ALA	CB-CA-C	-5.84	101.34	110.10
24	R	143	TYR	CD1-CE1-CZ	5.83	125.05	119.80
20	N	205	TYR	CB-CG-CD1	5.83	124.50	121.00
23	Q	201	TYR	CB-CG-CD1	5.83	124.50	121.00
24	R	177	ARG	NE-CZ-NH2	5.83	123.22	120.30
19	Z	469	TYR	CG-CD2-CE2	-5.83	116.64	121.30
21	S	320	PHE	CB-CG-CD1	5.83	124.88	120.80
8	1	122	ARG	NE-CZ-NH1	5.83	123.21	120.30
15	W	85	THR	N-CA-C	-5.83	95.27	111.00
24	R	231	LEU	CB-CG-CD2	5.82	120.90	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
26	O	173	TYR	CG-CD1-CE1	5.82	125.96	121.30
13	6	182	PHE	CB-CG-CD1	-5.82	116.73	120.80
5	E	63	SER	N-CA-CB	5.82	119.23	110.50
26	O	238	TYR	CZ-CE2-CD2	-5.82	114.56	119.80
31	M	63	LEU	CB-CG-CD2	5.82	120.89	111.00
7	G	245	LYS	CB-CA-C	5.82	122.03	110.40
17	T	347	ARG	NE-CZ-NH1	5.82	123.21	120.30
20	N	415	HIS	N-CA-C	-5.81	95.30	111.00
20	N	566	LEU	CB-CG-CD2	5.81	120.88	111.00
6	F	171	TYR	CD1-CE1-CZ	5.81	125.03	119.80
20	N	82	LEU	CB-CG-CD1	5.81	120.88	111.00
20	N	548	LEU	CB-CG-CD2	5.81	120.88	111.00
25	U	49	ASP	CB-CG-OD1	5.81	123.53	118.30
31	M	369	MET	CG-SD-CE	-5.81	90.91	100.20
31	M	413	ARG	CD-NE-CZ	-5.80	115.47	123.60
29	K	410	ASP	CB-CG-OD1	5.80	123.52	118.30
14	7	116	ILE	CA-CB-CG2	5.80	122.50	110.90
26	O	196	ARG	NE-CZ-NH2	-5.80	117.40	120.30
32	J	88	LYS	N-CA-CB	5.79	121.03	110.60
20	N	147	TYR	CB-CG-CD1	5.79	124.47	121.00
21	S	257	TYR	CB-CG-CD2	-5.79	117.53	121.00
31	M	195	ASP	CB-CG-OD1	5.79	123.51	118.30
22	P	324	TYR	CG-CD2-CE2	-5.79	116.67	121.30
24	R	368	GLU	N-CA-CB	5.79	121.02	110.60
28	I	75	GLU	OE1-CD-OE2	5.79	130.25	123.30
1	A	86	ASP	CB-CG-OD2	-5.79	113.09	118.30
8	1	123	TYR	CB-CG-CD2	-5.78	117.53	121.00
16	V	104	ARG	NE-CZ-NH2	-5.78	117.41	120.30
8	1	121	TYR	CD1-CG-CD2	5.78	124.26	117.90
23	Q	27	LEU	CB-CG-CD2	5.78	120.83	111.00
1	A	50	ILE	N-CA-CB	5.78	124.08	110.80
1	A	18	PRO	N-CA-CB	5.77	110.23	103.30
4	D	150	LEU	N-CA-C	-5.77	95.41	111.00
21	S	177	TYR	CG-CD2-CE2	-5.77	116.68	121.30
23	Q	208	ALA	CB-CA-C	-5.77	101.45	110.10
31	M	423	TYR	CB-CG-CD2	-5.77	117.54	121.00
31	M	139	VAL	CA-CB-CG1	5.77	119.55	110.90
8	1	161	GLY	N-CA-C	-5.76	98.69	113.10
9	2	91	THR	CA-CB-CG2	-5.76	104.33	112.40
14	7	170	ASP	CB-CG-OD2	5.76	123.49	118.30
19	Z	332	ALA	N-CA-C	-5.76	95.44	111.00
28	I	418	ASP	CB-CG-OD1	5.76	123.49	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	153	LEU	CB-CG-CD1	5.76	120.80	111.00
20	N	167	ILE	N-CA-C	-5.76	95.45	111.00
31	M	307	ARG	N-CA-CB	5.76	120.97	110.60
15	W	5	SER	N-CA-CB	5.76	119.14	110.50
17	T	247	VAL	C-N-CA	5.76	136.10	121.70
21	S	197	ARG	NE-CZ-NH1	-5.76	117.42	120.30
24	R	222	TYR	CB-CG-CD1	5.76	124.46	121.00
32	J	317	PHE	CB-CG-CD1	5.76	124.83	120.80
4	D	92	ARG	NE-CZ-NH2	-5.76	117.42	120.30
9	2	66	GLY	N-CA-C	-5.75	98.71	113.10
24	R	343	LEU	N-CA-C	-5.75	95.46	111.00
32	J	260	GLU	OE1-CD-OE2	5.75	130.20	123.30
7	G	114	ASP	CB-CG-OD2	5.75	123.48	118.30
5	E	59	MET	N-CA-C	-5.75	95.48	111.00
20	N	141	CYS	CA-CB-SG	-5.75	103.65	114.00
10	3	72	ASN	CB-CA-C	-5.74	98.91	110.40
20	N	253	TYR	CD1-CE1-CZ	5.74	124.97	119.80
31	M	285	ILE	N-CA-C	-5.74	95.50	111.00
21	S	341	ARG	CA-CB-CG	5.74	126.03	113.40
24	R	253	LEU	N-CA-C	5.74	126.49	111.00
5	E	84	ASP	CA-CB-CG	-5.74	100.78	113.40
19	Z	267	ARG	NE-CZ-NH1	-5.74	117.43	120.30
28	I	103	ARG	NE-CZ-NH1	5.74	123.17	120.30
32	J	217	SER	N-CA-CB	5.74	119.10	110.50
1	A	200	THR	N-CA-CB	5.73	121.19	110.30
12	5	166	ARG	NE-CZ-NH1	5.73	123.17	120.30
13	6	131	TYR	CB-CG-CD2	-5.73	117.56	121.00
14	7	95	LEU	N-CA-C	-5.73	95.53	111.00
19	Z	356	ASN	CA-CB-CG	5.73	126.01	113.40
23	Q	270	LEU	CB-CG-CD1	5.73	120.74	111.00
20	N	59	PHE	CB-CG-CD2	5.73	124.81	120.80
28	I	295	TYR	CB-CG-CD2	-5.73	117.56	121.00
19	Z	393	ASP	CB-CG-OD1	5.73	123.45	118.30
27	H	273	PHE	CB-CG-CD1	-5.72	116.79	120.80
2	B	190	THR	CA-CB-CG2	-5.72	104.39	112.40
19	Z	711	SER	N-CA-CB	5.72	119.08	110.50
26	O	179	PHE	CB-CG-CD2	5.72	124.80	120.80
16	V	65	TYR	N-CA-CB	5.72	120.89	110.60
20	N	743	ASN	CB-CA-C	-5.72	98.97	110.40
29	K	256	GLU	CA-CB-CG	5.72	125.98	113.40
12	5	147	TYR	CG-CD2-CE2	-5.71	116.73	121.30
25	U	101	LEU	CA-CB-CG	5.71	128.44	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	I	365	PHE	CB-CG-CD2	-5.71	116.80	120.80
3	C	184	MET	CG-SD-CE	-5.71	91.06	100.20
5	E	42	THR	N-CA-CB	5.71	121.15	110.30
13	6	91	LEU	CB-CG-CD2	5.71	120.71	111.00
19	Z	79	ARG	NE-CZ-NH1	5.71	123.16	120.30
31	M	106	ASP	CB-CG-OD2	-5.71	113.16	118.30
31	M	159	ASP	CB-CG-OD1	5.71	123.44	118.30
7	G	159	TYR	CB-CG-CD1	5.71	124.43	121.00
20	N	85	GLY	O-C-N	5.71	131.83	122.70
3	C	55	LEU	CB-CA-C	5.71	121.04	110.20
2	B	12	THR	N-CA-C	-5.71	95.60	111.00
6	F	123	TYR	CZ-CE2-CD2	-5.70	114.67	119.80
25	U	186	THR	CA-CB-CG2	-5.70	104.42	112.40
15	W	139	ASP	CB-CG-OD2	-5.70	113.17	118.30
19	Z	156	HIS	CA-C-O	5.70	132.07	120.10
17	T	148	ARG	NH1-CZ-NH2	5.70	125.67	119.40
3	C	6	ASP	CB-CG-OD1	5.70	123.42	118.30
27	H	407	LYS	CB-CA-C	-5.69	99.02	110.40
24	R	83	ARG	NE-CZ-NH1	5.69	123.14	120.30
25	U	94	TRP	CD1-CG-CD2	-5.69	101.75	106.30
20	N	490	ARG	NE-CZ-NH2	5.69	123.14	120.30
16	V	118	PHE	CZ-CE2-CD2	-5.69	113.28	120.10
3	C	143	TYR	CB-CG-CD2	-5.68	117.59	121.00
32	J	280	LEU	CB-CG-CD2	5.68	120.66	111.00
3	C	97	TYR	CG-CD2-CE2	5.68	125.84	121.30
20	N	361	ARG	NE-CZ-NH2	5.68	123.14	120.30
29	K	98	GLN	CB-CA-C	-5.68	99.04	110.40
26	O	51	ALA	CB-CA-C	-5.67	101.59	110.10
26	O	120	ALA	CB-CA-C	-5.67	101.59	110.10
32	J	382	ASP	CB-CG-OD1	5.67	123.40	118.30
2	B	128	ARG	NH1-CZ-NH2	-5.67	113.16	119.40
19	Z	239	TYR	CB-CG-CD1	5.67	124.40	121.00
20	N	921	ILE	CA-CB-CG1	5.67	121.77	111.00
9	2	85	TYR	CB-CG-CD2	5.67	124.40	121.00
9	2	133	TYR	CB-CG-CD1	5.66	124.40	121.00
23	Q	403	THR	CA-CB-CG2	-5.66	104.47	112.40
29	K	53	PHE	CB-CG-CD1	5.66	124.76	120.80
31	M	139	VAL	CA-CB-CG2	-5.66	102.41	110.90
32	J	285	ALA	N-CA-CB	5.66	118.02	110.10
7	G	221	THR	CA-CB-CG2	-5.66	104.48	112.40
8	1	94	TYR	CA-CB-CG	5.66	124.15	113.40
31	M	52	ASP	CB-CG-OD2	-5.66	113.21	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	M	323	PHE	CB-CG-CD1	-5.66	116.84	120.80
22	P	137	TYR	CB-CG-CD1	-5.66	117.61	121.00
31	M	91	TYR	CB-CG-CD1	5.66	124.39	121.00
32	J	39	SER	N-CA-CB	5.66	118.98	110.50
19	Z	508	SER	CB-CA-C	5.65	120.84	110.10
23	Q	330	LEU	CB-CG-CD2	5.65	120.61	111.00
20	N	938	GLU	OE1-CD-OE2	5.65	130.08	123.30
23	Q	177	TYR	CD1-CE1-CZ	-5.65	114.71	119.80
29	K	245	ARG	NH1-CZ-NH2	-5.65	113.18	119.40
19	Z	55	GLU	N-CA-CB	5.65	120.77	110.60
30	L	98	ARG	NE-CZ-NH2	-5.65	117.48	120.30
32	J	223	PHE	CB-CG-CD1	5.65	124.75	120.80
6	F	13	TRP	CB-CG-CD1	5.65	134.34	127.00
14	7	202	PRO	N-CA-CB	5.65	110.08	103.30
24	R	177	ARG	NE-CZ-NH1	5.65	123.12	120.30
12	5	157	GLY	N-CA-C	-5.64	98.99	113.10
20	N	49	TYR	CB-CG-CD1	-5.64	117.61	121.00
3	C	186	LEU	CB-CG-CD1	5.64	120.59	111.00
12	5	124	ILE	CA-CB-CG1	5.64	121.72	111.00
1	A	185	LYS	C-N-CA	5.64	135.80	121.70
20	N	557	TYR	CD1-CE1-CZ	5.64	124.88	119.80
6	F	73	SER	N-CA-CB	5.64	118.96	110.50
20	N	474	ARG	CD-NE-CZ	-5.64	115.71	123.60
20	N	392	TRP	CA-CB-CG	5.64	124.41	113.70
23	Q	11	ARG	NE-CZ-NH1	5.64	123.12	120.30
30	L	292	ALA	N-CA-CB	5.64	117.99	110.10
15	W	156	PHE	CB-CG-CD2	5.63	124.74	120.80
20	N	611	ASN	CB-CG-OD1	-5.63	110.33	121.60
25	U	204	LYS	CB-CA-C	-5.63	99.13	110.40
20	N	179	TYR	CD1-CG-CD2	-5.63	111.70	117.90
23	Q	85	ALA	N-CA-CB	5.63	117.98	110.10
20	N	751	ARG	NE-CZ-NH1	5.63	123.11	120.30
10	3	147	TYR	CB-CG-CD1	-5.63	117.62	121.00
4	D	17	PHE	CB-CA-C	-5.62	99.15	110.40
23	Q	324	ALA	N-CA-CB	5.62	117.98	110.10
28	I	294	ARG	NE-CZ-NH1	5.62	123.11	120.30
32	J	307	ARG	NE-CZ-NH1	5.62	123.11	120.30
20	N	106	ASP	CB-CG-OD2	5.62	123.36	118.30
30	L	289	MET	CG-SD-CE	-5.62	91.20	100.20
16	V	183	HIS	CA-CB-CG	5.62	123.16	113.60
29	K	41	TYR	CD1-CE1-CZ	-5.62	114.74	119.80
13	6	191	VAL	N-CA-C	-5.62	95.83	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	L	368	ALA	N-CA-CB	5.62	117.97	110.10
32	J	148	TYR	CB-CA-C	-5.62	99.17	110.40
10	3	118	LYS	N-CA-C	-5.62	95.84	111.00
11	4	43	LEU	CB-CA-C	-5.61	99.53	110.20
19	Z	751	TYR	CG-CD1-CE1	-5.61	116.81	121.30
6	F	227	ASP	CB-CG-OD1	5.61	123.35	118.30
20	N	553	ALA	CB-CA-C	-5.61	101.68	110.10
7	G	92	ALA	CB-CA-C	-5.61	101.69	110.10
12	5	118	LEU	CA-CB-CG	5.61	128.20	115.30
2	B	41	ALA	N-CA-CB	5.61	117.95	110.10
7	G	191	VAL	CG1-CB-CG2	-5.61	101.93	110.90
10	3	157	ASN	N-CA-C	-5.61	95.86	111.00
18	Y	65	TYR	CG-CD2-CE2	-5.61	116.81	121.30
28	I	67	ARG	NE-CZ-NH1	5.61	123.10	120.30
10	3	155	GLU	CA-C-N	5.61	132.79	117.10
12	5	208	VAL	CG1-CB-CG2	5.61	119.87	110.90
14	7	77	LEU	N-CA-CB	5.61	121.61	110.40
19	Z	834	ASP	CB-CG-OD2	-5.61	113.26	118.30
22	P	80	TRP	CD1-CG-CD2	-5.60	101.82	106.30
20	N	144	ASP	CB-CG-OD2	-5.60	113.26	118.30
8	1	230	VAL	CA-CB-CG1	-5.60	102.50	110.90
16	V	219	ASN	CB-CG-OD1	-5.60	110.41	121.60
25	U	261	TYR	CB-CG-CD2	-5.60	117.64	121.00
30	L	127	ARG	CD-NE-CZ	5.60	131.44	123.60
8	1	136	TRP	CB-CG-CD1	-5.59	119.73	127.00
10	3	41	LYS	N-CA-CB	5.59	120.67	110.60
23	Q	138	PHE	CB-CG-CD2	-5.59	116.88	120.80
31	M	76	ILE	CA-CB-CG2	-5.59	99.71	110.90
4	D	79	VAL	CA-CB-CG2	-5.59	102.51	110.90
5	E	156	MET	N-CA-C	-5.59	95.90	111.00
7	G	31	VAL	CA-CB-CG1	-5.59	102.51	110.90
26	O	172	TYR	CB-CG-CD2	5.59	124.36	121.00
26	O	63	PHE	CB-CG-CD1	5.59	124.71	120.80
32	J	311	ILE	N-CA-C	-5.58	95.92	111.00
20	N	460	TYR	CB-CG-CD1	5.58	124.35	121.00
24	R	312	ARG	NE-CZ-NH1	5.58	123.09	120.30
9	2	175	LEU	N-CA-CB	-5.58	99.24	110.40
7	G	141	TYR	CG-CD1-CE1	-5.58	116.84	121.30
15	W	54	LEU	C-N-CA	5.58	135.65	121.70
2	B	82	ASP	CB-CG-OD2	-5.58	113.28	118.30
19	Z	63	LEU	CB-CA-C	-5.58	99.60	110.20
20	N	225	ASP	CB-CG-OD2	5.58	123.32	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	K	170	MET	N-CA-CB	5.58	120.64	110.60
21	S	345	ARG	CA-CB-CG	5.58	125.67	113.40
26	O	330	ARG	NE-CZ-NH2	5.58	123.09	120.30
26	O	172	TYR	CB-CG-CD1	-5.57	117.66	121.00
13	6	133	VAL	CA-CB-CG2	5.57	119.26	110.90
22	P	47	LEU	CB-CG-CD1	5.57	120.47	111.00
26	O	321	ARG	NE-CZ-NH2	-5.57	117.52	120.30
2	B	156	PHE	N-CA-CB	5.57	120.62	110.60
11	4	118	MET	CG-SD-CE	-5.57	91.30	100.20
21	S	124	ARG	NE-CZ-NH2	5.57	123.08	120.30
22	P	436	MET	CG-SD-CE	-5.57	91.29	100.20
24	R	53	TYR	CB-CG-CD1	5.57	124.34	121.00
19	Z	865	PHE	CB-CG-CD2	-5.56	116.91	120.80
24	R	62	ASP	CB-CG-OD2	5.56	123.30	118.30
21	S	472	PHE	CB-CG-CD1	5.56	124.69	120.80
2	B	145	TYR	CB-CG-CD1	5.56	124.33	121.00
24	R	286	TRP	CB-CG-CD1	-5.56	119.78	127.00
31	M	334	ALA	N-CA-CB	5.56	117.88	110.10
19	Z	393	ASP	CB-CG-OD2	-5.55	113.30	118.30
29	K	268	ASP	CB-CG-OD2	-5.55	113.30	118.30
31	M	408	MET	CG-SD-CE	-5.55	91.31	100.20
17	T	318	TYR	CB-CG-CD2	5.55	124.33	121.00
28	I	410	ARG	NE-CZ-NH2	-5.55	117.53	120.30
10	3	48	ARG	NE-CZ-NH1	5.55	123.08	120.30
19	Z	746	ARG	NE-CZ-NH1	5.55	123.08	120.30
7	G	141	TYR	N-CA-CB	5.55	120.59	110.60
19	Z	71	TYR	CG-CD1-CE1	-5.55	116.86	121.30
19	Z	24	ALA	CB-CA-C	-5.54	101.78	110.10
6	F	13	TRP	CG-CD2-CE3	-5.54	128.91	133.90
19	Z	543	MET	CG-SD-CE	-5.54	91.33	100.20
11	4	104	LEU	CB-CA-C	-5.54	99.67	110.20
15	W	112	PHE	CB-CG-CD1	-5.54	116.92	120.80
28	I	438	LEU	CB-CG-CD1	-5.54	101.58	111.00
14	7	64	VAL	C-N-CA	5.54	135.55	121.70
20	N	590	TYR	CB-CG-CD2	-5.54	117.68	121.00
11	4	42	ILE	CA-CB-CG1	5.54	121.52	111.00
17	T	178	TYR	CG-CD1-CE1	-5.54	116.87	121.30
19	Z	510	SER	N-CA-CB	5.54	118.81	110.50
27	H	118	PHE	CB-CG-CD1	-5.54	116.92	120.80
15	W	170	LEU	CB-CA-C	-5.53	99.69	110.20
25	U	85	VAL	CA-CB-CG2	5.53	119.20	110.90
30	L	58	GLU	CA-CB-CG	-5.53	101.23	113.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	183	LYS	N-CA-CB	5.53	120.56	110.60
16	V	155	VAL	CA-CB-CG2	-5.53	102.60	110.90
16	V	202	SER	N-CA-CB	5.53	118.80	110.50
19	Z	758	ASN	CB-CA-C	5.53	121.46	110.40
20	N	88	PHE	CB-CG-CD2	-5.53	116.93	120.80
21	S	193	THR	CA-CB-CG2	-5.53	104.66	112.40
11	4	37	LYS	N-CA-C	-5.53	96.08	111.00
21	S	207	TYR	CG-CD2-CE2	-5.53	116.88	121.30
20	N	246	TYR	CA-CB-CG	-5.53	102.90	113.40
20	N	492	ASP	CB-CG-OD2	5.53	123.27	118.30
20	N	724	VAL	CA-CB-CG1	-5.53	102.61	110.90
1	A	27	TYR	CB-CG-CD2	5.52	124.31	121.00
31	M	170	GLU	N-CA-CB	5.52	120.54	110.60
16	V	82	VAL	CA-C-O	5.52	131.69	120.10
30	L	92	ARG	NE-CZ-NH1	-5.52	117.54	120.30
2	B	230	LEU	CB-CA-C	-5.52	99.71	110.20
3	C	12	PHE	CB-CG-CD2	-5.52	116.94	120.80
17	T	296	PHE	CB-CG-CD2	-5.52	116.94	120.80
1	A	136	CYS	CB-CA-C	-5.52	99.37	110.40
24	R	110	TYR	CZ-CE2-CD2	5.52	124.77	119.80
10	3	96	TYR	CB-CG-CD2	-5.52	117.69	121.00
17	T	231	HIS	CA-CB-CG	5.52	122.98	113.60
27	H	217	PRO	N-CD-CG	5.51	111.47	103.20
31	M	180	VAL	CA-CB-CG1	-5.51	102.63	110.90
31	M	339	ASP	CB-CG-OD1	5.51	123.26	118.30
13	6	157	TYR	CD1-CE1-CZ	5.51	124.76	119.80
28	I	203	LEU	CB-CG-CD1	-5.51	101.63	111.00
28	I	260	LEU	C-N-CA	5.51	133.88	122.30
30	L	175	ARG	NE-CZ-NH2	-5.51	117.55	120.30
10	3	140	GLY	N-CA-C	-5.51	99.33	113.10
19	Z	874	LEU	CB-CG-CD1	5.51	120.36	111.00
10	3	131	MET	CG-SD-CE	-5.50	91.39	100.20
31	M	274	ALA	CB-CA-C	-5.50	101.85	110.10
10	3	104	TYR	CD1-CG-CD2	5.50	123.95	117.90
19	Z	183	PRO	N-CD-CG	5.50	111.45	103.20
2	B	8	PHE	CB-CG-CD2	5.50	124.65	120.80
21	S	68	LEU	CB-CG-CD1	5.50	120.34	111.00
22	P	30	GLU	CA-CB-CG	5.50	125.49	113.40
22	P	226	TYR	CB-CG-CD2	-5.50	117.70	121.00
23	Q	360	ASP	CB-CG-OD2	5.49	123.24	118.30
28	I	164	MET	CG-SD-CE	-5.49	91.41	100.20
28	I	120	HIS	N-CA-C	-5.49	96.17	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Z	469	TYR	CZ-CE2-CD2	5.49	124.74	119.80
29	K	226	ALA	CB-CA-C	5.49	118.33	110.10
19	Z	341	GLU	N-CA-CB	5.49	120.48	110.60
30	L	256	ARG	NE-CZ-NH1	-5.49	117.56	120.30
4	D	38	ARG	NE-CZ-NH1	-5.49	117.56	120.30
19	Z	61	GLU	N-CA-CB	5.49	120.47	110.60
21	S	116	PHE	CB-CG-CD1	-5.49	116.96	120.80
8	1	41	PHE	CB-CG-CD1	5.48	124.64	120.80
27	H	367	ASP	CB-CG-OD1	-5.48	113.36	118.30
7	G	166	ILE	N-CA-C	-5.48	96.19	111.00
21	S	464	SER	N-CA-CB	5.48	118.72	110.50
28	I	127	VAL	CG1-CB-CG2	5.48	119.67	110.90
3	C	82	ASP	CB-CG-OD1	-5.48	113.37	118.30
16	V	200	TYR	CG-CD1-CE1	-5.48	116.92	121.30
28	I	295	TYR	CE1-CZ-CE2	-5.48	111.03	119.80
11	4	148	THR	CA-C-O	-5.48	108.60	120.10
6	F	128	TYR	CB-CG-CD2	5.48	124.29	121.00
4	D	162	TRP	CG-CD2-CE3	-5.47	128.97	133.90
12	5	252	ALA	N-CA-CB	5.47	117.76	110.10
7	G	182	MET	CG-SD-CE	-5.47	91.45	100.20
15	W	157	VAL	CA-CB-CG2	-5.47	102.69	110.90
24	R	286	TRP	CB-CG-CD2	5.47	133.71	126.60
12	5	220	TYR	CG-CD1-CE1	-5.47	116.93	121.30
20	N	557	TYR	CB-CG-CD2	5.47	124.28	121.00
21	S	119	SER	N-CA-CB	5.47	118.70	110.50
2	B	11	THR	N-CA-CB	5.46	120.68	110.30
9	2	154	TYR	CA-CB-CG	-5.46	103.02	113.40
20	N	194	ARG	NE-CZ-NH1	5.46	123.03	120.30
1	A	14	THR	C-N-CA	5.46	135.35	121.70
14	7	226	ARG	NE-CZ-NH1	-5.46	117.57	120.30
22	P	88	MET	CA-CB-CG	5.46	122.58	113.30
4	D	177	PHE	CB-CG-CD1	-5.46	116.98	120.80
12	5	114	TRP	CD1-NE1-CE2	5.46	113.91	109.00
20	N	719	ASP	CB-CG-OD2	5.46	123.21	118.30
10	3	99	ARG	NE-CZ-NH1	-5.45	117.57	120.30
32	J	378	VAL	CA-CB-CG1	-5.45	102.72	110.90
12	5	187	VAL	C-N-CA	5.45	133.75	122.30
23	Q	138	PHE	CB-CG-CD1	5.45	124.62	120.80
23	Q	397	TYR	CB-CG-CD1	5.45	124.27	121.00
7	G	239	TYR	CD1-CG-CD2	5.45	123.90	117.90
13	6	61	SER	CB-CA-C	5.45	120.45	110.10
23	Q	191	THR	CA-CB-CG2	-5.45	104.77	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	K	127	ASN	CB-CG-OD1	-5.45	110.70	121.60
5	E	18	GLU	N-CA-CB	-5.45	100.79	110.60
12	5	61	THR	C-N-CA	5.45	135.32	121.70
25	U	261	TYR	CD1-CG-CD2	5.45	123.89	117.90
30	L	265	ARG	CD-NE-CZ	5.45	131.23	123.60
15	W	159	THR	CA-CB-OG1	5.45	120.44	109.00
21	S	308	ALA	CB-CA-C	-5.45	101.93	110.10
6	F	171	TYR	CZ-CE2-CD2	5.45	124.70	119.80
11	4	123	ALA	C-N-CA	5.45	135.32	121.70
23	Q	233	TYR	CB-CG-CD1	5.45	124.27	121.00
14	7	206	GLN	CB-CA-C	5.44	121.29	110.40
19	Z	158	TYR	CG-CD1-CE1	5.44	125.66	121.30
19	Z	807	ARG	NE-CZ-NH2	5.44	123.02	120.30
10	3	193	ASP	CB-CG-OD1	-5.44	113.40	118.30
25	U	283	ARG	NE-CZ-NH2	-5.44	117.58	120.30
29	K	339	ARG	NH1-CZ-NH2	5.44	125.39	119.40
2	B	99	LEU	CB-CA-C	-5.44	99.86	110.20
2	B	199	PHE	CD1-CE1-CZ	5.44	126.63	120.10
7	G	214	LEU	N-CA-C	-5.44	96.31	111.00
29	K	410	ASP	CB-CG-OD2	-5.44	113.40	118.30
30	L	15	MET	CG-SD-CE	-5.44	91.50	100.20
4	D	124	TYR	CB-CG-CD1	5.44	124.26	121.00
7	G	111	HIS	CA-CB-CG	5.44	122.85	113.60
1	A	125	TYR	CG-CD2-CE2	-5.44	116.95	121.30
2	B	44	VAL	CA-CB-CG1	-5.44	102.74	110.90
30	L	272	MET	CG-SD-CE	-5.43	91.50	100.20
19	Z	103	TYR	CB-CG-CD1	5.43	124.26	121.00
22	P	274	VAL	CG1-CB-CG2	-5.43	102.21	110.90
14	7	215	ARG	NE-CZ-NH1	-5.43	117.59	120.30
19	Z	551	LYS	N-CA-CB	5.43	120.37	110.60
29	K	309	MET	CG-SD-CE	-5.43	91.52	100.20
23	Q	239	TYR	CB-CG-CD2	5.42	124.25	121.00
1	A	152	TYR	CD1-CE1-CZ	5.42	124.68	119.80
4	D	243	GLU	OE1-CD-OE2	5.42	129.80	123.30
29	K	249	ASP	CB-CG-OD1	5.42	123.18	118.30
15	W	24	THR	N-CA-C	-5.42	96.37	111.00
4	D	158	THR	N-CA-C	-5.42	96.38	111.00
20	N	388	ASP	CB-CG-OD2	-5.41	113.43	118.30
26	O	255	TRP	CE2-CD2-CG	-5.41	102.97	107.30
16	V	142	ALA	CB-CA-C	-5.41	101.98	110.10
22	P	201	ARG	NE-CZ-NH1	-5.41	117.59	120.30
6	F	120	THR	CA-CB-CG2	5.41	119.97	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	3	177	ARG	CG-CD-NE	-5.41	100.44	111.80
17	T	104	GLU	N-CA-CB	5.41	120.34	110.60
19	Z	744	MET	CG-SD-CE	-5.41	91.54	100.20
16	V	115	HIS	N-CA-CB	5.41	120.34	110.60
20	N	138	PHE	CG-CD1-CE1	-5.41	114.85	120.80
28	I	324	ASP	CB-CG-OD1	5.41	123.17	118.30
6	F	120	THR	O-C-N	5.41	131.35	122.70
12	5	113	PHE	CB-CG-CD2	-5.41	117.02	120.80
12	5	183	THR	N-CA-CB	5.41	120.57	110.30
16	V	32	TYR	CA-CB-CG	-5.41	103.13	113.40
5	E	108	THR	CA-CB-CG2	-5.40	104.83	112.40
21	S	237	ARG	NE-CZ-NH1	-5.40	117.60	120.30
22	P	400	LYS	N-CA-CB	5.40	120.32	110.60
20	N	202	VAL	CA-CB-CG2	-5.40	102.80	110.90
20	N	678	ASP	CB-CG-OD2	-5.40	113.44	118.30
21	S	432	PHE	CD1-CE1-CZ	-5.40	113.62	120.10
31	M	441	TYR	CB-CG-CD1	-5.40	117.76	121.00
2	B	26	LEU	N-CA-CB	5.40	121.20	110.40
14	7	80	PHE	CB-CG-CD2	-5.40	117.02	120.80
21	S	354	MET	N-CA-CB	5.40	120.31	110.60
22	P	186	ILE	CG1-CB-CG2	5.39	123.27	111.40
17	T	188	SER	N-CA-C	-5.39	96.44	111.00
29	K	120	ASP	C-N-CA	5.39	135.18	121.70
32	J	189	TYR	CB-CG-CD2	-5.39	117.76	121.00
12	5	67	PHE	CB-CG-CD1	-5.39	117.03	120.80
24	R	118	GLU	C-N-CA	5.39	133.62	122.30
1	A	190	THR	O-C-N	-5.39	114.08	122.70
5	E	163	VAL	CB-CA-C	5.39	121.64	111.40
17	T	181	TYR	CG-CD2-CE2	5.39	125.61	121.30
20	N	205	TYR	CG-CD1-CE1	-5.39	116.99	121.30
20	N	533	VAL	CA-CB-CG2	-5.39	102.82	110.90
21	S	387	THR	OG1-CB-CG2	-5.39	97.61	110.00
32	J	404	LEU	CB-CG-CD2	-5.39	101.84	111.00
29	K	409	LYS	N-CA-CB	5.38	120.29	110.60
1	A	221	THR	CA-CB-CG2	-5.38	104.87	112.40
2	B	194	THR	CA-CB-OG1	5.38	120.30	109.00
3	C	103	GLU	OE1-CD-OE2	5.38	129.76	123.30
4	D	173	SER	O-C-N	-5.38	114.09	122.70
12	5	239	ARG	NE-CZ-NH1	-5.38	117.61	120.30
23	Q	253	TYR	CB-CG-CD2	-5.38	117.77	121.00
28	I	71	TYR	CB-CG-CD1	-5.38	117.77	121.00
28	I	101	ASP	CB-CG-OD2	5.38	123.14	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	K	263	PHE	CB-CG-CD2	5.38	124.57	120.80
17	T	117	GLU	N-CA-CB	5.38	120.28	110.60
20	N	362	ASN	CB-CA-C	-5.38	99.64	110.40
29	K	41	TYR	CB-CG-CD1	-5.38	117.77	121.00
30	L	60	ASP	CB-CG-OD1	-5.38	113.46	118.30
31	M	309	VAL	CA-CB-CG1	-5.38	102.83	110.90
1	A	187	PHE	CB-CG-CD1	-5.38	117.04	120.80
20	N	788	ILE	CA-CB-CG1	5.38	121.21	111.00
16	V	112	TYR	CG-CD2-CE2	-5.37	117.00	121.30
17	T	244	TYR	CG-CD1-CE1	-5.37	117.00	121.30
28	I	370	SER	N-CA-CB	5.37	118.56	110.50
7	G	216	TRP	CB-CG-CD1	5.37	133.98	127.00
12	5	220	TYR	CZ-CE2-CD2	-5.37	114.97	119.80
21	S	224	ARG	NE-CZ-NH1	5.37	122.98	120.30
25	U	175	LEU	CB-CG-CD1	-5.37	101.88	111.00
12	5	250	ASN	N-CA-C	-5.36	96.52	111.00
13	6	30	SER	N-CA-C	-5.36	96.52	111.00
18	Y	57	ARG	NE-CZ-NH1	-5.36	117.62	120.30
19	Z	99	LEU	CB-CG-CD1	5.36	120.12	111.00
20	N	836	THR	CA-CB-CG2	-5.36	104.89	112.40
31	M	357	PHE	CB-CG-CD1	5.36	124.55	120.80
31	M	124	CYS	N-CA-CB	5.36	120.24	110.60
20	N	684	ARG	NE-CZ-NH1	-5.35	117.62	120.30
19	Z	879	ARG	N-CA-C	-5.35	96.55	111.00
20	N	69	TYR	CB-CG-CD2	-5.35	117.79	121.00
20	N	699	THR	N-CA-CB	5.35	120.47	110.30
21	S	263	ALA	CB-CA-C	-5.35	102.07	110.10
18	Y	67	MET	CA-CB-CG	5.35	122.40	113.30
20	N	559	ARG	NE-CZ-NH2	-5.35	117.62	120.30
19	Z	400	TYR	CB-CG-CD2	-5.35	117.79	121.00
22	P	389	SER	N-CA-CB	5.35	118.52	110.50
27	H	319	MET	CB-CA-C	-5.35	99.71	110.40
29	K	339	ARG	NE-CZ-NH1	-5.35	117.63	120.30
25	U	226	ILE	CA-CB-CG2	-5.35	100.21	110.90
8	1	67	LEU	N-CA-CB	5.34	121.09	110.40
28	I	317	ASP	CB-CG-OD2	5.34	123.11	118.30
12	5	62	THR	CA-CB-CG2	5.34	119.88	112.40
19	Z	849	ALA	N-CA-CB	5.34	117.58	110.10
1	A	107	TYR	CZ-CE2-CD2	-5.34	114.99	119.80
16	V	201	TYR	O-C-N	5.34	131.24	122.70
12	5	141	LEU	CB-CG-CD1	5.34	120.07	111.00
15	W	145	GLU	N-CA-CB	5.34	120.21	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Z	257	ARG	NE-CZ-NH1	5.34	122.97	120.30
6	F	126	ARG	NE-CZ-NH1	-5.34	117.63	120.30
17	T	273	GLU	CB-CG-CD	-5.34	99.79	114.20
20	N	36	ALA	CB-CA-C	-5.34	102.09	110.10
22	P	55	ARG	NE-CZ-NH2	5.34	122.97	120.30
14	7	181	LEU	CB-CA-C	-5.33	100.06	110.20
17	T	345	TYR	CD1-CE1-CZ	-5.33	115.00	119.80
22	P	127	THR	C-N-CA	5.33	135.03	121.70
22	P	251	TYR	CG-CD2-CE2	-5.33	117.03	121.30
22	P	279	PHE	CB-CG-CD1	-5.33	117.07	120.80
32	J	153	GLY	N-CA-C	-5.33	99.78	113.10
5	E	130	PRO	N-CD-CG	5.33	111.19	103.20
13	6	85	HIS	N-CA-CB	5.33	120.19	110.60
10	3	174	ALA	CB-CA-C	-5.33	102.11	110.10
23	Q	374	PHE	N-CA-CB	5.33	120.19	110.60
10	3	189	ILE	N-CA-C	-5.33	96.62	111.00
19	Z	794	ALA	CB-CA-C	-5.33	102.11	110.10
14	7	171	MET	CG-SD-CE	-5.32	91.68	100.20
22	P	104	MET	CG-SD-CE	-5.32	91.68	100.20
24	R	261	PHE	CB-CG-CD1	-5.32	117.07	120.80
32	J	369	TYR	CB-CG-CD1	-5.32	117.81	121.00
1	A	51	VAL	N-CA-C	-5.32	96.64	111.00
4	D	175	ARG	NE-CZ-NH1	5.32	122.96	120.30
16	V	140	ALA	N-CA-CB	5.32	117.55	110.10
2	B	146	LEU	N-CA-C	-5.32	96.65	111.00
3	C	116	ASP	CB-CA-C	-5.32	99.77	110.40
11	4	25	ILE	N-CA-C	-5.31	96.65	111.00
30	L	152	LEU	C-N-CA	5.31	134.99	121.70
3	C	120	ALA	O-C-N	5.31	131.20	122.70
6	F	225	ASP	CB-CG-OD1	-5.31	113.52	118.30
16	V	310	LYS	CB-CG-CD	5.31	125.42	111.60
20	N	690	ALA	CB-CA-C	-5.31	102.13	110.10
29	K	406	VAL	CA-CB-CG1	5.31	118.87	110.90
21	S	320	PHE	CZ-CE2-CD2	-5.31	113.73	120.10
29	K	88	VAL	CG1-CB-CG2	-5.31	102.40	110.90
2	B	58	ASP	CB-CG-OD1	5.31	123.08	118.30
5	E	140	ALA	N-CA-CB	5.31	117.53	110.10
9	2	148	VAL	CA-CB-CG1	5.31	118.86	110.90
13	6	205	VAL	CA-CB-CG2	5.31	118.86	110.90
27	H	105	ASP	CB-CG-OD1	5.31	123.08	118.30
28	I	144	LEU	N-CA-C	-5.31	96.66	111.00
20	N	586	VAL	CA-CB-CG2	5.31	118.86	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	U	164	ALA	CB-CA-C	-5.31	102.14	110.10
4	D	226	LEU	CB-CG-CD2	5.30	120.02	111.00
30	L	186	LEU	N-CA-CB	5.30	121.01	110.40
10	3	178	ASP	CB-CG-OD2	-5.30	113.53	118.30
19	Z	456	ARG	NE-CZ-NH1	-5.30	117.65	120.30
20	N	216	VAL	CG1-CB-CG2	5.30	119.38	110.90
19	Z	687	ARG	NE-CZ-NH1	5.30	122.95	120.30
26	O	134	THR	CA-CB-CG2	-5.30	104.98	112.40
14	7	141	TYR	CG-CD1-CE1	5.29	125.54	121.30
19	Z	226	TYR	CB-CG-CD2	5.29	124.18	121.00
22	P	40	LEU	CB-CG-CD2	5.29	120.00	111.00
25	U	209	ARG	O-C-N	5.29	131.17	122.70
29	K	178	ARG	NE-CZ-NH2	-5.29	117.65	120.30
25	U	122	VAL	N-CA-C	-5.29	96.71	111.00
16	V	255	TYR	CA-CB-CG	5.29	123.45	113.40
28	I	381	ASP	CB-CG-OD1	-5.29	113.54	118.30
15	W	150	THR	CA-CB-CG2	-5.29	105.00	112.40
12	5	220	TYR	CB-CG-CD1	-5.28	117.83	121.00
1	A	102	LYS	N-CA-CB	5.28	120.11	110.60
6	F	26	MET	N-CA-CB	5.28	120.11	110.60
10	3	166	THR	CA-CB-CG2	-5.28	105.00	112.40
14	7	135	TRP	CB-CG-CD2	-5.28	119.74	126.60
24	R	364	TRP	CD2-CE3-CZ3	5.28	125.67	118.80
21	S	281	TRP	CA-CB-CG	5.28	123.73	113.70
24	R	93	LYS	CA-CB-CG	5.28	125.01	113.40
24	R	276	ALA	CB-CA-C	-5.28	102.19	110.10
7	G	66	ARG	NE-CZ-NH2	-5.28	117.66	120.30
15	W	139	ASP	N-CA-C	-5.28	96.76	111.00
19	Z	875	ALA	CB-CA-C	-5.28	102.19	110.10
23	Q	261	LEU	C-N-CA	5.28	134.89	121.70
31	M	323	PHE	CB-CG-CD2	5.28	124.49	120.80
4	D	170	GLY	N-CA-C	-5.27	99.92	113.10
29	K	161	ASP	CB-CG-OD1	5.27	123.05	118.30
3	C	136	TYR	CB-CG-CD1	5.27	124.16	121.00
23	Q	167	VAL	CG1-CB-CG2	5.27	119.33	110.90
27	H	227	ARG	CD-NE-CZ	-5.27	116.22	123.60
21	S	454	VAL	O-C-N	-5.27	114.27	122.70
13	6	231	ARG	N-CA-CB	5.27	120.08	110.60
9	2	211	GLY	O-C-N	5.26	131.12	122.70
11	4	129	PHE	CB-CG-CD1	5.26	124.48	120.80
20	N	616	ARG	CD-NE-CZ	-5.26	116.23	123.60
22	P	268	LYS	CB-CA-C	-5.26	99.87	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	U	54	PHE	CZ-CE2-CD2	-5.26	113.78	120.10
21	S	340	ASP	N-CA-CB	5.26	120.07	110.60
31	M	115	ASP	CB-CG-OD1	5.26	123.04	118.30
2	B	143	ARG	NE-CZ-NH2	5.26	122.93	120.30
6	F	89	ARG	NE-CZ-NH1	5.26	122.93	120.30
13	6	88	CYS	C-N-CA	5.26	134.86	121.70
28	I	347	ILE	CA-CB-CG1	-5.26	101.00	111.00
32	J	299	ASP	CB-CG-OD1	-5.26	113.56	118.30
5	E	95	GLU	OE1-CD-OE2	5.26	129.61	123.30
5	E	55	THR	CA-CB-CG2	-5.26	105.04	112.40
2	B	76	TYR	CA-CB-CG	5.25	123.38	113.40
16	V	297	VAL	CA-CB-CG2	-5.25	103.02	110.90
17	T	294	LEU	N-CA-CB	5.25	120.90	110.40
20	N	105	ILE	CA-CB-CG1	5.25	120.97	111.00
5	E	10	ARG	CD-NE-CZ	-5.25	116.25	123.60
8	1	222	LEU	CB-CG-CD1	-5.25	102.08	111.00
22	P	285	ASP	CB-CG-OD1	-5.25	113.58	118.30
30	L	93	TYR	CB-CG-CD1	5.25	124.15	121.00
24	R	366	TYR	CB-CG-CD2	-5.25	117.85	121.00
13	6	196	ASP	CB-CA-C	-5.24	99.91	110.40
14	7	194	LEU	CB-CG-CD1	5.24	119.91	111.00
23	Q	39	ASP	CA-CB-CG	-5.24	101.86	113.40
24	R	177	ARG	NH1-CZ-NH2	-5.24	113.63	119.40
29	K	308	ILE	N-CA-C	-5.24	96.84	111.00
24	R	8	GLU	N-CA-CB	5.24	120.03	110.60
1	A	139	ILE	CA-CB-CG2	-5.24	100.42	110.90
20	N	161	ASP	CB-CG-OD2	-5.24	113.58	118.30
20	N	709	PHE	CD1-CE1-CZ	-5.24	113.82	120.10
4	D	112	TYR	CD1-CE1-CZ	5.24	124.51	119.80
20	N	650	TYR	CD1-CE1-CZ	5.24	124.51	119.80
21	S	147	THR	CA-CB-CG2	-5.24	105.07	112.40
31	M	96	VAL	CA-CB-CG2	-5.24	103.05	110.90
19	Z	385	PHE	CB-CG-CD1	5.23	124.46	120.80
10	3	145	GLN	C-N-CA	5.23	134.78	121.70
21	S	341	ARG	N-CA-CB	5.23	120.02	110.60
32	J	370	ALA	N-CA-CB	-5.23	102.78	110.10
7	G	44	ASP	CB-CG-OD1	-5.23	113.59	118.30
11	4	59	TYR	CB-CG-CD2	5.23	124.14	121.00
22	P	244	CYS	CA-CB-SG	-5.23	104.58	114.00
8	1	98	PHE	CG-CD1-CE1	-5.23	115.05	120.80
20	N	754	HIS	C-N-CA	5.23	134.77	121.70
5	E	83	ALA	CB-CA-C	-5.23	102.26	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	24	TYR	CG-CD2-CE2	-5.23	117.12	121.30
19	Z	489	TYR	CD1-CE1-CZ	5.23	124.50	119.80
6	F	171	TYR	CG-CD1-CE1	-5.23	117.12	121.30
31	M	58	MET	O-C-N	-5.23	114.34	122.70
19	Z	418	LEU	CB-CG-CD2	5.22	119.88	111.00
27	H	280	ILE	CA-CB-CG1	5.22	120.92	111.00
29	K	262	ILE	N-CA-C	-5.22	96.90	111.00
9	2	99	THR	O-C-N	-5.22	114.35	122.70
17	T	183	GLU	N-CA-C	-5.22	96.91	111.00
28	I	185	ALA	N-CA-CB	5.22	117.41	110.10
30	L	162	VAL	CA-CB-CG2	-5.22	103.07	110.90
20	N	919	GLU	CB-CA-C	-5.22	99.96	110.40
21	S	286	TYR	CD1-CE1-CZ	5.22	124.50	119.80
26	O	43	ASP	CB-CG-OD2	5.22	123.00	118.30
26	O	95	THR	CA-CB-CG2	-5.22	105.10	112.40
26	O	331	VAL	CB-CA-C	5.22	121.31	111.40
4	D	219	ARG	NE-CZ-NH2	-5.21	117.69	120.30
7	G	22	PHE	CZ-CE2-CD2	-5.21	113.84	120.10
30	L	291	MET	CG-SD-CE	-5.21	91.86	100.20
12	5	132	ARG	N-CA-CB	5.21	119.98	110.60
21	S	458	GLU	O-C-N	5.21	131.04	122.70
26	O	196	ARG	NE-CZ-NH1	-5.21	117.69	120.30
30	L	390	ASP	CB-CG-OD2	5.21	122.99	118.30
6	F	227	ASP	CB-CG-OD2	-5.21	113.61	118.30
10	3	136	PHE	CG-CD2-CE2	-5.21	115.07	120.80
19	Z	769	THR	N-CA-CB	5.21	120.20	110.30
27	H	311	PRO	N-CA-CB	5.21	109.55	103.30
32	J	49	ARG	NE-CZ-NH2	5.21	122.91	120.30
22	P	353	ASP	CB-CG-OD2	5.21	122.99	118.30
9	2	217	ASP	CB-CG-OD1	-5.21	113.61	118.30
20	N	147	TYR	CB-CG-CD2	-5.21	117.88	121.00
24	R	68	ASP	N-CA-CB	5.21	119.97	110.60
4	D	112	TYR	CG-CD2-CE2	-5.20	117.14	121.30
9	2	172	SER	N-CA-CB	5.20	118.31	110.50
11	4	148	THR	CA-C-N	5.20	131.67	117.10
11	4	180	VAL	O-C-N	-5.20	114.38	122.70
28	I	365	PHE	CB-CG-CD1	5.20	124.44	120.80
22	P	312	MET	O-C-N	5.20	131.02	122.70
1	A	178	PHE	CG-CD2-CE2	-5.20	115.08	120.80
11	4	83	PHE	CB-CG-CD1	5.20	124.44	120.80
17	T	311	TRP	CA-CB-CG	5.20	123.58	113.70
14	7	80	PHE	CD1-CG-CD2	5.20	125.06	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
20	N	229	VAL	CA-CB-CG1	5.20	118.69	110.90
21	S	102	ARG	NE-CZ-NH1	5.20	122.90	120.30
22	P	274	VAL	CA-CB-CG2	-5.20	103.11	110.90
24	R	264	TYR	CG-CD2-CE2	-5.20	117.14	121.30
10	3	47	ASP	CA-CB-CG	-5.19	101.98	113.40
15	W	38	HIS	CB-CA-C	-5.19	100.02	110.40
26	O	47	ASP	CA-C-O	-5.19	109.19	120.10
7	G	12	ALA	N-CA-CB	5.19	117.37	110.10
23	Q	415	TYR	CB-CG-CD2	-5.19	117.89	121.00
11	4	86	ARG	NE-CZ-NH2	-5.19	117.71	120.30
25	U	216	ALA	N-CA-CB	5.19	117.36	110.10
6	F	193	ARG	NH1-CZ-NH2	5.18	125.10	119.40
16	V	63	ASP	CB-CG-OD2	5.18	122.97	118.30
10	3	10	ALA	N-CA-CB	5.18	117.36	110.10
16	V	90	VAL	CB-CA-C	-5.18	101.55	111.40
22	P	12	ARG	O-C-N	5.18	130.99	122.70
28	I	184	TYR	C-N-CA	5.18	134.65	121.70
32	J	232	ARG	NE-CZ-NH2	-5.18	117.71	120.30
15	W	138	VAL	N-CA-C	-5.18	97.03	111.00
22	P	158	ASP	CB-CG-OD1	5.18	122.96	118.30
31	M	52	ASP	CB-CG-OD1	5.18	122.96	118.30
3	C	3	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
14	7	141	TYR	CZ-CE2-CD2	5.17	124.46	119.80
8	1	38	ALA	N-CA-C	-5.17	97.03	111.00
19	Z	271	MET	CG-SD-CE	-5.17	91.92	100.20
26	O	56	LEU	CB-CG-CD1	5.17	119.79	111.00
10	3	96	TYR	CB-CG-CD1	5.17	124.10	121.00
13	6	230	ILE	CA-CB-CG1	5.17	120.82	111.00
16	V	121	TRP	CE2-CD2-CG	5.17	111.44	107.30
20	N	883	ARG	NH1-CZ-NH2	-5.17	113.71	119.40
31	M	30	ASP	CB-CA-C	-5.17	100.06	110.40
9	2	174	SER	O-C-N	-5.17	114.43	122.70
31	M	312	THR	O-C-N	-5.17	114.43	122.70
32	J	41	ASN	CB-CA-C	-5.17	100.07	110.40
13	6	224	ILE	N-CA-C	-5.17	97.06	111.00
8	1	94	TYR	N-CA-CB	5.16	119.90	110.60
12	5	236	TYR	CB-CG-CD1	5.16	124.10	121.00
21	S	485	MET	CG-SD-CE	5.16	108.46	100.20
3	C	120	ALA	CB-CA-C	5.16	117.84	110.10
14	7	71	LEU	CB-CG-CD2	-5.16	102.22	111.00
20	N	738	ASP	CB-CG-OD1	5.16	122.95	118.30
9	2	91	THR	N-CA-CB	5.16	120.10	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
19	Z	680	ARG	NE-CZ-NH2	5.16	122.88	120.30
27	H	338	ASP	CB-CA-C	-5.16	100.08	110.40
31	M	161	TYR	O-C-N	5.16	130.96	122.70
19	Z	803	PHE	CB-CG-CD2	-5.16	117.19	120.80
19	Z	819	TYR	CB-CG-CD2	-5.16	117.91	121.00
19	Z	843	SER	CB-CA-C	-5.16	100.30	110.10
24	R	192	ARG	CB-CG-CD	5.16	125.01	111.60
29	K	283	ARG	NE-CZ-NH1	-5.16	117.72	120.30
30	L	400	TYR	CG-CD1-CE1	5.16	125.43	121.30
21	S	320	PHE	CB-CG-CD2	-5.16	117.19	120.80
1	A	96	TYR	CB-CG-CD1	-5.16	117.91	121.00
16	V	275	VAL	CA-CB-CG1	5.16	118.63	110.90
21	S	295	GLN	O-C-N	5.16	130.95	122.70
31	M	183	ARG	NE-CZ-NH1	5.16	122.88	120.30
19	Z	392	THR	O-C-N	5.15	130.95	122.70
29	K	355	SER	N-CA-CB	5.15	118.23	110.50
2	B	181	ASP	CB-CG-OD2	-5.15	113.66	118.30
8	1	227	ILE	CA-C-O	-5.15	109.28	120.10
26	O	176	ALA	CB-CA-C	5.15	117.83	110.10
30	L	160	ARG	NE-CZ-NH2	-5.15	117.72	120.30
27	H	70	THR	N-CA-C	-5.15	97.09	111.00
29	K	275	PHE	CD1-CE1-CZ	5.15	126.28	120.10
14	7	107	LEU	CB-CG-CD2	-5.15	102.25	111.00
16	V	208	ARG	NE-CZ-NH1	5.15	122.88	120.30
23	Q	93	LEU	CB-CG-CD1	5.15	119.75	111.00
25	U	272	LEU	CB-CG-CD2	5.15	119.75	111.00
10	3	71	LEU	CB-CG-CD1	5.15	119.75	111.00
26	O	284	ARG	NE-CZ-NH2	5.15	122.87	120.30
14	7	74	TYR	CD1-CE1-CZ	-5.14	115.17	119.80
19	Z	224	ASN	CB-CA-C	-5.14	100.11	110.40
32	J	6	PRO	N-CA-CB	5.14	109.47	103.30
17	T	105	TRP	CE2-CD2-CG	5.14	111.41	107.30
28	I	88	LEU	C-N-CA	5.14	134.55	121.70
21	S	222	VAL	CG1-CB-CG2	5.14	119.12	110.90
24	R	254	PRO	N-CA-C	5.14	125.45	112.10
21	S	348	SER	N-CA-CB	-5.13	102.80	110.50
27	H	86	THR	CA-CB-CG2	-5.13	105.21	112.40
30	L	18	PRO	N-CA-CB	5.13	109.46	103.30
6	F	62	LYS	O-C-N	-5.13	114.49	122.70
21	S	388	TYR	CB-CG-CD1	5.13	124.08	121.00
22	P	364	ARG	CG-CD-NE	-5.13	101.03	111.80
4	D	70	CYS	N-CA-CB	5.13	119.83	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	2	241	ARG	CD-NE-CZ	-5.13	116.42	123.60
22	P	353	ASP	CB-CG-OD1	-5.13	113.69	118.30
14	7	195	ARG	CB-CG-CD	5.12	124.92	111.60
4	D	51	ALA	N-CA-CB	5.12	117.27	110.10
20	N	769	PHE	CB-CG-CD1	-5.12	117.22	120.80
22	P	247	TYR	CD1-CG-CD2	5.12	123.53	117.90
28	I	411	ARG	NE-CZ-NH2	-5.12	117.74	120.30
23	Q	75	PRO	N-CD-CG	5.12	110.88	103.20
6	F	11	THR	CA-CB-CG2	-5.12	105.23	112.40
26	O	211	PHE	CZ-CE2-CD2	5.12	126.24	120.10
21	S	353	LEU	CB-CG-CD2	5.12	119.70	111.00
25	U	45	LYS	N-CA-CB	5.12	119.81	110.60
14	7	88	ARG	NE-CZ-NH1	5.11	122.86	120.30
16	V	167	MET	CG-SD-CE	-5.11	92.02	100.20
27	H	136	GLU	CB-CA-C	-5.11	100.18	110.40
32	J	236	VAL	CA-CB-CG1	5.11	118.57	110.90
22	P	341	PHE	N-CA-CB	5.11	119.80	110.60
3	C	148	TYR	N-CA-CB	5.11	119.79	110.60
14	7	235	THR	CA-CB-CG2	-5.11	105.25	112.40
20	N	829	SER	N-CA-CB	5.11	118.16	110.50
21	S	313	PRO	C-N-CA	5.11	134.47	121.70
23	Q	328	ASP	CB-CG-OD2	-5.11	113.70	118.30
24	R	329	PHE	CB-CG-CD1	5.11	124.37	120.80
14	7	242	GLU	N-CA-CB	5.10	119.79	110.60
30	L	338	GLY	O-C-N	5.10	130.87	122.70
10	3	120	PHE	CB-CG-CD1	-5.10	117.23	120.80
19	Z	175	ASP	CB-CG-OD2	-5.10	113.71	118.30
31	M	184	PRO	N-CA-C	-5.10	98.83	112.10
13	6	51	ALA	N-CA-C	-5.10	97.23	111.00
16	V	98	MET	CA-CB-CG	5.10	121.97	113.30
4	D	87	ARG	CD-NE-CZ	-5.10	116.46	123.60
14	7	104	PHE	CB-CG-CD2	-5.10	117.23	120.80
19	Z	717	ALA	N-CA-CB	5.10	117.24	110.10
21	S	113	VAL	CB-CA-C	5.10	121.09	111.40
21	S	287	TYR	CB-CG-CD2	-5.10	117.94	121.00
26	O	141	MET	N-CA-CB	5.10	119.78	110.60
28	I	182	GLU	CA-CB-CG	5.10	124.62	113.40
31	M	63	LEU	N-CA-CB	5.10	120.60	110.40
31	M	188	TYR	CG-CD2-CE2	-5.10	117.22	121.30
20	N	325	MET	CG-SD-CE	-5.10	92.04	100.20
22	P	146	THR	CA-CB-CG2	-5.10	105.26	112.40
25	U	94	TRP	CG-CD2-CE3	-5.10	129.31	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	U	144	VAL	CA-CB-CG2	5.10	118.55	110.90
30	L	400	TYR	CA-C-O	5.10	130.81	120.10
24	R	85	ASP	CB-CA-C	-5.10	100.21	110.40
30	L	143	ASN	N-CA-CB	5.10	119.77	110.60
7	G	141	TYR	CD1-CE1-CZ	5.09	124.39	119.80
9	2	197	LEU	CB-CG-CD2	-5.09	102.34	111.00
18	Y	57	ARG	NE-CZ-NH2	5.09	122.85	120.30
5	E	100	TRP	CB-CG-CD2	-5.09	119.98	126.60
14	7	223	ARG	NE-CZ-NH2	5.09	122.85	120.30
20	N	833	LEU	CB-CG-CD1	5.09	119.66	111.00
22	P	92	LYS	CB-CA-C	-5.09	100.22	110.40
27	H	296	GLN	CB-CA-C	-5.09	100.22	110.40
12	5	121	GLN	CA-CB-CG	5.09	124.60	113.40
15	W	92	VAL	CA-CB-CG2	-5.09	103.27	110.90
20	N	106	ASP	CB-CG-OD1	-5.09	113.72	118.30
22	P	131	VAL	CA-CB-CG1	5.09	118.53	110.90
17	T	254	ILE	CA-C-O	-5.09	109.42	120.10
19	Z	469	TYR	CD1-CE1-CZ	5.09	124.38	119.80
30	L	206	ASP	CB-CG-OD2	-5.09	113.72	118.30
23	Q	260	MET	O-C-N	5.08	130.84	122.70
4	D	186	ALA	N-CA-CB	5.08	117.22	110.10
19	Z	156	HIS	O-C-N	-5.08	114.57	122.70
12	5	147	TYR	CG-CD1-CE1	-5.08	117.23	121.30
15	W	7	MET	N-CA-CB	5.08	119.74	110.60
11	4	31	ASP	N-CA-C	-5.08	97.29	111.00
19	Z	139	CYS	CA-CB-SG	5.08	123.14	114.00
29	K	391	ARG	NE-CZ-NH1	5.08	122.84	120.30
8	1	58	TYR	CG-CD1-CE1	5.08	125.36	121.30
32	J	15	LYS	CA-CB-CG	5.08	124.57	113.40
6	F	195	LEU	CB-CG-CD2	5.08	119.63	111.00
20	N	546	ARG	NE-CZ-NH1	5.08	122.84	120.30
23	Q	343	SER	N-CA-C	-5.08	97.29	111.00
6	F	93	LEU	N-CA-CB	5.07	120.55	110.40
8	1	45	VAL	CG1-CB-CG2	5.07	119.02	110.90
17	T	188	SER	N-CA-CB	5.07	118.11	110.50
1	A	58	ASP	CB-CG-OD1	-5.07	113.73	118.30
13	6	157	TYR	CG-CD1-CE1	-5.07	117.24	121.30
28	I	105	THR	CA-CB-CG2	-5.07	105.30	112.40
29	K	191	TYR	CB-CG-CD2	-5.07	117.96	121.00
3	C	207	SER	N-CA-CB	5.07	118.10	110.50
19	Z	421	ASP	N-CA-CB	5.07	119.72	110.60
30	L	248	GLU	OE1-CD-OE2	5.07	129.38	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	103	TYR	CD1-CG-CD2	5.07	123.47	117.90
22	P	359	VAL	O-C-N	-5.07	114.59	122.70
29	K	340	GLN	CG-CD-OE1	-5.07	111.47	121.60
12	5	204	TYR	CG-CD1-CE1	-5.07	117.25	121.30
13	6	28	ARG	NE-CZ-NH2	5.07	122.83	120.30
23	Q	297	ARG	CD-NE-CZ	-5.07	116.51	123.60
32	J	358	GLU	OE1-CD-OE2	5.07	129.38	123.30
23	Q	118	LYS	N-CA-CB	5.06	119.72	110.60
11	4	140	LEU	CB-CA-C	-5.06	100.58	110.20
32	J	108	VAL	CA-CB-CG1	5.06	118.50	110.90
1	A	126	THR	CA-CB-CG2	5.06	119.49	112.40
2	B	103	GLU	N-CA-C	-5.06	97.34	111.00
14	7	141	TYR	CB-CG-CD1	5.06	124.03	121.00
14	7	224	ASP	CB-CG-OD2	-5.06	113.75	118.30
26	O	176	ALA	N-CA-CB	-5.06	103.02	110.10
22	P	358	VAL	CA-CB-CG2	5.06	118.49	110.90
3	C	151	ASP	CB-CG-OD1	-5.06	113.75	118.30
19	Z	643	PRO	O-C-N	5.06	130.79	122.70
21	S	196	ARG	NE-CZ-NH1	-5.05	117.77	120.30
27	H	107	GLU	N-CA-C	-5.05	97.36	111.00
28	I	162	VAL	N-CA-C	-5.05	97.36	111.00
32	J	372	ARG	NH1-CZ-NH2	-5.05	113.84	119.40
12	5	126	GLU	OE1-CD-OE2	5.05	129.36	123.30
20	N	838	LYS	CD-CE-NZ	5.05	123.32	111.70
29	K	303	VAL	C-N-CA	5.05	134.33	121.70
1	A	240	VAL	CA-CB-CG1	-5.05	103.33	110.90
26	O	278	MET	CG-SD-CE	-5.05	92.12	100.20
20	N	86	ASP	C-N-CA	5.05	134.32	121.70
20	N	900	TYR	N-CA-CB	5.05	119.69	110.60
11	4	31	ASP	CB-CG-OD1	5.04	122.84	118.30
15	W	170	LEU	N-CA-CB	5.04	120.49	110.40
5	E	11	GLY	CA-C-O	5.04	129.68	120.60
17	T	353	VAL	CA-CB-CG1	-5.04	103.33	110.90
22	P	117	ASP	CB-CG-OD2	5.04	122.84	118.30
25	U	224	HIS	CA-CB-CG	5.04	122.17	113.60
26	O	330	ARG	N-CA-CB	5.04	119.68	110.60
2	B	101	TYR	CG-CD1-CE1	5.04	125.33	121.30
4	D	191	ASP	CB-CG-OD2	-5.04	113.76	118.30
10	3	42	ILE	CG1-CB-CG2	5.04	122.49	111.40
17	T	126	LEU	CB-CA-C	-5.04	100.63	110.20
10	3	85	TYR	CD1-CG-CD2	-5.04	112.36	117.90
12	5	74	ALA	CB-CA-C	-5.04	102.55	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	H	320	ALA	N-CA-CB	5.04	117.15	110.10
11	4	113	PRO	N-CA-CB	5.03	109.34	103.30
16	V	65	TYR	CD1-CE1-CZ	-5.03	115.27	119.80
30	L	37	ASP	CB-CG-OD2	5.03	122.83	118.30
21	S	351	ARG	NH1-CZ-NH2	-5.03	113.87	119.40
22	P	319	THR	CA-CB-CG2	-5.03	105.36	112.40
12	5	241	ASP	CB-CG-OD1	-5.03	113.78	118.30
21	S	334	LEU	CB-CG-CD2	5.03	119.55	111.00
12	5	76	ASP	CB-CG-OD2	5.03	122.82	118.30
24	R	125	ARG	NE-CZ-NH1	5.03	122.81	120.30
27	H	210	LYS	N-CA-CB	5.03	119.64	110.60
5	E	170	ILE	CA-C-N	5.02	126.25	116.20
17	T	345	TYR	CZ-CE2-CD2	5.02	124.32	119.80
22	P	329	ARG	CD-NE-CZ	5.02	130.63	123.60
31	M	74	ASP	CB-CG-OD2	5.02	122.82	118.30
13	6	71	TYR	CG-CD1-CE1	-5.02	117.28	121.30
13	6	162	PHE	CG-CD2-CE2	5.02	126.33	120.80
15	W	172	THR	C-N-CA	5.02	134.25	121.70
21	S	304	THR	CA-CB-CG2	-5.02	105.37	112.40
23	Q	110	CYS	CA-CB-SG	-5.02	104.96	114.00
23	Q	243	ASP	CB-CG-OD2	-5.02	113.78	118.30
27	H	237	PHE	CB-CG-CD2	-5.02	117.28	120.80
3	C	112	THR	CA-CB-CG2	-5.02	105.37	112.40
3	C	136	TYR	CG-CD1-CE1	-5.02	117.28	121.30
19	Z	202	HIS	CB-CG-ND1	-5.02	110.65	123.20
19	Z	324	VAL	N-CA-CB	5.02	122.54	111.50
23	Q	192	SER	N-CA-CB	5.02	118.03	110.50
19	Z	40	ASP	CB-CG-OD1	-5.02	113.78	118.30
29	K	230	VAL	CA-CB-CG1	-5.02	103.37	110.90
32	J	3	LEU	C-N-CA	5.02	134.25	121.70
22	P	57	ALA	O-C-N	5.02	130.72	122.70
30	L	144	VAL	C-N-CA	5.01	134.24	121.70
3	C	87	THR	O-C-N	-5.01	114.68	122.70
5	E	103	TYR	CD1-CE1-CZ	-5.01	115.29	119.80
19	Z	479	LEU	CB-CG-CD1	5.01	119.52	111.00
20	N	179	TYR	CG-CD2-CE2	5.01	125.31	121.30
6	F	101	ARG	NE-CZ-NH1	5.01	122.81	120.30
6	F	234	ASP	N-CA-CB	5.01	119.62	110.60
11	4	144	ASP	CB-CG-OD1	5.01	122.81	118.30
20	N	425	THR	CA-CB-CG2	-5.01	105.38	112.40
21	S	248	ASN	N-CA-CB	5.01	119.62	110.60
22	P	129	ARG	NE-CZ-NH2	-5.01	117.80	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	F	108	LEU	CB-CG-CD1	5.01	119.52	111.00
6	F	118	ILE	CA-C-N	5.01	131.13	117.10
30	L	400	TYR	N-CA-CB	5.01	119.62	110.60
19	Z	732	VAL	CA-CB-CG2	5.01	118.41	110.90
22	P	252	ASP	N-CA-CB	5.01	119.61	110.60
29	K	90	GLY	N-CA-C	-5.01	100.58	113.10
19	Z	557	TRP	CE2-CD2-CG	-5.00	103.30	107.30
21	S	307	ASN	CB-CA-C	-5.00	100.39	110.40
29	K	135	HIS	CA-CB-CG	-5.00	105.09	113.60
32	J	376	VAL	CA-CB-CG1	5.00	118.40	110.90
4	D	159	TYR	CB-CG-CD2	5.00	124.00	121.00
13	6	132	TYR	CB-CG-CD2	-5.00	118.00	121.00
20	N	605	VAL	CB-CA-C	-5.00	101.90	111.40
26	O	24	ARG	CG-CD-NE	-5.00	101.30	111.80
30	L	310	ASP	CB-CG-OD2	5.00	122.80	118.30

There are no chirality outliers.

All (260) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	145	TYR	Sidechain
8	1	155	ARG	Sidechain
8	1	177	ARG	Sidechain
8	1	208	ARG	Sidechain
8	1	58	TYR	Sidechain
8	1	78	ARG	Sidechain
9	2	118	ARG	Sidechain
9	2	167	TYR	Sidechain
9	2	186	ARG	Sidechain
9	2	230	ARG	Sidechain
9	2	241	ARG	Sidechain
9	2	56	VAL	Mainchain
10	3	129	CYS	Peptide
10	3	147	TYR	Sidechain
10	3	3	VAL	Peptide
10	3	50	TYR	Sidechain
10	3	6	TYR	Sidechain
10	3	74	TYR	Sidechain
10	3	80	ARG	Sidechain
11	4	107	TYR	Sidechain
11	4	117	TYR	Sidechain
11	4	120	TYR	Sidechain

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Mol	Chain	Res	Type	Group
11	4	147	TYR	Sidechain
11	4	170	ARG	Sidechain
11	4	175	LEU	Peptide
11	4	178	PHE	Sidechain
11	4	19	ARG	Sidechain
11	4	3	TYR	Sidechain
11	4	73	TYR	Sidechain
12	5	113	PHE	Sidechain
12	5	125	TYR	Sidechain
12	5	132	ARG	Sidechain
12	5	171	TYR	Sidechain
12	5	172	TYR	Sidechain
12	5	193	TYR	Sidechain
12	5	61	THR	Mainchain
12	5	72	ILE	Mainchain
13	6	124	TYR	Sidechain
13	6	127	ARG	Sidechain
13	6	151	PHE	Sidechain
13	6	197	ARG	Sidechain
13	6	221	ARG	Sidechain
13	6	29	PHE	Sidechain
13	6	32	TYR	Sidechain
13	6	85	HIS	Sidechain
14	7	106	TYR	Sidechain
14	7	130	ARG	Sidechain
14	7	143	ARG	Sidechain
14	7	168	TYR	Sidechain
14	7	188	TYR	Sidechain
14	7	195	ARG	Sidechain
14	7	222	TYR	Sidechain
14	7	226	ARG	Sidechain
14	7	257	HIS	Sidechain
14	7	57	GLY	Mainchain
14	7	69	ASP	Mainchain
14	7	88	ARG	Sidechain
1	A	105	TYR	Sidechain
1	A	107	TYR	Sidechain
1	A	117	ARG	Sidechain
1	A	187	PHE	Sidechain
2	B	121	TYR	Sidechain
2	B	155	TYR	Sidechain
2	B	178	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	B	189	HIS	Sidechain
2	B	57	TYR	Sidechain
2	B	6	TYR	Sidechain
2	B	84	ARG	Sidechain
3	C	136	TYR	Sidechain
3	C	143	TYR	Sidechain
3	C	19	TYR	Sidechain
3	C	218	ARG	Sidechain
3	C	49	ARG	Sidechain
3	C	5	TYR	Sidechain
4	D	101	ARG	Sidechain
4	D	112	TYR	Sidechain
4	D	131	ARG	Sidechain
4	D	151	TYR	Sidechain
4	D	159	TYR	Sidechain
4	D	169	ARG	Sidechain
4	D	3	TYR	Sidechain
4	D	38	ARG	Sidechain
4	D	74	ALA	Peptide
4	D	76	VAL	Peptide
4	D	87	ARG	Sidechain
5	E	20	ARG	Sidechain
5	E	99	HIS	Sidechain
6	F	137	TYR	Sidechain
6	F	154	PHE	Sidechain
6	F	171	TYR	Sidechain
6	F	193	ARG	Sidechain
6	F	224	TYR	Sidechain
6	F	65	HIS	Peptide
7	G	119	TYR	Sidechain
7	G	150	TYR	Sidechain
7	G	199	TYR	Sidechain
7	G	233	ARG	Sidechain
7	G	26	TYR	Sidechain
7	G	8	TYR	Sidechain
27	H	111	TYR	Sidechain
27	H	147	TYR	Sidechain
27	H	150	HIS	Sidechain
27	H	232	ARG	Sidechain
27	H	258	ARG	Sidechain
27	H	339	ARG	Sidechain
27	H	386	ARG	Sidechain

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Mol	Chain	Res	Type	Group
28	I	131	HIS	Sidechain
28	I	132	TYR	Sidechain
28	I	138	PHE	Sidechain
28	I	225	TYR	Sidechain
28	I	249	ARG	Sidechain
28	I	268	ARG	Sidechain
28	I	439	TYR	Sidechain
32	J	148	TYR	Sidechain
32	J	258	ARG	Sidechain
32	J	313	ARG	Sidechain
32	J	369	TYR	Sidechain
32	J	43	ARG	Sidechain
29	K	114	ARG	Sidechain
29	K	178	ARG	Sidechain
29	K	205	TYR	Sidechain
29	K	263	PHE	Sidechain
29	K	313	ARG	Sidechain
29	K	323	ARG	Sidechain
29	K	363	TYR	Sidechain
29	K	417	TYR	Sidechain
29	K	44	TYR	Sidechain
29	K	81	ARG	Sidechain
30	L	111	ARG	Sidechain
30	L	124	TYR	Sidechain
30	L	187	TYR	Sidechain
30	L	19	ARG	Sidechain
30	L	237	ARG	Sidechain
30	L	265	ARG	Sidechain
30	L	269	ARG	Sidechain
30	L	311	ARG	Sidechain
30	L	400	TYR	Sidechain
31	M	133	GLN	Sidechain
31	M	135	TYR	Sidechain
31	M	183	ARG	Sidechain
31	M	307	ARG	Sidechain
31	M	347	ARG	Sidechain
31	M	384	TYR	Sidechain
31	M	412	ARG	Sidechain
31	M	441	TYR	Sidechain
31	M	49	ARG	Sidechain
20	N	147	TYR	Sidechain
20	N	159	ARG	Sidechain

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Mol	Chain	Res	Type	Group
20	N	193	PHE	Sidechain
20	N	22	PHE	Sidechain
20	N	246	TYR	Sidechain
20	N	253	TYR	Sidechain
20	N	269	ARG	Sidechain
20	N	34	PHE	Sidechain
20	N	344	ARG	Sidechain
20	N	460	TYR	Sidechain
20	N	474	ARG	Sidechain
20	N	49	TYR	Sidechain
20	N	494	TYR	Sidechain
20	N	541	HIS	Sidechain
20	N	55	ARG	Sidechain
20	N	57	ARG	Sidechain
20	N	601	ARG	Sidechain
20	N	650	TYR	Sidechain
20	N	68	PHE	Sidechain
20	N	709	PHE	Sidechain
20	N	778	PHE	Sidechain
20	N	80	TYR	Sidechain
20	N	813	TYR	Sidechain
20	N	88	PHE	Sidechain
20	N	881	PRO	Mainchain
20	N	899	ARG	Sidechain
20	N	96	TYR	Sidechain
26	O	173	TYR	Sidechain
26	O	24	ARG	Sidechain
26	O	29	TYR	Sidechain
26	O	63	PHE	Sidechain
22	P	114	GLU	Peptide
22	P	137	TYR	Sidechain
22	P	199	TYR	Sidechain
22	P	227	TYR	Sidechain
22	P	247	TYR	Sidechain
22	P	27	ARG	Sidechain
22	P	279	PHE	Sidechain
22	P	302	TYR	Sidechain
22	P	322	GLU	Sidechain
22	P	324	TYR	Sidechain
22	P	370	TYR	Sidechain
22	P	38	GLY	Mainchain
22	P	75	TYR	Sidechain

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Mol	Chain	Res	Type	Group
23	Q	126	ARG	Sidechain
23	Q	177	TYR	Sidechain
23	Q	231	TYR	Sidechain
23	Q	233	TYR	Sidechain
23	Q	344	ARG	Sidechain
23	Q	72	TYR	Sidechain
23	Q	96	PHE	Sidechain
24	R	110	TYR	Sidechain
24	R	183	TYR	Sidechain
24	R	216	TYR	Sidechain
24	R	225	TYR	Sidechain
24	R	24	PHE	Sidechain
24	R	259	TYR	Sidechain
24	R	304	TYR	Sidechain
24	R	366	TYR	Sidechain
24	R	53	TYR	Sidechain
24	R	83	ARG	Sidechain
21	S	146	ARG	Sidechain
21	S	162	TYR	Sidechain
21	S	196	ARG	Sidechain
21	S	209	TYR	Sidechain
21	S	214	TYR	Sidechain
21	S	257	TYR	Sidechain
21	S	283	ARG	Sidechain
21	S	325	HIS	Sidechain
21	S	356	TYR	Sidechain
21	S	388	TYR	Sidechain
21	S	410	TYR	Sidechain
21	S	497	TYR	Sidechain
21	S	76	ARG	Sidechain
21	S	95	ARG	Sidechain
17	T	177	TYR	Sidechain
17	T	282	TYR	Sidechain
17	T	292	ARG	Sidechain
17	T	305	TYR	Sidechain
17	T	321	PHE	Sidechain
17	T	91	LEU	Peptide
25	U	145	HIS	Sidechain
25	U	190	ARG	Sidechain
25	U	211	TYR	Sidechain
25	U	69	PHE	Sidechain
25	U	72	HIS	Sidechain

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Mol	Chain	Res	Type	Group
25	U	88	ARG	Sidechain
16	V	104	ARG	Sidechain
16	V	175	ARG	Sidechain
16	V	207	TYR	Sidechain
16	V	65	TYR	Sidechain
16	V	68	ARG	Sidechain
15	W	105	HIS	Sidechain
15	W	130	ARG	Sidechain
15	W	156	PHE	Sidechain
15	W	25	ARG	Sidechain
15	W	91	ARG	Sidechain
18	Y	65	TYR	Sidechain
19	Z	103	TYR	Sidechain
19	Z	158	TYR	Sidechain
19	Z	181	ARG	Sidechain
19	Z	202	HIS	Sidechain
19	Z	261	ARG	Sidechain
19	Z	267	ARG	Sidechain
19	Z	400	TYR	Sidechain
19	Z	469	TYR	Sidechain
19	Z	489	TYR	Sidechain
19	Z	554	TYR	Sidechain
19	Z	673	ARG	Sidechain
19	Z	687	ARG	Sidechain
19	Z	719	PRO	Peptide
19	Z	781	TYR	Sidechain
19	Z	845	ARG	Sidechain
19	Z	865	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

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
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
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%)	226 (93%)	14 (6%)	4 (2%)	9	44
2	B	232/234 (99%)	210 (90%)	19 (8%)	3 (1%)	12	48
3	C	247/261 (95%)	229 (93%)	16 (6%)	2 (1%)	19	60
4	D	244/254 (96%)	218 (89%)	21 (9%)	5 (2%)	7	38
5	E	231/241 (96%)	220 (95%)	10 (4%)	1 (0%)	34	72
6	F	236/263 (90%)	219 (93%)	17 (7%)	0	100	100
7	G	243/255 (95%)	220 (90%)	19 (8%)	4 (2%)	9	44
8	1	200/238 (84%)	173 (86%)	13 (6%)	14 (7%)	1	14
9	2	217/277 (78%)	181 (83%)	16 (7%)	20 (9%)	1	11
10	3	203/205 (99%)	169 (83%)	19 (9%)	15 (7%)	1	14
11	4	194/201 (96%)	175 (90%)	10 (5%)	9 (5%)	2	21
12	5	199/263 (76%)	176 (88%)	17 (8%)	6 (3%)	4	28
13	6	211/240 (88%)	180 (85%)	16 (8%)	15 (7%)	1	14
14	7	214/263 (81%)	187 (87%)	15 (7%)	12 (6%)	2	19
15	W	193/377 (51%)	178 (92%)	8 (4%)	7 (4%)	3	25
16	V	287/310 (93%)	258 (90%)	17 (6%)	12 (4%)	3	22
17	T	261/353 (74%)	233 (89%)	22 (8%)	6 (2%)	6	34
18	Y	22/70 (31%)	21 (96%)	1 (4%)	0	100	100
19	Z	894/908 (98%)	800 (90%)	71 (8%)	23 (3%)	5	31
20	N	901/953 (94%)	823 (91%)	58 (6%)	20 (2%)	6	35
21	S	474/530 (89%)	425 (90%)	33 (7%)	16 (3%)	3	26
22	P	454/456 (100%)	419 (92%)	22 (5%)	13 (3%)	4	29
23	Q	420/422 (100%)	388 (92%)	24 (6%)	8 (2%)	8	38
24	R	387/389 (100%)	360 (93%)	21 (5%)	6 (2%)	9	44
25	U	286/320 (89%)	261 (91%)	15 (5%)	10 (4%)	3	25
26	O	374/376 (100%)	347 (93%)	18 (5%)	9 (2%)	6	33
27	H	394/433 (91%)	350 (89%)	27 (7%)	17 (4%)	2	22
28	I	383/440 (87%)	359 (94%)	15 (4%)	9 (2%)	6	34
29	K	389/418 (93%)	356 (92%)	26 (7%)	7 (2%)	8	40
30	L	387/403 (96%)	356 (92%)	19 (5%)	12 (3%)	4	27

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
31	M	413/442 (93%)	381 (92%)	18 (4%)	14 (3%)	3	26
32	J	404/406 (100%)	365 (90%)	31 (8%)	8 (2%)	7	38
All	All	10438/11447 (91%)	9463 (91%)	668 (6%)	307 (3%)	7	29

All (307) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
7	G	35	SER
8	1	45	VAL
8	1	105	GLU
8	1	153	MET
8	1	163	SER
8	1	217	VAL
9	2	81	SER
9	2	91	THR
9	2	166	PRO
9	2	172	SER
9	2	224	SER
9	2	248	GLU
10	3	5	SER
10	3	41	LYS
10	3	57	ALA
10	3	142	CYS
10	3	204	MET
11	4	22	ALA
11	4	50	ALA
11	4	114	ALA
12	5	62	THR
12	5	72	ILE
13	6	57	SER
13	6	85	HIS
13	6	129	PHE
13	6	168	ALA
13	6	231	ARG
14	7	64	VAL
14	7	65	VAL
14	7	175	ALA
14	7	242	GLU
15	W	17	ARG
16	V	26	ASP
16	V	147	PRO

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Mol	Chain	Res	Type
16	V	189	ILE
16	V	199	HIS
17	T	220	ALA
19	Z	147	SER
19	Z	241	PRO
19	Z	310	ASP
19	Z	324	VAL
19	Z	614	HIS
19	Z	810	ILE
19	Z	814	SER
19	Z	843	SER
20	N	119	PRO
20	N	165	LYS
20	N	453	HIS
20	N	471	ASP
20	N	881	PRO
20	N	899	ARG
21	S	54	ALA
21	S	108	VAL
21	S	142	GLN
21	S	270	SER
21	S	296	LEU
21	S	314	GLN
22	P	3	ASP
22	P	13	ILE
22	P	341	PHE
22	P	344	THR
22	P	400	LYS
23	Q	3	ALA
23	Q	43	VAL
23	Q	102	ALA
24	R	17	LEU
24	R	289	ALA
25	U	5	ALA
25	U	164	ALA
25	U	219	LYS
25	U	237	LEU
26	O	47	ASP
27	H	65	ILE
27	H	94	GLN
27	H	128	GLN
27	H	280	ILE

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Mol	Chain	Res	Type
27	H	347	ASP
28	I	87	PRO
28	I	118	ASP
28	I	278	ALA
28	I	391	SER
32	J	152	GLY
1	A	57	PRO
1	A	186	LYS
2	B	41	ALA
2	B	207	ASN
3	C	58	GLU
4	D	29	GLY
4	D	80	SER
8	1	136	TRP
8	1	164	GLY
8	1	206	VAL
8	1	226	GLN
9	2	161	SER
9	2	187	PRO
9	2	189	MET
9	2	250	GLY
10	3	31	GLN
10	3	137	VAL
10	3	186	ILE
11	4	124	LEU
12	5	63	LEU
12	5	233	VAL
13	6	33	ALA
13	6	39	VAL
14	7	77	LEU
14	7	101	TYR
15	W	104	ASN
15	W	148	VAL
16	V	148	ILE
16	V	202	SER
16	V	232	GLN
19	Z	173	LEU
19	Z	178	LYS
19	Z	837	LEU
19	Z	849	ALA
20	N	87	LEU
20	N	123	LYS

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Mol	Chain	Res	Type
20	N	431	THR
20	N	489	ALA
20	N	755	THR
20	N	817	LEU
21	S	82	VAL
21	S	184	SER
21	S	185	ASP
22	P	136	ILE
22	P	419	LYS
22	P	452	ILE
23	Q	280	ALA
24	R	16	ASP
24	R	191	ILE
24	R	215	ASP
26	O	49	CYS
26	O	51	ALA
26	O	341	LEU
27	H	118	PHE
27	H	147	TYR
27	H	276	GLU
27	H	403	ILE
29	K	269	ALA
29	K	304	ASN
30	L	118	THR
30	L	144	VAL
31	M	106	ASP
31	M	187	GLN
31	M	298	ARG
32	J	220	VAL
32	J	223	PHE
1	A	4	GLY
4	D	13	ASP
4	D	76	VAL
7	G	73	HIS
7	G	217	VAL
8	1	51	SER
9	2	215	ASN
9	2	232	TYR
10	3	43	PHE
10	3	50	TYR
10	3	127	ILE
10	3	159	ASP

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Mol	Chain	Res	Type
10	3	185	VAL
11	4	32	HIS
12	5	88	GLN
13	6	47	PHE
13	6	77	THR
14	7	202	PRO
15	W	46	GLU
15	W	181	ASP
17	T	93	ALA
19	Z	190	GLU
19	Z	293	GLN
19	Z	384	ALA
19	Z	459	CYS
20	N	348	THR
20	N	560	MET
20	N	944	PRO
21	S	80	LYS
21	S	127	LEU
22	P	402	ILE
22	P	454	ASN
23	Q	141	LYS
23	Q	262	ASN
25	U	186	THR
25	U	247	LYS
26	O	14	SER
26	O	103	LYS
26	O	286	ALA
26	O	287	ASN
27	H	171	ASP
27	H	173	THR
27	H	281	GLY
27	H	312	ARG
28	I	89	GLU
28	I	185	ALA
28	I	410	ARG
29	K	390	ASN
30	L	81	GLU
30	L	127	ARG
30	L	143	ASN
30	L	193	GLY
31	M	306	ASP
31	M	307	ARG

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Mol	Chain	Res	Type
31	M	326	ASN
31	M	436	ALA
32	J	10	GLU
32	J	80	MET
32	J	354	ALA
4	D	169	ARG
7	G	43	LYS
9	2	67	MET
9	2	136	TYR
9	2	188	ASP
9	2	225	LYS
10	3	130	PRO
13	6	32	TYR
13	6	34	PHE
13	6	220	LEU
14	7	252	ASN
15	W	178	SER
16	V	116	PRO
16	V	183	HIS
16	V	266	THR
17	T	287	PHE
19	Z	490	ALA
19	Z	802	SER
20	N	524	LYS
20	N	772	TRP
20	N	819	VAL
21	S	149	LYS
21	S	339	PRO
22	P	93	ARG
22	P	95	SER
22	P	340	VAL
24	R	50	MET
25	U	31	ASN
25	U	66	SER
27	H	337	LEU
28	I	431	GLN
29	K	317	LEU
29	K	408	LYS
30	L	372	ASP
31	M	160	SER
31	M	290	GLU
32	J	111	ASN

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Mol	Chain	Res	Type
1	A	209	ASP
2	B	202	GLN
5	E	73	HIS
8	1	231	THR
9	2	148	VAL
9	2	167	TYR
11	4	4	LEU
11	4	101	ASN
12	5	232	ALA
13	6	157	TYR
14	7	56	LEU
14	7	191	GLN
16	V	187	PRO
17	T	258	SER
17	T	286	LEU
20	N	490	ARG
20	N	903	PHE
21	S	131	LEU
21	S	134	PRO
21	S	136	ASP
30	L	258	SER
30	L	341	ASP
31	M	114	ILE
32	J	192	PRO
3	C	8	ARG
8	1	138	PRO
8	1	141	GLY
8	1	148	PRO
9	2	231	PRO
14	7	151	TRP
19	Z	175	ASP
19	Z	622	SER
19	Z	642	ALA
25	U	244	GLU
27	H	106	SER
27	H	311	PRO
28	I	127	VAL
30	L	297	ASP
15	W	45	PRO
16	V	155	VAL
19	Z	311	VAL
23	Q	341	PRO

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Mol	Chain	Res	Type
27	H	378	PRO
30	L	318	PRO
31	M	184	PRO
9	2	261	PRO
10	3	119	PRO
11	4	13	VAL
13	6	37	GLY
13	6	62	ILE
26	O	183	VAL
14	7	246	PRO
19	Z	115	PRO
31	M	102	VAL
31	M	340	ILE
11	4	26	VAL
17	T	255	PRO
23	Q	391	PRO
25	U	179	ILE
29	K	199	PRO
29	K	406	VAL
30	L	183	GLY
31	M	32	ILE

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%)	198 (94%)	12 (6%)	20	45
2	B	191/191 (100%)	181 (95%)	10 (5%)	23	48
3	C	209/221 (95%)	200 (96%)	9 (4%)	29	53
4	D	208/215 (97%)	195 (94%)	13 (6%)	18	43
5	E	195/203 (96%)	186 (95%)	9 (5%)	27	52
6	F	204/224 (91%)	193 (95%)	11 (5%)	22	47
7	G	202/212 (95%)	191 (95%)	11 (5%)	22	47
8	1	160/185 (86%)	138 (86%)	22 (14%)	3	17

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
9	2	180/227 (79%)	162 (90%)	18 (10%)	7	26
10	3	175/175 (100%)	161 (92%)	14 (8%)	12	35
11	4	167/172 (97%)	154 (92%)	13 (8%)	12	36
12	5	158/205 (77%)	143 (90%)	15 (10%)	8	27
13	6	179/200 (90%)	160 (89%)	19 (11%)	6	24
14	7	178/215 (83%)	159 (89%)	19 (11%)	6	23
15	W	168/312 (54%)	160 (95%)	8 (5%)	25	51
16	V	253/268 (94%)	236 (93%)	17 (7%)	16	41
17	T	233/298 (78%)	221 (95%)	12 (5%)	23	48
18	Y	22/63 (35%)	21 (96%)	1 (4%)	27	52
19	Z	753/765 (98%)	699 (93%)	54 (7%)	14	39
20	N	776/814 (95%)	727 (94%)	49 (6%)	18	43
21	S	414/458 (90%)	394 (95%)	20 (5%)	25	51
22	P	419/419 (100%)	393 (94%)	26 (6%)	18	43
23	Q	362/362 (100%)	344 (95%)	18 (5%)	24	49
24	R	345/345 (100%)	324 (94%)	21 (6%)	18	44
25	U	259/289 (90%)	243 (94%)	16 (6%)	18	43
26	O	334/334 (100%)	315 (94%)	19 (6%)	20	45
27	H	341/372 (92%)	327 (96%)	14 (4%)	30	55
28	I	341/385 (89%)	318 (93%)	23 (7%)	16	41
29	K	343/367 (94%)	324 (94%)	19 (6%)	21	47
30	L	341/353 (97%)	319 (94%)	22 (6%)	17	42
31	M	357/382 (94%)	338 (95%)	19 (5%)	22	47
32	J	352/352 (100%)	334 (95%)	18 (5%)	24	48
All	All	9029/9793 (92%)	8458 (94%)	571 (6%)	21	43

All (571) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	13	ILE
1	A	15	ILE
1	A	58	ASP
1	A	93	ARG
1	A	107	TYR

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Mol	Chain	Res	Type
1	A	121	ILE
1	A	143	ILE
1	A	161	CYS
1	A	166	THR
1	A	187	PHE
1	A	193	GLN
1	A	222	VAL
2	B	45	VAL
2	B	79	MET
2	B	127	VAL
2	B	128	ARG
2	B	192	ILE
2	B	193	LEU
2	B	199	PHE
2	B	205	GLU
2	B	208	ILE
2	B	220	ARG
3	C	35	LEU
3	C	43	VAL
3	C	44	LEU
3	C	82	ASP
3	C	103	GLU
3	C	137	ILE
3	C	140	ASP
3	C	180	LYS
3	C	225	ILE
4	D	3	TYR
4	D	9	VAL
4	D	10	PHE
4	D	13	ASP
4	D	75	VAL
4	D	79	VAL
4	D	102	LEU
4	D	150	LEU
4	D	152	GLN
4	D	154	ASP
4	D	219	ARG
4	D	225	ILE
4	D	235	VAL
5	E	41	GLN
5	E	69	GLU
5	E	101	PHE

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Mol	Chain	Res	Type
5	E	162	PHE
5	E	201	ILE
5	E	209	LYS
5	E	211	ASN
5	E	215	ILE
5	E	217	LEU
6	F	4	ASN
6	F	38	LEU
6	F	74	ILE
6	F	103	LEU
6	F	104	PRO
6	F	120	THR
6	F	125	ARG
6	F	130	VAL
6	F	208	LYS
6	F	215	VAL
6	F	230	SER
7	G	20	ARG
7	G	64	ASN
7	G	67	LEU
7	G	136	PHE
7	G	140	SER
7	G	166	ILE
7	G	171	GLN
7	G	198	ILE
7	G	205	VAL
7	G	226	GLU
7	G	230	LYS
8	1	36	ILE
8	1	45	VAL
8	1	46	VAL
8	1	52	ARG
8	1	71	HIS
8	1	84	ASP
8	1	94	TYR
8	1	121	TYR
8	1	122	ARG
8	1	136	TRP
8	1	137	ASP
8	1	147	VAL
8	1	153	MET
8	1	171	TYR

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Mol	Chain	Res	Type
8	1	173	ASP
8	1	177	ARG
8	1	181	THR
8	1	183	ASP
8	1	186	LEU
8	1	199	ARG
8	1	219	ARG
8	1	230	VAL
9	2	50	VAL
9	2	68	VAL
9	2	108	LEU
9	2	111	LEU
9	2	119	VAL
9	2	125	MET
9	2	128	GLN
9	2	131	PHE
9	2	149	THR
9	2	154	TYR
9	2	162	THR
9	2	170	MET
9	2	184	LYS
9	2	190	GLU
9	2	195	LYS
9	2	230	ARG
9	2	246	ARG
9	2	248	GLU
10	3	15	LYS
10	3	28	PHE
10	3	30	ILE
10	3	47	ASP
10	3	60	VAL
10	3	80	ARG
10	3	95	LEU
10	3	102	PRO
10	3	124	LEU
10	3	156	PRO
10	3	161	GLU
10	3	187	VAL
10	3	189	ILE
10	3	200	LEU
11	4	4	LEU
11	4	41	LYS

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Mol	Chain	Res	Type
11	4	42	ILE
11	4	61	GLN
11	4	68	LYS
11	4	69	MET
11	4	115	LEU
11	4	116	TYR
11	4	138	LEU
11	4	145	ARG
11	4	153	ARG
11	4	154	GLU
11	4	168	GLN
12	5	90	VAL
12	5	104	MET
12	5	113	PHE
12	5	114	TRP
12	5	116	ARG
12	5	124	ILE
12	5	125	TYR
12	5	135	VAL
12	5	149	TYR
12	5	165	LYS
12	5	193	TYR
12	5	200	ARG
12	5	205	ASP
12	5	221	GLN
12	5	245	ARG
13	6	35	ASN
13	6	38	THR
13	6	42	ILE
13	6	46	ASP
13	6	55	ARG
13	6	60	PHE
13	6	77	THR
13	6	78	VAL
13	6	88	CYS
13	6	119	LEU
13	6	137	ILE
13	6	140	LEU
13	6	159	ARG
13	6	162	PHE
13	6	171	MET
13	6	176	LEU

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Mol	Chain	Res	Type
13	6	186	GLN
13	6	193	LEU
13	6	212	ARG
14	7	49	MET
14	7	59	LYS
14	7	61	ASP
14	7	71	LEU
14	7	87	MET
14	7	94	MET
14	7	103	ASP
14	7	104	PHE
14	7	117	ASP
14	7	133	HIS
14	7	135	TRP
14	7	138	ARG
14	7	150	LEU
14	7	177	GLU
14	7	204	LEU
14	7	221	TYR
14	7	236	VAL
14	7	252	ASN
14	7	257	HIS
15	W	17	ARG
15	W	34	ASN
15	W	49	VAL
15	W	54	LEU
15	W	62	THR
15	W	63	THR
15	W	71	ILE
15	W	143	PHE
16	V	65	TYR
16	V	95	MET
16	V	100	LYS
16	V	130	GLN
16	V	163	ILE
16	V	178	THR
16	V	203	ILE
16	V	220	LEU
16	V	231	LEU
16	V	255	TYR
16	V	257	LYS
16	V	265	MET

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Mol	Chain	Res	Type
16	V	288	VAL
16	V	300	LEU
16	V	303	MET
16	V	304	LEU
16	V	310	LYS
17	T	105	TRP
17	T	107	ARG
17	T	127	LEU
17	T	215	LEU
17	T	216	GLU
17	T	221	LYS
17	T	245	ASN
17	T	247	VAL
17	T	248	PHE
17	T	303	THR
17	T	316	ASN
17	T	319	TYR
18	Y	61	GLU
19	Z	6	ARG
19	Z	31	LYS
19	Z	45	LEU
19	Z	52	LEU
19	Z	66	LYS
19	Z	99	LEU
19	Z	108	GLU
19	Z	110	TYR
19	Z	115	PRO
19	Z	143	ARG
19	Z	158	TYR
19	Z	181	ARG
19	Z	189	LYS
19	Z	190	GLU
19	Z	192	VAL
19	Z	202	HIS
19	Z	214	VAL
19	Z	222	ASP
19	Z	233	LEU
19	Z	237	VAL
19	Z	278	VAL
19	Z	309	GLU
19	Z	312	GLU
19	Z	313	GLU

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Mol	Chain	Res	Type
19	Z	317	LEU
19	Z	329	ASN
19	Z	340	MET
19	Z	345	PRO
19	Z	356	ASN
19	Z	421	ASP
19	Z	436	SER
19	Z	445	LEU
19	Z	451	VAL
19	Z	452	ASN
19	Z	456	ARG
19	Z	477	MET
19	Z	552	ASP
19	Z	553	THR
19	Z	613	LEU
19	Z	614	HIS
19	Z	635	LYS
19	Z	639	LYS
19	Z	675	PHE
19	Z	701	ASN
19	Z	719	PRO
19	Z	740	ARG
19	Z	741	LEU
19	Z	763	ARG
19	Z	764	LEU
19	Z	776	LEU
19	Z	851	ASP
19	Z	872	VAL
19	Z	879	ARG
19	Z	886	GLU
20	N	1	MET
20	N	55	ARG
20	N	82	LEU
20	N	96	TYR
20	N	120	GLU
20	N	140	ARG
20	N	143	ASP
20	N	190	ASN
20	N	200	VAL
20	N	213	PHE
20	N	243	LEU
20	N	250	PHE

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Mol	Chain	Res	Type
20	N	266	GLN
20	N	269	ARG
20	N	323	LEU
20	N	333	MET
20	N	349	ASP
20	N	353	LEU
20	N	367	THR
20	N	390	LEU
20	N	391	GLU
20	N	402	PHE
20	N	407	SER
20	N	422	LEU
20	N	423	MET
20	N	465	LEU
20	N	472	ILE
20	N	474	ARG
20	N	479	LEU
20	N	552	ILE
20	N	554	LEU
20	N	561	GLU
20	N	572	ARG
20	N	573	ASP
20	N	601	ARG
20	N	627	PHE
20	N	670	ASN
20	N	732	LEU
20	N	746	ILE
20	N	756	HIS
20	N	766	PHE
20	N	770	TRP
20	N	792	ASN
20	N	877	LEU
20	N	889	LEU
20	N	908	ILE
20	N	913	ILE
20	N	921	ILE
20	N	928	VAL
21	S	32	ASP
21	S	38	GLU
21	S	155	LEU
21	S	163	LEU
21	S	188	MET

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Mol	Chain	Res	Type
21	S	208	TYR
21	S	217	LEU
21	S	248	ASN
21	S	281	TRP
21	S	305	MET
21	S	341	ARG
21	S	397	ASN
21	S	411	SER
21	S	415	LEU
21	S	447	ILE
21	S	463	TYR
21	S	472	PHE
21	S	488	LYS
21	S	491	ARG
21	S	495	LYS
22	P	7	GLU
22	P	12	ARG
22	P	18	VAL
22	P	24	VAL
22	P	41	GLN
22	P	55	ARG
22	P	65	ARG
22	P	66	ILE
22	P	78	LYS
22	P	129	ARG
22	P	136	ILE
22	P	138	VAL
22	P	186	ILE
22	P	198	ASP
22	P	206	SER
22	P	250	ILE
22	P	259	GLU
22	P	276	LEU
22	P	283	GLN
22	P	299	ILE
22	P	316	ARG
22	P	323	ASP
22	P	345	GLU
22	P	364	ARG
22	P	380	GLN
22	P	446	ILE
23	Q	15	LEU

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Mol	Chain	Res	Type
23	Q	27	LEU
23	Q	32	LYS
23	Q	77	LEU
23	Q	172	LEU
23	Q	183	LEU
23	Q	196	THR
23	Q	200	ILE
23	Q	229	TYR
23	Q	252	LYS
23	Q	306	LEU
23	Q	319	ILE
23	Q	337	ARG
23	Q	353	LEU
23	Q	363	ARG
23	Q	377	ILE
23	Q	388	PHE
23	Q	407	MET
24	R	5	ASN
24	R	18	ARG
24	R	23	ARG
24	R	34	ASP
24	R	41	LEU
24	R	42	MET
24	R	50	MET
24	R	53	TYR
24	R	84	LEU
24	R	88	LEU
24	R	134	LEU
24	R	146	ARG
24	R	176	ARG
24	R	214	MET
24	R	225	TYR
24	R	259	TYR
24	R	286	TRP
24	R	299	MET
24	R	314	LEU
24	R	331	ASP
24	R	366	TYR
25	U	7	GLN
25	U	11	VAL
25	U	15	VAL
25	U	35	VAL

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Mol	Chain	Res	Type
25	U	39	LEU
25	U	67	VAL
25	U	81	MET
25	U	118	ASN
25	U	131	LEU
25	U	174	HIS
25	U	181	ASP
25	U	201	LEU
25	U	249	PHE
25	U	261	TYR
25	U	273	HIS
25	U	284	ASP
26	O	8	LEU
26	O	9	GLN
26	O	44	PHE
26	O	73	PRO
26	O	76	LEU
26	O	79	ILE
26	O	81	LEU
26	O	115	LYS
26	O	133	GLU
26	O	138	VAL
26	O	155	PHE
26	O	187	ASP
26	O	210	VAL
26	O	240	PHE
26	O	255	TRP
26	O	272	ILE
26	O	294	GLU
26	O	344	GLN
26	O	350	LYS
27	H	68	SER
27	H	91	GLN
27	H	105	ASP
27	H	149	ILE
27	H	165	GLN
27	H	240	VAL
27	H	297	ARG
27	H	316	LYS
27	H	328	ASP
27	H	346	PRO
27	H	355	PHE

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Mol	Chain	Res	Type
27	H	371	GLU
27	H	380	SER
27	H	385	ILE
28	I	62	LEU
28	I	64	LYS
28	I	85	MET
28	I	90	GLU
28	I	107	MET
28	I	117	ASP
28	I	134	SER
28	I	148	CYS
28	I	178	LYS
28	I	210	TYR
28	I	214	MET
28	I	216	ILE
28	I	253	SER
28	I	257	GLN
28	I	265	LYS
28	I	285	ASP
28	I	294	ARG
28	I	360	THR
28	I	365	PHE
28	I	405	MET
28	I	408	ARG
28	I	410	ARG
28	I	439	TYR
29	K	30	LEU
29	K	33	GLU
29	K	51	LEU
29	K	72	PHE
29	K	80	LYS
29	K	120	ASP
29	K	121	ARG
29	K	125	LYS
29	K	154	LEU
29	K	198	PRO
29	K	212	LYS
29	K	234	GLU
29	K	242	GLU
29	K	274	ARG
29	K	276	ASP
29	K	284	GLU

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Mol	Chain	Res	Type
29	K	309	MET
29	K	361	GLU
29	K	399	PHE
30	L	84	ILE
30	L	106	LEU
30	L	114	LEU
30	L	129	VAL
30	L	130	ASP
30	L	182	LYS
30	L	217	ILE
30	L	222	ILE
30	L	242	CYS
30	L	244	ILE
30	L	265	ARG
30	L	290	ILE
30	L	293	THR
30	L	318	PRO
30	L	341	ASP
30	L	343	GLU
30	L	352	PHE
30	L	360	VAL
30	L	374	ASP
30	L	375	PHE
30	L	381	PHE
30	L	390	ASP
31	M	30	ASP
31	M	50	LEU
31	M	55	ILE
31	M	102	VAL
31	M	109	GLU
31	M	137	LEU
31	M	144	ASP
31	M	147	LYS
31	M	149	LYS
31	M	170	GLU
31	M	191	ILE
31	M	206	VAL
31	M	213	GLU
31	M	262	MET
31	M	335	THR
31	M	342	ASP
31	M	365	ARG

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Mol	Chain	Res	Type
31	M	383	ASN
31	M	417	GLU
32	J	10	GLU
32	J	12	GLU
32	J	15	LYS
32	J	56	VAL
32	J	126	ILE
32	J	132	ASP
32	J	134	LEU
32	J	187	LEU
32	J	206	HIS
32	J	251	ILE
32	J	260	GLU
32	J	276	LEU
32	J	287	LYS
32	J	298	ILE
32	J	336	MET
32	J	339	THR
32	J	358	GLU
32	J	379	THR

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.

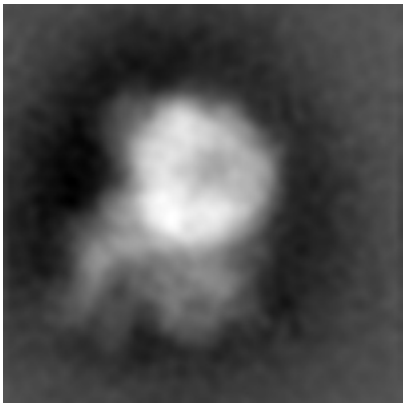
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-3913. These allow visual inspection of the internal detail of the map and identification of artifacts.

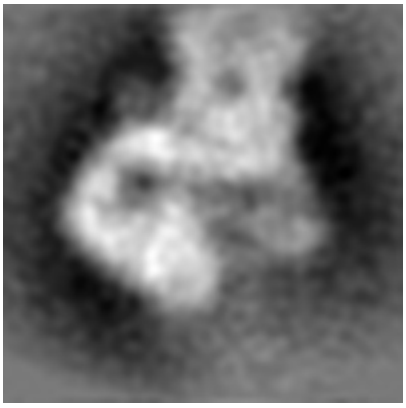
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

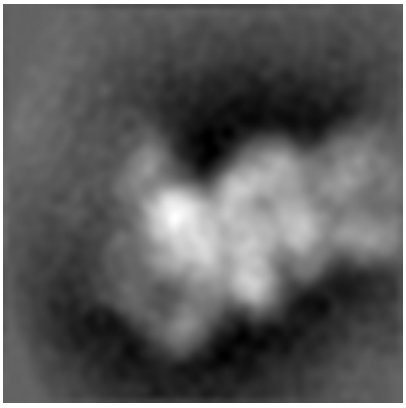
6.1.1 Primary map



X



Y

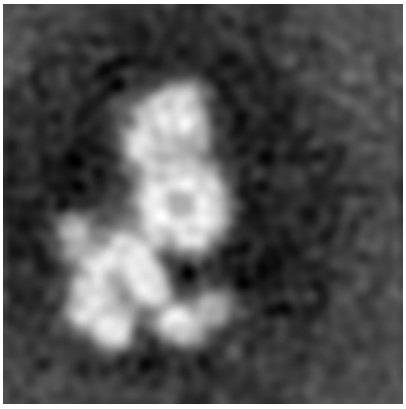


Z

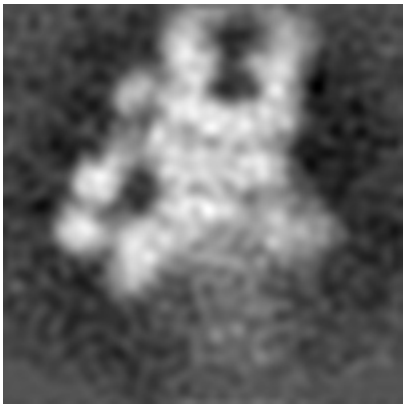
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



X Index: 45



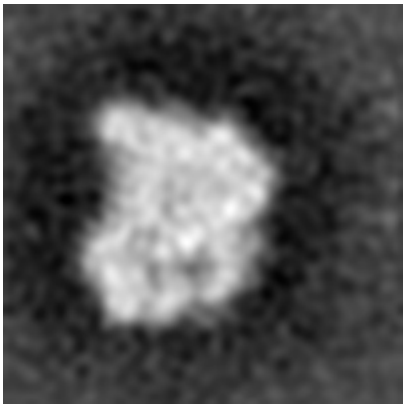
Y Index: 45

Z Index: 45

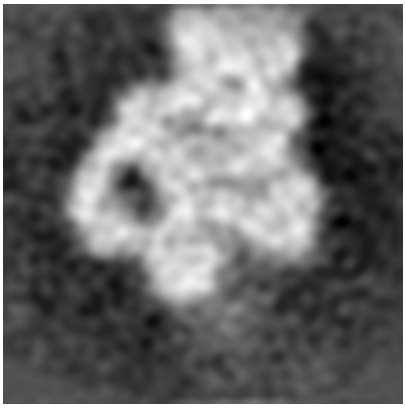
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

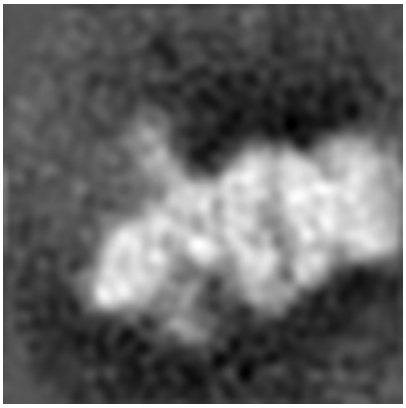
6.3.1 Primary map



X Index: 55



Y Index: 37

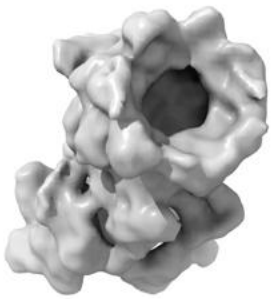


Z Index: 42

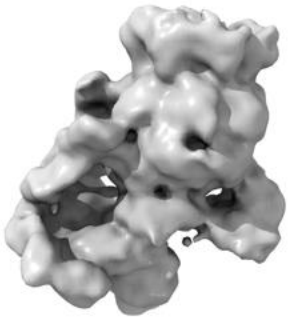
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

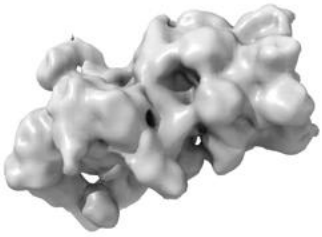
6.4.1 Primary map



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.

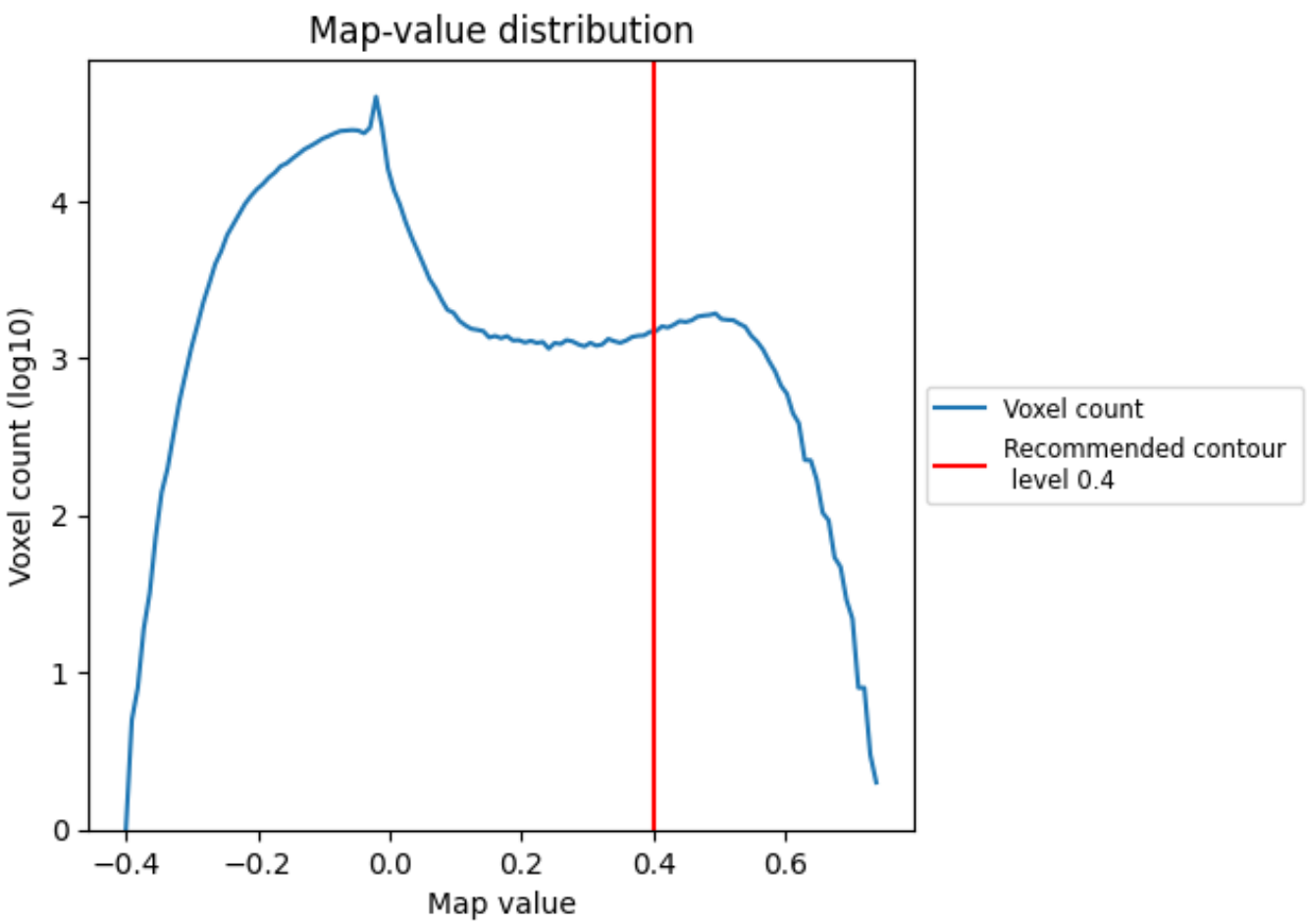
6.5 Mask visualisation (i)

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

7 Map analysis (i)

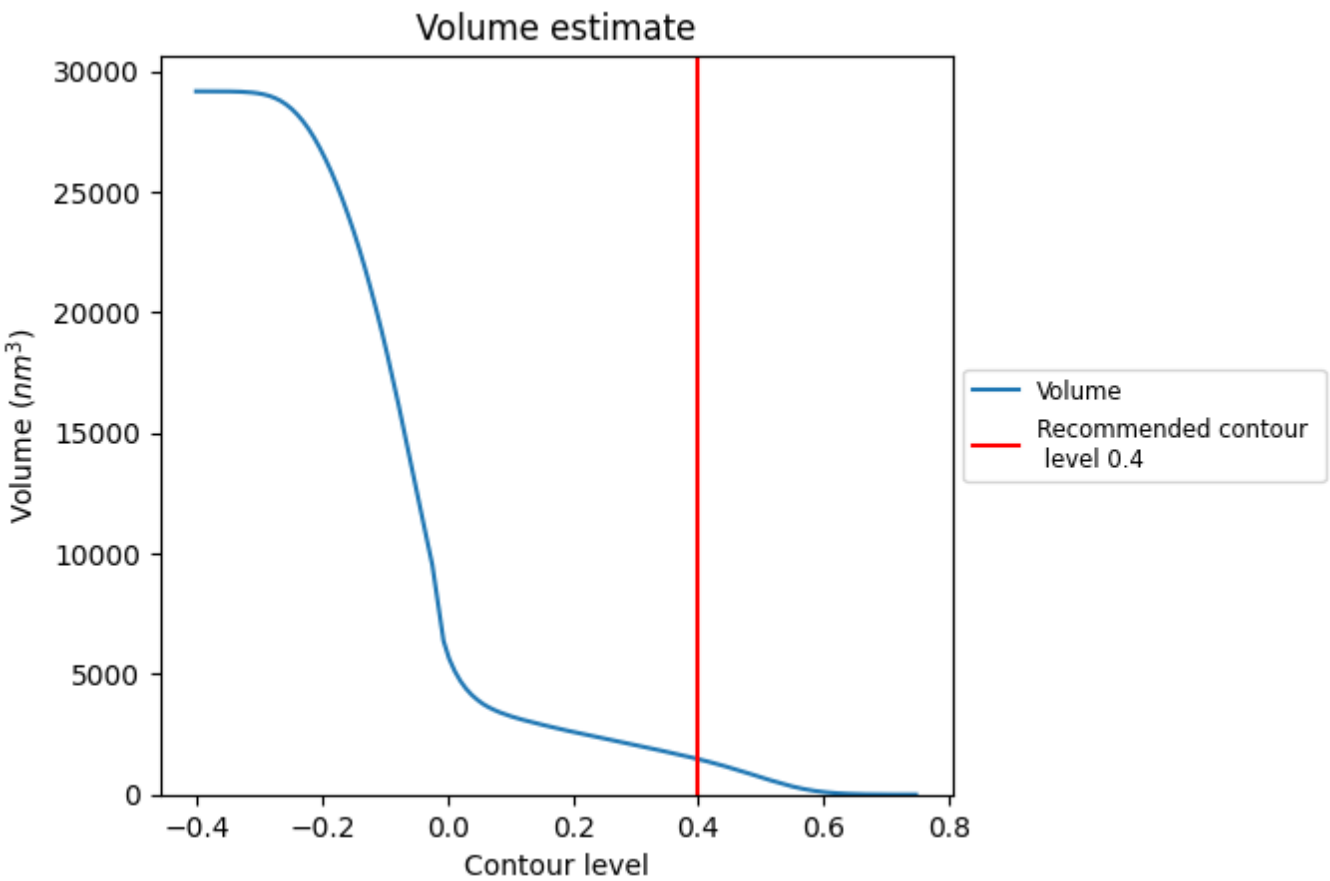
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution (i)



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

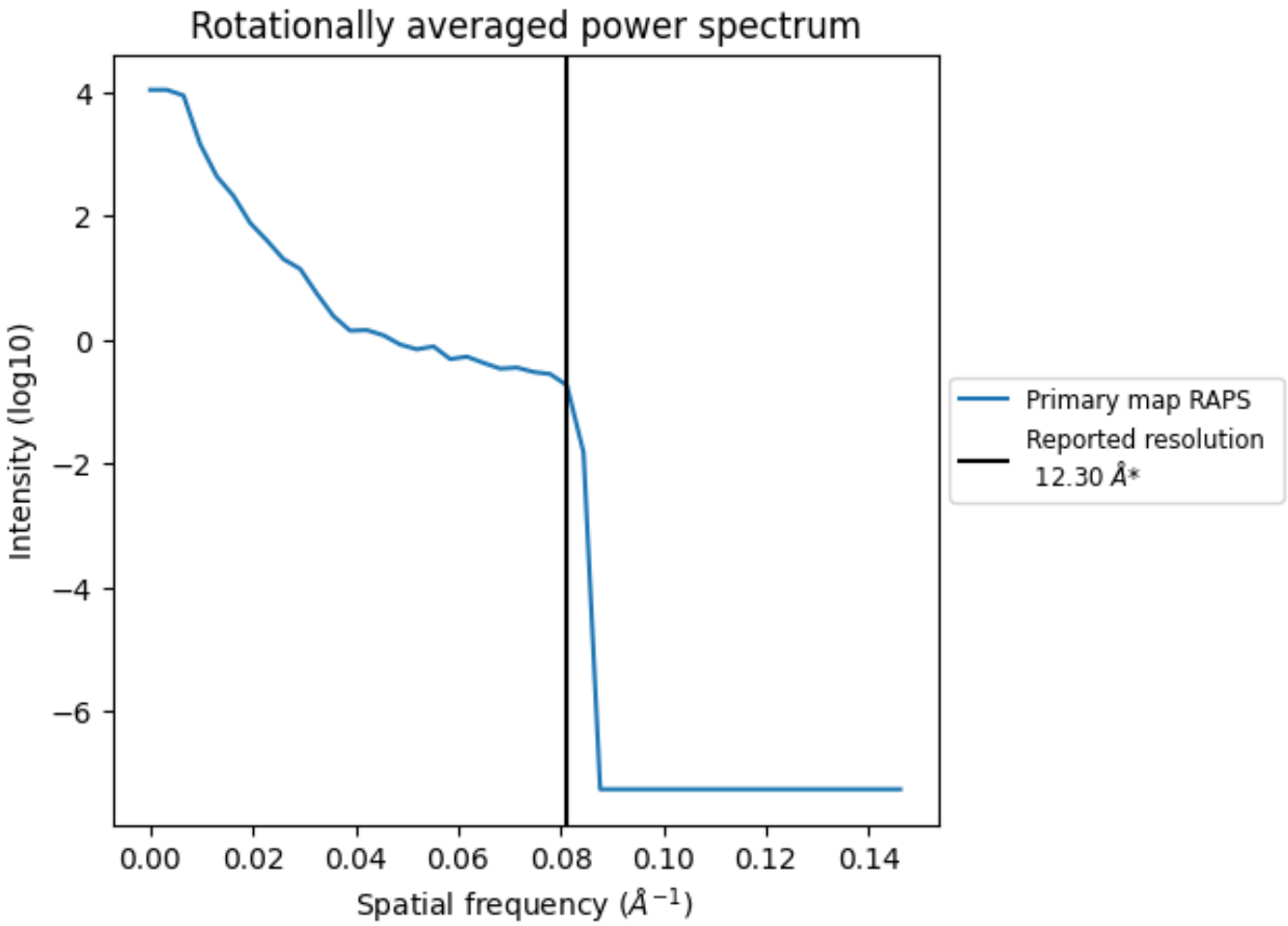
7.2 Volume estimate (i)



The volume at the recommended contour level is 1469 nm^3; this corresponds to an approximate mass of 1327 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 0.081 Å^{-1}

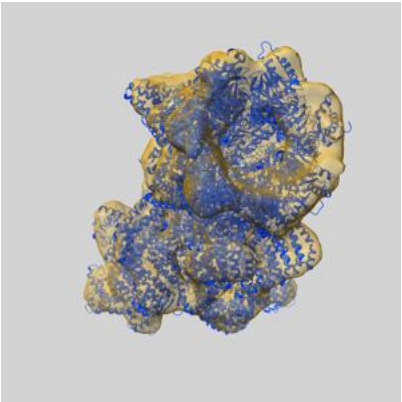
8 Fourier-Shell correlation (i)

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

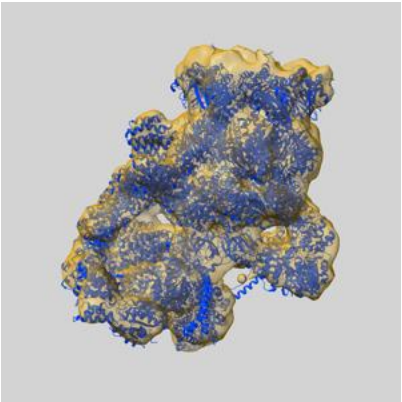
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-3913 and PDB model 6EPC. Per-residue inclusion information can be found in section 3 on page 9.

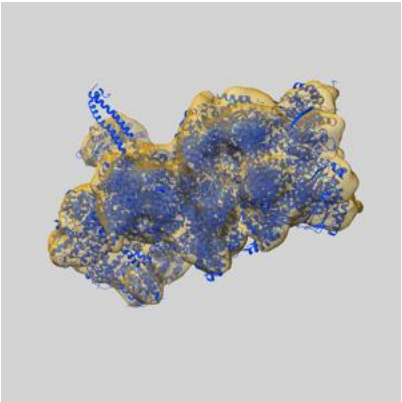
9.1 Map-model overlay (i)



X



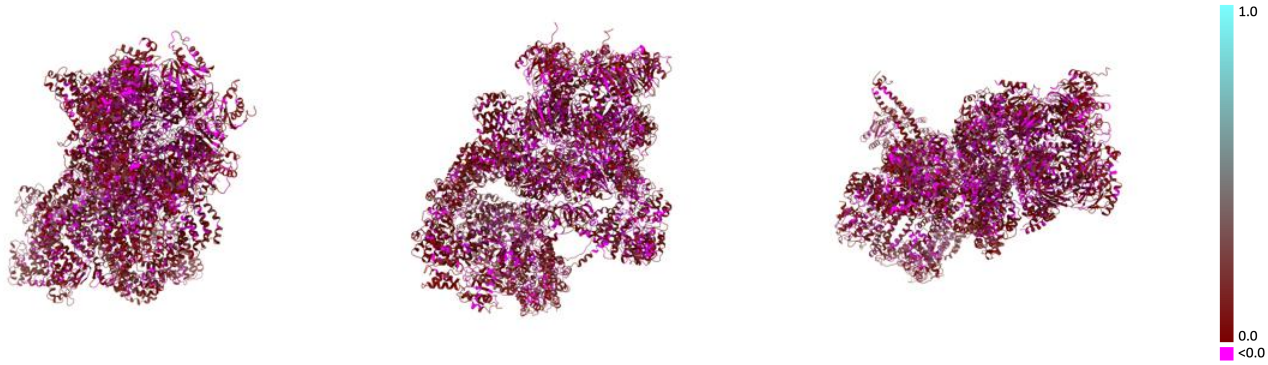
Y



Z

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

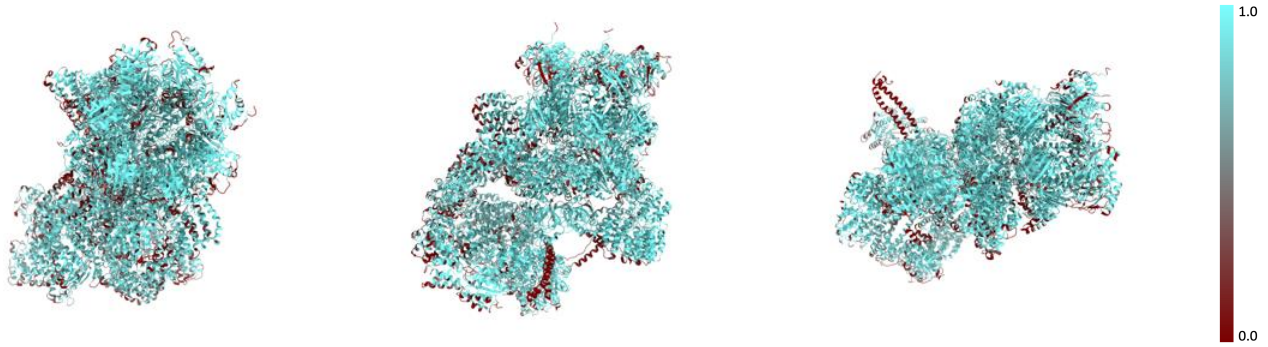
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

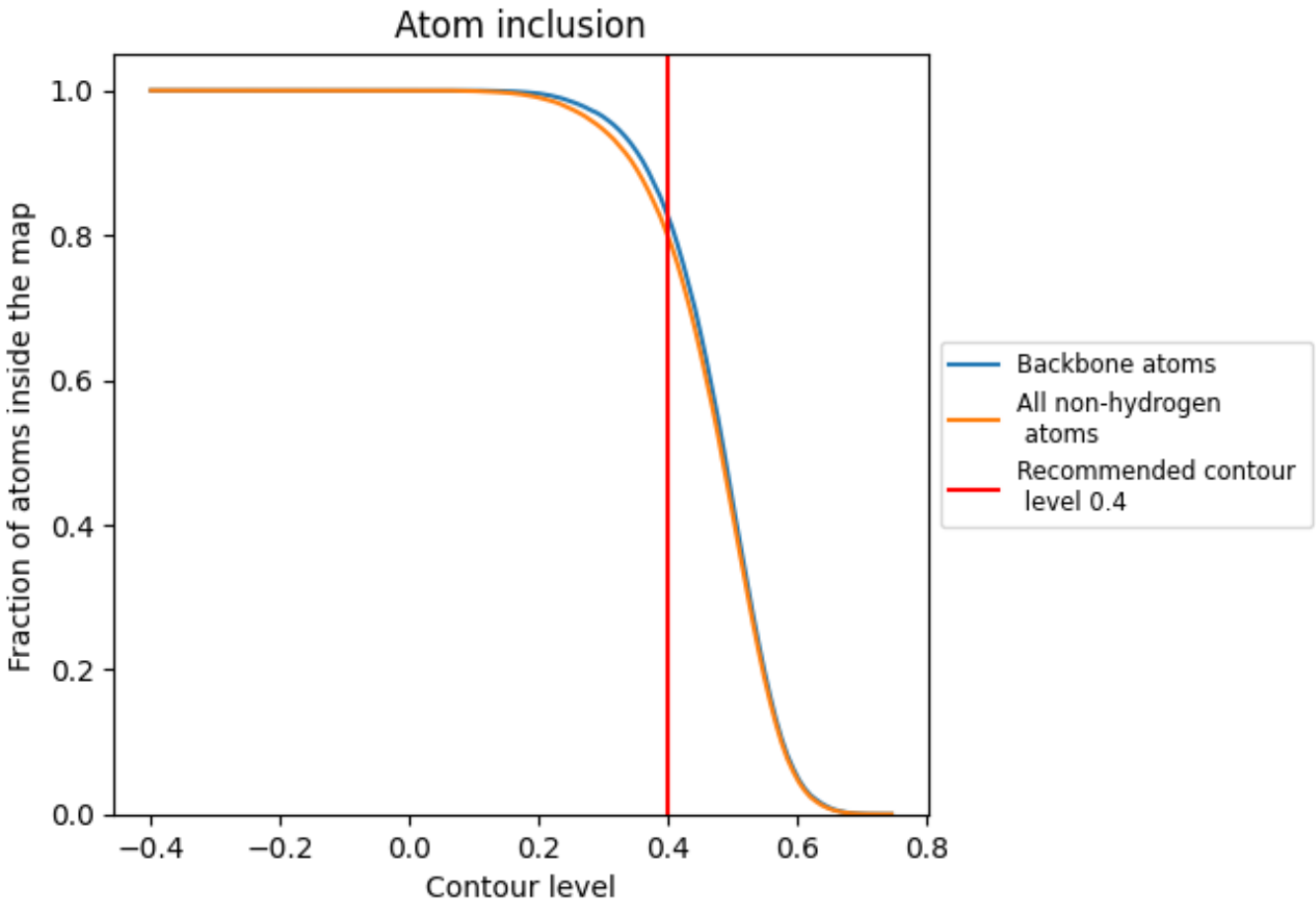
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.4).

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 (i)

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	0.7995	0.0520
1	0.7719	0.0430
2	0.6973	0.0440
3	0.7314	0.0290
4	0.7199	0.0570
5	0.7726	0.0470
6	0.6821	0.0410
7	0.7707	0.0470
A	0.8818	0.0400
B	0.8322	0.0450
C	0.7820	0.0460
D	0.8378	0.0440
E	0.8905	0.0340
F	0.9333	0.0470
G	0.9225	0.0310
H	0.9377	0.0420
I	0.8127	0.0420
J	0.7937	0.0550
K	0.8542	0.0490
L	0.8229	0.0480
M	0.8080	0.0480
N	0.8136	0.0560
O	0.6493	0.0690
P	0.7407	0.0740
Q	0.7924	0.0640
R	0.7357	0.0610
S	0.7939	0.0570
T	0.6814	0.0690
U	0.7446	0.0460
V	0.9238	0.0570
W	0.7211	0.0720
Y	0.5408	0.0380
Z	0.8267	0.0470