Full wwPDB EM Validation Report (i)

Nov 20, 2022 – 12:59 am GMT

PDB ID	:	6FVV
EMDB ID	:	EMD-4321
Title	:	26S proteasome, s3 state
Authors	:	Eisele, M.R.; Reed, R.G.; Rudack, T.; Schweitzer, A.; Beck, F.; Nagy, I.; Pfeifer, G.; Plitzko, J.M.; Baumeister, W.; Tomko, R.J.; Sakata, E.
Deposited on	:	2018-03-05
Resolution	:	5.40 Å(reported)

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

We welcome your comments at *validation@mail.wwpdb.org*
A user guide is available at
https://www.wwpdb.org/validation/2017/EMValidationReportHelp
with specific help available everywhere you see the (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 (1)) were used in the production of this report:

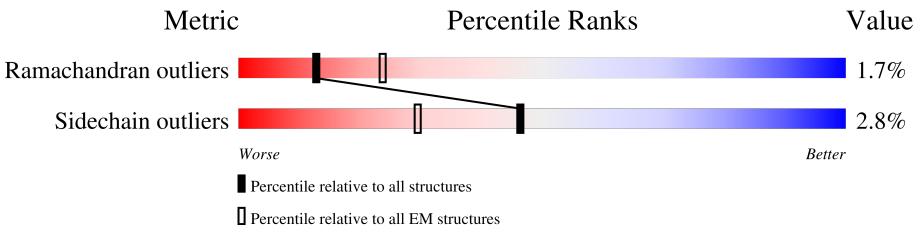
EMDB validation analysis	:	0.0.1.dev43
Mogul	:	1.8.4, CSD as541be (2020)
MolProbity	:	4.02b-467
buster-report	:	1.1.7 (2018)
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)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

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 5.40 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	241	99%
1	a	241	32%, 80%, 17%
2	B	249	98%
2	b	249	40%, 82%, 16%
3	C	244	99%
3	c	244	37%, 76%, 23%
4	D	251	92%, 6%
4	d	251	38%, 80%, 18%
5	E	244	7%, 95%, 5%

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Mol	Chain	Length	Quality of chain
5	e	244	42% 78% 20%
6	F	231	97%
6	f	231	29% 74% 21%
7	G	242	96%
7	g	242	33% 74% 21% 5%
8	1	196	82% 15%
8	h	196	75% 21%
9	2	226	83% 16%
9	i	226	5% 80% 16%
10	3	204	7% 76% 22%
10	j	204	8% 77% 20%
11	4	195	79% 19%
11	k	195	7% 75% 21%
12	5	212	75% 23%
12	l	212	6% 77% 21%
13	6	222	74% 23%
13	m	222	12% 74% 23%
14	7	232	70% 25%
14	n	232	6% 76% 18% 6%
15	W	197	18% 76% 20%
16	V	289	9% 75% 21%
17	T	266	14% 81% 17%
18	X	127	73% 74% 22%
19	Y	89	46% 78% 19%
20	Z	970	59% 86% 6% 7%

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Mol	Chain	Length	Quality of chain
21	N	922	12% 81% 16%
22	S	475	15% 78% 18%
23	P	440	81% 17%
24	Q	434	7% 77% 18%
25	R	405	7% 77% 20%
26	U	304	14% 81% 17%
27	O	388	7% 76% 21%
28	H	417	23% 74% 23%
29	I	385	23% 78% 19%
30	K	394	18% 72% 23%
31	L	388	13% 77% 18%
32	M	421	21% 78% 19%
33	J	405	23% 74% 21%

2 Entry composition (i)

There are 36 unique types of molecules in this entry. The entry contains 110420 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	a	241	1908	1214	320	366	8	0	0
1	A	241	1908	1214	320	366	8	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	249	1907	1214	314	376	3	0	0
2	B	249	1907	1214	314	376	3	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	d	251	1982	1235	350	393	4	0	0
4	D	237	1859	1164	325	366	4	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	244	1883	1176	316	384	7	0	0
5	E	244	1883	1176	316	384	7	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
7	g	242	1886	1199	328	355	4	0	0
7	G	242	1886	1199	328	355	4	0	0

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
9	i	226	1720	1082	298	333	7	0	0
9	2	226	1720	1082	298	333	7	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	j	204	1581	1010	258	305	8	0	0

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
11	k	195	1562	992	264	300	6	0	0
11	4	195	1562	992	264	300	6	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	l	212	1644	1045	280	312	7	0	0
12	5	212	1644	1045	280	312	7	0	0

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
28	H	417	3234	2008	578	632	16	0	0

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

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

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

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

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

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

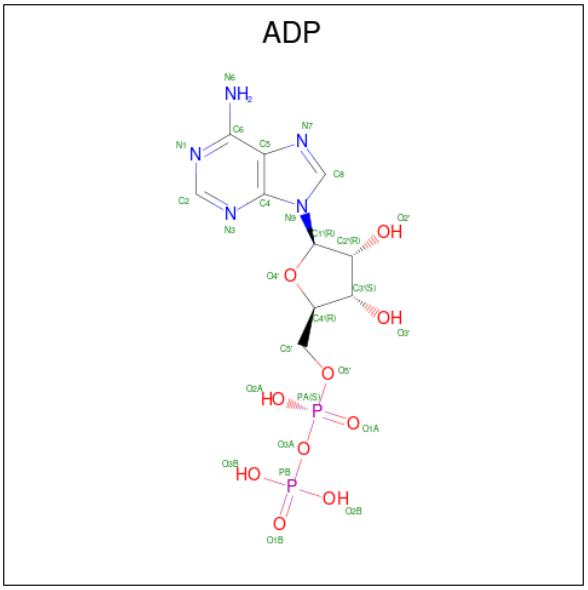
- Molecule 32 is a protein called 26S proteasome regulatory subunit 6A.

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

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

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

- Molecule 34 is ADENOSINE-5'-DIPHOSPHATE (three-letter code: ADP) (formula: $C_{10}H_{15}N_5O_{10}P_2$).



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

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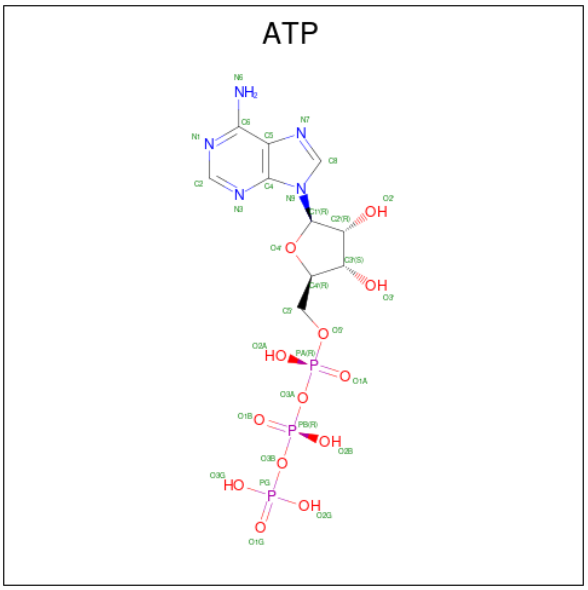
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
34	M	1	27	10	5	10	2	0

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

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

- Molecule 36 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



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

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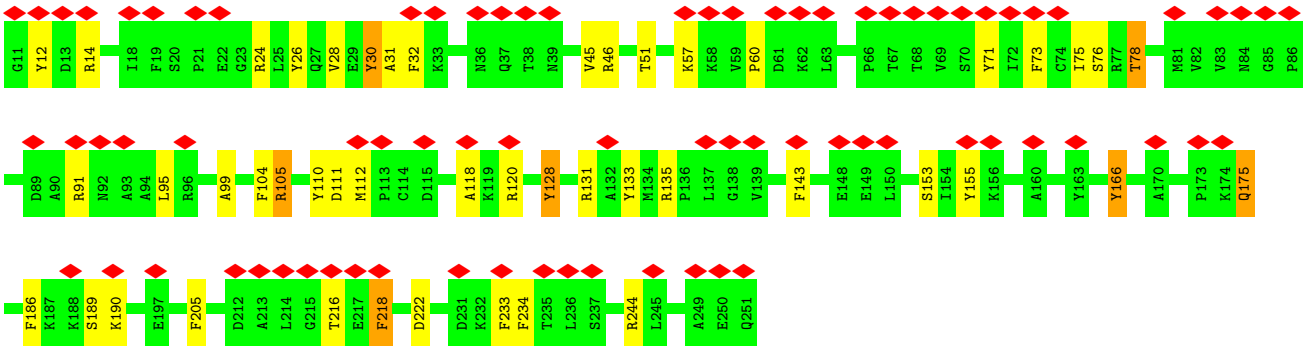
Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
36	L	1	31	10	5	13	3	0
			Total	C	N	O	P	
36	J	1	31	10	5	13	3	0

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.

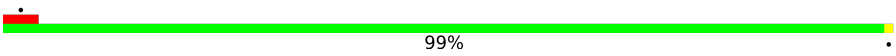
- Molecule 1: Proteasome subunit alpha type-1

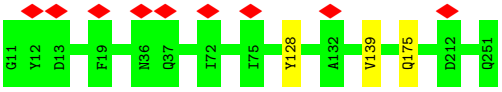
Chain a:



- Molecule 1: Proteasome subunit alpha type-1

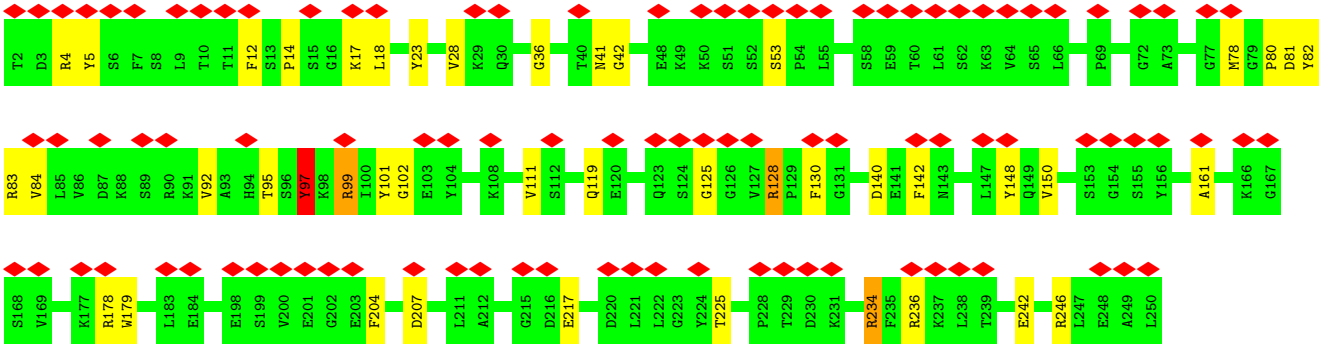
Chain A:





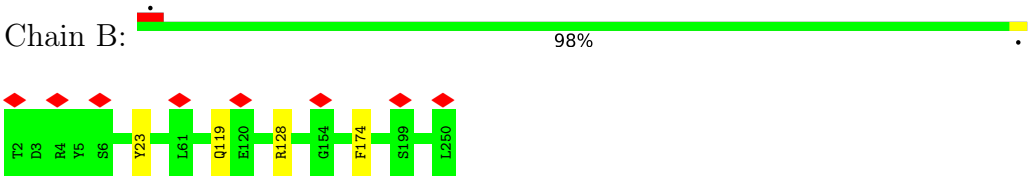
- Molecule 2: Proteasome subunit alpha type-2

Chain b:



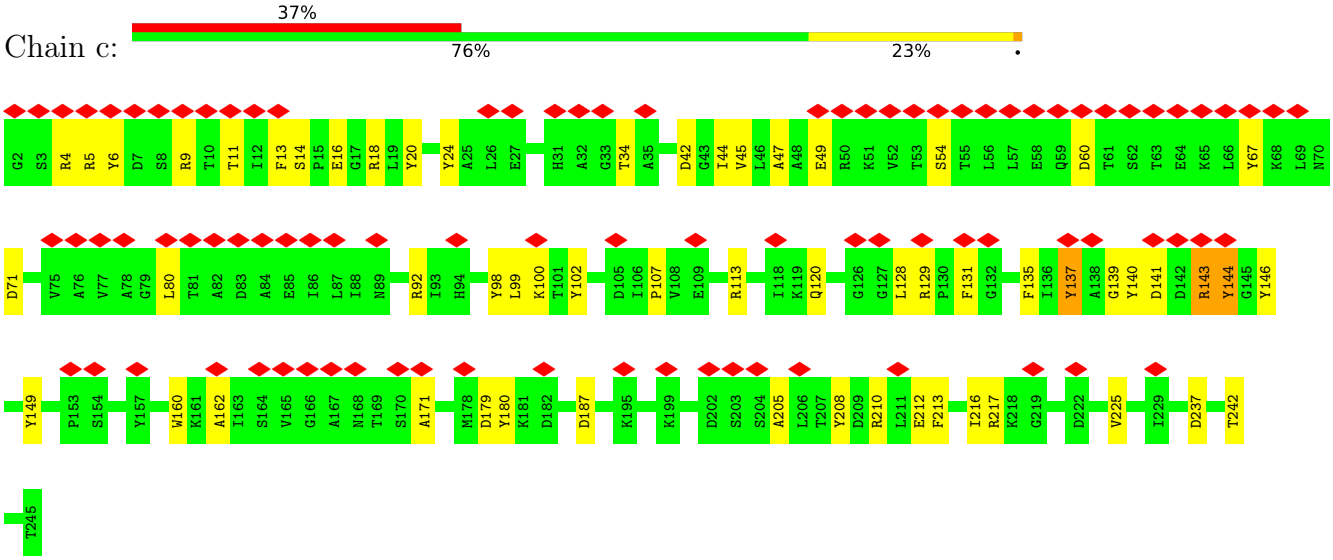
- Molecule 2: Proteasome subunit alpha type-2

Chain B:



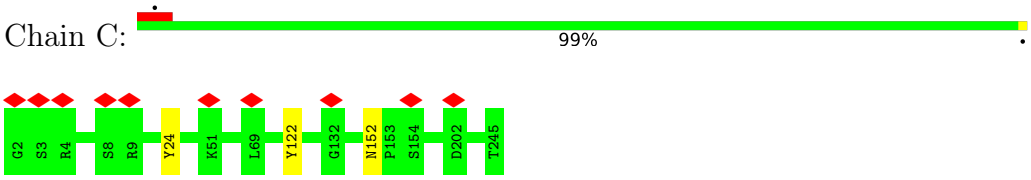
- Molecule 3: Proteasome subunit alpha type-3

Chain c:



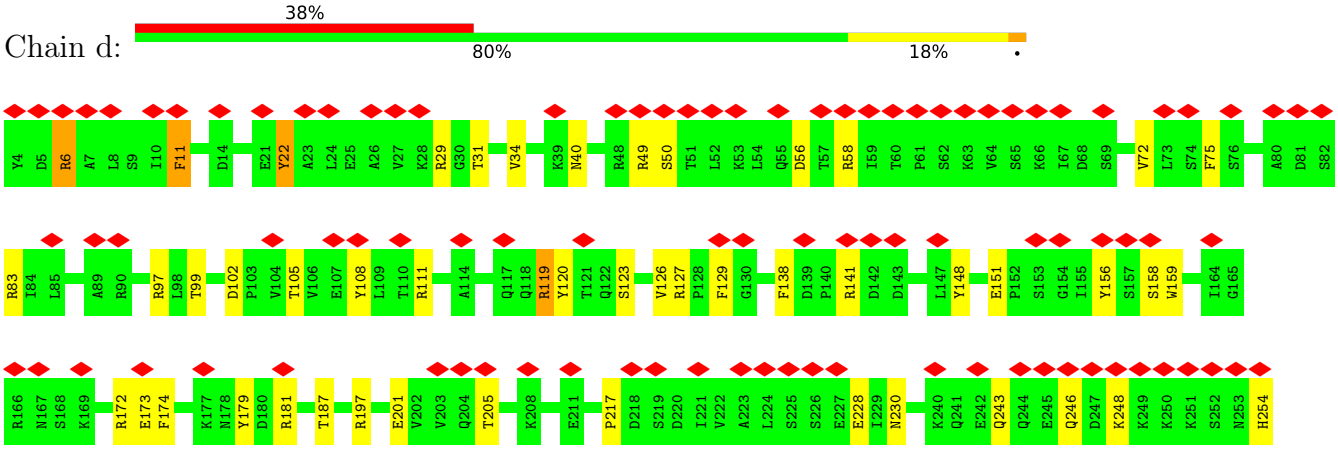
- Molecule 3: Proteasome subunit alpha type-3

Chain C:



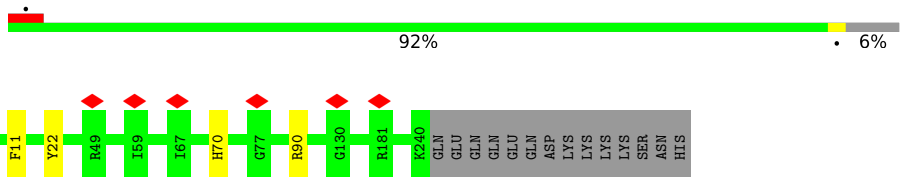
- Molecule 4: Proteasome subunit alpha type-4

Chain d:



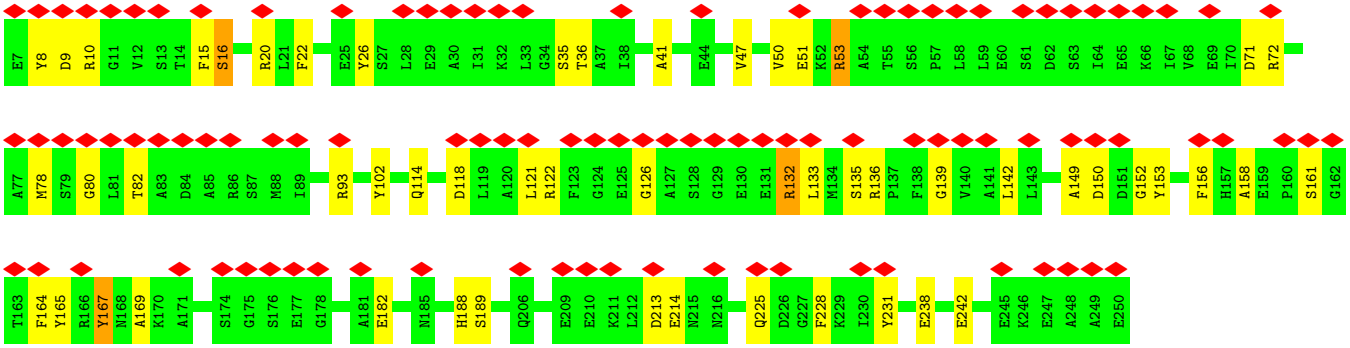
- Molecule 4: Proteasome subunit alpha type-4

Chain D:



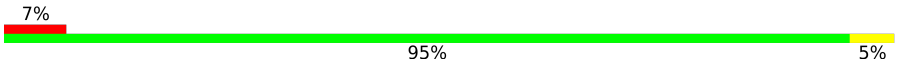
• Molecule 5: Proteasome subunit alpha type-5

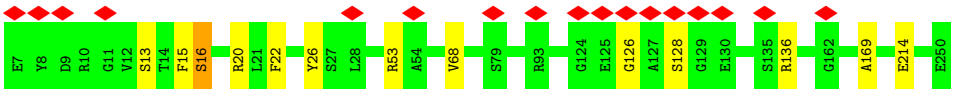
Chain e:



• Molecule 5: Proteasome subunit alpha type-5

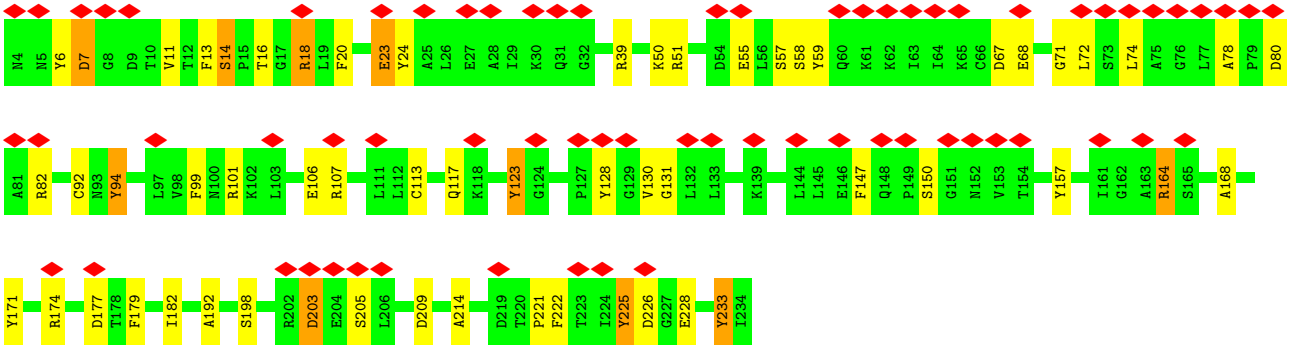
Chain E:





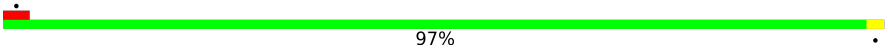
• Molecule 6: Proteasome subunit alpha type-6

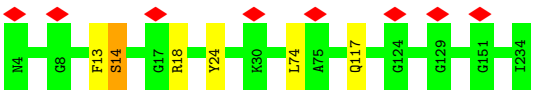
Chain f:



• Molecule 6: Proteasome subunit alpha type-6

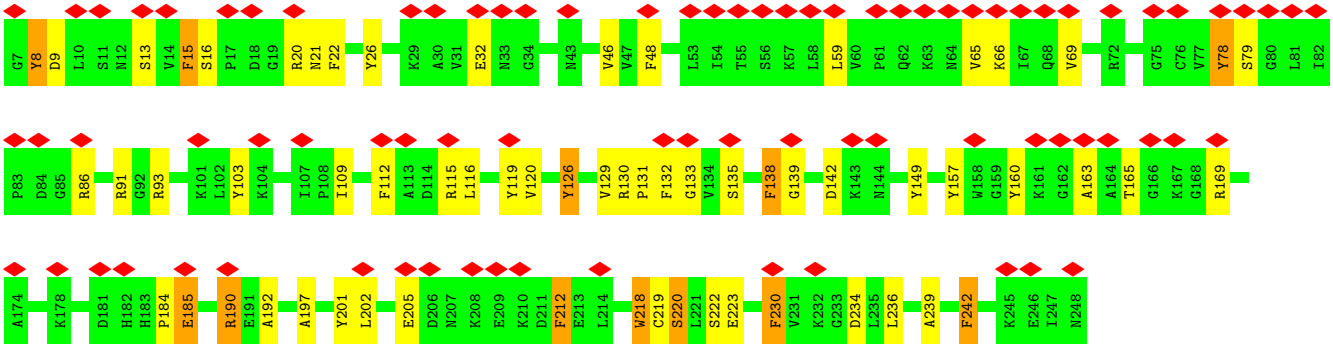
Chain F:





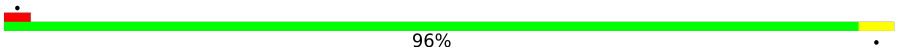
• Molecule 7: Probable proteasome subunit alpha type-7

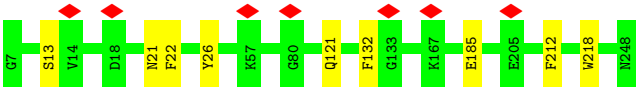
Chain g:



• Molecule 7: Probable proteasome subunit alpha type-7

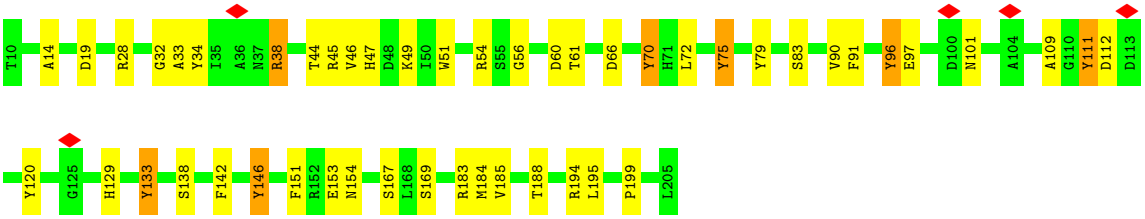
Chain G:





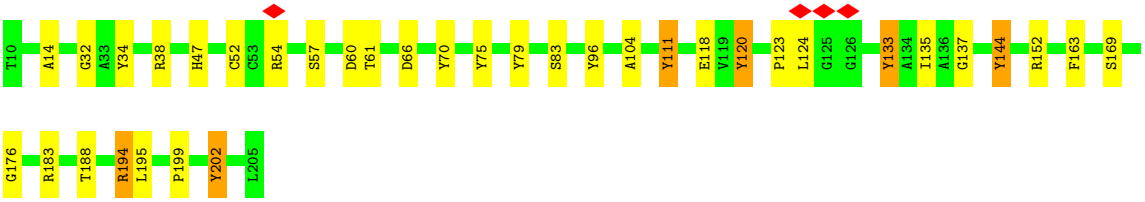
• Molecule 8: Proteasome subunit beta type-1

Chain h:



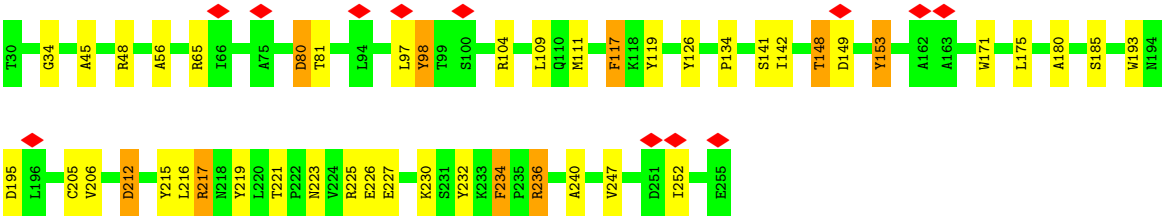
• Molecule 8: Proteasome subunit beta type-1

Chain 1:



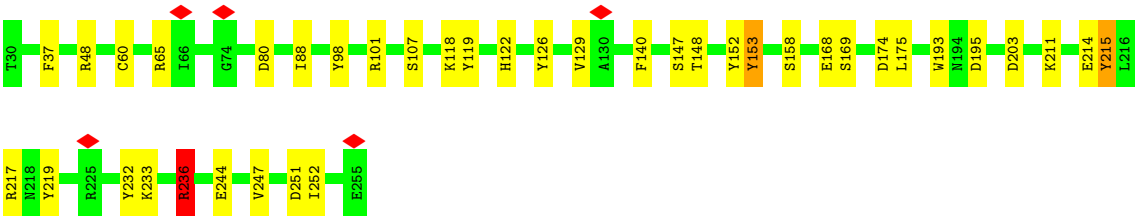
• Molecule 9: Proteasome subunit beta type-2

Chain i:



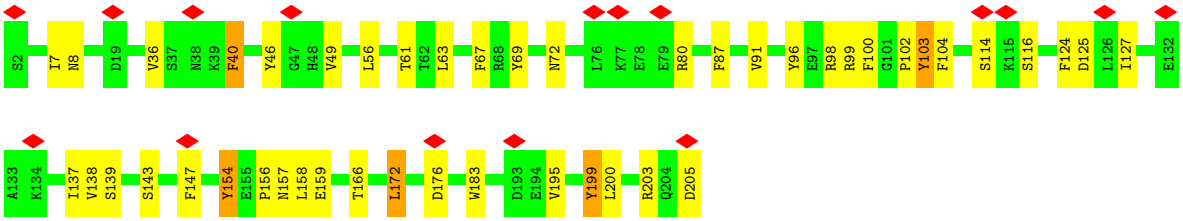
• Molecule 9: Proteasome subunit beta type-2

Chain 2:



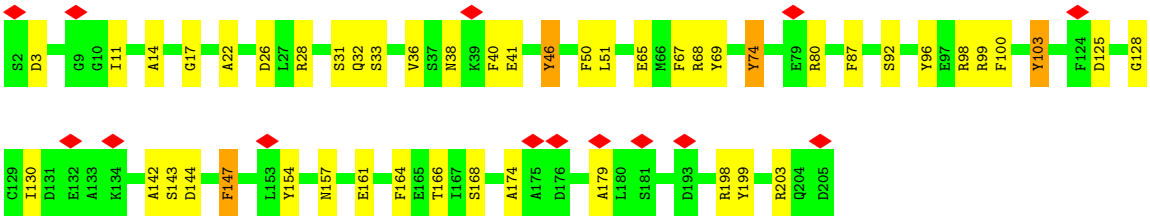
• Molecule 10: Proteasome subunit beta type-3

Chain j:



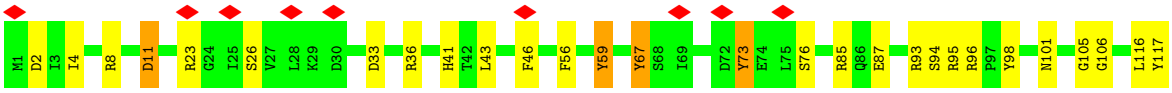
• Molecule 10: Proteasome subunit beta type-3

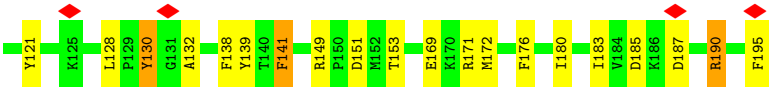
Chain 3:



• Molecule 11: Proteasome subunit beta type-4

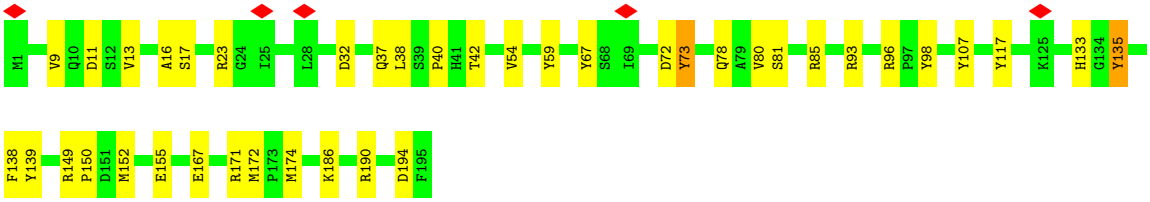
Chain k:





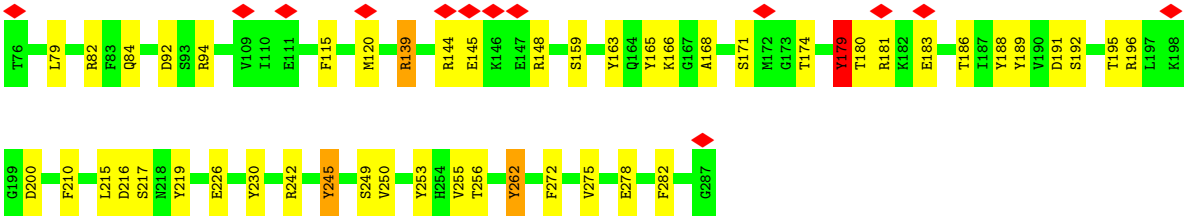
• Molecule 11: Proteasome subunit beta type-4

Chain 4:



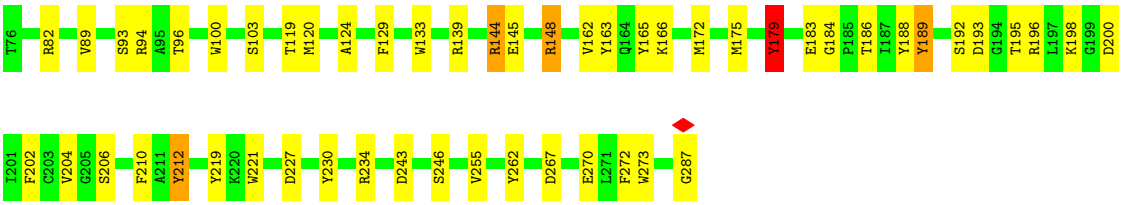
• Molecule 12: Proteasome subunit beta type-5

Chain l:



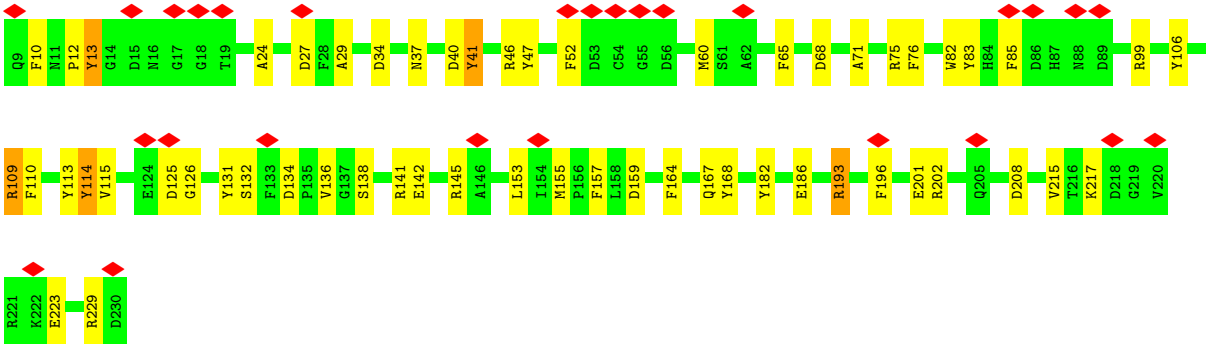
• Molecule 12: Proteasome subunit beta type-5

Chain 5:



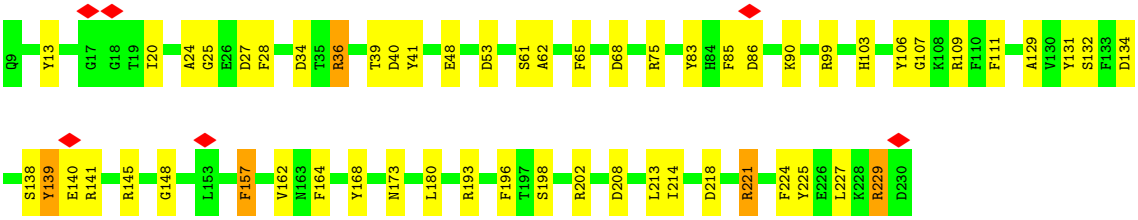
• Molecule 13: Proteasome subunit beta type-6

Chain m:



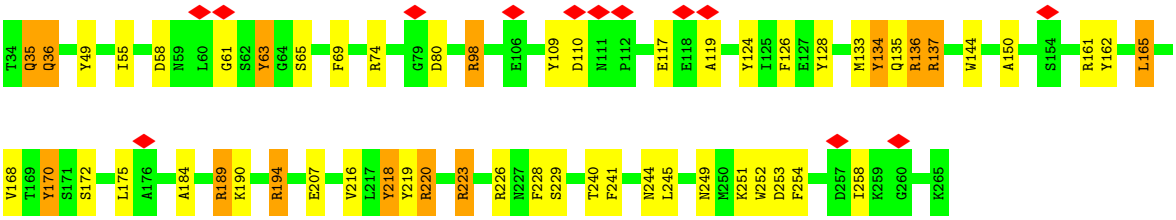
• Molecule 13: Proteasome subunit beta type-6

Chain 6:



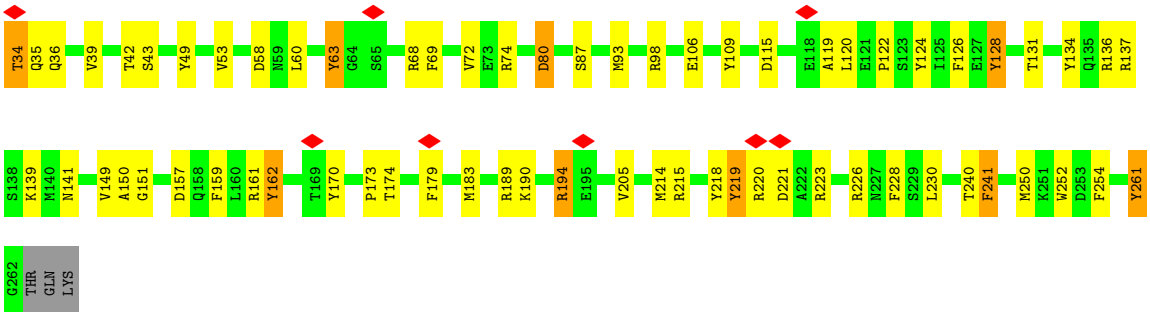
• Molecule 14: Proteasome subunit beta type-7

Chain n:



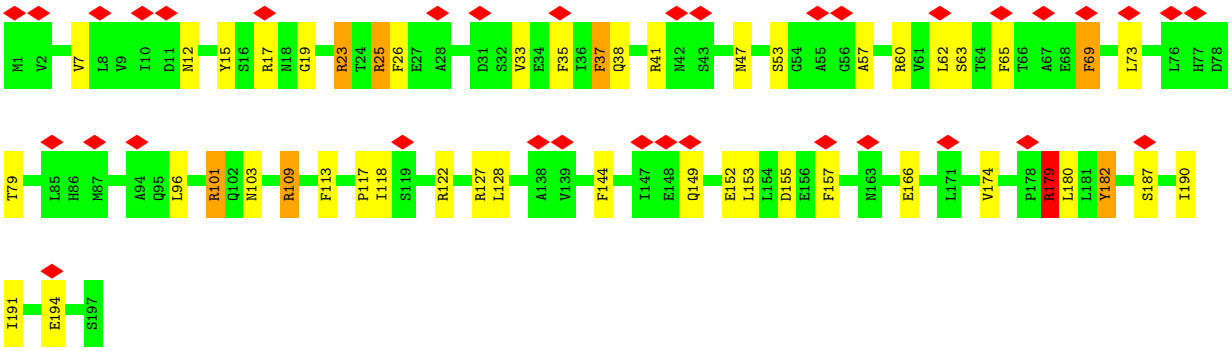
• Molecule 14: Proteasome subunit beta type-7

Chain 7:



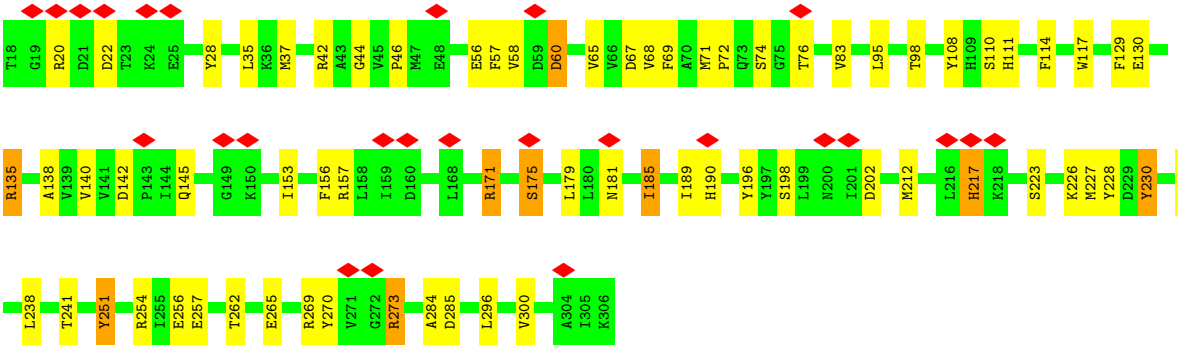
• Molecule 15: 26S proteasome regulatory subunit RPN10

Chain W:



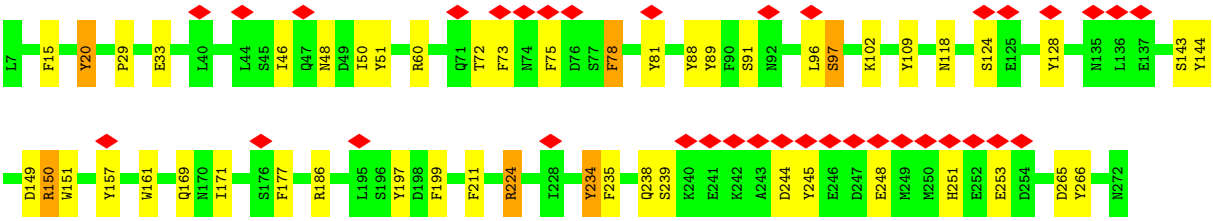
• Molecule 16: Ubiquitin carboxyl-terminal hydrolase RPN11

Chain V:



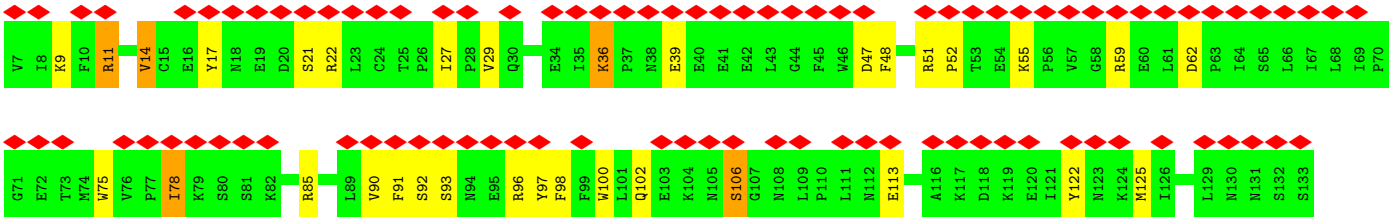
• Molecule 17: 26S proteasome regulatory subunit RPN12

Chain T:



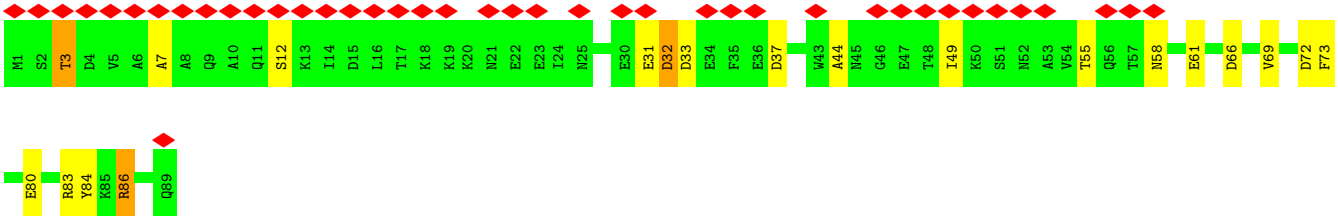
• Molecule 18: 26S proteasome regulatory subunit RPN13

Chain X:



• Molecule 19: 26S proteasome complex subunit SEM1

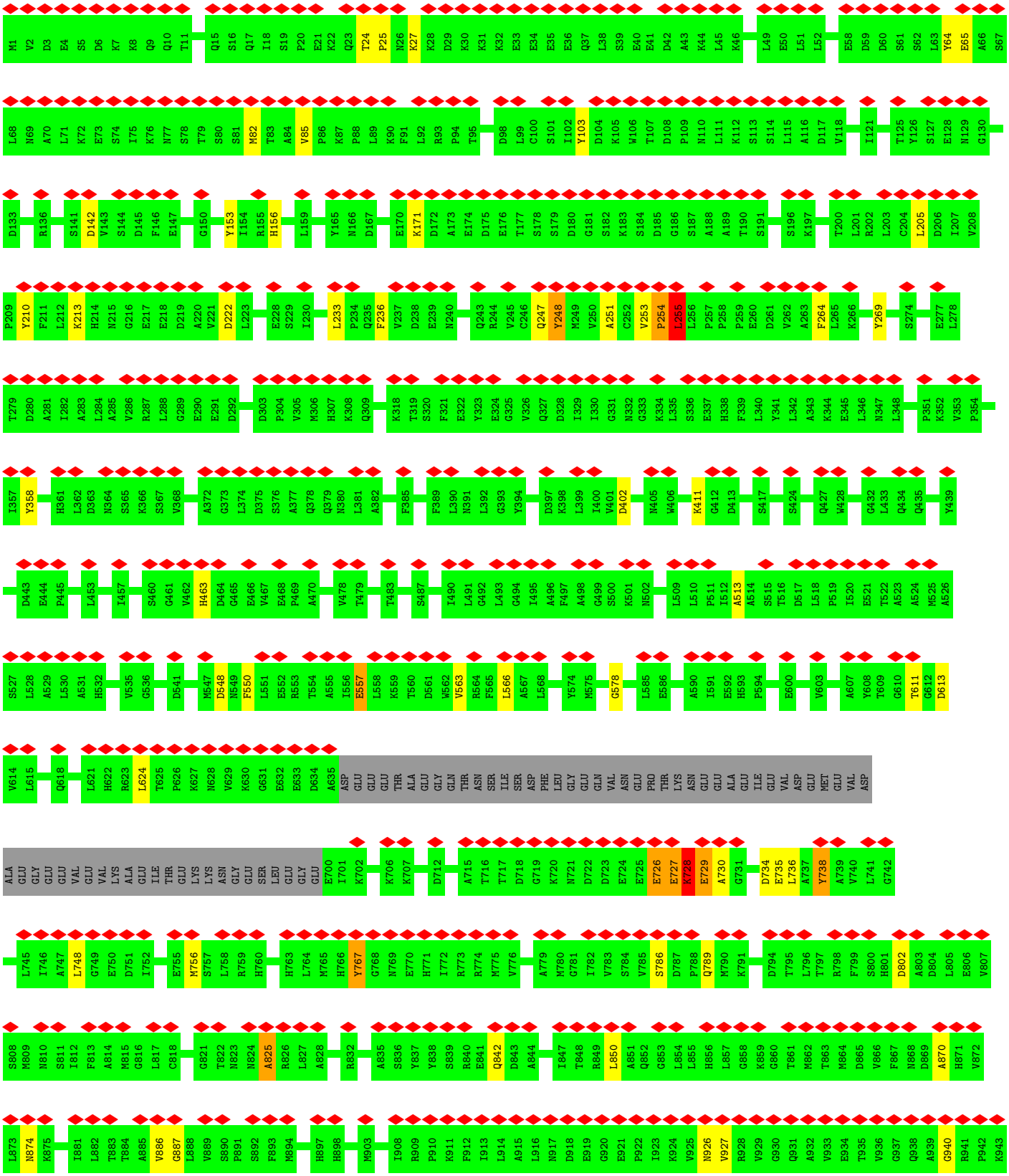
Chain Y:

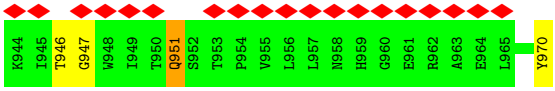


• Molecule 20: 26S proteasome regulatory subunit RPN1

Chain Z:

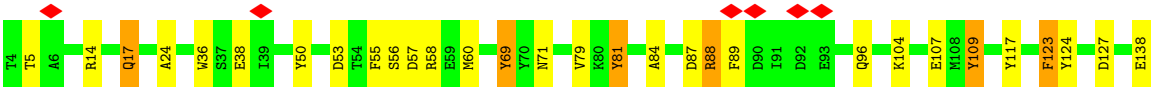
59%
86%
6%
7%

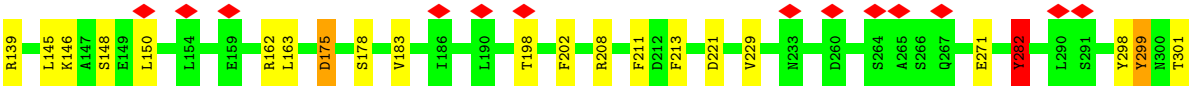

M1 V2 D3 E4 S5 D6 K7 K8 Q9 Q10 T11 Q15 S16 Q17 T18 S19 P20 E21 K22 Q23 T24 P25 N26 K27 K28 D29 K30 K31 K32 E33 E34 E35 E36 Q37 L38 S39 E40 E41 D42 A43 K44 L45 K46 L49 E50 L51 L52 E58 D59 D60 S61 S62 L63 Y64 E65 A66 S67
L68 N69 A70 L71 K72 E73 S74 I75 K76 N77 S78 T79 S80 S81 M82 T83 A84 V85 P86 K87 P88 L89 K90 F91 L92 R93 P94 T95 D98 L99 C100 S101 I102 Y103 D104 K105 W106 T107 D108 P109 N110 L111 K112 S113 S114 L115 A116 D117 V118 I121 T125 Y126 S127 E128 N129 G130
D133 R136 S141 D142 V143 S144 D145 F146 E147 G150 Y153 I154 R155 H156 L159 Y165 N166 D167 E170 K171 D172 A173 E174 D175 E176 T177 S178 S179 D180 G181 S182 K183 S184 D185 G186 S187 A188 A189 T190 S191 S196 K197 T200 L201 R202 L203 C204 L205 D206 I207 V208
P209 Y210 F211 L212 K213 H214 N215 G216 E217 E218 D219 A220 V221 D222 L223 E228 S229 I230 L233 P234 Q235 F236 V237 D238 E239 N240 Q243 R244 V245 C246 Q247 Y248 M249 V250 A251 C252 V253 P254 L255 L256 P257 P258 P259 E260 D261 V262 A263 F264 L265 K266 Y269 S274 E277 L278
T279 D280 A281 I282 A283 L284 A285 V286 R287 L288 G289 E290 E291 D292 D303 P304 V305 M306 H307 K308 Q309 K318 T319 S320 F321 E322 Y323 E324 G325 V326 Q327 D328 I329 I330 G331 N332 G333 K334 L335 S336 E337 H338 F339 L340 Y341 L342 A343 K344 E345 L346 N347 L348 P351 K352 V353 P354
I357 Y358 H361 L362 D363 N364 S365 K366 S367 V368 A372 G373 L374 D375 S376 A377 Q378 Q379 N380 L381 A382 F385 F389 L390 N391 L392 G393 Y394 D397 K398 L399 I400 V401 D402 N405 W406 K411 G412 D413 S417 S424 Q427 W428 G432 L433 Q434 Q435 Y439
D443 E444 P445 L453 I457 S460 G461 V462 H463 D464 G465 E466 V467 E468 P469 A470 V478 T479 T483 S487 I490 L491 G492 L493 G494 I495 A496 F497 A498 G499 S500 K501 N502 L509 L510 P511 I512 A513 A514 S515 T516 D517 L518 P519 I520 E521 T522 A523 A524 M525 A526
S527 L528 A529 L530 A531 H532 V535 G536 D541 M547 D548 N549 F550 L551 E552 R553 T554 A555 I556 E557 L558 K559 T560 D561 W562 V563 R564 F565 L566 A567 L568 Y574 M575 G578 L585 E586 A590 I591 E592 H593 P594 E600 V603 A607 Y608 T609 G610 T611 G612 D613
V614 L615 Q618 L621 H622 R623 L624 T625 P626 K627 N628 V629 K630 G631 E632 E633 D634 A635 ASP GLU GLU GLU THR ALA GLU GLY GLN THR ASN SER ILE SER ASP PHE LEU GLY GLU GLN VAL ASN GLU PRO THR LYS ASN GLU GLU ALA GLU ILE GLU VAL ASP GLU MET GLU VAL ASP
ALA GLU GLY GLU GLU VAL GLU VAL LYS ALA GLU ILE THR GLU LYS LYS ASN GLY GLU SER LEU GLU GLY GLU E700 I701 K702 K706 K707 D712 A715 T716 T717 D718 G719 K720 N721 D722 D723 E724 E725 E726 E727 K728 E729 A730 G731 D734 E735 L736 A737 Y738 A739 V740 L741 G742
L745 I746 A747 L748 G749 E750 D751 I752 E755 M756 S757 L758 R759 H760 H763 L764 M765 H766 Y767 G768 N769 E770 H771 I772 R773 R774 M775 V776 A779 M780 G781 I782 V783 S784 V785 S786 D787 P788 Q789 M790 K791 D794 T795 L796 T797 R798 F799 S800 H801 D802 A803 D804 L805 E806 V807
S808 M809 N810 S811 I812 F813 A814 M815 G816 L817 C818 G821 T822 N823 N824 A825 R826 L827 A828 R832 A835 S836 Y837 Y838 S839 R840 E841 Q842 D843 A844 I847 T848 R849 L850 A851 Q852 G853 L854 L855 H856 L857 G858 K859 G860 T861 M862 T863 M864 D865 V866 F867 N868 D869 A870 H871 V872
L873 N874 K875 I881 L882 T883 T884 A885 V886 G887 L888 V889 S890 P891 S892 F893 M894 H897 H898 M903 I908 R909 P910 K911 F912 I913 L914 A915 L916 N917 D918 E919 G920 E921 P922 I923 K924 V925 N926 V927 R928 V929 G930 Q931 A932 V933 E934 T935 V936 G937 Q938 A939 G940 R941 P942 K943

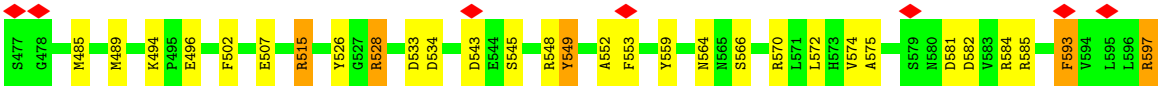


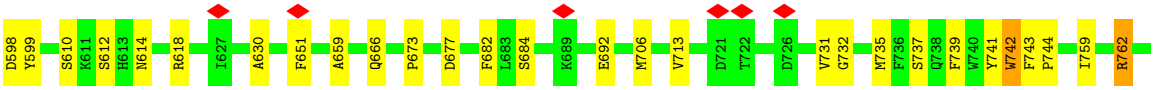
• Molecule 21: 26S proteasome regulatory subunit RPN2

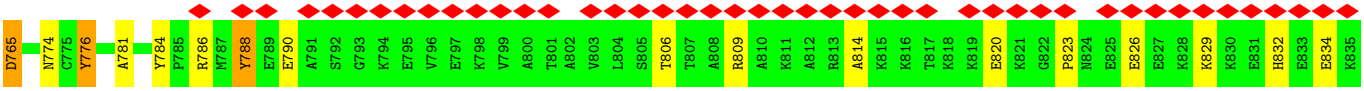
Chain N:

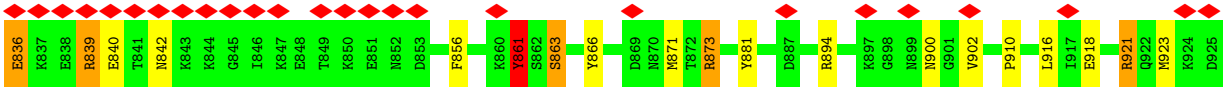






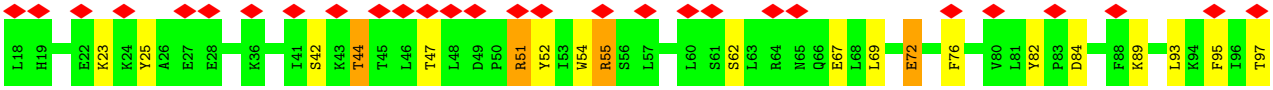


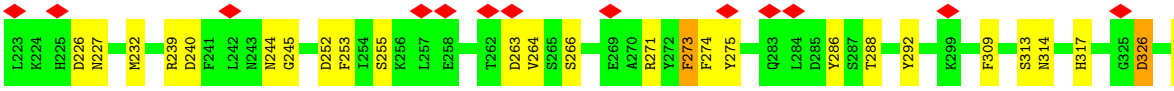


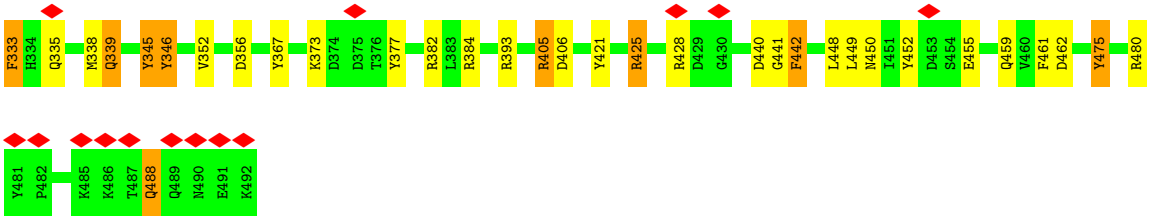


• Molecule 22: 26S proteasome regulatory subunit RPN3

Chain S:

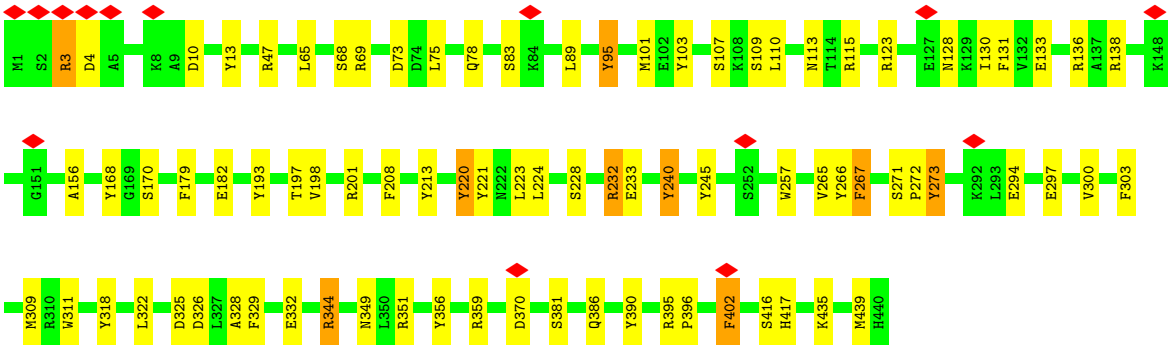






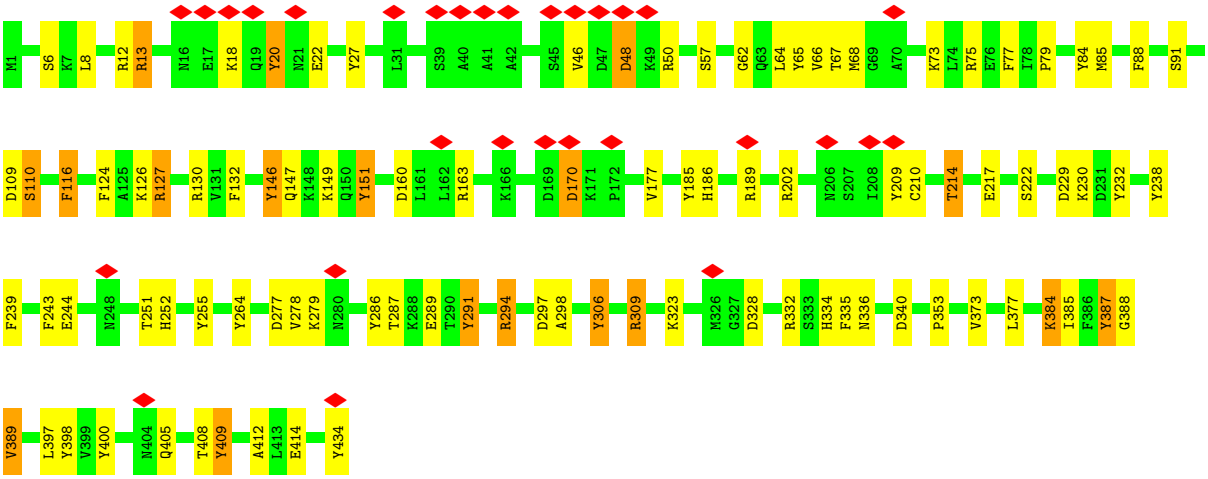
• Molecule 23: 26S proteasome regulatory subunit RPN5

Chain P:



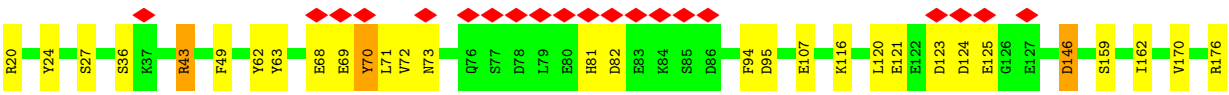
• Molecule 24: 26S proteasome regulatory subunit RPN6

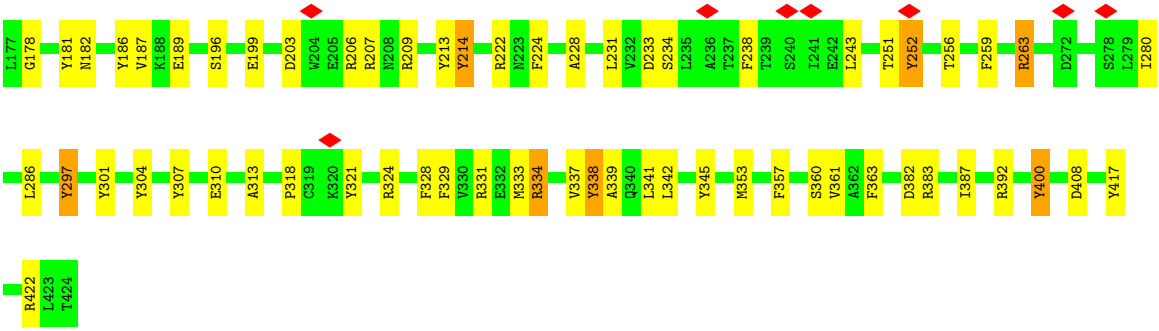
Chain Q:



• Molecule 25: 26S proteasome regulatory subunit RPN7

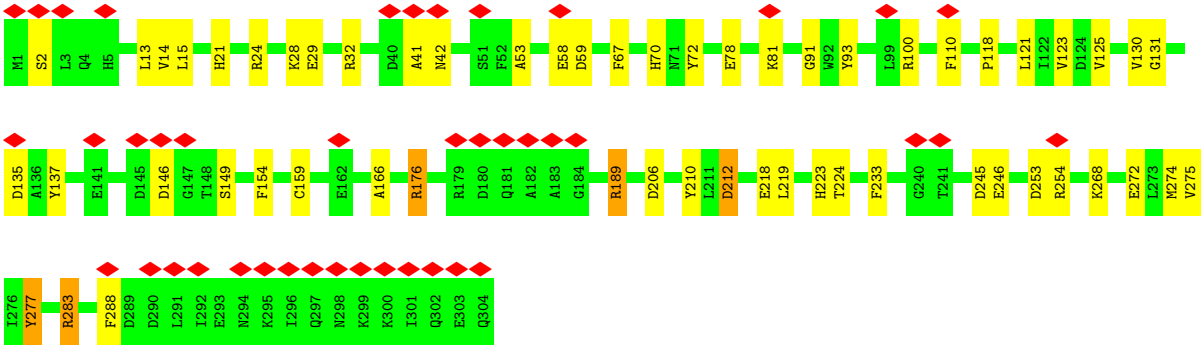
Chain R:





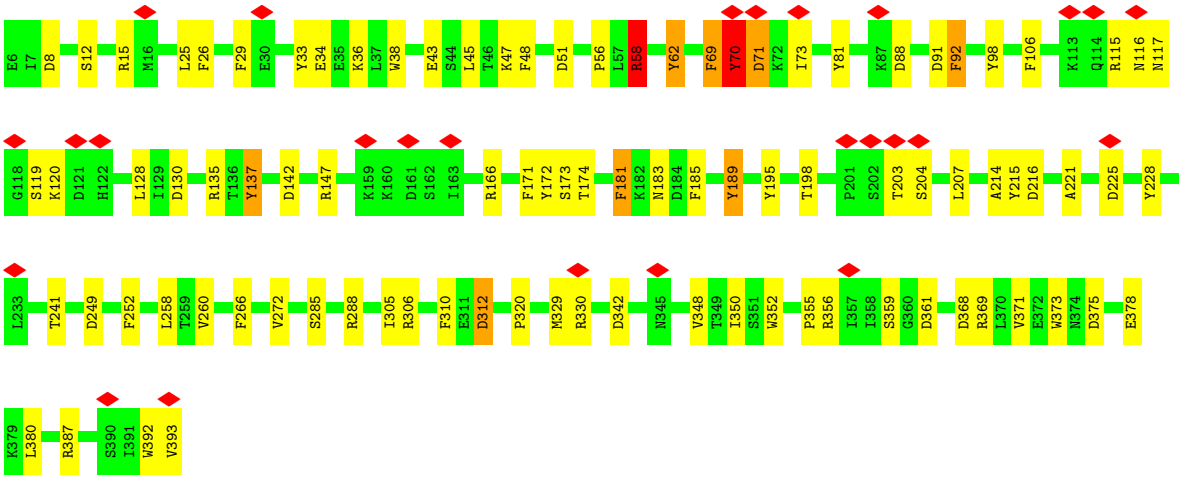
- Molecule 26: 26S proteasome regulatory subunit RPN8

Chain U:



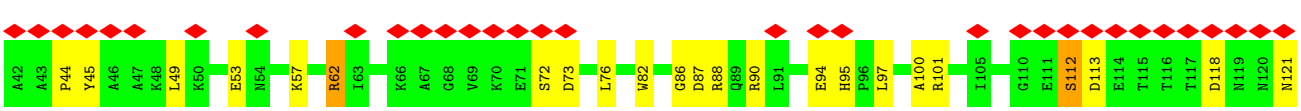
- Molecule 27: 26S proteasome regulatory subunit RPN9

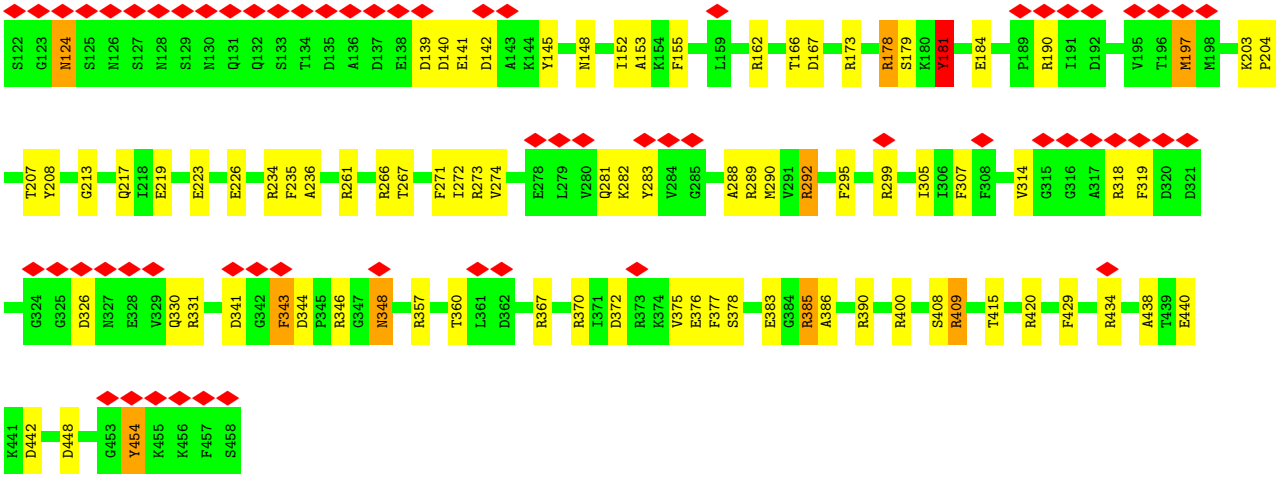
Chain O:



- Molecule 28: 26S proteasome regulatory subunit 7 homolog

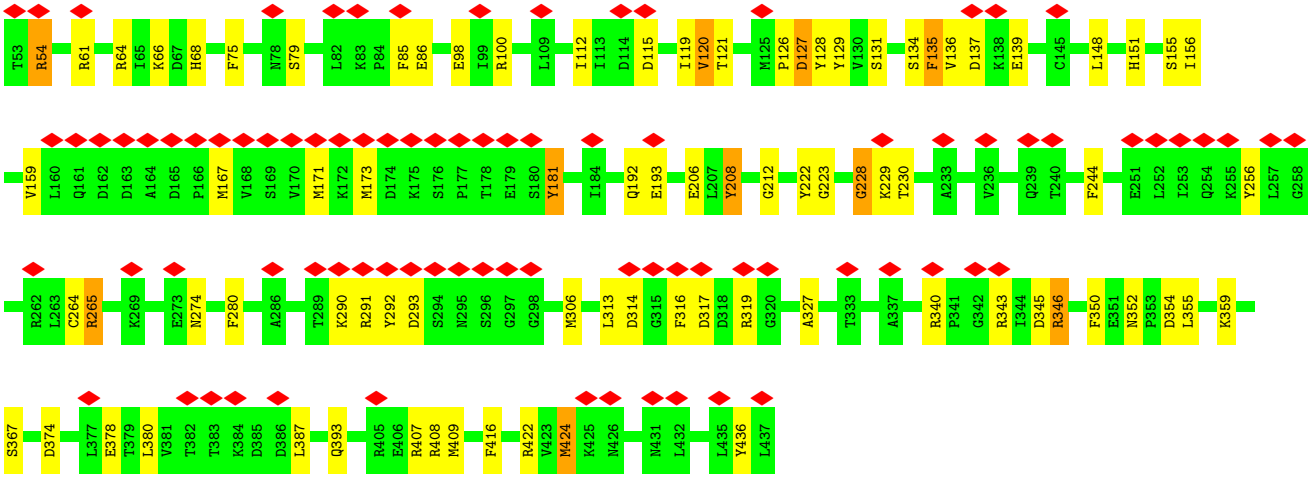
Chain H:





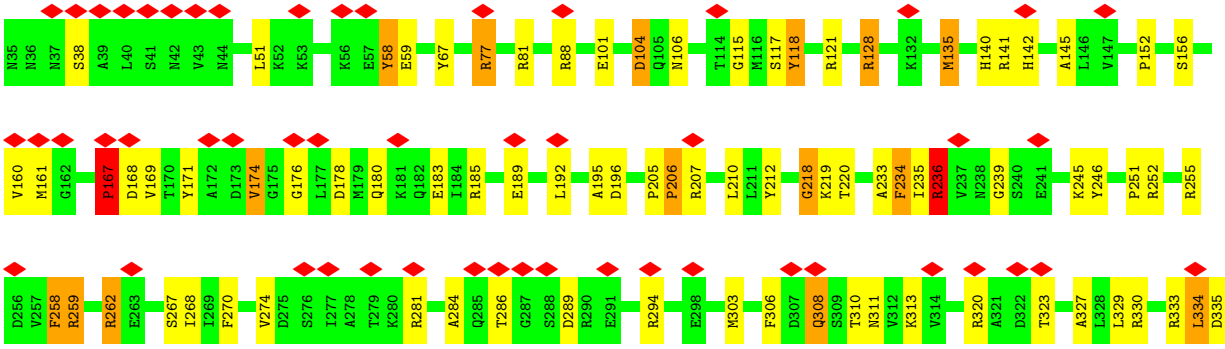
• Molecule 29: 26S proteasome regulatory subunit 4 homolog

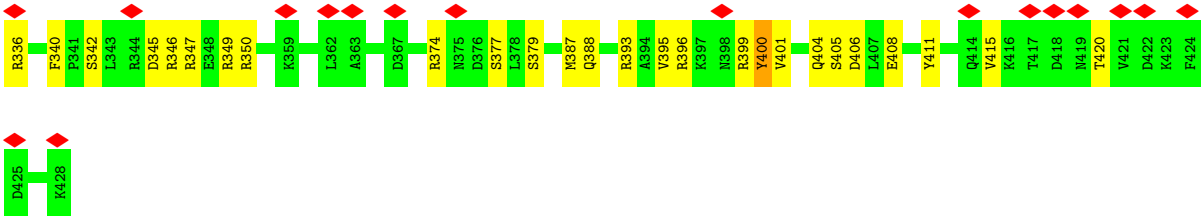
Chain I:



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

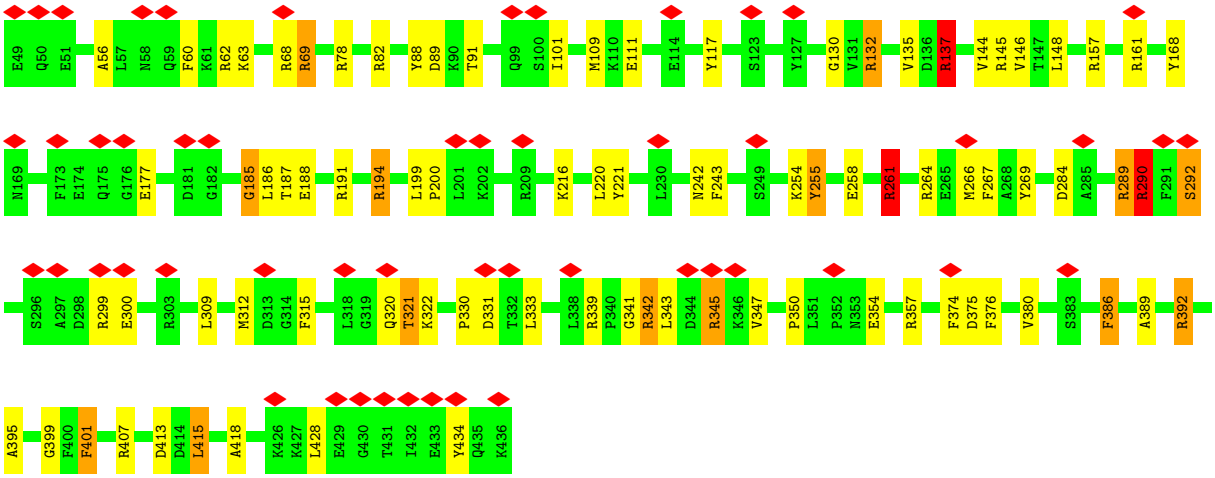
Chain K:





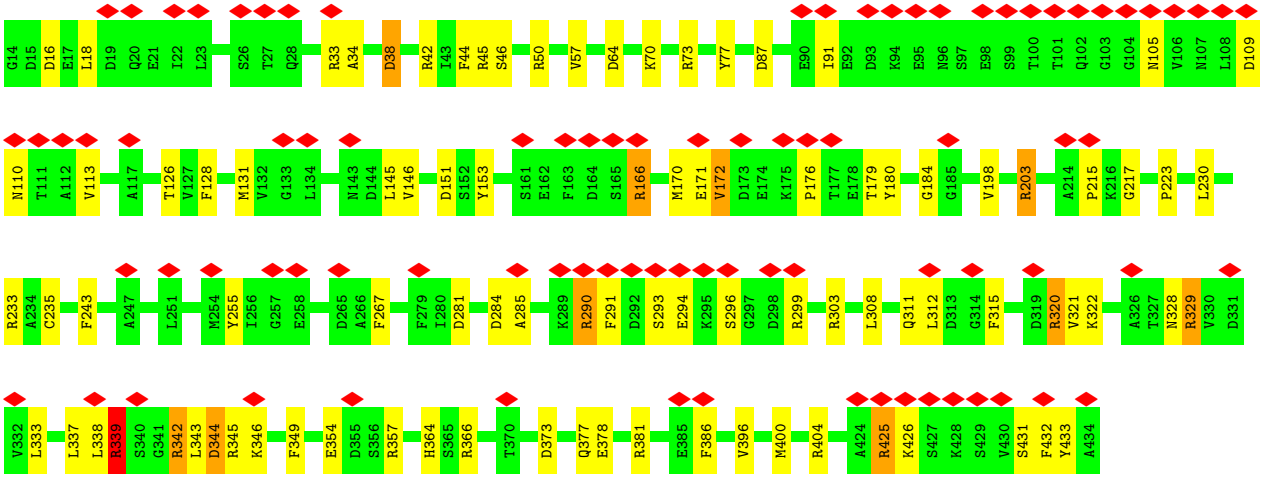
• Molecule 31: 26S proteasome subunit RPT4

Chain L:



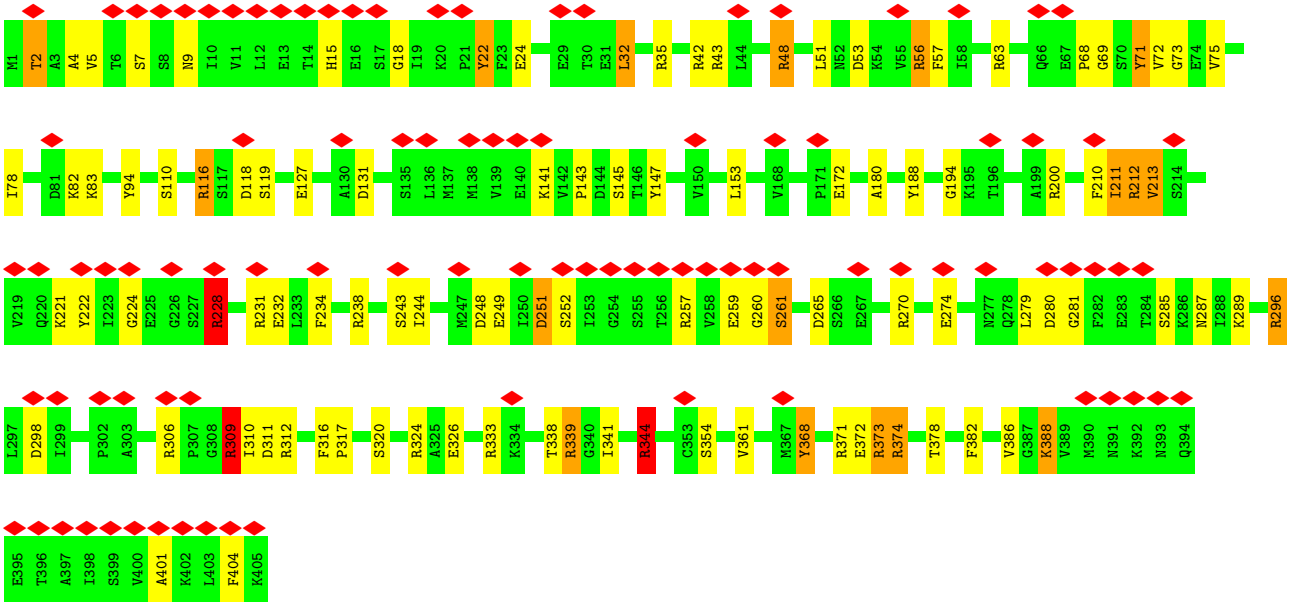
• Molecule 32: 26S proteasome regulatory subunit 6A

Chain M:



• Molecule 33: 26S proteasome regulatory subunit 8 homolog

Chain J:


M1 T2 A3 A4 V5 T6 S7 S8 N9 I10 V11 L12 E13 T14 H15 E16 S17 G18 I19 K20 P21 Y22 F23 E24 E29 T30 E31 L32 R35 R42 R43 L44 R48 L51 N52 D53 K54 V55 R56 F57 I58 R63 Q66 E67 P68 G69 S70 Y71 V72 G73 E74 V75
I78 D81 K82 K83 Y94 S110 R116 S117 D118 S119 E127 A130 D131 S135 L136 M137 M138 V139 E140 K141 V142 P143 D144 S145 T146 Y147 V150 L153 V168 P171 E172 A180 Y188 G194 K195 T196 A199 R200 F210 I211 R212 V213 S214
V219 Q220 K221 Y222 I223 G224 E225 G226 S227 R228 R231 E232 L233 F234 R238 S243 I244 M247 D248 E249 I250 D251 S252 I253 G254 S255 T256 R257 V258 E259 G260 S261 D265 S266 E267 R270 E274 N277 Q278 L279 D280 G281 F282 E283 T284 S285 K286 N287 I288 K289 R296
L297 D298 I299 P302 A303 R306 P307 G308 R309 I310 D311 R312 F316 P317 S320 R324 A325 E326 R333 K334 T338 R339 G340 I341 R344 C353 S354 V361 M367 Y368 R371 E372 R373 R374 T378 F382 V386 G387 K388 V389 M390 N391 K392 N393 Q394
E395 T396 A397 I398 S399 V400 A401 K402 L403 F404 K405

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	292279	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	35	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.086	Depositor
Minimum map value	-0.048	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.01	Depositor
Map size (Å)	529.92, 529.92, 529.92	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.38, 1.38, 1.38	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.93	0/1946	0.97	2/2634 (0.1%)
1	a	1.71	14/1946 (0.7%)	1.88	37/2634 (1.4%)
2	B	0.91	0/1944	0.96	1/2632 (0.0%)
2	b	1.73	15/1944 (0.8%)	1.90	44/2632 (1.7%)
3	C	0.94	0/1935	0.96	4/2618 (0.2%)
3	c	1.77	20/1935 (1.0%)	2.02	58/2618 (2.2%)
4	D	0.96	0/1888	0.96	2/2557 (0.1%)
4	d	1.75	19/2012 (0.9%)	1.93	38/2718 (1.4%)
5	E	1.70	2/1909 (0.1%)	1.32	7/2571 (0.3%)
5	e	1.71	23/1909 (1.2%)	1.86	34/2571 (1.3%)
6	F	0.95	0/1800	0.97	3/2433 (0.1%)
6	f	1.76	23/1800 (1.3%)	1.99	52/2433 (2.1%)
7	G	0.93	0/1926	1.20	6/2599 (0.2%)
7	g	1.73	21/1926 (1.1%)	2.10	54/2599 (2.1%)
8	1	1.72	16/1541 (1.0%)	1.85	25/2087 (1.2%)
8	h	1.73	14/1541 (0.9%)	1.90	41/2087 (2.0%)
9	2	1.74	21/1751 (1.2%)	1.87	31/2373 (1.3%)
9	i	1.75	17/1751 (1.0%)	1.93	35/2373 (1.5%)
10	3	1.74	18/1611 (1.1%)	1.94	42/2174 (1.9%)
10	j	1.71	10/1611 (0.6%)	1.94	41/2174 (1.9%)
11	4	1.73	9/1590 (0.6%)	1.90	28/2142 (1.3%)
11	k	1.76	19/1590 (1.2%)	1.95	39/2142 (1.8%)
12	5	1.75	23/1681 (1.4%)	1.92	41/2274 (1.8%)
12	l	1.77	16/1681 (1.0%)	2.05	48/2274 (2.1%)
13	6	1.76	16/1795 (0.9%)	2.00	51/2420 (2.1%)
13	m	1.74	20/1795 (1.1%)	2.05	52/2420 (2.1%)
14	7	1.72	15/1821 (0.8%)	2.03	61/2470 (2.5%)
14	n	1.73	18/1847 (1.0%)	2.07	52/2503 (2.1%)
15	W	1.71	16/1558 (1.0%)	1.94	39/2111 (1.8%)
16	V	1.69	21/2309 (0.9%)	1.95	61/3115 (2.0%)
17	T	1.70	16/2236 (0.7%)	1.89	44/3017 (1.5%)
18	X	1.74	6/1059 (0.6%)	1.98	33/1432 (2.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
19	Y	1.65	4/741 (0.5%)	1.98	15/1000 (1.5%)
20	Z	1.34	16/7123 (0.2%)	1.29	62/9645 (0.6%)
21	N	1.71	48/7273 (0.7%)	1.89	159/9822 (1.6%)
22	S	1.69	32/3967 (0.8%)	1.87	81/5355 (1.5%)
23	P	1.66	25/3664 (0.7%)	1.87	71/4940 (1.4%)
24	Q	1.70	30/3556 (0.8%)	1.93	88/4787 (1.8%)
25	R	1.72	26/3314 (0.8%)	1.97	93/4469 (2.1%)
26	U	1.67	16/2461 (0.7%)	1.82	42/3327 (1.3%)
27	O	1.70	30/3247 (0.9%)	1.95	82/4380 (1.9%)
28	H	1.73	29/3282 (0.9%)	1.94	88/4423 (2.0%)
29	I	1.69	28/3059 (0.9%)	1.87	66/4115 (1.6%)
30	K	1.75	37/3156 (1.2%)	2.19	89/4261 (2.1%)
31	L	1.73	33/3128 (1.1%)	2.22	90/4201 (2.1%)
32	M	2.68	30/3323 (0.9%)	2.13	81/4478 (1.8%)
33	J	1.91	44/3212 (1.4%)	2.14	86/4316 (2.0%)
All	All	1.68	856/112094 (0.8%)	1.84	2299/151356 (1.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	a	0	9
2	b	0	3
3	c	0	5
4	D	0	1
4	d	0	5
5	e	0	3
6	F	0	1
6	f	0	6
7	G	0	2
7	g	0	12
8	1	0	6
8	h	0	8
9	2	0	4
9	i	0	6
10	3	0	4
10	j	0	4
11	4	0	6
11	k	0	4
12	5	0	6

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Mol	Chain	#Chirality outliers	#Planarity outliers
12	l	0	5
13	6	0	9
13	m	0	6
14	7	0	5
14	n	0	12
15	W	0	7
16	V	0	6
17	T	0	10
18	X	0	2
19	Y	0	1
20	Z	0	9
21	N	0	24
22	S	0	18
23	P	0	16
24	Q	0	13
25	R	0	11
26	U	0	6
27	O	0	9
28	H	0	13
29	I	0	9
30	K	0	19
31	L	0	18
32	M	0	13
33	J	0	15
All	All	0	351

All (856) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	E	20	ARG	NE-CZ	62.28	2.14	1.33
32	M	433	TYR	CE2-CZ	51.52	2.05	1.38
32	M	433	TYR	CG-CD1	51.22	2.05	1.39
32	M	433	TYR	CG-CD2	50.39	2.04	1.39
32	M	433	TYR	CE1-CZ	48.44	2.01	1.38
20	Z	728	LYS	CG-CD	46.45	3.10	1.52
32	M	433	TYR	CD2-CE2	45.63	2.07	1.39
32	M	433	TYR	CD1-CE1	45.25	2.07	1.39
20	Z	738	TYR	CZ-OH	43.53	2.11	1.37
33	J	211	ILE	C-N	-35.48	0.52	1.34
20	Z	728	LYS	CA-CB	27.41	2.14	1.53
33	J	309	ARG	CA-CB	-21.10	1.07	1.53
20	Z	255	LEU	CB-CG	20.29	2.11	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
20	Z	728	LYS	CD-CE	19.80	2.00	1.51
30	K	220	THR	C-N	-18.57	0.91	1.34
20	Z	728	LYS	CB-CG	18.10	2.01	1.52
20	Z	728	LYS	CA-C	16.67	1.96	1.52
32	M	338	LEU	C-N	15.23	1.69	1.34
33	J	212	ARG	C-N	14.86	1.68	1.34
20	Z	728	LYS	CE-NZ	14.81	1.86	1.49
14	n	252	TRP	NE1-CE2	10.33	1.50	1.37
11	k	94	SER	CA-CB	9.50	1.67	1.52
32	M	303	ARG	NE-CZ	9.45	1.45	1.33
9	2	107	SER	CA-CB	9.34	1.67	1.52
20	Z	728	LYS	C-N	9.13	1.55	1.34
20	Z	729	GLU	N-CA	9.11	1.64	1.46
30	K	294	ARG	NE-CZ	9.07	1.44	1.33
3	c	5	ARG	NE-CZ	9.02	1.44	1.33
25	R	43	ARG	NE-CZ	9.01	1.44	1.33
29	I	367	SER	CA-CB	8.96	1.66	1.52
3	c	20	TYR	CG-CD1	8.92	1.50	1.39
19	Y	12	SER	CA-CB	8.91	1.66	1.52
24	Q	62	GLY	N-CA	-8.90	1.32	1.46
17	T	124	SER	CA-CB	8.87	1.66	1.52
20	Z	255	LEU	CG-CD1	-8.79	1.19	1.51
24	Q	238	TYR	CZ-OH	8.75	1.52	1.37
10	3	92	SER	CA-CB	8.71	1.66	1.52
5	E	20	ARG	CD-NE	8.68	1.61	1.46
24	Q	309	ARG	NE-CZ	8.55	1.44	1.33
21	N	178	SER	CA-CB	8.50	1.65	1.52
9	2	126	TYR	CG-CD1	8.29	1.50	1.39
21	N	836	GLU	CD-OE1	8.25	1.34	1.25
17	T	199	PHE	CG-CD2	8.21	1.51	1.38
22	S	196	ARG	CZ-NH1	8.21	1.43	1.33
28	H	273	ARG	NE-CZ	8.07	1.43	1.33
11	k	105	GLY	CA-C	-8.03	1.39	1.51
9	i	126	TYR	CB-CG	-8.03	1.39	1.51
14	7	106	GLU	CD-OE1	7.95	1.34	1.25
26	U	272	GLU	CD-OE2	7.94	1.34	1.25
4	d	97	ARG	CD-NE	7.81	1.59	1.46
2	b	242	GLU	CG-CD	7.78	1.63	1.51
11	k	106	GLY	CA-C	-7.77	1.39	1.51
9	i	141	SER	CA-CB	7.62	1.64	1.52
10	3	128	GLY	CA-C	-7.62	1.39	1.51
7	g	201	TYR	CE1-CZ	7.55	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	243	SER	CA-CB	7.54	1.64	1.52
3	c	92	ARG	CZ-NH2	7.53	1.42	1.33
24	Q	202	ARG	CD-NE	7.50	1.59	1.46
23	P	294	GLU	CG-CD	7.49	1.63	1.51
18	X	92	SER	CA-CB	7.48	1.64	1.52
26	U	176	ARG	CZ-NH2	7.47	1.42	1.33
6	f	101	ARG	CZ-NH2	7.45	1.42	1.33
31	L	185	GLY	C-N	7.41	1.51	1.34
15	W	15	TYR	CG-CD2	7.40	1.48	1.39
23	P	3	ARG	NE-CZ	7.40	1.42	1.33
28	H	385	ARG	CZ-NH1	7.37	1.42	1.33
7	g	16	SER	CA-CB	7.35	1.64	1.52
6	f	71	GLY	N-CA	-7.33	1.35	1.46
22	S	345	TYR	CG-CD2	-7.31	1.29	1.39
12	5	183	GLU	CG-CD	7.27	1.62	1.51
22	S	271	ARG	CD-NE	7.26	1.58	1.46
23	P	332	GLU	CB-CG	7.23	1.65	1.52
32	M	299	ARG	CZ-NH2	7.20	1.42	1.33
11	k	139	TYR	CE2-CZ	7.20	1.48	1.38
32	M	42	ARG	NE-CZ	7.17	1.42	1.33
9	i	48	ARG	NE-CZ	7.14	1.42	1.33
32	M	293	SER	CA-CB	7.12	1.63	1.52
28	H	434	ARG	CZ-NH1	7.11	1.42	1.33
27	O	147	ARG	CZ-NH1	7.10	1.42	1.33
29	I	79	SER	CA-CB	7.10	1.63	1.52
17	T	248	GLU	CB-CG	7.09	1.65	1.52
28	H	378	SER	CA-CB	7.09	1.63	1.52
21	N	394	ARG	NE-CZ	7.06	1.42	1.33
5	e	132	ARG	CD-NE	7.06	1.58	1.46
9	2	158	SER	CA-CB	7.04	1.63	1.52
30	K	212	TYR	CG-CD2	7.03	1.48	1.39
29	I	64	ARG	NE-CZ	7.02	1.42	1.33
14	n	98	ARG	CZ-NH1	7.01	1.42	1.33
12	5	196	ARG	CZ-NH1	6.98	1.42	1.33
21	N	737	SER	CA-CB	6.98	1.63	1.52
32	M	342	ARG	C-N	-6.96	1.18	1.34
12	5	100	TRP	CB-CG	6.94	1.62	1.50
4	d	6	ARG	CD-NE	6.94	1.58	1.46
23	P	3	ARG	CZ-NH2	6.94	1.42	1.33
3	c	18	ARG	NE-CZ	6.93	1.42	1.33
5	e	139	GLY	N-CA	-6.93	1.35	1.46
9	i	225	ARG	NE-CZ	6.92	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	S	119	TYR	CZ-OH	6.91	1.49	1.37
21	N	84	ALA	N-CA	-6.90	1.32	1.46
8	h	51	TRP	CD2-CE3	-6.90	1.30	1.40
22	S	441	GLY	N-CA	-6.89	1.35	1.46
30	K	349	ARG	NE-CZ	6.89	1.42	1.33
31	L	132	ARG	CZ-NH2	6.88	1.42	1.33
21	N	549	TYR	CG-CD1	6.88	1.48	1.39
29	I	61	ARG	CZ-NH2	6.88	1.42	1.33
1	a	186	PHE	CG-CD1	6.84	1.49	1.38
3	c	143	ARG	NE-CZ	6.84	1.42	1.33
32	M	354	GLU	CG-CD	6.84	1.62	1.51
29	I	422	ARG	NE-CZ	6.84	1.42	1.33
11	4	17	SER	CA-CB	6.83	1.63	1.52
8	h	38	ARG	CZ-NH2	6.82	1.42	1.33
7	g	184	PRO	N-CD	-6.78	1.38	1.47
10	3	98	ARG	NE-CZ	6.76	1.41	1.33
9	2	119	TYR	CE2-CZ	6.75	1.47	1.38
12	5	129	PHE	CG-CD1	6.75	1.48	1.38
23	P	103	TYR	CE2-CZ	6.75	1.47	1.38
29	I	193	GLU	CG-CD	6.75	1.62	1.51
30	K	128	ARG	CZ-NH1	6.74	1.41	1.33
6	f	39	ARG	NE-CZ	6.73	1.41	1.33
33	J	238	ARG	NE-CZ	6.72	1.41	1.33
13	m	182	TYR	CG-CD2	6.71	1.47	1.39
21	N	585	ARG	NE-CZ	6.70	1.41	1.33
25	R	27	SER	CA-CB	6.69	1.62	1.52
29	I	222	TYR	CE2-CZ	6.69	1.47	1.38
31	L	290	ARG	NE-CZ	6.67	1.41	1.33
20	Z	738	TYR	CD2-CE2	6.66	1.49	1.39
21	N	36	TRP	CD2-CE2	-6.65	1.33	1.41
1	a	26	TYR	CE1-CZ	6.65	1.47	1.38
28	H	289	ARG	CZ-NH1	6.64	1.41	1.33
16	V	265	GLU	CB-CG	6.62	1.64	1.52
27	O	359	SER	CA-CB	6.61	1.62	1.52
12	l	139	ARG	CZ-NH1	6.61	1.41	1.33
25	R	178	GLY	N-CA	-6.61	1.36	1.46
6	f	106	GLU	CG-CD	6.60	1.61	1.51
21	N	916	LEU	N-CA	-6.58	1.33	1.46
29	I	64	ARG	CZ-NH1	6.58	1.41	1.33
33	J	127	GLU	CG-CD	6.58	1.61	1.51
30	K	115	GLY	CA-C	-6.57	1.41	1.51
10	3	69	TYR	CG-CD1	6.55	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	J	231	ARG	CZ-NH1	6.54	1.41	1.33
28	H	289	ARG	NE-CZ	6.53	1.41	1.33
24	Q	286	TYR	CD2-CE2	6.53	1.49	1.39
8	h	38	ARG	CZ-NH1	6.53	1.41	1.33
23	P	182	GLU	CG-CD	6.52	1.61	1.51
23	P	193	TYR	CZ-OH	6.50	1.48	1.37
1	a	91	ARG	CD-NE	6.49	1.57	1.46
24	Q	387	TYR	CB-CG	6.49	1.61	1.51
27	O	195	TYR	CZ-OH	6.48	1.48	1.37
14	n	69	PHE	CG-CD1	6.47	1.48	1.38
27	O	58	ARG	CD-NE	6.47	1.57	1.46
28	H	299	ARG	NE-CZ	6.46	1.41	1.33
33	J	24	GLU	CD-OE1	6.46	1.32	1.25
30	K	330	ARG	CD-NE	6.45	1.57	1.46
1	a	76	SER	CA-CB	6.45	1.62	1.52
21	N	673	PRO	CA-C	-6.45	1.40	1.52
11	4	135	TYR	CE2-CZ	6.44	1.47	1.38
12	l	94	ARG	CZ-NH1	6.44	1.41	1.33
28	H	383	GLU	CD-OE1	6.44	1.32	1.25
29	I	359	LYS	CD-CE	6.44	1.67	1.51
2	b	53	SER	CA-CB	6.43	1.62	1.52
25	R	360	SER	CA-CB	6.43	1.62	1.52
2	b	82	TYR	CB-CG	6.43	1.61	1.51
22	S	275	TYR	CE1-CZ	6.42	1.46	1.38
8	h	97	GLU	CD-OE1	6.42	1.32	1.25
21	N	298	TYR	CG-CD1	6.41	1.47	1.39
5	e	149	ALA	CA-CB	6.40	1.65	1.52
14	7	218	TYR	CB-CG	-6.40	1.42	1.51
33	J	306	ARG	CZ-NH1	6.40	1.41	1.33
22	S	62	SER	CA-CB	6.38	1.62	1.52
10	3	28	ARG	CD-NE	6.37	1.57	1.46
10	3	147	PHE	C-N	6.37	1.44	1.33
24	Q	12	ARG	CZ-NH1	6.37	1.41	1.33
11	k	85	ARG	CZ-NH1	6.36	1.41	1.33
17	T	143	SER	CA-CB	6.36	1.62	1.52
10	j	96	TYR	CZ-OH	6.35	1.48	1.37
27	O	12	SER	CA-CB	6.34	1.62	1.52
16	V	130	GLU	CB-CG	6.34	1.64	1.52
16	V	44	GLY	N-CA	-6.33	1.36	1.46
4	d	29	ARG	NE-CZ	6.33	1.41	1.33
19	Y	80	GLU	CG-CD	6.32	1.61	1.51
26	U	246	GLU	CD-OE1	6.31	1.32	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	b	4	ARG	CZ-NH2	6.31	1.41	1.33
11	k	121	TYR	CE1-CZ	6.31	1.46	1.38
8	1	111	TYR	N-CA	-6.31	1.33	1.46
13	m	202	ARG	CD-NE	6.30	1.57	1.46
30	K	59	GLU	CG-CD	6.30	1.61	1.51
30	K	152	PRO	N-CD	-6.29	1.39	1.47
11	4	155	GLU	CD-OE1	6.29	1.32	1.25
16	V	20	ARG	NE-CZ	6.29	1.41	1.33
28	H	223	GLU	CA-CB	6.29	1.67	1.53
31	L	111	GLU	CG-CD	-6.29	1.42	1.51
5	e	102	TYR	CZ-OH	6.28	1.48	1.37
33	J	110	SER	CA-CB	6.28	1.62	1.52
9	i	142	ILE	N-CA	-6.28	1.33	1.46
1	a	110	TYR	CG-CD1	6.27	1.47	1.39
3	c	92	ARG	CZ-NH1	6.26	1.41	1.33
21	N	873	ARG	CD-NE	6.25	1.57	1.46
10	3	41	GLU	CD-OE1	6.25	1.32	1.25
24	Q	294	ARG	CZ-NH2	6.25	1.41	1.33
21	N	682	PHE	CG-CD2	6.24	1.48	1.38
1	a	128	TYR	CE1-CZ	6.24	1.46	1.38
29	I	222	TYR	CB-CG	6.24	1.61	1.51
31	L	299	ARG	NE-CZ	6.24	1.41	1.33
5	e	152	GLY	CA-C	-6.23	1.41	1.51
5	e	93	ARG	NE-CZ	6.23	1.41	1.33
30	K	118	TYR	CB-CG	-6.23	1.42	1.51
1	a	57	LYS	CA-CB	6.22	1.67	1.53
12	5	246	SER	CB-OG	6.22	1.50	1.42
23	P	359	ARG	CZ-NH2	6.22	1.41	1.33
26	U	2	SER	CA-CB	6.22	1.62	1.52
33	J	270	ARG	NE-CZ	6.22	1.41	1.33
22	S	442	PHE	CE1-CZ	6.22	1.49	1.37
5	e	80	GLY	N-CA	-6.21	1.36	1.46
12	5	165	TYR	CB-CG	-6.21	1.42	1.51
24	Q	130	ARG	CD-NE	6.20	1.56	1.46
14	n	194	ARG	NE-CZ	6.19	1.41	1.33
32	M	46	SER	CA-CB	6.18	1.62	1.52
30	K	349	ARG	CZ-NH2	6.18	1.41	1.33
31	L	161	ARG	NE-CZ	6.18	1.41	1.33
30	K	255	ARG	NE-CZ	6.17	1.41	1.33
33	J	344	ARG	CD-NE	6.17	1.56	1.46
22	S	425	ARG	CZ-NH2	6.16	1.41	1.33
18	X	17	TYR	CB-CG	6.16	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
13	m	157	PHE	CG-CD1	6.15	1.48	1.38
21	N	507	GLU	CA-C	-6.15	1.36	1.52
13	m	113	TYR	CE2-CZ	6.15	1.46	1.38
9	2	244	GLU	CD-OE1	-6.14	1.18	1.25
12	5	188	TYR	CG-CD2	6.14	1.47	1.39
4	d	108	TYR	CG-CD1	6.14	1.47	1.39
7	g	103	TYR	CE1-CZ	6.14	1.46	1.38
22	S	137	PHE	CG-CD1	6.13	1.48	1.38
28	H	226	GLU	CG-CD	6.13	1.61	1.51
32	M	381	ARG	NE-CZ	6.13	1.41	1.33
13	m	99	ARG	CZ-NH1	6.13	1.41	1.33
3	c	14	SER	CA-CB	6.11	1.62	1.52
7	g	222	SER	C-N	6.11	1.48	1.34
21	N	409	GLY	N-CA	-6.11	1.36	1.46
23	P	272	PRO	CA-CB	6.10	1.65	1.53
6	f	57	SER	CB-OG	6.10	1.50	1.42
33	J	43	ARG	NE-CZ	6.10	1.41	1.33
30	K	141	ARG	CZ-NH1	6.09	1.41	1.33
30	K	101	GLU	CD-OE2	6.09	1.32	1.25
30	K	117	SER	CA-CB	6.09	1.62	1.52
10	j	99	ARG	NE-CZ	6.09	1.41	1.33
9	i	185	SER	CA-CB	6.09	1.62	1.52
13	m	52	PHE	CG-CD2	6.08	1.47	1.38
9	2	219	TYR	CE2-CZ	6.08	1.46	1.38
30	K	330	ARG	NE-CZ	6.08	1.41	1.33
3	c	135	PHE	CG-CD2	6.07	1.47	1.38
23	P	69	ARG	NE-CZ	6.05	1.41	1.33
1	a	120	ARG	NE-CZ	6.05	1.41	1.33
22	S	271	ARG	NE-CZ	6.04	1.41	1.33
31	L	78	ARG	NE-CZ	6.04	1.41	1.33
25	R	159	SER	CA-CB	6.04	1.62	1.52
12	l	226	GLU	CD-OE2	6.03	1.32	1.25
18	X	17	TYR	CE2-CZ	6.03	1.46	1.38
9	2	236	ARG	CZ-NH1	6.03	1.40	1.33
11	4	167	GLU	CD-OE1	-6.03	1.19	1.25
32	M	432	PHE	CG-CD2	6.01	1.47	1.38
20	Z	729	GLU	CA-C	6.01	1.68	1.52
12	l	139	ARG	CZ-NH2	6.01	1.40	1.33
16	V	175	SER	CA-CB	6.01	1.61	1.52
6	f	128	TYR	CG-CD2	6.00	1.47	1.39
17	T	51	TYR	CG-CD1	6.00	1.47	1.39
17	T	224	ARG	CZ-NH1	6.00	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	1	202	TYR	CE2-CZ	5.99	1.46	1.38
21	N	398	ARG	CZ-NH2	5.99	1.40	1.33
29	I	319	ARG	CZ-NH1	5.99	1.40	1.33
33	J	43	ARG	CZ-NH2	5.98	1.40	1.33
26	U	233	PHE	CE1-CZ	5.98	1.48	1.37
33	J	326	GLU	CB-CG	5.98	1.63	1.52
16	V	230	TYR	CG-CD1	5.98	1.47	1.39
5	e	189	SER	CA-CB	5.97	1.61	1.52
5	e	161	SER	CA-CB	5.97	1.61	1.52
33	J	5	VAL	CA-CB	-5.96	1.42	1.54
13	m	99	ARG	CZ-NH2	5.96	1.40	1.33
9	i	34	GLY	N-CA	-5.96	1.37	1.46
8	h	167	SER	CA-CB	5.96	1.61	1.52
25	R	121	GLU	CD-OE2	-5.95	1.19	1.25
21	N	50	TYR	CG-CD1	5.95	1.46	1.39
20	Z	254	PRO	N-CA	-5.94	1.37	1.47
25	R	206	ARG	NE-CZ	5.94	1.40	1.33
14	7	215	ARG	CD-NE	5.94	1.56	1.46
5	e	122	ARG	CZ-NH2	5.93	1.40	1.33
25	R	334	ARG	CD-NE	5.93	1.56	1.46
9	2	152	TYR	CZ-OH	5.93	1.48	1.37
8	1	169	SER	CA-CB	5.93	1.61	1.52
8	1	152	ARG	CD-NE	5.93	1.56	1.46
13	m	46	ARG	NE-CZ	5.93	1.40	1.33
31	L	161	ARG	CD-NE	5.93	1.56	1.46
6	f	82	ARG	CD-NE	5.92	1.56	1.46
23	P	297	GLU	CB-CG	5.92	1.63	1.52
27	O	369	ARG	CZ-NH1	5.92	1.40	1.33
3	c	143	ARG	CZ-NH1	5.91	1.40	1.33
32	M	294	GLU	CB-CG	5.90	1.63	1.52
30	K	262	ARG	NE-CZ	5.90	1.40	1.33
24	Q	388	GLY	N-CA	-5.89	1.37	1.46
5	e	53	ARG	NE-CZ	5.89	1.40	1.33
8	1	176	GLY	CA-C	5.89	1.61	1.51
10	j	114	SER	CA-CB	5.88	1.61	1.52
8	1	137	GLY	CA-C	-5.88	1.42	1.51
25	R	301	TYR	CB-CG	5.88	1.60	1.51
31	L	345	ARG	CZ-NH2	5.87	1.40	1.33
14	n	65	SER	CB-OG	5.87	1.49	1.42
8	h	91	PHE	CG-CD2	5.86	1.47	1.38
31	L	331	ASP	CA-C	-5.86	1.37	1.52
14	n	229	SER	CA-CB	5.85	1.61	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
21	N	528	ARG	CZ-NH1	5.85	1.40	1.33
9	i	48	ARG	CD-NE	5.85	1.56	1.46
22	S	51	ARG	CD-NE	5.85	1.56	1.46
26	U	149	SER	CA-CB	5.84	1.61	1.52
3	c	180	TYR	CE2-CZ	5.84	1.46	1.38
7	g	165	THR	C-N	5.84	1.43	1.33
33	J	73	GLY	N-CA	-5.84	1.37	1.46
6	f	157	TYR	CB-CG	5.84	1.60	1.51
14	7	74	ARG	NE-CZ	5.84	1.40	1.33
2	b	42	GLY	CA-C	-5.83	1.42	1.51
21	N	81	TYR	CB-CG	-5.83	1.43	1.51
12	l	278	GLU	CA-CB	5.83	1.66	1.53
10	3	143	SER	CA-CB	5.83	1.61	1.52
20	Z	738	TYR	CG-CD2	5.83	1.46	1.39
16	V	269	ARG	CD-NE	5.83	1.56	1.46
15	W	63	SER	CA-CB	5.83	1.61	1.52
31	L	188	GLU	N-CA	-5.82	1.34	1.46
31	L	258	GLU	CG-CD	-5.82	1.43	1.51
3	c	139	GLY	CA-C	5.82	1.61	1.51
26	U	283	ARG	CZ-NH2	5.82	1.40	1.33
12	l	82	ARG	CZ-NH1	5.81	1.40	1.33
4	d	111	ARG	NE-CZ	5.81	1.40	1.33
13	m	114	TYR	CG-CD1	5.81	1.46	1.39
22	S	239	ARG	CZ-NH2	5.81	1.40	1.33
8	1	83	SER	CA-CB	5.81	1.61	1.52
11	k	23	ARG	NE-CZ	5.81	1.40	1.33
31	L	82	ARG	NE-CZ	5.81	1.40	1.33
14	7	219	TYR	CE2-CZ	5.80	1.46	1.38
18	X	85	ARG	NE-CZ	5.80	1.40	1.33
12	l	217	SER	CB-OG	-5.79	1.34	1.42
16	V	108	TYR	CG-CD1	5.79	1.46	1.39
7	g	190	ARG	CZ-NH1	5.79	1.40	1.33
11	k	121	TYR	CG-CD1	5.78	1.46	1.39
27	O	310	PHE	CA-CB	5.78	1.66	1.53
33	J	339	ARG	NE-CZ	5.78	1.40	1.33
23	P	266	TYR	CE1-CZ	5.77	1.46	1.38
13	6	132	SER	CA-CB	5.77	1.61	1.52
30	K	205	PRO	N-CD	5.77	1.55	1.47
28	H	57	LYS	N-CA	-5.76	1.34	1.46
31	L	264	ARG	CZ-NH2	5.76	1.40	1.33
21	N	856	PHE	CG-CD2	5.76	1.47	1.38
4	d	58	ARG	CD-NE	5.75	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	k	141	PHE	CB-CG	5.75	1.61	1.51
13	6	221	ARG	CZ-NH2	5.75	1.40	1.33
32	M	345	ARG	CZ-NH2	5.75	1.40	1.33
26	U	159	CYS	CB-SG	5.74	1.92	1.82
14	n	61	GLY	N-CA	-5.74	1.37	1.46
22	S	245	GLY	N-CA	-5.74	1.37	1.46
4	d	58	ARG	NE-CZ	5.74	1.40	1.33
15	W	101	ARG	CZ-NH1	5.73	1.40	1.33
31	L	267	PHE	CG-CD2	5.72	1.47	1.38
22	S	286	TYR	CB-CG	-5.72	1.43	1.51
24	Q	13	ARG	CA-CB	5.72	1.66	1.53
15	W	41	ARG	CD-NE	5.72	1.56	1.46
13	m	83	TYR	CE2-CZ	5.72	1.46	1.38
27	O	48	PHE	CG-CD2	5.72	1.47	1.38
12	l	144	ARG	CZ-NH2	5.71	1.40	1.33
31	L	130	GLY	N-CA	-5.71	1.37	1.46
4	d	151	GLU	CD-OE1	5.71	1.31	1.25
13	6	13	TYR	CG-CD1	5.71	1.46	1.39
13	6	221	ARG	CD-NE	5.71	1.56	1.46
33	J	238	ARG	CZ-NH2	5.71	1.40	1.33
8	h	83	SER	CA-CB	5.70	1.61	1.52
9	i	227	GLU	CD-OE2	5.70	1.31	1.25
15	W	25	ARG	CD-NE	5.70	1.56	1.46
23	P	103	TYR	CG-CD1	5.70	1.46	1.39
15	W	179	ARG	NE-CZ	5.69	1.40	1.33
30	K	350	ARG	NE-CZ	5.69	1.40	1.33
2	b	128	ARG	CZ-NH1	5.69	1.40	1.33
1	a	189	SER	CA-CB	5.68	1.61	1.52
22	S	275	TYR	CZ-OH	5.68	1.47	1.37
11	k	41	HIS	CA-CB	5.68	1.66	1.53
21	N	515	ARG	CD-NE	5.68	1.56	1.46
25	R	209	ARG	NE-CZ	5.68	1.40	1.33
27	O	81	TYR	CE2-CZ	5.68	1.46	1.38
4	d	248	LYS	CD-CE	5.67	1.65	1.51
30	K	259	ARG	CZ-NH2	5.67	1.40	1.33
14	n	252	TRP	CE3-CZ3	5.66	1.48	1.38
12	5	234	ARG	CZ-NH1	5.66	1.40	1.33
22	S	266	SER	CA-CB	5.66	1.61	1.52
27	O	378	GLU	CD-OE1	5.66	1.31	1.25
1	a	14	ARG	CZ-NH1	5.66	1.40	1.33
29	I	61	ARG	CD-NE	5.66	1.56	1.46
29	I	407	ARG	CD-NE	5.65	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	L	354	GLU	CD-OE1	5.65	1.31	1.25
7	g	205	GLU	CD-OE1	-5.64	1.19	1.25
29	I	378	GLU	CG-CD	5.63	1.60	1.51
9	2	65	ARG	NE-CZ	5.63	1.40	1.33
7	g	15	PHE	CG-CD1	5.63	1.47	1.38
25	R	252	TYR	CG-CD1	5.62	1.46	1.39
16	V	196	TYR	CZ-OH	5.62	1.47	1.37
23	P	201	ARG	CZ-NH1	5.62	1.40	1.33
22	S	313	SER	CB-OG	-5.62	1.34	1.42
3	c	120	GLN	C-N	5.61	1.43	1.33
5	e	72	ARG	CZ-NH2	5.61	1.40	1.33
21	N	58	ARG	NE-CZ	5.61	1.40	1.33
1	a	24	ARG	CZ-NH1	5.61	1.40	1.33
11	k	87	GLU	CG-CD	5.61	1.60	1.51
9	2	169	SER	CA-CB	5.61	1.61	1.52
12	5	272	PHE	CA-CB	5.61	1.66	1.53
4	d	111	ARG	CD-NE	5.60	1.55	1.46
5	e	242	GLU	CB-CG	5.60	1.62	1.52
33	J	368	TYR	CZ-OH	5.60	1.47	1.37
15	W	53	SER	CB-OG	-5.59	1.34	1.42
2	b	236	ARG	NE-CZ	5.59	1.40	1.33
27	O	166	ARG	CZ-NH2	5.59	1.40	1.33
21	N	826	GLU	CB-CG	5.59	1.62	1.52
31	L	221	TYR	CD1-CE1	5.59	1.47	1.39
7	g	132	PHE	CA-CB	5.59	1.66	1.53
11	k	195	PHE	CE1-CZ	5.59	1.48	1.37
8	1	79	TYR	CZ-OH	5.58	1.47	1.37
16	V	269	ARG	CZ-NH2	5.58	1.40	1.33
25	R	176	ARG	NE-CZ	5.58	1.40	1.33
29	I	291	ARG	CZ-NH1	5.58	1.40	1.33
32	M	378	GLU	CG-CD	5.58	1.60	1.51
12	l	84	GLN	C-N	5.58	1.43	1.33
24	Q	222	SER	CA-CB	5.58	1.61	1.52
10	3	198	ARG	CZ-NH2	5.58	1.40	1.33
6	f	55	GLU	CB-CG	5.58	1.62	1.52
5	e	164	PHE	CB-CG	5.58	1.60	1.51
12	l	181	ARG	CD-NE	5.58	1.55	1.46
12	l	159	SER	CA-CB	5.57	1.61	1.52
9	i	119	TYR	CZ-OH	5.57	1.47	1.37
21	N	584	ARG	CZ-NH1	5.57	1.40	1.33
21	N	873	ARG	NE-CZ	5.57	1.40	1.33
28	H	292	ARG	CZ-NH1	5.57	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	i	219	TYR	CB-CG	5.57	1.60	1.51
13	6	75	ARG	NE-CZ	5.57	1.40	1.33
13	m	85	PHE	CE1-CZ	5.56	1.48	1.37
8	1	183	ARG	NE-CZ	5.56	1.40	1.33
27	O	36	LYS	CB-CG	5.56	1.67	1.52
28	H	376	GLU	CD-OE1	5.56	1.31	1.25
4	d	228	GLU	CB-CG	5.55	1.62	1.52
6	f	51	ARG	CZ-NH1	5.55	1.40	1.33
11	4	171	ARG	CZ-NH2	5.55	1.40	1.33
24	Q	126	LYS	N-CA	-5.55	1.35	1.46
20	Z	738	TYR	CA-CB	5.55	1.66	1.53
24	Q	210	CYS	CB-SG	-5.55	1.72	1.81
14	n	170	TYR	CE1-CZ	5.55	1.45	1.38
12	5	270	GLU	CB-CG	5.54	1.62	1.52
25	R	400	TYR	CB-CG	5.54	1.59	1.51
18	X	59	ARG	CZ-NH1	5.54	1.40	1.33
5	e	135	SER	CB-OG	5.54	1.49	1.42
12	l	282	PHE	CG-CD1	5.54	1.47	1.38
27	O	285	SER	CA-CB	5.54	1.61	1.52
31	L	300	GLU	CD-OE1	5.54	1.31	1.25
13	6	193	ARG	NE-CZ	5.53	1.40	1.33
21	N	507	GLU	CB-CG	5.53	1.62	1.52
23	P	233	GLU	CG-CD	5.53	1.60	1.51
7	g	91	ARG	CZ-NH1	5.53	1.40	1.33
13	6	109	ARG	CD-NE	5.53	1.55	1.46
16	V	269	ARG	NE-CZ	5.53	1.40	1.33
25	R	383	ARG	CZ-NH1	5.53	1.40	1.33
29	I	61	ARG	CZ-NH1	5.53	1.40	1.33
16	V	285	ASP	N-CA	-5.52	1.35	1.46
17	T	161	TRP	N-CA	-5.52	1.35	1.46
12	5	184	GLY	N-CA	-5.52	1.37	1.46
23	P	265	VAL	CB-CG2	5.52	1.64	1.52
24	Q	130	ARG	NE-CZ	5.52	1.40	1.33
4	d	119	ARG	CZ-NH2	5.51	1.40	1.33
15	W	41	ARG	NE-CZ	5.51	1.40	1.33
26	U	58	GLU	CB-CG	5.51	1.62	1.52
6	f	131	GLY	CA-C	-5.51	1.43	1.51
1	a	175	GLN	CD-NE2	5.50	1.46	1.32
10	j	143	SER	CA-CB	5.50	1.61	1.52
3	c	67	TYR	CE2-CZ	5.50	1.45	1.38
5	e	165	TYR	CZ-OH	5.50	1.47	1.37
12	5	145	GLU	CD-OE1	5.50	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	151	GLY	N-CA	-5.50	1.37	1.46
6	f	228	GLU	CD-OE1	5.50	1.31	1.25
16	V	56	GLU	CD-OE2	5.50	1.31	1.25
24	Q	398	TYR	CE1-CZ	5.49	1.45	1.38
22	S	72	GLU	CD-OE2	5.49	1.31	1.25
16	V	234	GLU	N-CA	-5.49	1.35	1.46
29	I	151	HIS	CB-CG	5.49	1.59	1.50
3	c	9	ARG	NE-CZ	5.48	1.40	1.33
19	Y	83	ARG	CZ-NH1	5.48	1.40	1.33
27	O	34	GLU	CB-CG	5.48	1.62	1.52
25	R	176	ARG	CZ-NH2	5.48	1.40	1.33
2	b	99	ARG	NE-CZ	5.48	1.40	1.33
9	i	65	ARG	NE-CZ	5.48	1.40	1.33
21	N	921	ARG	CZ-NH2	5.48	1.40	1.33
32	M	34	ALA	N-CA	-5.48	1.35	1.46
8	1	57	SER	CA-CB	5.47	1.61	1.52
16	V	270	TYR	CG-CD1	5.47	1.46	1.39
9	2	168	GLU	CD-OE1	5.47	1.31	1.25
12	5	166	LYS	C-N	5.47	1.42	1.33
16	V	74	SER	CA-CB	5.47	1.61	1.52
23	P	349	ASN	N-CA	-5.47	1.35	1.46
14	n	220	ARG	CZ-NH2	5.46	1.40	1.33
12	5	82	ARG	CD-NE	5.46	1.55	1.46
16	V	198	SER	CA-CB	5.46	1.61	1.52
21	N	599	TYR	CE1-CZ	5.46	1.45	1.38
33	J	145	SER	CA-CB	5.46	1.61	1.52
12	5	163	TYR	CE1-CZ	5.46	1.45	1.38
33	J	231	ARG	NE-CZ	5.46	1.40	1.33
22	S	227	ASN	CB-CG	5.45	1.63	1.51
25	R	36	SER	CB-OG	-5.45	1.35	1.42
17	T	186	ARG	NE-CZ	5.45	1.40	1.33
33	J	371	ARG	NE-CZ	5.45	1.40	1.33
27	O	172	TYR	N-CA	-5.44	1.35	1.46
10	3	68	ARG	CZ-NH1	5.44	1.40	1.33
17	T	20	TYR	CE2-CZ	5.44	1.45	1.38
8	h	133	TYR	CE2-CZ	5.44	1.45	1.38
21	N	834	GLU	CD-OE1	5.43	1.31	1.25
18	X	52	PRO	N-CA	-5.43	1.38	1.47
26	U	91	GLY	N-CA	-5.43	1.38	1.46
27	O	45	LEU	C-N	5.42	1.46	1.34
27	O	288	ARG	NE-CZ	5.42	1.40	1.33
14	7	220	ARG	CD-NE	5.42	1.55	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	156	SER	CA-CB	5.42	1.61	1.52
21	N	81	TYR	CZ-OH	5.42	1.47	1.37
10	3	100	PHE	C-N	5.42	1.42	1.33
23	P	107	SER	CB-OG	5.42	1.49	1.42
31	L	315	PHE	CG-CD1	5.42	1.46	1.38
32	M	217	GLY	CA-C	5.42	1.60	1.51
14	n	74	ARG	NE-CZ	5.41	1.40	1.33
2	b	148	TYR	CG-CD1	5.41	1.46	1.39
10	j	159	GLU	CG-CD	5.41	1.60	1.51
9	2	119	TYR	CE1-CZ	5.41	1.45	1.38
32	M	33	ARG	CZ-NH1	5.41	1.40	1.33
25	R	310	GLU	CB-CG	5.41	1.62	1.52
15	W	19	GLY	CA-C	-5.40	1.43	1.51
30	K	167	PRO	C-N	-5.40	1.21	1.34
7	g	218	TRP	CE3-CZ3	5.40	1.47	1.38
25	R	345	TYR	CB-CG	5.40	1.59	1.51
28	H	213	GLY	N-CA	-5.40	1.38	1.46
4	d	173	GLU	CB-CG	5.40	1.62	1.52
24	Q	57	SER	CB-OG	5.40	1.49	1.42
32	M	110	ASN	CA-CB	5.39	1.67	1.53
13	m	76	PHE	CG-CD2	5.39	1.46	1.38
13	6	148	GLY	CA-C	-5.39	1.43	1.51
12	5	124	ALA	CA-C	-5.39	1.39	1.52
5	e	102	TYR	CA-CB	5.39	1.65	1.53
21	N	881	TYR	CE1-CZ	5.39	1.45	1.38
10	j	80	ARG	CZ-NH1	5.38	1.40	1.33
11	k	76	SER	CA-CB	5.38	1.61	1.52
9	2	236	ARG	NE-CZ	5.38	1.40	1.33
27	O	137	TYR	CE1-CZ	5.38	1.45	1.38
14	7	74	ARG	CZ-NH2	5.38	1.40	1.33
6	f	18	ARG	NE-CZ	5.38	1.40	1.33
24	Q	243	PHE	CG-CD1	5.38	1.46	1.38
27	O	147	ARG	CZ-NH2	5.38	1.40	1.33
29	I	313	LEU	CA-CB	5.38	1.66	1.53
30	K	189	GLU	CG-CD	-5.38	1.43	1.51
7	g	112	PHE	CG-CD1	5.38	1.46	1.38
8	h	109	ALA	N-CA	-5.37	1.35	1.46
13	m	13	TYR	CE1-CZ	5.37	1.45	1.38
21	N	732	GLY	CA-C	-5.37	1.43	1.51
10	3	65	GLU	CB-CG	5.37	1.62	1.52
24	Q	186	HIS	CB-CG	-5.37	1.40	1.50
6	f	233	TYR	CE1-CZ	5.37	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	d	83	ARG	CZ-NH1	5.37	1.40	1.33
33	J	257	ARG	NE-CZ	5.37	1.40	1.33
21	N	162	ARG	NE-CZ	5.36	1.40	1.33
30	K	400	TYR	CZ-OH	5.36	1.47	1.37
8	1	75	TYR	CE2-CZ	-5.36	1.31	1.38
33	J	42	ARG	CZ-NH2	5.36	1.40	1.33
27	O	330	ARG	CZ-NH2	5.36	1.40	1.33
2	b	102	GLY	CA-C	-5.35	1.43	1.51
32	M	433	TYR	CB-CG	-5.35	1.43	1.51
7	g	133	GLY	N-CA	-5.35	1.38	1.46
23	P	123	ARG	CZ-NH2	5.35	1.40	1.33
7	g	78	TYR	CE1-CZ	5.35	1.45	1.38
17	T	157	TYR	CZ-OH	5.35	1.47	1.37
4	d	179	TYR	CG-CD1	5.35	1.46	1.39
13	m	193	ARG	CZ-NH2	5.35	1.40	1.33
16	V	223	SER	CA-CB	5.35	1.60	1.52
33	J	56	ARG	CD-NE	5.35	1.55	1.46
28	H	330	GLN	CA-CB	5.34	1.65	1.53
33	J	116	ARG	CD-NE	5.34	1.55	1.46
13	6	107	GLY	N-CA	-5.34	1.38	1.46
30	K	251	PRO	CA-C	-5.34	1.42	1.52
14	7	189	ARG	NE-CZ	5.33	1.40	1.33
31	L	130	GLY	CA-C	-5.33	1.43	1.51
33	J	404	PHE	CE1-CZ	5.33	1.47	1.37
3	c	225	VAL	CA-CB	5.33	1.66	1.54
6	f	113	CYS	CB-SG	5.33	1.91	1.82
10	j	49	VAL	C-N	5.33	1.46	1.34
21	N	762	ARG	CD-NE	5.33	1.55	1.46
8	1	79	TYR	CE2-CZ	5.33	1.45	1.38
27	O	172	TYR	CE1-CZ	5.33	1.45	1.38
3	c	107	PRO	N-CD	-5.33	1.40	1.47
9	2	101	ARG	NE-CZ	5.33	1.40	1.33
17	T	33	GLU	CB-CG	5.32	1.62	1.52
27	O	33	TYR	CG-CD1	5.32	1.46	1.39
30	K	142	HIS	CB-CG	5.32	1.59	1.50
31	L	399	GLY	CA-C	-5.32	1.43	1.51
13	m	215	VAL	CA-CB	-5.32	1.43	1.54
10	3	161	GLU	CD-OE1	5.32	1.31	1.25
17	T	60	ARG	CD-NE	5.32	1.55	1.46
32	M	113	VAL	CB-CG1	5.32	1.64	1.52
16	V	228	TYR	CE1-CZ	5.32	1.45	1.38
6	f	198	SER	CB-OG	5.32	1.49	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	137	ARG	CZ-NH1	5.32	1.40	1.33
29	I	100	ARG	CZ-NH2	5.32	1.40	1.33
31	L	345	ARG	CD-NE	5.32	1.55	1.46
25	R	383	ARG	CD-NE	5.31	1.55	1.46
4	d	141	ARG	CZ-NH1	5.31	1.40	1.33
9	i	149	ASP	CB-CG	5.31	1.62	1.51
26	U	189	ARG	CZ-NH2	5.31	1.40	1.33
24	Q	151	TYR	CE2-CZ	5.31	1.45	1.38
13	m	186	GLU	CD-OE2	5.31	1.31	1.25
21	N	572	LEU	N-CA	-5.31	1.35	1.46
8	h	120	TYR	CE1-CZ	5.30	1.45	1.38
26	U	275	VAL	CB-CG2	5.30	1.64	1.52
1	a	233	PHE	CB-CG	5.30	1.60	1.51
14	n	218	TYR	CB-CG	-5.30	1.43	1.51
12	5	188	TYR	CG-CD1	5.29	1.46	1.39
33	J	317	PRO	CA-CB	5.29	1.64	1.53
30	K	38	SER	CA-CB	5.29	1.60	1.52
15	W	113	PHE	CG-CD1	5.29	1.46	1.38
32	M	184	GLY	C-N	5.29	1.42	1.33
11	k	26	SER	CA-CB	5.29	1.60	1.52
14	7	122	PRO	N-CD	-5.29	1.40	1.47
6	f	198	SER	CA-CB	5.28	1.60	1.52
21	N	545	SER	CA-CB	5.28	1.60	1.52
15	W	25	ARG	CZ-NH2	5.28	1.40	1.33
12	l	168	ALA	C-N	5.28	1.42	1.33
33	J	265	ASP	CB-CG	5.28	1.62	1.51
13	6	34	ASP	CA-CB	5.27	1.65	1.53
23	P	115	ARG	CZ-NH2	5.27	1.40	1.33
33	J	354	SER	CA-CB	5.27	1.60	1.52
10	j	116	SER	C-N	5.27	1.42	1.33
13	6	65	PHE	CD1-CE1	5.27	1.49	1.39
13	m	126	GLY	CA-C	5.26	1.60	1.51
29	I	407	ARG	CZ-NH2	5.26	1.39	1.33
33	J	18	GLY	N-CA	-5.26	1.38	1.46
22	S	377	TYR	CA-CB	5.26	1.65	1.53
24	Q	232	TYR	CD1-CE1	5.26	1.47	1.39
3	c	160	TRP	CZ2-CH2	5.26	1.47	1.37
6	f	101	ARG	CZ-NH1	5.26	1.39	1.33
10	j	36	VAL	CB-CG2	5.26	1.63	1.52
21	N	271	GLU	CD-OE1	-5.26	1.19	1.25
29	I	274	ASN	CB-CG	5.26	1.63	1.51
31	L	289	ARG	CZ-NH1	5.26	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	7	35	GLN	CA-CB	5.25	1.65	1.53
25	R	69	GLU	CA-CB	5.25	1.65	1.53
6	f	82	ARG	CZ-NH1	5.25	1.39	1.33
28	H	145	TYR	CZ-OH	5.25	1.46	1.37
14	n	251	LYS	CD-CE	5.25	1.64	1.51
21	N	56	SER	CB-OG	-5.25	1.35	1.42
8	h	146	TYR	CG-CD1	5.25	1.46	1.39
11	4	190	ARG	CZ-NH1	5.25	1.39	1.33
28	H	76	LEU	N-CA	-5.25	1.35	1.46
31	L	194	ARG	CZ-NH2	5.25	1.39	1.33
14	7	194	ARG	CZ-NH2	5.24	1.39	1.33
17	T	151	TRP	NE1-CE2	-5.24	1.30	1.37
28	H	190	ARG	CD-NE	-5.24	1.37	1.46
15	W	37	PHE	CE1-CZ	5.24	1.47	1.37
19	Y	84	TYR	CG-CD1	5.24	1.46	1.39
15	W	96	LEU	CA-C	-5.23	1.39	1.52
5	e	136	ARG	NE-CZ	5.23	1.39	1.33
23	P	201	ARG	CD-NE	5.23	1.55	1.46
30	K	239	GLY	N-CA	5.23	1.53	1.46
21	N	784	TYR	CG-CD2	5.23	1.46	1.39
10	j	203	ARG	NE-CZ	5.22	1.39	1.33
22	S	393	ARG	CZ-NH1	5.22	1.39	1.33
9	i	119	TYR	CE2-CZ	5.22	1.45	1.38
11	k	43	LEU	N-CA	-5.22	1.35	1.46
15	W	157	PHE	CG-CD1	5.22	1.46	1.38
24	Q	73	LYS	CD-CE	5.22	1.64	1.51
2	b	5	TYR	CZ-OH	5.21	1.46	1.37
31	L	242	ASN	CA-CB	5.21	1.66	1.53
11	k	169	GLU	CD-OE1	5.21	1.31	1.25
15	W	101	ARG	NE-CZ	5.21	1.39	1.33
10	3	203	ARG	CD-NE	5.21	1.55	1.46
12	5	94	ARG	NE-CZ	5.21	1.39	1.33
3	c	212	GLU	CG-CD	5.21	1.59	1.51
22	S	384	ARG	NE-CZ	5.21	1.39	1.33
28	H	90	ARG	NE-CZ	5.21	1.39	1.33
33	J	35	ARG	CZ-NH2	5.21	1.39	1.33
33	J	222	TYR	CE1-CZ	5.21	1.45	1.38
7	g	126	TYR	CE1-CZ	-5.21	1.31	1.38
9	i	221	THR	C-N	5.21	1.44	1.34
21	N	107	GLU	CD-OE2	5.21	1.31	1.25
33	J	386	VAL	C-N	5.21	1.42	1.33
4	d	97	ARG	CZ-NH2	5.20	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	K	77	ARG	CZ-NH1	5.20	1.39	1.33
30	K	333	ARG	NE-CZ	5.20	1.39	1.33
3	c	49	GLU	CG-CD	5.20	1.59	1.51
16	V	171	ARG	NE-CZ	5.20	1.39	1.33
24	Q	124	PHE	CG-CD1	5.20	1.46	1.38
25	R	224	PHE	CG-CD2	5.20	1.46	1.38
29	I	212	GLY	CA-C	-5.19	1.43	1.51
29	I	408	ARG	NE-CZ	5.19	1.39	1.33
8	1	194	ARG	CZ-NH1	5.19	1.39	1.33
22	S	118	PHE	CE1-CZ	5.19	1.47	1.37
27	O	181	PHE	CE1-CZ	5.19	1.47	1.37
31	L	261	ARG	CZ-NH1	5.19	1.39	1.33
28	H	86	GLY	CA-C	-5.19	1.43	1.51
13	m	71	ALA	CA-CB	5.18	1.63	1.52
22	S	255	SER	CA-CB	5.18	1.60	1.52
24	Q	84	TYR	CD2-CE2	5.18	1.47	1.39
26	U	210	TYR	CZ-OH	5.18	1.46	1.37
9	i	217	ARG	NE-CZ	5.18	1.39	1.33
22	S	67	GLU	N-CA	-5.18	1.35	1.46
25	R	214	TYR	CG-CD1	5.18	1.45	1.39
7	g	223	GLU	CB-CG	5.18	1.61	1.52
29	I	131	SER	CB-OG	-5.18	1.35	1.42
25	R	186	TYR	CD1-CE1	5.18	1.47	1.39
31	L	145	ARG	NE-CZ	5.18	1.39	1.33
12	5	212	TYR	CZ-OH	5.17	1.46	1.37
24	Q	146	TYR	CE1-CZ	5.17	1.45	1.38
11	4	98	TYR	CE1-CZ	5.17	1.45	1.38
5	e	114	GLN	CA-CB	5.17	1.65	1.53
13	6	145	ARG	CD-NE	5.17	1.55	1.46
14	7	98	ARG	CZ-NH1	5.17	1.39	1.33
4	d	172	ARG	CD-NE	5.16	1.55	1.46
9	2	152	TYR	CE1-CZ	5.16	1.45	1.38
17	T	73	PHE	CG-CD2	5.16	1.46	1.38
9	2	48	ARG	NE-CZ	5.16	1.39	1.33
30	K	171	TYR	CE2-CZ	5.16	1.45	1.38
28	H	145	TYR	CE2-CZ	5.16	1.45	1.38
13	m	37	ASN	CG-ND2	5.16	1.45	1.32
8	1	32	GLY	N-CA	-5.16	1.38	1.46
22	S	384	ARG	CZ-NH1	5.16	1.39	1.33
30	K	346	ARG	NE-CZ	5.15	1.39	1.33
14	n	194	ARG	CD-NE	5.15	1.55	1.46
8	h	28	ARG	CZ-NH1	5.15	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
10	3	168	SER	N-CA	-5.15	1.36	1.46
22	S	421	TYR	CG-CD2	5.15	1.45	1.39
30	K	252	ARG	CZ-NH1	5.15	1.39	1.33
2	b	234	ARG	CZ-NH2	5.14	1.39	1.33
6	f	150	SER	CB-OG	-5.14	1.35	1.42
17	T	224	ARG	NE-CZ	5.14	1.39	1.33
27	O	119	SER	CA-CB	5.14	1.60	1.52
27	O	392	TRP	CD2-CE2	5.14	1.47	1.41
6	f	94	TYR	CB-CG	5.14	1.59	1.51
5	e	15	PHE	CB-CG	-5.13	1.42	1.51
16	V	256	GLU	CG-CD	5.13	1.59	1.51
28	H	53	GLU	CD-OE2	5.13	1.31	1.25
29	I	244	PHE	CG-CD2	5.13	1.46	1.38
22	S	475	TYR	CE1-CZ	5.13	1.45	1.38
12	l	192	SER	CB-OG	5.13	1.49	1.42
10	3	80	ARG	NE-CZ	5.13	1.39	1.33
25	R	338	TYR	CZ-OH	5.12	1.46	1.37
14	n	252	TRP	CB-CG	5.12	1.59	1.50
9	2	193	TRP	CB-CG	5.12	1.59	1.50
13	6	99	ARG	NE-CZ	5.12	1.39	1.33
27	O	98	TYR	CE2-CZ	5.12	1.45	1.38
33	J	232	GLU	CD-OE1	5.12	1.31	1.25
11	4	54	VAL	CB-CG1	5.12	1.63	1.52
24	Q	353	PRO	N-CD	-5.12	1.40	1.47
31	L	88	TYR	CA-CB	5.12	1.65	1.53
32	M	70	LYS	CD-CE	5.12	1.64	1.51
33	J	15	HIS	N-CA	-5.12	1.36	1.46
30	K	185	ARG	NE-CZ	5.11	1.39	1.33
31	L	380	VAL	CB-CG1	5.11	1.63	1.52
7	g	32	GLU	CD-OE2	5.11	1.31	1.25
28	H	236	ALA	N-CA	-5.11	1.36	1.46
2	b	246	ARG	NE-CZ	5.11	1.39	1.33
7	g	126	TYR	CD1-CE1	5.11	1.47	1.39
21	N	784	TYR	CZ-OH	5.11	1.46	1.37
28	H	101	ARG	NE-CZ	5.11	1.39	1.33
23	P	381	SER	N-CA	-5.11	1.36	1.46
32	M	328	ASN	CA-C	-5.11	1.39	1.52
12	l	145	GLU	CD-OE1	5.11	1.31	1.25
24	Q	239	PHE	CB-CG	-5.11	1.42	1.51
21	N	684	SER	CB-OG	5.10	1.48	1.42
26	U	24	ARG	CZ-NH1	5.10	1.39	1.33
23	P	133	GLU	CD-OE1	5.10	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	123	ASP	CB-CG	5.10	1.62	1.51
5	e	10	ARG	CZ-NH2	5.10	1.39	1.33
33	J	224	GLY	N-CA	-5.10	1.38	1.46
33	J	324	ARG	CD-NE	5.10	1.55	1.46
27	O	195	TYR	CA-CB	5.10	1.65	1.53
26	U	218	GLU	CG-CD	5.09	1.59	1.51
30	K	393	ARG	CZ-NH2	5.09	1.39	1.33
14	7	36	GLN	CD-NE2	5.09	1.45	1.32
21	N	918	GLU	CG-CD	5.09	1.59	1.51
23	P	128	ASN	CB-CG	5.09	1.62	1.51
14	n	172	SER	CA-C	-5.09	1.39	1.52
9	2	217	ARG	CZ-NH2	5.09	1.39	1.33
13	6	140	GLU	CD-OE2	5.09	1.31	1.25
27	O	260	VAL	C-N	5.08	1.42	1.33
21	N	839	ARG	NE-CZ	5.08	1.39	1.33
8	1	144	TYR	CG-CD2	5.08	1.45	1.39
15	W	109	ARG	CZ-NH2	5.08	1.39	1.33
32	M	381	ARG	CD-NE	5.08	1.55	1.46
12	5	273	TRP	NE1-CE2	5.08	1.44	1.37
24	Q	22	GLU	CD-OE1	5.08	1.31	1.25
8	h	45	ARG	CD-NE	5.08	1.55	1.46
30	K	396	ARG	CZ-NH2	5.08	1.39	1.33
6	f	107	ARG	CZ-NH2	5.08	1.39	1.33
14	n	194	ARG	CZ-NH1	5.08	1.39	1.33
10	3	33	SER	CA-CB	5.08	1.60	1.52
12	5	89	VAL	N-CA	-5.08	1.36	1.46
21	N	398	ARG	CZ-NH1	5.08	1.39	1.33
23	P	198	VAL	N-CA	-5.08	1.36	1.46
26	U	29	GLU	CD-OE2	5.08	1.31	1.25
27	O	43	GLU	CD-OE1	5.08	1.31	1.25
4	d	111	ARG	CZ-NH1	5.07	1.39	1.33
12	l	272	PHE	CG-CD2	5.07	1.46	1.38
30	K	405	SER	CA-CB	5.07	1.60	1.52
31	L	62	ARG	NE-CZ	5.07	1.39	1.33
11	k	2	ASP	CB-CG	5.07	1.62	1.51
21	N	88	ARG	CZ-NH1	5.07	1.39	1.33
33	J	259	GLU	CD-OE2	5.07	1.31	1.25
29	I	206	GLU	CD-OE2	5.07	1.31	1.25
7	g	78	TYR	CB-CG	-5.07	1.44	1.51
13	6	145	ARG	CZ-NH1	5.07	1.39	1.33
29	I	208	TYR	CE1-CZ	5.07	1.45	1.38
11	k	85	ARG	NE-CZ	5.07	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
17	T	248	GLU	CD-OE1	5.07	1.31	1.25
22	S	326	ASP	CB-CG	5.07	1.62	1.51
11	4	138	PHE	CG-CD1	5.06	1.46	1.38
12	5	212	TYR	CE2-CZ	5.06	1.45	1.38
33	J	194	GLY	C-N	-5.06	1.22	1.34
9	2	195	ASP	N-CA	-5.06	1.36	1.46
9	2	214	GLU	CD-OE1	5.06	1.31	1.25
14	n	36	GLN	CD-NE2	5.06	1.45	1.32
10	3	87	PHE	CE1-CZ	5.06	1.47	1.37
21	N	692	GLU	CA-CB	5.06	1.65	1.53
9	i	134	PRO	N-CD	5.06	1.54	1.47
7	g	120	VAL	C-O	5.05	1.32	1.23
33	J	372	GLU	CD-OE2	-5.05	1.20	1.25
1	a	99	ALA	CA-CB	5.05	1.63	1.52
12	5	144	ARG	NE-CZ	5.05	1.39	1.33
22	S	175	SER	CA-CB	5.04	1.60	1.52
31	L	309	LEU	CA-CB	5.04	1.65	1.53
2	b	12	PHE	CE2-CZ	5.04	1.47	1.37
13	6	106	TYR	CZ-OH	5.04	1.46	1.37
28	H	367	ARG	CD-NE	5.04	1.55	1.46
28	H	357	ARG	NE-CZ	5.03	1.39	1.33
13	m	145	ARG	NE-CZ	5.03	1.39	1.33
24	Q	27	TYR	CE1-CZ	5.03	1.45	1.38
28	H	261	ARG	CZ-NH1	5.03	1.39	1.33
2	b	125	GLY	CA-C	-5.03	1.43	1.51
5	e	228	PHE	CG-CD2	5.03	1.46	1.38
28	H	273	ARG	CZ-NH1	5.03	1.39	1.33
31	L	330	PRO	N-CD	-5.02	1.40	1.47
33	J	143	PRO	N-CD	-5.02	1.40	1.47
29	I	98	GLU	CD-OE1	5.02	1.31	1.25
25	R	196	SER	CA-CB	5.02	1.60	1.52
32	M	16	ASP	CB-CG	5.02	1.62	1.51
5	e	238	GLU	CG-CD	5.01	1.59	1.51
8	1	133	TYR	CG-CD2	5.01	1.45	1.39
22	S	239	ARG	CD-NE	5.01	1.54	1.46
3	c	217	ARG	CZ-NH2	5.01	1.39	1.33
9	2	126	TYR	CB-CG	-5.01	1.44	1.51
27	O	15	ARG	CD-NE	5.01	1.54	1.46
33	J	238	ARG	CZ-NH1	5.01	1.39	1.33
24	Q	8	LEU	CA-CB	5.01	1.65	1.53
28	H	88	ARG	CZ-NH2	5.01	1.39	1.33
6	f	182	ILE	CA-C	-5.00	1.40	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	h	46	VAL	CB-CG1	5.00	1.63	1.52
11	k	130	TYR	CE2-CZ	5.00	1.45	1.38
21	N	462	VAL	CB-CG2	5.00	1.63	1.52

All (2299) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	185	GLY	O-C-N	-66.69	16.00	122.70
30	K	167	PRO	O-C-N	-47.18	47.21	122.70
33	J	211	ILE	O-C-N	-47.12	47.31	122.70
32	M	338	LEU	O-C-N	-33.56	69.00	122.70
20	Z	728	LYS	CG-CD-CE	-29.48	23.45	111.90
7	g	22	PHE	O-C-N	29.09	169.25	122.70
7	G	22	PHE	O-C-N	28.32	168.02	122.70
32	M	342	ARG	C-N-CA	-27.38	53.25	121.70
5	E	20	ARG	NE-CZ-NH1	25.65	133.13	120.30
20	Z	738	TYR	CB-CG-CD2	23.18	134.91	121.00
5	E	20	ARG	NE-CZ-NH2	22.69	131.64	120.30
5	E	20	ARG	NH1-CZ-NH2	-21.99	95.22	119.40
30	K	167	PRO	CA-C-N	21.97	165.53	117.20
32	M	338	LEU	CA-C-N	21.43	164.35	117.20
20	Z	728	LYS	CA-CB-CG	20.75	159.06	113.40
7	g	149	TYR	CB-CG-CD1	-20.47	108.72	121.00
33	J	212	ARG	O-C-N	19.80	154.37	122.70
5	E	20	ARG	CD-NE-CZ	19.44	150.82	123.60
32	M	342	ARG	CA-C-N	-19.33	74.67	117.20
20	Z	738	TYR	CD1-CE1-CZ	19.01	136.91	119.80
7	g	22	PHE	CA-C-O	-18.68	80.86	120.10
7	G	22	PHE	CA-C-O	-18.44	81.38	120.10
13	m	202	ARG	NE-CZ-NH2	-17.67	111.47	120.30
12	l	179	TYR	CB-CG-CD2	-17.55	110.47	121.00
30	K	220	THR	O-C-N	-17.49	94.72	122.70
14	n	220	ARG	NE-CZ-NH1	17.48	129.04	120.30
27	O	171	PHE	CB-CG-CD1	-17.15	108.79	120.80
30	K	58	TYR	CB-CG-CD2	-17.01	110.79	121.00
20	Z	738	TYR	CB-CG-CD1	-16.98	110.81	121.00
5	e	53	ARG	NE-CZ-NH1	16.95	128.77	120.30
33	J	309	ARG	CB-CA-C	-16.84	76.72	110.40
14	n	136	ARG	NE-CZ-NH1	16.83	128.71	120.30
30	K	167	PRO	C-N-CA	16.66	163.35	121.70
27	O	81	TYR	CB-CG-CD2	-16.60	111.04	121.00
32	M	42	ARG	NE-CZ-NH2	-16.56	112.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	P	318	TYR	CB-CG-CD2	-16.45	111.13	121.00
28	H	62	ARG	NE-CZ-NH2	-15.80	112.40	120.30
32	M	180	TYR	CB-CG-CD2	15.65	130.39	121.00
14	n	170	TYR	CB-CG-CD1	-15.53	111.68	121.00
23	P	136	ARG	NE-CZ-NH1	15.44	128.02	120.30
11	4	190	ARG	NE-CZ-NH2	-15.25	112.67	120.30
15	W	109	ARG	NE-CZ-NH1	15.10	127.85	120.30
32	M	33	ARG	NE-CZ-NH2	14.96	127.78	120.30
9	i	225	ARG	NE-CZ-NH1	14.95	127.78	120.30
23	P	318	TYR	CB-CG-CD1	14.90	129.94	121.00
9	i	225	ARG	NE-CZ-NH2	-14.80	112.90	120.30
20	Z	255	LEU	CA-CB-CG	14.63	148.96	115.30
7	g	149	TYR	CB-CG-CD2	14.60	129.76	121.00
14	7	124	TYR	CB-CG-CD2	-14.57	112.26	121.00
12	l	179	TYR	CB-CG-CD1	14.52	129.71	121.00
23	P	123	ARG	NE-CZ-NH1	14.44	127.52	120.30
23	P	266	TYR	CB-CG-CD2	-14.36	112.38	121.00
22	S	273	PHE	CB-CG-CD2	-14.33	110.77	120.80
33	J	309	ARG	N-CA-CB	14.33	136.40	110.60
19	Y	83	ARG	NE-CZ-NH1	14.27	127.43	120.30
30	K	294	ARG	NE-CZ-NH2	-14.18	113.21	120.30
2	b	23	TYR	CB-CG-CD1	14.14	129.49	121.00
13	m	85	PHE	CB-CG-CD2	-14.14	110.90	120.80
33	J	48	ARG	NE-CZ-NH1	13.99	127.30	120.30
7	G	22	PHE	CA-C-N	-13.87	86.68	117.20
30	K	281	ARG	NE-CZ-NH2	-13.86	113.37	120.30
20	Z	255	LEU	CB-CG-CD2	13.83	134.51	111.00
11	k	59	TYR	CB-CG-CD1	-13.77	112.74	121.00
25	R	321	TYR	CB-CG-CD1	13.75	129.25	121.00
14	n	136	ARG	NE-CZ-NH2	-13.66	113.47	120.30
4	d	119	ARG	NE-CZ-NH2	-13.64	113.48	120.30
31	L	290	ARG	NE-CZ-NH1	-13.59	113.50	120.30
32	M	299	ARG	NE-CZ-NH1	13.55	127.07	120.30
30	K	141	ARG	NE-CZ-NH2	13.51	127.06	120.30
28	H	370	ARG	NE-CZ-NH1	13.45	127.02	120.30
25	R	417	TYR	CB-CG-CD1	-13.44	112.94	121.00
1	a	30	TYR	CB-CG-CD2	-13.42	112.95	121.00
8	1	152	ARG	NE-CZ-NH1	13.37	126.98	120.30
28	H	370	ARG	NE-CZ-NH2	-13.28	113.66	120.30
30	K	220	THR	C-N-CA	13.25	154.82	121.70
25	R	214	TYR	CB-CG-CD2	-13.21	113.07	121.00
31	L	78	ARG	NE-CZ-NH1	-13.20	113.70	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	77	ARG	NE-CZ-NH2	-13.20	113.70	120.30
25	R	259	PHE	CB-CG-CD2	13.14	130.00	120.80
33	J	270	ARG	NE-CZ-NH1	13.12	126.86	120.30
19	Y	86	ARG	NE-CZ-NH2	-13.06	113.77	120.30
22	S	367	TYR	CB-CG-CD1	-13.04	113.17	121.00
24	Q	189	ARG	NE-CZ-NH1	12.97	126.78	120.30
22	S	346	TYR	CB-CG-CD1	12.90	128.74	121.00
23	P	220	TYR	CB-CG-CD2	-12.90	113.26	121.00
30	K	347	ARG	NE-CZ-NH2	-12.84	113.88	120.30
30	K	88	ARG	NE-CZ-NH2	-12.80	113.90	120.30
3	c	98	TYR	CB-CG-CD1	-12.78	113.33	121.00
30	K	281	ARG	NE-CZ-NH1	12.73	126.67	120.30
31	L	299	ARG	NE-CZ-NH1	12.69	126.64	120.30
6	f	107	ARG	NE-CZ-NH2	-12.64	113.98	120.30
25	R	307	TYR	CB-CG-CD1	12.57	128.54	121.00
9	2	236	ARG	NE-CZ-NH2	-12.50	114.05	120.30
20	Z	728	LYS	CB-CA-C	12.50	135.39	110.40
11	4	171	ARG	NE-CZ-NH1	12.46	126.53	120.30
33	J	238	ARG	NE-CZ-NH1	12.44	126.52	120.30
33	J	212	ARG	CA-C-N	-12.43	89.85	117.20
27	O	135	ARG	NE-CZ-NH2	-12.42	114.09	120.30
4	d	108	TYR	CB-CG-CD1	-12.42	113.55	121.00
32	M	342	ARG	O-C-N	-12.42	102.83	122.70
7	g	22	PHE	CA-C-N	-12.40	89.92	117.20
10	3	103	TYR	CB-CG-CD1	12.37	128.42	121.00
22	S	286	TYR	CB-CG-CD2	-12.30	113.62	121.00
21	N	597	ARG	NE-CZ-NH1	12.23	126.42	120.30
10	j	104	PHE	CB-CG-CD2	12.22	129.35	120.80
33	J	211	ILE	CA-C-N	12.22	144.08	117.20
33	J	188	TYR	CB-CG-CD1	-12.15	113.71	121.00
14	7	241	PHE	CB-CG-CD1	12.10	129.27	120.80
21	N	548	ARG	NE-CZ-NH1	12.09	126.35	120.30
25	R	49	PHE	CB-CG-CD2	-12.08	112.34	120.80
19	Y	86	ARG	NE-CZ-NH1	12.07	126.33	120.30
7	g	160	TYR	CB-CG-CD2	-12.06	113.76	121.00
11	k	149	ARG	NE-CZ-NH2	-12.05	114.28	120.30
13	m	113	TYR	CB-CG-CD1	12.03	128.22	121.00
14	7	124	TYR	CB-CG-CD1	12.00	128.20	121.00
27	O	166	ARG	NE-CZ-NH1	11.99	126.30	120.30
3	c	140	TYR	CB-CG-CD2	-11.93	113.84	121.00
1	a	135	ARG	NE-CZ-NH2	-11.91	114.35	120.30
29	I	228	GLY	O-C-N	-11.90	103.66	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	108	TYR	CB-CG-CD2	-11.88	113.87	121.00
22	S	345	TYR	CB-CG-CD1	-11.77	113.94	121.00
32	M	180	TYR	CB-CG-CD1	-11.76	113.95	121.00
21	N	422	TYR	CB-CG-CD2	11.74	128.04	121.00
21	N	739	PHE	CB-CG-CD2	-11.74	112.58	120.80
17	T	235	PHE	CB-CG-CD2	-11.72	112.60	120.80
21	N	58	ARG	NE-CZ-NH2	-11.70	114.45	120.30
25	R	307	TYR	CB-CG-CD2	-11.68	114.00	121.00
13	6	28	PHE	CB-CG-CD2	-11.67	112.63	120.80
28	H	409	ARG	NE-CZ-NH1	11.65	126.12	120.30
27	O	171	PHE	CB-CG-CD2	11.64	128.95	120.80
24	Q	209	TYR	CB-CG-CD1	-11.63	114.02	121.00
29	I	100	ARG	NE-CZ-NH1	-11.59	114.50	120.30
1	a	133	TYR	CB-CG-CD2	-11.58	114.05	121.00
2	b	83	ARG	NE-CZ-NH1	11.58	126.09	120.30
26	U	210	TYR	CB-CG-CD2	-11.55	114.07	121.00
31	L	261	ARG	NE-CZ-NH2	-11.53	114.54	120.30
11	k	130	TYR	CB-CG-CD2	-11.50	114.10	121.00
18	X	48	PHE	CB-CG-CD2	-11.50	112.75	120.80
7	g	230	PHE	CB-CG-CD2	-11.47	112.77	120.80
4	d	129	PHE	CB-CG-CD1	11.44	128.81	120.80
9	i	219	TYR	CB-CG-CD2	-11.43	114.14	121.00
14	7	134	TYR	CB-CG-CD1	11.39	127.83	121.00
32	M	73	ARG	NE-CZ-NH2	-11.36	114.62	120.30
23	P	220	TYR	CB-CG-CD1	11.33	127.80	121.00
30	K	81	ARG	NE-CZ-NH1	11.32	125.96	120.30
25	R	329	PHE	CB-CG-CD1	-11.29	112.90	120.80
31	L	299	ARG	NE-CZ-NH2	-11.29	114.66	120.30
13	6	41	TYR	CB-CG-CD1	-11.28	114.23	121.00
17	T	234	TYR	CB-CG-CD1	11.27	127.76	121.00
31	L	82	ARG	NE-CZ-NH2	-11.27	114.67	120.30
20	Z	254	PRO	C-N-CA	11.26	149.84	121.70
3	c	143	ARG	NE-CZ-NH2	-11.22	114.69	120.30
27	O	135	ARG	NE-CZ-NH1	11.22	125.91	120.30
20	Z	728	LYS	CD-CE-NZ	11.16	137.38	111.70
24	Q	294	ARG	NE-CZ-NH2	-11.14	114.73	120.30
24	Q	50	ARG	NE-CZ-NH2	-11.12	114.74	120.30
26	U	277	TYR	CB-CG-CD2	-11.06	114.37	121.00
27	O	137	TYR	CB-CG-CD2	-11.00	114.40	121.00
29	I	280	PHE	CB-CG-CD2	-10.98	113.11	120.80
28	H	367	ARG	NE-CZ-NH2	-10.98	114.81	120.30
15	W	23	ARG	NE-CZ-NH2	-10.96	114.82	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	85	PHE	CB-CG-CD1	10.95	128.47	120.80
30	K	220	THR	CA-C-N	10.94	141.27	117.20
21	N	597	ARG	NE-CZ-NH2	-10.93	114.83	120.30
21	N	117	TYR	CB-CG-CD2	-10.92	114.45	121.00
24	Q	77	PHE	CB-CG-CD1	-10.91	113.16	120.80
32	M	77	TYR	CB-CG-CD2	-10.91	114.45	121.00
12	l	163	TYR	CB-CG-CD1	10.91	127.54	121.00
22	S	309	PHE	CB-CG-CD1	10.89	128.42	120.80
2	b	236	ARG	NE-CZ-NH1	10.88	125.74	120.30
14	7	134	TYR	CB-CG-CD2	-10.86	114.48	121.00
4	d	181	ARG	NE-CZ-NH2	-10.84	114.88	120.30
13	6	229	ARG	NE-CZ-NH2	-10.83	114.89	120.30
21	N	389	TYR	CB-CG-CD1	-10.81	114.51	121.00
23	P	266	TYR	CB-CG-CD1	10.81	127.49	121.00
22	S	239	ARG	NE-CZ-NH1	10.81	125.70	120.30
27	O	81	TYR	CB-CG-CD1	10.78	127.47	121.00
10	3	50	PHE	CB-CG-CD2	-10.77	113.27	120.80
11	4	107	TYR	CB-CG-CD2	-10.76	114.55	121.00
24	Q	77	PHE	CB-CG-CD2	10.75	128.33	120.80
30	K	333	ARG	NE-CZ-NH2	-10.75	114.92	120.30
21	N	553	PHE	CB-CG-CD1	-10.71	113.31	120.80
32	M	349	PHE	CB-CG-CD1	10.70	128.29	120.80
31	L	191	ARG	NE-CZ-NH2	-10.69	114.95	120.30
33	J	324	ARG	NE-CZ-NH1	10.65	125.62	120.30
24	Q	335	PHE	CB-CG-CD1	10.64	128.25	120.80
11	4	171	ARG	NE-CZ-NH2	-10.59	115.00	120.30
6	f	59	TYR	CB-CG-CD2	10.58	127.35	121.00
22	S	309	PHE	CB-CG-CD2	-10.56	113.41	120.80
13	m	110	PHE	CB-CG-CD2	10.54	128.18	120.80
18	X	122	TYR	CB-CG-CD1	10.53	127.32	121.00
30	K	350	ARG	NE-CZ-NH2	-10.53	115.04	120.30
24	Q	132	PHE	CB-CG-CD1	-10.52	113.44	120.80
25	R	203	ASP	CB-CG-OD2	10.52	127.76	118.30
12	l	144	ARG	NE-CZ-NH1	-10.49	115.05	120.30
25	R	62	TYR	CB-CG-CD1	-10.49	114.70	121.00
22	S	292	TYR	CB-CG-CD2	-10.49	114.71	121.00
33	J	312	ARG	NE-CZ-NH2	-10.49	115.06	120.30
31	L	82	ARG	NE-CZ-NH1	10.47	125.54	120.30
3	c	24	TYR	CB-CG-CD2	-10.45	114.73	121.00
4	d	22	TYR	CB-CG-CD1	10.45	127.27	121.00
32	M	77	TYR	CB-CG-CD1	10.43	127.26	121.00
33	J	333	ARG	NE-CZ-NH1	-10.43	115.08	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	124	TYR	CB-CG-CD1	-10.42	114.75	121.00
9	2	152	TYR	CB-CG-CD2	10.41	127.25	121.00
10	j	176	ASP	CB-CG-OD2	10.41	127.67	118.30
13	m	159	ASP	CB-CG-OD1	-10.40	108.94	118.30
16	V	129	PHE	CB-CG-CD1	10.36	128.05	120.80
12	l	191	ASP	CB-CG-OD2	-10.35	108.99	118.30
29	I	61	ARG	NE-CZ-NH1	10.31	125.45	120.30
10	j	176	ASP	CB-CG-OD1	-10.29	109.04	118.30
25	R	63	TYR	CB-CG-CD2	-10.29	114.83	121.00
20	Z	729	GLU	N-CA-CB	10.29	129.12	110.60
22	S	346	TYR	CB-CG-CD2	-10.27	114.84	121.00
32	M	203	ARG	NE-CZ-NH2	10.26	125.43	120.30
6	f	59	TYR	CB-CG-CD1	-10.26	114.84	121.00
33	J	43	ARG	NE-CZ-NH2	-10.21	115.20	120.30
26	U	233	PHE	CB-CG-CD2	-10.17	113.68	120.80
16	V	129	PHE	CB-CG-CD2	-10.12	113.72	120.80
29	I	343	ARG	NE-CZ-NH2	-10.10	115.25	120.30
24	Q	13	ARG	NE-CZ-NH2	-10.08	115.26	120.30
8	h	142	PHE	CB-CG-CD2	10.08	127.85	120.80
20	Z	255	LEU	CD1-CG-CD2	-10.07	80.30	110.50
14	7	226	ARG	NE-CZ-NH1	-10.06	115.27	120.30
16	V	254	ARG	NE-CZ-NH2	-10.06	115.27	120.30
2	b	142	PHE	CB-CG-CD1	10.05	127.84	120.80
14	7	254	PHE	CB-CG-CD2	-10.05	113.76	120.80
20	Z	247	GLN	CB-CA-C	10.05	130.50	110.40
22	S	452	TYR	CB-CG-CD1	-10.04	114.97	121.00
14	n	223	ARG	NE-CZ-NH2	-9.99	115.30	120.30
10	3	74	TYR	CB-CG-CD2	9.99	126.99	121.00
22	S	273	PHE	CB-CG-CD1	9.99	127.79	120.80
21	N	298	TYR	CB-CG-CD1	9.98	126.99	121.00
12	5	179	TYR	CB-CG-CD1	9.98	126.99	121.00
22	S	377	TYR	CB-CG-CD2	-9.98	115.01	121.00
5	e	213	ASP	CB-CG-OD2	-9.97	109.33	118.30
28	H	162	ARG	NE-CZ-NH2	-9.96	115.32	120.30
7	g	20	ARG	NE-CZ-NH1	9.95	125.28	120.30
8	h	96	TYR	CB-CG-CD1	9.92	126.95	121.00
27	O	356	ARG	NE-CZ-NH1	-9.92	115.34	120.30
24	Q	400	TYR	CB-CG-CD2	-9.91	115.06	121.00
29	I	75	PHE	CB-CG-CD1	9.88	127.72	120.80
22	S	184	TRP	CB-CG-CD2	-9.88	113.75	126.60
12	l	181	ARG	NE-CZ-NH2	-9.87	115.37	120.30
32	M	339	ARG	NE-CZ-NH2	-9.85	115.38	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	d	156	TYR	CB-CG-CD1	-9.84	115.09	121.00
24	Q	309	ARG	NE-CZ-NH1	-9.84	115.38	120.30
28	H	283	TYR	CB-CG-CD2	-9.84	115.10	121.00
23	P	267	PHE	CB-CG-CD2	-9.82	113.92	120.80
24	Q	20	TYR	CB-CG-CD1	-9.82	115.11	121.00
20	Z	729	GLU	CB-CA-C	-9.82	90.77	110.40
6	f	174	ARG	NE-CZ-NH1	9.81	125.21	120.30
20	Z	738	TYR	CE1-CZ-CE2	-9.80	104.12	119.80
11	k	36	ARG	NE-CZ-NH1	9.80	125.20	120.30
14	n	80	ASP	CB-CG-OD1	9.79	127.11	118.30
18	X	17	TYR	CB-CG-CD1	-9.77	115.14	121.00
10	3	26	ASP	CB-CG-OD2	9.76	127.08	118.30
3	c	67	TYR	CB-CG-CD2	-9.73	115.16	121.00
7	g	138	PHE	CB-CG-CD2	-9.72	113.99	120.80
31	L	243	PHE	CB-CG-CD1	-9.72	114.00	120.80
12	5	212	TYR	CB-CG-CD1	-9.72	115.17	121.00
24	Q	116	PHE	CB-CG-CD2	-9.72	114.00	120.80
9	2	152	TYR	CB-CG-CD1	-9.70	115.18	121.00
3	c	20	TYR	CB-CG-CD1	-9.69	115.19	121.00
6	f	128	TYR	CB-CG-CD2	9.67	126.80	121.00
9	i	236	ARG	NE-CZ-NH1	-9.67	115.47	120.30
1	a	205	PHE	CB-CG-CD1	-9.66	114.04	120.80
10	3	203	ARG	NE-CZ-NH2	-9.66	115.47	120.30
3	c	149	TYR	CB-CG-CD1	-9.63	115.22	121.00
3	c	137	TYR	CB-CG-CD1	-9.62	115.22	121.00
4	d	22	TYR	CB-CG-CD2	-9.62	115.23	121.00
13	m	109	ARG	NE-CZ-NH1	9.62	125.11	120.30
20	Z	728	LYS	O-C-N	-9.62	107.31	122.70
32	M	45	ARG	NE-CZ-NH2	-9.62	115.49	120.30
14	n	63	TYR	CB-CG-CD1	-9.61	115.24	121.00
20	Z	738	TYR	OH-CZ-CE2	9.61	146.03	120.10
24	Q	400	TYR	CB-CG-CD1	9.60	126.76	121.00
25	R	62	TYR	CB-CG-CD2	9.60	126.76	121.00
21	N	861	TYR	CB-CG-CD2	-9.60	115.24	121.00
12	l	148	ARG	NE-CZ-NH2	-9.58	115.51	120.30
25	R	186	TYR	CB-CG-CD2	-9.57	115.26	121.00
12	l	139	ARG	NE-CZ-NH2	9.57	125.09	120.30
27	O	58	ARG	NE-CZ-NH1	-9.55	115.52	120.30
29	I	135	PHE	CB-CG-CD2	-9.55	114.11	120.80
13	6	99	ARG	NE-CZ-NH1	9.53	125.07	120.30
32	M	128	PHE	CB-CG-CD2	9.53	127.47	120.80
3	c	102	TYR	CB-CG-CD2	-9.53	115.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	a	244	ARG	NE-CZ-NH1	9.51	125.05	120.30
6	f	164	ARG	NE-CZ-NH1	9.51	125.05	120.30
7	g	157	TYR	CB-CG-CD1	9.50	126.70	121.00
9	2	98	TYR	CB-CG-CD2	9.46	126.68	121.00
28	H	390	ARG	NE-CZ-NH2	-9.45	115.57	120.30
31	L	339	ARG	NE-CZ-NH2	-9.45	115.58	120.30
16	V	269	ARG	NE-CZ-NH1	9.44	125.02	120.30
13	m	141	ARG	NE-CZ-NH1	-9.43	115.59	120.30
14	n	49	TYR	CB-CG-CD2	9.42	126.65	121.00
16	V	22	ASP	CB-CG-OD1	-9.41	109.83	118.30
11	4	93	ARG	NE-CZ-NH2	-9.40	115.60	120.30
17	T	60	ARG	NE-CZ-NH1	9.40	125.00	120.30
12	l	242	ARG	NE-CZ-NH2	-9.40	115.60	120.30
24	Q	286	TYR	CB-CG-CD2	-9.40	115.36	121.00
26	U	100	ARG	NE-CZ-NH1	9.40	125.00	120.30
31	L	60	PHE	CB-CG-CD2	-9.39	114.23	120.80
25	R	181	TYR	CB-CG-CD2	-9.35	115.39	121.00
33	J	270	ARG	NE-CZ-NH2	-9.35	115.63	120.30
12	5	272	PHE	CB-CG-CD2	9.34	127.34	120.80
22	S	184	TRP	CB-CG-CD1	9.34	139.14	127.00
4	d	119	ARG	NE-CZ-NH1	9.33	124.97	120.30
24	Q	335	PHE	CB-CG-CD2	-9.33	114.27	120.80
30	K	330	ARG	NE-CZ-NH1	9.32	124.96	120.30
33	J	257	ARG	NE-CZ-NH2	-9.32	115.64	120.30
28	H	343	PHE	CB-CG-CD1	-9.30	114.29	120.80
13	6	193	ARG	NE-CZ-NH1	-9.30	115.65	120.30
8	h	75	TYR	CG-CD2-CE2	-9.29	113.87	121.30
17	T	60	ARG	NE-CZ-NH2	-9.28	115.66	120.30
22	S	55	ARG	NE-CZ-NH1	9.23	124.91	120.30
25	R	345	TYR	CB-CG-CD1	9.22	126.53	121.00
10	j	147	PHE	CB-CG-CD1	-9.20	114.36	120.80
9	2	153	TYR	CB-CG-CD1	-9.20	115.48	121.00
15	W	60	ARG	NE-CZ-NH2	9.20	124.90	120.30
30	K	118	TYR	CB-CG-CD2	-9.20	115.48	121.00
31	L	357	ARG	NE-CZ-NH2	-9.19	115.71	120.30
17	T	157	TYR	CB-CG-CD2	9.16	126.50	121.00
8	h	38	ARG	NE-CZ-NH2	9.16	124.88	120.30
23	P	232	ARG	NE-CZ-NH1	9.16	124.88	120.30
30	K	233	ALA	CB-CA-C	-9.15	96.37	110.10
23	P	395	ARG	NE-CZ-NH2	-9.14	115.73	120.30
28	H	346	ARG	NE-CZ-NH1	9.13	124.87	120.30
32	M	338	LEU	C-N-CA	9.12	144.50	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
18	X	98	PHE	CB-CG-CD2	-9.12	114.42	120.80
12	l	115	PHE	CB-CG-CD2	-9.12	114.42	120.80
3	c	146	TYR	CB-CG-CD1	-9.11	115.53	121.00
16	V	270	TYR	CG-CD2-CE2	-9.11	114.01	121.30
31	L	191	ARG	NE-CZ-NH1	9.11	124.85	120.30
6	f	39	ARG	NE-CZ-NH1	9.10	124.85	120.30
32	M	349	PHE	CB-CG-CD2	-9.09	114.44	120.80
12	5	196	ARG	NE-CZ-NH2	-9.08	115.76	120.30
26	U	277	TYR	CB-CG-CD1	9.08	126.45	121.00
30	K	393	ARG	NE-CZ-NH2	-9.06	115.77	120.30
25	R	263	ARG	NE-CZ-NH1	9.05	124.83	120.30
15	W	65	PHE	CB-CG-CD2	-9.05	114.46	120.80
16	V	212	MET	CG-SD-CE	-9.04	85.74	100.20
31	L	342	ARG	NE-CZ-NH2	-9.04	115.78	120.30
32	M	425	ARG	NE-CZ-NH1	-9.01	115.80	120.30
33	J	22	TYR	CG-CD1-CE1	-9.00	114.10	121.30
7	g	78	TYR	CB-CG-CD2	-9.00	115.60	121.00
3	c	129	ARG	NE-CZ-NH2	-8.99	115.80	120.30
6	f	164	ARG	NE-CZ-NH2	-8.99	115.80	120.30
15	W	144	PHE	CB-CG-CD1	-8.98	114.51	120.80
11	k	2	ASP	CB-CG-OD2	-8.98	110.22	118.30
17	T	199	PHE	CB-CG-CD2	-8.97	114.52	120.80
26	U	283	ARG	NE-CZ-NH1	8.96	124.78	120.30
17	T	234	TYR	CB-CG-CD2	-8.95	115.63	121.00
13	6	131	TYR	CB-CG-CD2	-8.95	115.63	121.00
12	l	262	TYR	CB-CG-CD1	-8.95	115.63	121.00
21	N	599	TYR	CG-CD1-CE1	-8.95	114.14	121.30
8	1	144	TYR	CB-CG-CD2	8.94	126.36	121.00
24	Q	332	ARG	NE-CZ-NH2	8.92	124.76	120.30
22	S	171	TYR	CB-CG-CD1	8.92	126.35	121.00
28	H	190	ARG	NE-CZ-NH1	8.91	124.76	120.30
8	h	194	ARG	NE-CZ-NH2	-8.90	115.85	120.30
13	m	68	ASP	CB-CG-OD2	8.90	126.31	118.30
17	T	149	ASP	CB-CG-OD1	8.90	126.31	118.30
14	n	226	ARG	NE-CZ-NH1	8.89	124.75	120.30
19	Y	44	ALA	N-CA-CB	8.89	122.55	110.10
3	c	140	TYR	CB-CG-CD1	8.89	126.33	121.00
33	J	374	ARG	NE-CZ-NH2	-8.88	115.86	120.30
27	O	92	PHE	CB-CG-CD1	8.88	127.01	120.80
12	5	200	ASP	CB-CG-OD1	-8.87	110.32	118.30
3	c	6	TYR	CB-CG-CD1	-8.86	115.68	121.00
14	7	241	PHE	CB-CG-CD2	-8.86	114.60	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	270	TYR	CB-CG-CD2	-8.85	115.69	121.00
5	e	20	ARG	NE-CZ-NH2	8.85	124.72	120.30
25	R	181	TYR	CB-CG-CD1	8.81	126.29	121.00
29	I	127	ASP	CB-CG-OD2	-8.79	110.39	118.30
24	Q	297	ASP	CB-CG-OD2	8.78	126.21	118.30
20	Z	248	TYR	N-CA-CB	8.77	126.39	110.60
21	N	743	PHE	CB-CG-CD1	8.77	126.94	120.80
21	N	762	ARG	NE-CZ-NH1	8.77	124.69	120.30
6	f	24	TYR	CZ-CE2-CD2	-8.77	111.91	119.80
16	V	22	ASP	CB-CG-OD2	8.77	126.19	118.30
17	T	245	TYR	CB-CG-CD1	8.77	126.26	121.00
25	R	321	TYR	CB-CG-CD2	-8.76	115.74	121.00
28	H	442	ASP	CB-CG-OD2	-8.76	110.42	118.30
28	H	420	ARG	NE-CZ-NH1	8.76	124.68	120.30
29	I	256	TYR	CB-CG-CD1	-8.75	115.75	121.00
8	1	111	TYR	CB-CG-CD2	8.75	126.25	121.00
21	N	109	TYR	CB-CG-CD1	8.74	126.25	121.00
18	X	122	TYR	CB-CG-CD2	-8.72	115.77	121.00
30	K	258	PHE	CB-CG-CD2	-8.70	114.71	120.80
4	d	148	TYR	CB-CG-CD2	-8.69	115.79	121.00
5	e	53	ARG	NE-CZ-NH2	-8.68	115.96	120.30
33	J	257	ARG	NE-CZ-NH1	8.68	124.64	120.30
29	I	293	ASP	CB-CG-OD1	8.67	126.11	118.30
4	d	6	ARG	NE-CZ-NH2	-8.67	115.97	120.30
26	U	254	ARG	NE-CZ-NH1	8.65	124.63	120.30
6	f	177	ASP	CB-CG-OD1	8.65	126.09	118.30
2	b	97	TYR	CB-CG-CD2	-8.65	115.81	121.00
2	b	204	PHE	CB-CG-CD1	-8.65	114.75	120.80
10	3	87	PHE	CB-CG-CD1	8.65	126.85	120.80
32	M	381	ARG	NE-CZ-NH1	-8.62	115.99	120.30
12	l	230	TYR	CB-CG-CD2	-8.62	115.83	121.00
15	W	26	PHE	CB-CG-CD1	-8.61	114.77	120.80
18	X	11	ARG	NE-CZ-NH2	8.58	124.59	120.30
29	I	291	ARG	NE-CZ-NH2	8.57	124.59	120.30
21	N	735	MET	CG-SD-CE	-8.57	86.49	100.20
17	T	235	PHE	CB-CG-CD1	8.55	126.79	120.80
11	k	95	ARG	NE-CZ-NH2	8.54	124.57	120.30
17	T	97	SER	N-CA-CB	8.54	123.31	110.50
32	M	233	ARG	NE-CZ-NH1	8.54	124.57	120.30
25	R	214	TYR	CB-CG-CD1	8.51	126.10	121.00
21	N	109	TYR	CB-CG-CD2	-8.50	115.90	121.00
21	N	202	PHE	CB-CG-CD1	8.48	126.74	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	144	TYR	CB-CG-CD1	-8.48	115.91	121.00
12	l	82	ARG	NE-CZ-NH1	-8.48	116.06	120.30
31	L	145	ARG	NE-CZ-NH1	8.48	124.54	120.30
26	U	100	ARG	NE-CZ-NH2	-8.47	116.06	120.30
33	J	131	ASP	CB-CG-OD1	-8.46	110.68	118.30
31	L	88	TYR	CB-CG-CD1	-8.45	115.93	121.00
12	5	189	TYR	CB-CG-CD1	-8.45	115.93	121.00
1	a	110	TYR	CB-CG-CD1	8.44	126.07	121.00
24	Q	202	ARG	NE-CZ-NH1	8.44	124.52	120.30
12	5	188	TYR	CB-CG-CD2	8.44	126.06	121.00
11	k	59	TYR	CB-CG-CD2	8.44	126.06	121.00
31	L	345	ARG	NE-CZ-NH1	8.41	124.51	120.30
25	R	383	ARG	NE-CZ-NH1	8.41	124.51	120.30
25	R	49	PHE	CB-CG-CD1	8.41	126.69	120.80
13	m	109	ARG	NE-CZ-NH2	-8.40	116.10	120.30
11	4	85	ARG	NE-CZ-NH1	8.39	124.50	120.30
10	3	203	ARG	NE-CZ-NH1	8.38	124.49	120.30
2	b	128	ARG	NE-CZ-NH2	8.38	124.49	120.30
13	m	113	TYR	CG-CD1-CE1	8.38	128.00	121.30
14	n	109	TYR	CB-CG-CD2	-8.38	115.97	121.00
7	g	163	ALA	N-CA-CB	8.38	121.83	110.10
18	X	96	ARG	NE-CZ-NH1	8.37	124.48	120.30
7	g	8	TYR	CB-CG-CD1	-8.36	115.98	121.00
21	N	399	PHE	CB-CG-CD1	-8.36	114.95	120.80
27	O	137	TYR	CB-CG-CD1	8.35	126.01	121.00
30	K	335	ASP	CB-CG-OD1	-8.35	110.78	118.30
29	I	340	ARG	NE-CZ-NH1	8.34	124.47	120.30
31	L	194	ARG	NE-CZ-NH1	-8.32	116.14	120.30
15	W	69	PHE	CB-CG-CD2	-8.31	114.98	120.80
33	J	228	ARG	NE-CZ-NH2	-8.31	116.15	120.30
14	n	49	TYR	CB-CG-CD1	-8.29	116.03	121.00
13	m	13	TYR	CB-CG-CD1	-8.29	116.03	121.00
22	S	345	TYR	CB-CG-CD2	8.27	125.96	121.00
4	d	120	TYR	CB-CG-CD1	8.26	125.96	121.00
14	n	253	ASP	CB-CG-OD1	-8.26	110.87	118.30
21	N	117	TYR	CB-CG-CD1	8.24	125.94	121.00
33	J	22	TYR	CB-CG-CD2	-8.22	116.07	121.00
13	6	36	ARG	NE-CZ-NH1	8.21	124.40	120.30
15	W	25	ARG	NE-CZ-NH2	8.21	124.40	120.30
13	6	68	ASP	CB-CG-OD1	8.20	125.68	118.30
12	5	219	TYR	CB-CG-CD1	8.19	125.91	121.00
14	n	63	TYR	CB-CG-CD2	8.19	125.91	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
30	K	218	GLY	C-N-CA	-8.19	101.24	121.70
3	c	24	TYR	CB-CG-CD1	8.17	125.90	121.00
5	e	158	ALA	N-CA-CB	8.17	121.54	110.10
9	2	140	PHE	CB-CG-CD1	8.17	126.52	120.80
13	6	41	TYR	CB-CG-CD2	8.17	125.90	121.00
24	Q	88	PHE	CB-CG-CD1	-8.17	115.08	120.80
2	b	4	ARG	NE-CZ-NH2	-8.16	116.22	120.30
4	d	148	TYR	CD1-CE1-CZ	-8.16	112.46	119.80
7	g	78	TYR	CB-CG-CD1	8.13	125.88	121.00
14	n	109	TYR	CB-CG-CD1	8.13	125.88	121.00
15	W	127	ARG	NE-CZ-NH2	-8.11	116.24	120.30
25	R	329	PHE	CB-CG-CD2	8.11	126.48	120.80
32	M	400	MET	CG-SD-CE	-8.11	87.22	100.20
21	N	861	TYR	CB-CG-CD1	8.10	125.86	121.00
20	Z	255	LEU	CB-CG-CD1	8.10	124.77	111.00
21	N	552	ALA	N-CA-CB	8.07	121.40	110.10
3	c	20	TYR	CB-CG-CD2	8.07	125.84	121.00
27	O	342	ASP	CB-CG-OD2	-8.06	111.04	118.30
6	f	16	THR	CA-CB-CG2	-8.06	101.12	112.40
10	j	195	VAL	CA-CB-CG2	-8.05	98.82	110.90
13	m	65	PHE	CB-CG-CD1	8.04	126.43	120.80
13	6	24	ALA	CB-CA-C	-8.04	98.04	110.10
1	a	233	PHE	CB-CG-CD2	-8.02	115.18	120.80
11	k	187	ASP	CB-CG-OD1	8.02	125.52	118.30
21	N	873	ARG	NE-CZ-NH2	-8.02	116.29	120.30
30	K	58	TYR	CB-CG-CD1	8.02	125.81	121.00
16	V	20	ARG	NE-CZ-NH2	-8.02	116.29	120.30
31	L	200	PRO	N-CA-CB	8.01	112.91	103.30
20	Z	255	LEU	CB-CA-C	8.00	125.40	110.20
33	J	261	SER	N-CA-CB	8.00	122.50	110.50
21	N	162	ARG	NE-CZ-NH2	-7.99	116.31	120.30
16	V	114	PHE	CB-CG-CD1	-7.99	115.21	120.80
22	S	332	PHE	CB-CG-CD1	-7.98	115.21	120.80
30	K	345	ASP	CB-CG-OD1	-7.98	111.12	118.30
12	5	272	PHE	CB-CG-CD1	-7.97	115.22	120.80
32	M	128	PHE	CB-CG-CD1	-7.97	115.22	120.80
33	J	231	ARG	NE-CZ-NH1	-7.97	116.32	120.30
2	b	23	TYR	CB-CG-CD2	-7.96	116.23	121.00
23	P	344	ARG	NE-CZ-NH1	-7.95	116.33	120.30
31	L	315	PHE	CB-CG-CD1	7.94	126.36	120.80
11	4	152	MET	CG-SD-CE	-7.94	87.50	100.20
28	H	62	ARG	NE-CZ-NH1	7.94	124.27	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	208	ARG	NE-CZ-NH1	-7.93	116.33	120.30
1	a	30	TYR	CG-CD1-CE1	-7.93	114.95	121.30
10	j	203	ARG	NE-CZ-NH1	7.92	124.26	120.30
19	Y	73	PHE	CB-CG-CD2	-7.91	115.26	120.80
33	J	296	ARG	NE-CZ-NH2	-7.91	116.35	120.30
5	e	136	ARG	NE-CZ-NH2	-7.89	116.36	120.30
23	P	359	ARG	NE-CZ-NH1	7.88	124.24	120.30
33	J	382	PHE	CB-CG-CD1	-7.87	115.29	120.80
11	4	23	ARG	NE-CZ-NH1	-7.87	116.36	120.30
33	J	35	ARG	NE-CZ-NH1	7.87	124.24	120.30
8	1	54	ARG	NE-CZ-NH1	7.85	124.22	120.30
27	O	356	ARG	NE-CZ-NH2	7.84	124.22	120.30
7	g	242	PHE	CB-CG-CD2	-7.84	115.31	120.80
10	j	205	ASP	CB-CG-OD1	7.84	125.35	118.30
10	3	103	TYR	CB-CG-CD2	-7.83	116.30	121.00
17	T	149	ASP	CB-CG-OD2	-7.83	111.25	118.30
26	U	93	TYR	CB-CG-CD2	-7.82	116.31	121.00
29	I	127	ASP	CB-CG-OD1	7.82	125.34	118.30
28	H	341	ASP	CB-CG-OD1	7.82	125.33	118.30
3	c	208	TYR	CB-CG-CD2	-7.80	116.32	121.00
28	H	434	ARG	NE-CZ-NH2	7.79	124.20	120.30
29	I	181	TYR	CB-CG-CD2	7.79	125.68	121.00
24	Q	163	ARG	NE-CZ-NH1	7.79	124.19	120.30
18	X	48	PHE	CB-CG-CD1	7.79	126.25	120.80
16	V	171	ARG	NE-CZ-NH1	7.78	124.19	120.30
25	R	222	ARG	NE-CZ-NH2	-7.77	116.42	120.30
10	3	14	ALA	N-CA-CB	7.76	120.97	110.10
12	l	181	ARG	NE-CZ-NH1	7.75	124.18	120.30
10	3	3	ASP	CB-CG-OD2	7.75	125.28	118.30
29	I	291	ARG	NE-CZ-NH1	-7.75	116.43	120.30
33	J	251	ASP	N-CA-CB	7.75	124.55	110.60
27	O	26	PHE	CB-CG-CD1	7.73	126.21	120.80
5	e	167	TYR	CB-CG-CD2	7.70	125.62	121.00
13	m	110	PHE	CB-CG-CD1	-7.70	115.41	120.80
17	T	150	ARG	NE-CZ-NH1	7.69	124.14	120.30
21	N	894	ARG	NE-CZ-NH1	7.69	124.14	120.30
28	H	118	ASP	CB-CG-OD2	-7.69	111.38	118.30
32	M	42	ARG	NE-CZ-NH1	7.68	124.14	120.30
6	f	123	TYR	CB-CG-CD2	-7.68	116.39	121.00
33	J	316	PHE	CB-CG-CD1	7.68	126.17	120.80
33	J	32	LEU	CB-CG-CD1	7.67	124.05	111.00
7	g	20	ARG	NE-CZ-NH2	-7.67	116.46	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
15	W	35	PHE	CB-CG-CD2	7.66	126.16	120.80
21	N	123	PHE	CB-CG-CD1	7.66	126.17	120.80
23	P	65	LEU	CB-CG-CD2	7.65	124.00	111.00
27	O	98	TYR	CB-CG-CD2	7.64	125.58	121.00
3	c	67	TYR	CB-CG-CD1	7.63	125.58	121.00
22	S	442	PHE	CB-CG-CD1	-7.63	115.46	120.80
26	U	137	TYR	CB-CG-CD2	-7.62	116.42	121.00
20	Z	970	TYR	CB-CG-CD2	-7.62	116.43	121.00
27	O	29	PHE	CB-CG-CD1	7.62	126.13	120.80
24	Q	306	TYR	CB-CG-CD1	-7.61	116.44	121.00
31	L	145	ARG	NE-CZ-NH2	-7.60	116.50	120.30
29	I	436	TYR	CB-CG-CD1	-7.60	116.44	121.00
23	P	115	ARG	NE-CZ-NH2	7.59	124.10	120.30
25	R	382	ASP	CB-CG-OD2	7.59	125.13	118.30
25	R	259	PHE	CB-CG-CD1	-7.58	115.50	120.80
33	J	368	TYR	CB-CG-CD1	-7.58	116.45	121.00
28	H	400	ARG	NE-CZ-NH2	-7.57	116.51	120.30
12	5	96	THR	CA-CB-CG2	-7.57	101.80	112.40
24	Q	309	ARG	N-CA-CB	7.57	124.23	110.60
24	Q	412	ALA	N-CA-CB	7.57	120.70	110.10
15	W	179	ARG	NE-CZ-NH2	-7.57	116.52	120.30
33	J	200	ARG	NE-CZ-NH2	-7.57	116.52	120.30
29	I	129	TYR	CG-CD1-CE1	-7.55	115.26	121.30
4	d	141	ARG	NE-CZ-NH1	7.55	124.07	120.30
12	l	249	SER	N-CA-CB	7.55	121.82	110.50
14	7	261	TYR	CB-CG-CD1	7.55	125.53	121.00
14	n	170	TYR	CG-CD1-CE1	-7.54	115.26	121.30
3	c	131	PHE	CB-CG-CD2	7.54	126.08	120.80
12	l	200	ASP	CB-CG-OD2	-7.54	111.51	118.30
20	Z	253	VAL	CA-CB-CG2	7.54	122.21	110.90
22	S	452	TYR	CB-CG-CD2	7.54	125.52	121.00
32	M	303	ARG	NE-CZ-NH1	7.53	124.06	120.30
32	M	87	ASP	CB-CG-OD2	-7.52	111.53	118.30
32	M	243	PHE	CB-CG-CD1	-7.52	115.54	120.80
11	4	190	ARG	NH1-CZ-NH2	7.52	127.67	119.40
13	m	60	MET	CG-SD-CE	-7.52	88.17	100.20
21	N	221	ASP	CB-CG-OD2	-7.52	111.54	118.30
21	N	471	TYR	CB-CG-CD2	7.52	125.51	121.00
14	7	261	TYR	CB-CG-CD2	-7.51	116.50	121.00
23	P	136	ARG	NE-CZ-NH2	-7.51	116.55	120.30
23	P	138	ARG	NE-CZ-NH1	7.50	124.05	120.30
29	I	327	ALA	CB-CA-C	-7.50	98.85	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
16	V	76	THR	CA-CB-CG2	-7.49	101.91	112.40
20	Z	951	GLN	N-CA-CB	7.49	124.09	110.60
28	H	385	ARG	NE-CZ-NH1	-7.49	116.55	120.30
14	7	87	SER	N-CA-CB	7.49	121.74	110.50
14	n	170	TYR	CZ-CE2-CD2	-7.49	113.06	119.80
20	Z	970	TYR	CB-CG-CD1	7.49	125.49	121.00
27	O	91	ASP	CB-CG-OD1	7.49	125.04	118.30
13	6	221	ARG	NE-CZ-NH2	-7.49	116.56	120.30
22	S	292	TYR	CB-CG-CD1	7.48	125.49	121.00
21	N	553	PHE	CB-CG-CD2	7.48	126.04	120.80
25	R	63	TYR	CB-CG-CD1	7.48	125.49	121.00
14	n	226	ARG	NE-CZ-NH2	-7.47	116.56	120.30
27	O	312	ASP	CB-CG-OD2	-7.47	111.58	118.30
21	N	784	TYR	CB-CG-CD2	-7.46	116.52	121.00
13	6	157	PHE	CB-CG-CD2	-7.46	115.58	120.80
30	K	395	VAL	CA-CB-CG2	-7.46	99.71	110.90
20	Z	253	VAL	CG1-CB-CG2	-7.46	98.96	110.90
24	Q	291	TYR	CB-CG-CD1	-7.46	116.53	121.00
5	E	16	SER	N-CA-CB	7.46	121.68	110.50
26	U	59	ASP	CB-CG-OD2	-7.45	111.59	118.30
21	N	776	TYR	CB-CG-CD2	-7.45	116.53	121.00
22	S	186	TYR	CB-CG-CD2	7.45	125.47	121.00
30	K	255	ARG	NE-CZ-NH2	-7.45	116.58	120.30
8	h	75	TYR	CB-CG-CD2	-7.44	116.53	121.00
25	R	422	ARG	NE-CZ-NH2	-7.44	116.58	120.30
23	P	95	TYR	CZ-CE2-CD2	-7.44	113.11	119.80
22	S	346	TYR	CD1-CE1-CZ	7.43	126.49	119.80
27	O	252	PHE	CB-CG-CD1	-7.43	115.60	120.80
11	k	67	TYR	CB-CG-CD2	7.42	125.45	121.00
16	V	202	ASP	CB-CG-OD1	-7.42	111.62	118.30
33	J	228	ARG	NE-CZ-NH1	7.42	124.01	120.30
32	M	404	ARG	NE-CZ-NH1	-7.42	116.59	120.30
21	N	421	ASP	CB-CG-OD2	-7.41	111.63	118.30
13	m	52	PHE	CB-CG-CD2	7.41	125.99	120.80
27	O	62	TYR	CB-CG-CD1	7.41	125.45	121.00
14	7	58	ASP	CB-CG-OD2	-7.41	111.63	118.30
32	M	38	ASP	N-CA-CB	7.41	123.94	110.60
21	N	415	PHE	CB-CG-CD2	-7.41	115.61	120.80
10	j	87	PHE	CB-CG-CD2	-7.41	115.62	120.80
27	O	369	ARG	NE-CZ-NH1	-7.40	116.60	120.30
22	S	333	PHE	CB-CG-CD1	-7.40	115.62	120.80
24	Q	84	TYR	CB-CG-CD1	7.40	125.44	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	b	4	ARG	NE-CZ-NH1	7.40	124.00	120.30
16	V	228	TYR	CB-CG-CD2	-7.39	116.57	121.00
13	6	109	ARG	NE-CZ-NH1	7.39	124.00	120.30
24	Q	294	ARG	NE-CZ-NH1	7.37	123.99	120.30
6	f	13	PHE	C-N-CA	7.37	140.12	121.70
26	U	253	ASP	CB-CG-OD1	7.37	124.93	118.30
16	V	156	PHE	CB-CG-CD2	7.37	125.96	120.80
20	Z	255	LEU	N-CA-CB	7.37	125.14	110.40
28	H	90	ARG	NE-CZ-NH2	-7.37	116.62	120.30
24	Q	160	ASP	CB-CG-OD1	-7.36	111.68	118.30
30	K	340	PHE	CB-CG-CD2	-7.35	115.65	120.80
23	P	69	ARG	NE-CZ-NH1	7.35	123.97	120.30
28	H	181	TYR	CD1-CE1-CZ	-7.34	113.20	119.80
21	N	422	TYR	CB-CG-CD1	-7.33	116.60	121.00
31	L	258	GLU	OE1-CD-OE2	-7.33	114.50	123.30
31	L	292	SER	N-CA-CB	7.33	121.50	110.50
18	X	22	ARG	NE-CZ-NH2	-7.33	116.64	120.30
6	f	99	PHE	CB-CG-CD1	-7.33	115.67	120.80
5	e	26	TYR	CB-CG-CD1	7.32	125.39	121.00
25	R	417	TYR	CG-CD1-CE1	-7.32	115.44	121.30
2	b	142	PHE	CB-CG-CD2	-7.32	115.68	120.80
10	3	3	ASP	CB-CG-OD1	-7.31	111.72	118.30
16	V	135	ARG	NE-CZ-NH1	7.31	123.96	120.30
22	S	393	ARG	NE-CZ-NH2	7.31	123.95	120.30
30	K	218	GLY	O-C-N	-7.31	111.01	122.70
33	J	248	ASP	CB-CG-OD1	7.30	124.87	118.30
31	L	339	ARG	NE-CZ-NH1	7.30	123.95	120.30
14	7	150	ALA	N-CA-CB	7.30	120.31	110.10
21	N	543	ASP	CB-CG-OD2	-7.30	111.73	118.30
9	i	232	TYR	CB-CG-CD1	7.29	125.38	121.00
24	Q	127	ARG	NE-CZ-NH2	-7.29	116.65	120.30
33	J	222	TYR	CB-CG-CD2	-7.28	116.63	121.00
20	Z	730	ALA	N-CA-C	7.28	130.65	111.00
1	a	244	ARG	NE-CZ-NH2	-7.28	116.66	120.30
6	f	157	TYR	CB-CG-CD1	-7.28	116.64	121.00
9	2	140	PHE	CB-CG-CD2	-7.28	115.71	120.80
30	K	306	PHE	N-CA-CB	7.28	123.70	110.60
33	J	75	VAL	CA-CB-CG2	-7.28	99.99	110.90
28	H	167	ASP	CB-CG-OD2	-7.27	111.75	118.30
31	L	117	TYR	CB-CG-CD2	-7.27	116.64	121.00
24	Q	110	SER	N-CA-CB	7.27	121.41	110.50
21	N	163	LEU	CB-CG-CD1	7.27	123.36	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	116	PHE	CB-CG-CD1	7.27	125.89	120.80
8	h	133	TYR	CB-CG-CD1	-7.26	116.64	121.00
8	1	163	PHE	CB-CG-CD2	-7.26	115.72	120.80
24	Q	297	ASP	CB-CG-OD1	-7.26	111.76	118.30
14	7	157	ASP	CB-CG-OD1	7.26	124.84	118.30
8	h	79	TYR	CB-CG-CD1	7.26	125.35	121.00
20	Z	735	GLU	N-CA-CB	7.25	123.66	110.60
32	M	255	TYR	CB-CG-CD1	7.25	125.35	121.00
2	b	130	PHE	CB-CG-CD1	-7.24	115.73	120.80
13	m	136	VAL	CA-CB-CG1	-7.24	100.04	110.90
1	a	110	TYR	CG-CD2-CE2	7.23	127.08	121.30
25	R	338	TYR	CB-CG-CD2	7.23	125.34	121.00
2	b	80	PRO	N-CA-CB	7.21	111.95	103.30
13	m	202	ARG	NH1-CZ-NH2	7.21	127.33	119.40
21	N	581	ASP	CB-CG-OD1	7.21	124.79	118.30
20	Z	726	GLU	N-CA-C	7.20	130.43	111.00
22	S	275	TYR	CB-CG-CD1	-7.20	116.68	121.00
6	f	20	PHE	CB-CG-CD1	-7.19	115.77	120.80
28	H	88	ARG	NE-CZ-NH2	7.19	123.89	120.30
28	H	235	PHE	CB-CG-CD2	-7.19	115.77	120.80
26	U	245	ASP	CB-CG-OD2	-7.18	111.83	118.30
10	3	28	ARG	NE-CZ-NH2	7.18	123.89	120.30
27	O	368	ASP	CB-CG-OD2	-7.18	111.84	118.30
31	L	161	ARG	NE-CZ-NH1	-7.18	116.71	120.30
24	Q	264	TYR	CB-CG-CD1	7.17	125.30	121.00
14	7	69	PHE	CB-CG-CD1	-7.17	115.78	120.80
21	N	139	ARG	NE-CZ-NH2	-7.16	116.72	120.30
22	S	188	TYR	CB-CG-CD2	-7.16	116.70	121.00
6	f	94	TYR	CB-CG-CD2	-7.16	116.70	121.00
32	M	109	ASP	CB-CG-OD2	7.16	124.74	118.30
31	L	413	ASP	CB-CG-OD2	7.16	124.74	118.30
6	f	82	ARG	NE-CZ-NH1	7.16	123.88	120.30
1	a	32	PHE	CB-CG-CD2	-7.15	115.79	120.80
1	a	135	ARG	NE-CZ-NH1	7.15	123.88	120.30
22	S	55	ARG	NE-CZ-NH2	-7.15	116.72	120.30
24	Q	50	ARG	NE-CZ-NH1	7.15	123.88	120.30
6	f	24	TYR	CG-CD2-CE2	7.14	127.01	121.30
12	l	180	THR	CA-CB-CG2	-7.14	102.41	112.40
15	W	37	PHE	CB-CG-CD1	7.14	125.80	120.80
7	g	212	PHE	CB-CG-CD1	7.13	125.79	120.80
9	i	219	TYR	CB-CG-CD1	7.13	125.28	121.00
8	h	66	ASP	CB-CG-OD2	7.13	124.72	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	134	ASP	CB-CG-OD1	7.13	124.72	118.30
6	f	13	PHE	CB-CG-CD1	-7.13	115.81	120.80
7	g	26	TYR	CB-CG-CD2	-7.13	116.72	121.00
13	m	41	TYR	CB-CG-CD1	-7.12	116.72	121.00
14	7	261	TYR	CZ-CE2-CD2	-7.12	113.39	119.80
28	H	372	ASP	CB-CG-OD2	-7.12	111.89	118.30
32	M	433	TYR	CB-CG-CD1	-7.12	116.73	121.00
2	b	5	TYR	CZ-CE2-CD2	-7.12	113.39	119.80
20	Z	248	TYR	CB-CG-CD2	-7.12	116.73	121.00
19	Y	72	ASP	CB-CG-OD1	-7.12	111.89	118.30
11	k	98	TYR	CB-CG-CD1	7.12	125.27	121.00
10	j	158	LEU	CB-CG-CD2	7.11	123.09	111.00
30	K	118	TYR	CB-CG-CD1	7.11	125.27	121.00
5	e	8	TYR	CB-CG-CD2	7.11	125.27	121.00
33	J	118	ASP	CB-CG-OD2	-7.11	111.91	118.30
10	j	166	THR	CA-CB-CG2	-7.10	102.46	112.40
8	h	169	SER	N-CA-CB	7.10	121.15	110.50
13	6	202	ARG	NE-CZ-NH2	-7.10	116.75	120.30
23	P	115	ARG	NE-CZ-NH1	-7.10	116.75	120.30
3	c	20	TYR	CG-CD1-CE1	-7.09	115.62	121.30
14	7	68	ARG	NE-CZ-NH2	-7.09	116.75	120.30
25	R	307	TYR	CD1-CE1-CZ	7.09	126.18	119.80
33	J	312	ARG	NE-CZ-NH1	7.09	123.85	120.30
17	T	89	TYR	CB-CG-CD2	-7.09	116.75	121.00
18	X	22	ARG	N-CA-CB	7.09	123.36	110.60
23	P	232	ARG	NE-CZ-NH2	-7.08	116.76	120.30
23	P	329	PHE	CB-CG-CD2	7.08	125.76	120.80
21	N	89	PHE	CB-CG-CD1	-7.08	115.84	120.80
7	g	91	ARG	NE-CZ-NH1	7.08	123.84	120.30
21	N	502	PHE	CB-CG-CD1	-7.08	115.85	120.80
4	d	120	TYR	CB-CG-CD2	-7.07	116.76	121.00
22	S	240	ASP	CB-CG-OD2	7.07	124.66	118.30
9	i	148	THR	CA-CB-CG2	-7.07	102.50	112.40
28	H	207	THR	CA-CB-CG2	-7.07	102.51	112.40
33	J	234	PHE	CB-CG-CD2	-7.07	115.85	120.80
13	m	82	TRP	CB-CG-CD2	-7.06	117.42	126.60
21	N	682	PHE	CB-CG-CD2	-7.06	115.86	120.80
11	k	46	PHE	CB-CG-CD1	-7.06	115.86	120.80
24	Q	132	PHE	CB-CG-CD2	7.06	125.74	120.80
3	c	113	ARG	NE-CZ-NH2	7.05	123.83	120.30
10	j	69	TYR	CB-CG-CD2	-7.05	116.77	121.00
33	J	131	ASP	CB-CG-OD2	7.05	124.64	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	20	TYR	CB-CG-CD2	7.05	125.23	121.00
26	U	110	PHE	CB-CG-CD1	-7.04	115.87	120.80
32	M	233	ARG	NE-CZ-NH2	-7.04	116.78	120.30
17	T	88	TYR	CB-CG-CD2	-7.03	116.78	121.00
27	O	228	TYR	CB-CG-CD2	-7.03	116.78	121.00
27	O	8	ASP	CB-CG-OD1	-7.03	111.98	118.30
12	5	262	TYR	CG-CD1-CE1	7.02	126.92	121.30
28	H	113	ASP	CB-CG-OD2	-7.02	111.98	118.30
11	4	117	TYR	CA-CB-CG	-7.01	100.07	113.40
33	J	306	ARG	NE-CZ-NH2	7.01	123.81	120.30
30	K	323	THR	CA-CB-CG2	-7.01	102.59	112.40
10	3	68	ARG	NE-CZ-NH1	7.01	123.80	120.30
29	I	422	ARG	NE-CZ-NH2	-7.01	116.80	120.30
21	N	322	ASP	CB-CG-OD2	7.00	124.60	118.30
33	J	298	ASP	CB-CG-OD2	-7.00	112.00	118.30
2	b	234	ARG	NE-CZ-NH2	6.99	123.80	120.30
29	I	422	ARG	NE-CZ-NH1	-6.99	116.80	120.30
21	N	528	ARG	NE-CZ-NH2	-6.99	116.80	120.30
10	3	67	PHE	CB-CG-CD1	-6.99	115.91	120.80
14	n	126	PHE	CB-CG-CD1	6.98	125.68	120.80
20	Z	253	VAL	N-CA-CB	6.98	126.85	111.50
21	N	145	LEU	CB-CG-CD1	6.97	122.85	111.00
15	W	182	TYR	CB-CG-CD2	-6.96	116.83	121.00
21	N	476	THR	CA-CB-CG2	-6.95	102.67	112.40
11	k	172	MET	CG-SD-CE	-6.95	89.08	100.20
14	n	134	TYR	CB-CG-CD1	6.95	125.17	121.00
24	Q	88	PHE	CB-CG-CD2	6.95	125.66	120.80
4	d	179	TYR	CG-CD1-CE1	-6.94	115.74	121.30
29	I	314	ASP	CB-CG-OD2	-6.94	112.05	118.30
33	J	71	TYR	CB-CG-CD2	-6.94	116.83	121.00
9	i	117	PHE	CB-CG-CD2	-6.93	115.95	120.80
8	h	79	TYR	CB-CG-CD2	-6.93	116.84	121.00
20	Z	213	LYS	N-CA-CB	-6.93	98.13	110.60
21	N	81	TYR	CB-CG-CD1	6.93	125.16	121.00
26	U	233	PHE	CB-CG-CD1	6.92	125.65	120.80
13	6	129	ALA	N-CA-CB	6.92	119.79	110.10
30	K	185	ARG	NE-CZ-NH1	6.92	123.76	120.30
11	k	43	LEU	CB-CG-CD1	6.92	122.76	111.00
21	N	211	PHE	CB-CG-CD2	-6.92	115.96	120.80
22	S	211	ARG	NE-CZ-NH1	6.92	123.76	120.30
14	7	220	ARG	NE-CZ-NH1	-6.91	116.84	120.30
8	h	38	ARG	NH1-CZ-NH2	-6.90	111.81	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	409	ARG	NE-CZ-NH2	-6.90	116.85	120.30
3	c	71	ASP	CB-CG-OD1	6.89	124.50	118.30
14	n	252	TRP	CD1-NE1-CE2	-6.89	102.80	109.00
17	T	89	TYR	CB-CG-CD1	6.89	125.14	121.00
1	a	111	ASP	CB-CG-OD2	6.89	124.50	118.30
13	m	196	PHE	CB-CG-CD1	6.89	125.62	120.80
10	j	67	PHE	CG-CD1-CE1	-6.88	113.23	120.80
10	j	100	PHE	CB-CG-CD2	6.88	125.61	120.80
33	J	210	PHE	CB-CG-CD2	-6.88	115.99	120.80
9	2	215	TYR	CB-CG-CD1	-6.87	116.88	121.00
32	M	131	MET	CG-SD-CE	-6.87	89.20	100.20
1	a	12	TYR	CB-CG-CD2	-6.87	116.88	121.00
30	K	218	GLY	CA-C-N	-6.87	102.09	117.20
25	R	301	TYR	CB-CG-CD2	-6.87	116.88	121.00
14	7	223	ARG	NE-CZ-NH2	-6.87	116.87	120.30
29	I	387	LEU	N-CA-CB	6.87	124.13	110.40
4	d	108	TYR	CG-CD1-CE1	-6.86	115.81	121.30
32	M	366	ARG	NE-CZ-NH1	6.86	123.73	120.30
29	I	208	TYR	CB-CG-CD2	-6.85	116.89	121.00
31	L	331	ASP	CB-CG-OD1	6.85	124.47	118.30
8	h	90	VAL	O-C-N	-6.85	111.74	122.70
21	N	412	TYR	CB-CG-CD2	6.85	125.11	121.00
3	C	24	TYR	CB-CG-CD2	-6.85	116.89	121.00
16	V	270	TYR	CZ-CE2-CD2	6.85	125.96	119.80
33	J	147	TYR	CG-CD1-CE1	-6.85	115.82	121.30
21	N	127	ASP	CB-CG-OD1	-6.84	112.14	118.30
4	d	174	PHE	CB-CG-CD2	6.83	125.58	120.80
10	j	103	TYR	CD1-CE1-CZ	-6.82	113.66	119.80
8	h	151	PHE	CZ-CE2-CD2	-6.82	111.92	120.10
21	N	741	TYR	CB-CG-CD1	6.81	125.09	121.00
25	R	297	TYR	CB-CG-CD2	-6.81	116.91	121.00
32	M	320	ARG	NE-CZ-NH2	6.81	123.70	120.30
24	Q	336	ASN	N-CA-CB	6.81	122.85	110.60
29	I	128	TYR	CG-CD2-CE2	-6.80	115.86	121.30
15	W	179	ARG	NE-CZ-NH1	6.79	123.70	120.30
7	g	212	PHE	CB-CG-CD2	-6.79	116.05	120.80
31	L	418	ALA	CB-CA-C	-6.79	99.91	110.10
11	k	130	TYR	CB-CG-CD1	6.79	125.07	121.00
13	6	145	ARG	NE-CZ-NH1	6.78	123.69	120.30
30	K	77	ARG	NE-CZ-NH1	6.78	123.69	120.30
28	H	438	ALA	N-CA-CB	6.78	119.59	110.10
33	J	9	ASN	N-CA-CB	6.77	122.79	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	J	316	PHE	CB-CG-CD2	-6.77	116.06	120.80
4	d	29	ARG	NE-CZ-NH1	-6.77	116.92	120.30
9	i	232	TYR	CZ-CE2-CD2	-6.76	113.72	119.80
28	H	153	ALA	N-CA-CB	6.76	119.57	110.10
9	i	98	TYR	CB-CG-CD1	-6.74	116.95	121.00
10	3	69	TYR	CG-CD2-CE2	-6.74	115.91	121.30
20	Z	727	GLU	C-N-CA	6.74	138.56	121.70
10	3	103	TYR	CZ-CE2-CD2	-6.74	113.73	119.80
5	e	50	VAL	CG1-CB-CG2	6.74	121.68	110.90
6	F	14	SER	N-CA-CB	6.74	120.60	110.50
17	T	265	ASP	CB-CG-OD2	-6.74	112.24	118.30
29	I	54	ARG	NE-CZ-NH2	6.73	123.67	120.30
6	f	203	ASP	N-CA-CB	6.73	122.72	110.60
12	l	275	VAL	CA-CB-CG2	-6.73	100.81	110.90
12	5	243	ASP	CB-CG-OD1	6.73	124.36	118.30
15	W	122	ARG	NE-CZ-NH1	6.73	123.66	120.30
14	n	162	TYR	CA-CB-CG	6.73	126.18	113.40
4	d	99	THR	CA-CB-CG2	-6.72	102.99	112.40
30	K	174	VAL	C-N-CA	6.72	136.42	122.30
13	m	182	TYR	CG-CD2-CE2	-6.71	115.93	121.30
14	7	126	PHE	CB-CG-CD1	6.71	125.50	120.80
28	H	454	TYR	CB-CG-CD1	6.71	125.03	121.00
6	f	18	ARG	NE-CZ-NH2	-6.71	116.95	120.30
14	7	189	ARG	NE-CZ-NH1	-6.70	116.95	120.30
13	m	106	TYR	CB-CG-CD1	6.70	125.02	121.00
21	N	328	PHE	CB-CG-CD2	-6.70	116.11	120.80
17	T	51	TYR	CB-CG-CD2	-6.69	116.98	121.00
32	M	431	SER	N-CA-CB	6.69	120.54	110.50
13	m	10	PHE	CB-CG-CD2	-6.69	116.12	120.80
26	U	288	PHE	CB-CG-CD1	-6.69	116.12	120.80
33	J	374	ARG	NE-CZ-NH1	6.69	123.64	120.30
9	2	37	PHE	CB-CG-CD1	6.69	125.48	120.80
22	S	170	TYR	CB-CG-CD2	6.69	125.01	121.00
28	H	295	PHE	CB-CG-CD1	-6.69	116.12	120.80
23	P	123	ARG	NE-CZ-NH2	-6.68	116.96	120.30
3	c	60	ASP	CB-CG-OD2	-6.68	112.28	118.30
8	h	19	ASP	O-C-N	-6.68	111.84	123.20
14	n	137	ARG	NE-CZ-NH1	6.68	123.64	120.30
14	7	254	PHE	CG-CD1-CE1	-6.67	113.46	120.80
1	a	71	TYR	CB-CG-CD2	-6.67	117.00	121.00
21	N	559	TYR	CD1-CE1-CZ	-6.67	113.80	119.80
32	M	290	ARG	NE-CZ-NH2	-6.67	116.97	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	O	128	LEU	CB-CG-CD1	6.66	122.33	111.00
24	Q	151	TYR	CB-CG-CD2	-6.66	117.00	121.00
8	1	47	HIS	N-CA-CB	6.64	122.56	110.60
6	f	14	SER	N-CA-CB	6.64	120.46	110.50
15	W	37	PHE	CG-CD1-CE1	6.63	128.10	120.80
3	C	122	TYR	CB-CG-CD1	6.63	124.98	121.00
31	L	357	ARG	NE-CZ-NH1	6.63	123.61	120.30
2	b	83	ARG	NE-CZ-NH2	-6.63	116.99	120.30
4	d	75	PHE	CB-CG-CD1	6.63	125.44	120.80
30	K	420	THR	CA-CB-CG2	-6.63	103.12	112.40
3	c	149	TYR	CB-CG-CD2	6.62	124.97	121.00
27	O	69	PHE	CB-CG-CD2	-6.62	116.16	120.80
1	a	30	TYR	CD1-CG-CD2	6.61	125.17	117.90
27	O	36	LYS	N-CA-CB	6.61	122.50	110.60
14	n	228	PHE	CB-CG-CD2	-6.61	116.17	120.80
21	N	362	TRP	CZ3-CH2-CZ2	-6.60	113.68	121.60
27	O	330	ARG	NE-CZ-NH1	6.59	123.60	120.30
33	J	378	THR	CA-CB-CG2	-6.59	103.17	112.40
9	i	153	TYR	CB-CG-CD2	-6.59	117.05	121.00
2	b	236	ARG	NE-CZ-NH2	-6.59	117.01	120.30
25	R	338	TYR	CB-CG-CD1	-6.59	117.05	121.00
27	O	71	ASP	CB-CG-OD2	-6.59	112.37	118.30
11	k	73	TYR	CB-CG-CD1	-6.58	117.05	121.00
13	6	193	ARG	NE-CZ-NH2	6.58	123.59	120.30
3	c	129	ARG	NE-CZ-NH1	6.58	123.59	120.30
31	L	68	ARG	NE-CZ-NH1	6.57	123.59	120.30
21	N	14	ARG	NE-CZ-NH1	6.57	123.58	120.30
21	N	713	VAL	CA-CB-CG2	6.57	120.75	110.90
21	N	124	TYR	CB-CG-CD2	6.57	124.94	121.00
26	U	118	PRO	N-CA-CB	6.57	111.18	103.30
21	N	282	TYR	CB-CG-CD2	6.56	124.94	121.00
8	h	66	ASP	CB-CG-OD1	-6.56	112.40	118.30
21	N	533	ASP	CB-CG-OD2	-6.56	112.40	118.30
24	Q	146	TYR	CG-CD1-CE1	-6.55	116.06	121.30
1	a	24	ARG	NE-CZ-NH2	-6.55	117.03	120.30
25	R	107	GLU	OE1-CD-OE2	-6.55	115.44	123.30
30	K	195	ALA	C-N-CA	6.55	138.07	121.70
14	n	216	VAL	CA-CB-CG1	6.55	120.72	110.90
11	4	54	VAL	CA-CB-CG1	-6.55	101.08	110.90
10	3	40	PHE	CB-CG-CD1	-6.54	116.22	120.80
2	b	23	TYR	CG-CD2-CE2	6.54	126.53	121.30
13	6	111	PHE	CB-CG-CD1	-6.54	116.22	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
17	T	51	TYR	CB-CG-CD1	6.54	124.92	121.00
1	a	28	VAL	CA-CB-CG2	-6.54	101.09	110.90
10	j	46	TYR	CB-CG-CD2	-6.54	117.08	121.00
21	N	593	PHE	CB-CG-CD2	6.54	125.38	120.80
14	n	168	VAL	CA-CB-CG1	6.54	120.70	110.90
29	I	409	MET	CG-SD-CE	-6.53	89.75	100.20
6	f	18	ARG	NE-CZ-NH1	6.53	123.57	120.30
14	7	250	MET	CG-SD-CE	-6.53	89.75	100.20
25	R	68	GLU	OE1-CD-OE2	6.53	131.13	123.30
21	N	14	ARG	NE-CZ-NH2	-6.53	117.04	120.30
25	R	170	VAL	CA-CB-CG2	-6.53	101.11	110.90
27	O	221	ALA	CB-CA-C	-6.53	100.31	110.10
3	c	102	TYR	CB-CG-CD1	6.52	124.91	121.00
23	P	103	TYR	CZ-CE2-CD2	6.52	125.67	119.80
8	h	151	PHE	CB-CG-CD2	-6.52	116.24	120.80
13	6	141	ARG	NE-CZ-NH1	-6.52	117.04	120.30
7	g	169	ARG	NE-CZ-NH2	-6.52	117.04	120.30
11	4	139	TYR	CB-CG-CD2	-6.52	117.09	121.00
22	S	286	TYR	CG-CD2-CE2	-6.52	116.09	121.30
21	N	17	GLN	N-CA-C	-6.51	93.41	111.00
14	7	161	ARG	NE-CZ-NH1	6.51	123.56	120.30
25	R	82	ASP	CB-CG-OD2	-6.51	112.44	118.30
21	N	809	ARG	NE-CZ-NH2	6.51	123.56	120.30
18	X	47	ASP	CB-CG-OD2	-6.51	112.44	118.30
31	L	221	TYR	N-CA-CB	6.51	122.31	110.60
2	b	97	TYR	CB-CG-CD1	6.51	124.90	121.00
3	c	113	ARG	NH1-CZ-NH2	-6.51	112.24	119.40
24	Q	217	GLU	OE1-CD-OE2	6.51	131.11	123.30
13	m	99	ARG	NE-CZ-NH2	6.50	123.55	120.30
12	5	267	ASP	CB-CG-OD2	-6.50	112.45	118.30
14	n	150	ALA	CB-CA-C	-6.49	100.36	110.10
5	e	82	THR	CA-CB-CG2	-6.49	103.31	112.40
13	m	138	SER	N-CA-CB	6.49	120.23	110.50
17	T	239	SER	N-CA-CB	6.49	120.23	110.50
23	P	416	SER	N-CA-CB	6.48	120.23	110.50
10	j	200	LEU	CB-CG-CD2	6.48	122.02	111.00
26	U	274	MET	CG-SD-CE	-6.48	89.84	100.20
8	1	118	GLU	N-CA-CB	6.47	122.25	110.60
13	6	28	PHE	CB-CG-CD1	6.47	125.33	120.80
23	P	73	ASP	CB-CG-OD1	6.47	124.13	118.30
20	Z	358	TYR	CB-CG-CD2	-6.47	117.12	121.00
21	N	301	THR	CA-CB-CG2	-6.47	103.34	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	85	PHE	CB-CG-CD2	6.47	125.33	120.80
30	K	236	ARG	NE-CZ-NH2	-6.46	117.07	120.30
31	L	186	LEU	N-CA-C	-6.46	93.55	111.00
27	O	310	PHE	CB-CG-CD1	-6.46	116.28	120.80
1	a	216	THR	CA-CB-CG2	-6.46	103.36	112.40
31	L	185	GLY	C-N-CA	6.46	137.84	121.70
12	l	255	VAL	CG1-CB-CG2	6.45	121.23	110.90
21	N	682	PHE	CB-CG-CD1	6.45	125.32	120.80
33	J	312	ARG	N-CA-CB	6.45	122.21	110.60
14	7	228	PHE	CB-CG-CD1	-6.45	116.28	120.80
25	R	146	ASP	N-CA-C	-6.45	93.60	111.00
9	i	111	MET	CG-SD-CE	-6.44	89.90	100.20
8	1	188	THR	CA-CB-CG2	-6.44	103.39	112.40
26	U	212	ASP	CB-CG-OD1	-6.44	112.51	118.30
30	K	270	PHE	CB-CG-CD2	6.44	125.31	120.80
13	m	47	TYR	CB-CG-CD2	-6.44	117.14	121.00
28	H	289	ARG	NE-CZ-NH1	-6.42	117.09	120.30
12	5	120	MET	CG-SD-CE	-6.42	89.93	100.20
32	M	243	PHE	CB-CG-CD2	6.42	125.30	120.80
3	C	24	TYR	CB-CG-CD1	6.42	124.85	121.00
22	S	69	LEU	N-CA-CB	6.42	123.23	110.40
9	i	215	TYR	CB-CG-CD1	-6.41	117.15	121.00
17	T	128	TYR	CG-CD2-CE2	-6.41	116.17	121.30
28	H	429	PHE	CB-CG-CD2	-6.41	116.31	120.80
10	3	74	TYR	CB-CG-CD1	-6.41	117.16	121.00
18	X	11	ARG	NH1-CZ-NH2	-6.41	112.36	119.40
12	l	253	TYR	CB-CG-CD2	6.40	124.84	121.00
21	N	322	ASP	CB-CG-OD1	-6.40	112.54	118.30
27	O	310	PHE	CB-CG-CD2	6.39	125.28	120.80
20	Z	728	LYS	CB-CG-CD	6.39	128.21	111.60
20	Z	153	TYR	C-N-CA	6.39	137.67	121.70
3	c	6	TYR	CG-CD2-CE2	-6.38	116.19	121.30
10	j	104	PHE	CB-CG-CD1	-6.38	116.33	120.80
8	1	96	TYR	CB-CG-CD1	-6.38	117.17	121.00
7	g	79	SER	N-CA-CB	6.38	120.07	110.50
17	T	20	TYR	CG-CD2-CE2	6.38	126.40	121.30
25	R	297	TYR	CB-CG-CD1	6.38	124.83	121.00
2	b	178	ARG	NE-CZ-NH1	6.37	123.48	120.30
3	c	60	ASP	CB-CG-OD1	6.37	124.03	118.30
33	J	265	ASP	CB-CG-OD1	-6.37	112.57	118.30
28	H	87	ASP	CB-CG-OD2	6.36	124.03	118.30
29	I	422	ARG	NH1-CZ-NH2	6.36	126.40	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	348	PHE	CB-CG-CD2	-6.36	116.35	120.80
25	R	71	LEU	CB-CG-CD1	6.35	121.80	111.00
28	H	178	ARG	NE-CZ-NH1	-6.35	117.13	120.30
24	Q	12	ARG	NE-CZ-NH1	-6.35	117.13	120.30
31	L	137	ARG	NE-CZ-NH1	6.34	123.47	120.30
4	d	72	VAL	CA-CB-CG1	-6.34	101.39	110.90
14	n	134	TYR	CB-CG-CD2	-6.34	117.20	121.00
25	R	124	ASP	CB-CG-OD2	-6.34	112.59	118.30
27	O	106	PHE	CB-CG-CD2	-6.34	116.36	120.80
25	R	233	ASP	CB-CG-OD1	6.34	124.00	118.30
32	M	170	MET	CG-SD-CE	-6.34	90.06	100.20
6	f	147	PHE	CB-CG-CD1	-6.33	116.37	120.80
3	C	122	TYR	CB-CG-CD2	-6.33	117.20	121.00
16	V	254	ARG	NE-CZ-NH1	6.33	123.47	120.30
8	1	120	TYR	CB-CG-CD2	-6.33	117.20	121.00
9	i	180	ALA	N-CA-CB	6.33	118.96	110.10
20	Z	247	GLN	CA-CB-CG	6.32	127.30	113.40
23	P	138	ARG	NE-CZ-NH2	-6.32	117.14	120.30
21	N	549	TYR	CG-CD2-CE2	-6.32	116.25	121.30
25	R	345	TYR	CB-CG-CD2	-6.31	117.21	121.00
14	n	175	LEU	CA-C-O	6.31	133.36	120.10
13	6	36	ARG	NH1-CZ-NH2	-6.31	112.46	119.40
29	I	155	SER	N-CA-CB	6.31	119.97	110.50
3	c	205	ALA	N-CA-CB	6.31	118.93	110.10
8	1	60	ASP	CB-CG-OD2	-6.31	112.62	118.30
33	J	42	ARG	NE-CZ-NH2	-6.31	117.15	120.30
24	Q	414	GLU	OE1-CD-OE2	-6.31	115.73	123.30
27	O	305	ILE	CA-CB-CG2	-6.30	98.29	110.90
29	I	136	VAL	CA-CB-CG2	-6.30	101.44	110.90
13	m	75	ARG	NE-CZ-NH2	-6.30	117.15	120.30
21	N	574	VAL	CA-CB-CG2	-6.30	101.45	110.90
31	L	216	LYS	N-CA-CB	6.30	121.94	110.60
12	5	82	ARG	NE-CZ-NH2	-6.30	117.15	120.30
15	W	12	ASN	N-CA-CB	6.30	121.94	110.60
6	f	192	ALA	CB-CA-C	-6.29	100.66	110.10
28	H	420	ARG	NE-CZ-NH2	-6.29	117.15	120.30
3	c	171	ALA	CB-CA-C	-6.29	100.66	110.10
7	g	234	ASP	CB-CG-OD2	6.29	123.96	118.30
16	V	157	ARG	NE-CZ-NH2	-6.29	117.15	120.30
27	O	387	ARG	NE-CZ-NH2	-6.29	117.15	120.30
16	V	227	MET	CG-SD-CE	-6.29	90.14	100.20
4	d	230	ASN	CB-CA-C	-6.29	97.82	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	g	163	ALA	CB-CA-C	-6.29	100.67	110.10
31	L	392	ARG	CG-CD-NE	-6.29	98.60	111.80
33	J	71	TYR	CA-CB-CG	-6.29	101.46	113.40
28	H	281	GLN	N-CA-CB	6.28	121.91	110.60
24	Q	185	TYR	CB-CG-CD2	-6.28	117.23	121.00
30	K	58	TYR	CG-CD1-CE1	-6.28	116.28	121.30
4	d	49	ARG	NE-CZ-NH1	6.27	123.44	120.30
12	5	204	VAL	CA-CB-CG2	-6.27	101.49	110.90
8	h	194	ARG	NE-CZ-NH1	6.27	123.43	120.30
7	g	112	PHE	CB-CG-CD1	-6.27	116.41	120.80
13	6	24	ALA	N-CA-CB	6.27	118.87	110.10
26	U	78	GLU	OE1-CD-OE2	-6.26	115.78	123.30
10	3	198	ARG	NE-CZ-NH1	-6.26	117.17	120.30
6	f	94	TYR	CB-CG-CD1	6.26	124.75	121.00
3	c	205	ALA	CB-CA-C	-6.26	100.72	110.10
22	S	111	ARG	NE-CZ-NH2	6.26	123.43	120.30
23	P	179	PHE	CB-CG-CD1	6.26	125.18	120.80
25	R	224	PHE	CB-CG-CD2	6.26	125.18	120.80
21	N	598	ASP	CB-CG-OD1	-6.25	112.68	118.30
30	K	262	ARG	NE-CZ-NH2	-6.25	117.18	120.30
12	5	210	PHE	CG-CD1-CE1	6.24	127.67	120.80
21	N	354	PRO	N-CA-CB	6.24	110.79	103.30
31	L	56	ALA	CB-CA-C	-6.24	100.73	110.10
27	O	116	ASN	CB-CG-OD1	-6.24	109.12	121.60
33	J	296	ARG	NH1-CZ-NH2	6.24	126.26	119.40
3	c	92	ARG	NE-CZ-NH2	-6.24	117.18	120.30
10	j	99	ARG	NE-CZ-NH1	-6.24	117.18	120.30
27	O	25	LEU	CB-CG-CD1	6.23	121.60	111.00
3	c	242	THR	CA-CB-CG2	-6.23	103.68	112.40
18	X	100	TRP	N-CA-C	-6.23	94.17	111.00
29	I	355	LEU	CB-CG-CD1	6.23	121.59	111.00
30	K	286	THR	N-CA-C	-6.23	94.18	111.00
33	J	22	TYR	CD1-CG-CD2	6.23	124.75	117.90
2	b	5	TYR	CB-CG-CD2	-6.23	117.26	121.00
3	c	45	VAL	CG1-CB-CG2	6.22	120.86	110.90
10	j	91	VAL	CA-CB-CG2	-6.22	101.56	110.90
31	L	91	THR	N-CA-CB	6.22	122.13	110.30
15	W	57	ALA	CB-CA-C	-6.22	100.77	110.10
20	Z	728	LYS	N-CA-C	-6.22	94.21	111.00
24	Q	264	TYR	CB-CG-CD2	-6.22	117.27	121.00
30	K	286	THR	CA-CB-CG2	-6.22	103.70	112.40
22	S	421	TYR	CB-CG-CD1	6.21	124.73	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	144	TYR	CB-CG-CD2	-6.21	117.27	121.00
10	3	199	TYR	CB-CG-CD1	6.21	124.72	121.00
14	7	136	ARG	NE-CZ-NH1	6.20	123.40	120.30
21	N	5	THR	CA-CB-CG2	-6.20	103.72	112.40
31	L	345	ARG	NE-CZ-NH2	-6.20	117.20	120.30
10	j	87	PHE	CB-CG-CD1	6.20	125.14	120.80
12	l	255	VAL	CA-CB-CG2	-6.20	101.60	110.90
26	U	67	PHE	CB-CG-CD1	6.20	125.14	120.80
3	c	210	ARG	NE-CZ-NH1	6.20	123.40	120.30
10	3	174	ALA	N-CA-CB	-6.20	101.43	110.10
21	N	139	ARG	NE-CZ-NH1	6.20	123.40	120.30
22	S	367	TYR	CB-CG-CD2	6.20	124.72	121.00
4	D	22	TYR	CB-CG-CD1	6.19	124.72	121.00
21	N	229	VAL	CG1-CB-CG2	6.19	120.81	110.90
28	H	283	TYR	CG-CD1-CE1	-6.19	116.35	121.30
11	k	151	ASP	CB-CG-OD1	6.19	123.87	118.30
24	Q	147	GLN	O-C-N	-6.19	112.79	122.70
4	d	179	TYR	CB-CG-CD1	-6.19	117.29	121.00
6	f	177	ASP	CB-CG-OD2	-6.19	112.73	118.30
16	V	145	GLN	O-C-N	6.19	132.60	122.70
31	L	220	LEU	CB-CG-CD1	-6.18	100.49	111.00
22	S	76	PHE	CB-CG-CD2	-6.18	116.47	120.80
2	b	5	TYR	CB-CG-CD1	6.18	124.71	121.00
25	R	304	TYR	CB-CG-CD1	6.17	124.70	121.00
14	7	254	PHE	CD1-CE1-CZ	6.17	127.50	120.10
10	j	104	PHE	CG-CD1-CE1	6.16	127.58	120.80
32	M	315	PHE	CB-CG-CD1	-6.16	116.49	120.80
11	k	33	ASP	CB-CG-OD2	-6.16	112.76	118.30
15	W	152	GLU	OE1-CD-OE2	6.16	130.69	123.30
21	N	338	PHE	CB-CG-CD2	-6.16	116.49	120.80
5	e	16	SER	N-CA-CB	6.16	119.73	110.50
12	5	210	PHE	CB-CG-CD1	6.16	125.11	120.80
13	m	82	TRP	CB-CG-CD1	6.15	135.00	127.00
22	S	274	PHE	CB-CG-CD2	-6.15	116.49	120.80
31	L	375	ASP	CB-CG-OD1	6.15	123.83	118.30
22	S	356	ASP	CB-CG-OD2	6.15	123.83	118.30
14	n	220	ARG	NE-CZ-NH2	-6.15	117.23	120.30
27	O	225	ASP	CB-CG-OD2	-6.15	112.77	118.30
28	H	375	VAL	CA-CB-CG1	6.15	120.12	110.90
12	5	230	TYR	CB-CG-CD1	6.15	124.69	121.00
20	Z	727	GLU	N-CA-C	6.14	127.59	111.00
4	d	246	GLN	CG-CD-OE1	6.14	133.88	121.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	165	TYR	CB-CG-CD2	-6.14	117.32	121.00
23	P	101	MET	CG-SD-CE	-6.14	90.38	100.20
25	R	233	ASP	CB-CG-OD2	-6.14	112.78	118.30
30	K	178	ASP	CB-CG-OD2	-6.13	112.78	118.30
5	e	153	TYR	CD1-CE1-CZ	-6.13	114.29	119.80
7	g	239	ALA	CB-CA-C	-6.13	100.91	110.10
29	I	316	PHE	CB-CG-CD1	-6.13	116.51	120.80
13	6	139	TYR	CB-CG-CD1	-6.12	117.33	121.00
17	T	48	ASN	N-CA-CB	6.12	121.62	110.60
17	T	144	TYR	CG-CD1-CE1	-6.12	116.40	121.30
21	N	399	PHE	CB-CG-CD2	6.12	125.09	120.80
22	S	252	ASP	CB-CG-OD2	-6.12	112.79	118.30
23	P	221	TYR	CB-CG-CD1	-6.12	117.33	121.00
26	U	206	ASP	CB-CG-OD2	-6.12	112.79	118.30
3	c	146	TYR	CB-CG-CD2	6.12	124.67	121.00
21	N	57	ASP	CB-CG-OD2	-6.12	112.79	118.30
4	d	230	ASN	N-CA-CB	6.12	121.61	110.60
9	i	80	ASP	CB-CG-OD2	-6.12	112.79	118.30
32	M	255	TYR	CB-CG-CD2	-6.12	117.33	121.00
5	e	133	LEU	CB-CG-CD1	-6.12	100.60	111.00
21	N	81	TYR	CB-CG-CD2	-6.12	117.33	121.00
6	f	6	TYR	CB-CG-CD1	-6.11	117.33	121.00
17	T	157	TYR	CB-CG-CD1	-6.11	117.33	121.00
14	7	170	TYR	CD1-CE1-CZ	-6.11	114.30	119.80
1	a	78	THR	CA-CB-CG2	-6.11	103.85	112.40
21	N	549	TYR	CZ-CE2-CD2	6.11	125.30	119.80
22	S	170	TYR	CB-CG-CD1	-6.11	117.34	121.00
20	Z	358	TYR	CB-CG-CD1	6.10	124.66	121.00
12	5	148	ARG	NE-CZ-NH1	-6.10	117.25	120.30
12	5	198	LYS	N-CA-CB	6.10	121.57	110.60
18	X	78	ILE	CA-CB-CG1	6.10	122.59	111.00
33	J	401	ALA	N-CA-CB	6.09	118.63	110.10
5	e	20	ARG	N-CA-CB	6.09	121.57	110.60
31	L	146	VAL	CB-CA-C	-6.09	99.83	111.40
2	b	161	ALA	N-CA-CB	6.09	118.62	110.10
21	N	415	PHE	CB-CG-CD1	6.09	125.06	120.80
14	7	189	ARG	NE-CZ-NH2	6.08	123.34	120.30
22	S	405	ARG	NE-CZ-NH2	-6.08	117.26	120.30
31	L	407	ARG	NE-CZ-NH2	-6.08	117.26	120.30
10	j	138	VAL	CA-CB-CG1	-6.08	101.77	110.90
17	T	144	TYR	CB-CG-CD2	6.08	124.65	121.00
29	I	167	MET	CA-CB-CG	6.08	123.64	113.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	128	TYR	CB-CG-CD2	-6.08	117.35	121.00
9	2	129	VAL	CG1-CB-CG2	6.08	120.62	110.90
30	K	349	ARG	NE-CZ-NH2	-6.08	117.26	120.30
3	c	162	ALA	N-CA-CB	6.08	118.61	110.10
13	m	29	ALA	N-CA-CB	6.07	118.60	110.10
21	N	38	GLU	CB-CG-CD	-6.07	97.80	114.20
24	Q	306	TYR	CG-CD1-CE1	-6.07	116.44	121.30
3	c	137	TYR	CB-CG-CD2	6.07	124.64	121.00
12	5	221	TRP	CG-CD2-CE3	-6.07	128.44	133.90
8	1	111	TYR	CB-CG-CD1	-6.07	117.36	121.00
25	R	341	LEU	CB-CG-CD1	6.07	121.32	111.00
10	j	139	SER	N-CA-CB	6.07	119.60	110.50
1	a	31	ALA	CB-CA-C	-6.07	101.00	110.10
7	g	48	PHE	CB-CG-CD1	-6.07	116.56	120.80
14	7	63	TYR	CG-CD2-CE2	-6.07	116.45	121.30
21	N	682	PHE	CB-CA-C	-6.07	98.27	110.40
31	L	321	THR	CA-CB-CG2	-6.07	103.91	112.40
7	g	201	TYR	CB-CG-CD2	-6.06	117.36	121.00
26	U	135	ASP	N-CA-CB	6.06	121.51	110.60
22	S	271	ARG	NE-CZ-NH1	-6.06	117.27	120.30
11	4	172	MET	CG-SD-CE	-6.06	90.51	100.20
24	Q	309	ARG	NH1-CZ-NH2	6.06	126.06	119.40
31	L	386	PHE	CB-CG-CD1	-6.06	116.56	120.80
14	7	72	VAL	CA-CB-CG1	6.05	119.98	110.90
25	R	94	PHE	CB-CG-CD2	6.05	125.03	120.80
21	N	299	TYR	CB-CG-CD1	-6.05	117.37	121.00
21	N	630	ALA	CB-CA-C	-6.05	101.03	110.10
5	e	118	ASP	N-CA-CB	6.05	121.48	110.60
26	U	275	VAL	CA-CB-CG1	6.04	119.97	110.90
32	M	285	ALA	CB-CA-C	-6.04	101.04	110.10
27	O	70	TYR	N-CA-CB	6.04	121.47	110.60
10	j	154	TYR	CD1-CE1-CZ	6.04	125.23	119.80
30	K	234	PHE	CB-CG-CD2	6.04	125.03	120.80
9	i	234	PHE	CZ-CE2-CD2	-6.03	112.86	120.10
17	T	245	TYR	CZ-CE2-CD2	6.03	125.23	119.80
11	k	59	TYR	CZ-CE2-CD2	-6.03	114.37	119.80
14	n	74	ARG	N-CA-CB	6.03	121.46	110.60
14	n	254	PHE	CB-CG-CD1	-6.03	116.58	120.80
30	K	235	ILE	C-N-CA	6.03	136.77	121.70
3	c	100	LYS	O-C-N	-6.03	113.06	122.70
31	L	395	ALA	N-CA-CB	-6.03	101.67	110.10
18	X	91	PHE	CB-CG-CD1	-6.02	116.58	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
21	N	471	TYR	CB-CG-CD1	-6.02	117.39	121.00
28	H	272	ILE	N-CA-C	-6.01	94.76	111.00
18	X	106	SER	N-CA-CB	6.01	119.52	110.50
11	4	80	VAL	CA-CB-CG1	6.01	119.91	110.90
10	3	154	TYR	CZ-CE2-CD2	6.00	125.20	119.80
21	N	618	ARG	NE-CZ-NH1	6.00	123.30	120.30
21	N	731	VAL	CA-C-N	6.00	128.21	116.20
21	N	24	ALA	N-CA-CB	6.00	118.50	110.10
27	O	387	ARG	NE-CZ-NH1	6.00	123.30	120.30
33	J	344	ARG	N-CA-CB	6.00	121.40	110.60
30	K	168	ASP	CB-CG-OD1	6.00	123.70	118.30
13	6	157	PHE	CB-CG-CD1	5.99	125.00	120.80
16	V	285	ASP	CB-CG-OD1	-5.99	112.91	118.30
21	N	548	ARG	NE-CZ-NH2	-5.99	117.30	120.30
13	6	227	LEU	CB-CG-CD1	-5.99	100.81	111.00
30	K	210	LEU	CB-CG-CD1	5.99	121.19	111.00
12	l	216	ASP	CB-CG-OD2	-5.99	112.91	118.30
14	7	179	PHE	CB-CG-CD1	-5.99	116.61	120.80
32	M	337	LEU	CB-CG-CD1	5.99	121.18	111.00
16	V	138	ALA	N-CA-C	-5.99	94.84	111.00
27	O	215	TYR	CB-CG-CD2	-5.99	117.41	121.00
3	c	216	ILE	N-CA-C	-5.98	94.85	111.00
12	l	262	TYR	CB-CG-CD2	5.98	124.59	121.00
4	D	22	TYR	CB-CG-CD2	-5.98	117.41	121.00
10	3	99	ARG	NE-CZ-NH2	5.98	123.29	120.30
30	K	306	PHE	N-CA-C	-5.98	94.86	111.00
6	f	51	ARG	CA-CB-CG	5.98	126.55	113.40
22	S	263	ASP	N-CA-CB	5.98	121.36	110.60
7	G	26	TYR	CB-CG-CD2	-5.97	117.42	121.00
13	m	196	PHE	CB-CG-CD2	-5.97	116.62	120.80
32	M	303	ARG	NE-CZ-NH2	-5.97	117.31	120.30
16	V	300	VAL	CB-CA-C	5.97	122.75	111.40
30	K	270	PHE	CB-CG-CD1	-5.97	116.62	120.80
32	M	333	LEU	CB-CG-CD2	5.97	121.15	111.00
33	J	310	ILE	N-CA-C	-5.97	94.88	111.00
10	3	50	PHE	CB-CG-CD1	5.97	124.98	120.80
14	7	179	PHE	CB-CG-CD2	5.97	124.98	120.80
22	S	286	TYR	CD1-CG-CD2	5.97	124.46	117.90
22	S	264	VAL	CG1-CB-CG2	5.96	120.44	110.90
28	H	100	ALA	N-CA-CB	-5.96	101.75	110.10
31	L	389	ALA	N-CA-CB	5.96	118.45	110.10
32	M	357	ARG	CG-CD-NE	-5.96	99.27	111.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	180	THR	N-CA-CB	5.96	121.63	110.30
2	b	92	VAL	CG1-CB-CG2	5.96	120.44	110.90
9	2	80	ASP	CB-CG-OD1	5.96	123.66	118.30
16	V	273	ARG	CG-CD-NE	-5.96	99.29	111.80
13	6	86	ASP	CB-CG-OD2	5.96	123.66	118.30
23	P	329	PHE	CB-CG-CD1	-5.96	116.63	120.80
26	U	131	GLY	N-CA-C	-5.96	98.21	113.10
31	L	191	ARG	CA-CB-CG	5.95	126.50	113.40
32	M	281	ASP	CB-CG-OD2	5.95	123.66	118.30
9	i	195	ASP	CB-CG-OD1	-5.95	112.95	118.30
14	n	58	ASP	CB-CG-OD2	-5.95	112.95	118.30
14	n	223	ARG	NH1-CZ-NH2	5.95	125.94	119.40
21	N	788	TYR	CB-CG-CD1	-5.95	117.43	121.00
24	Q	209	TYR	CG-CD2-CE2	-5.95	116.54	121.30
8	h	54	ARG	NE-CZ-NH2	-5.95	117.33	120.30
23	P	4	ASP	CB-CG-OD2	-5.95	112.95	118.30
28	H	331	ARG	NE-CZ-NH2	-5.95	117.33	120.30
20	Z	738	TYR	CE1-CZ-OH	-5.95	104.05	120.10
3	c	98	TYR	CB-CG-CD2	5.94	124.56	121.00
13	6	180	LEU	CB-CG-CD2	5.94	121.10	111.00
14	7	93	MET	CG-SD-CE	-5.94	90.70	100.20
21	N	910	PRO	N-CD-CG	5.94	112.11	103.20
27	O	70	TYR	CG-CD1-CE1	5.94	126.05	121.30
21	N	585	ARG	NE-CZ-NH2	5.93	123.27	120.30
17	T	161	TRP	CA-CB-CG	5.93	124.97	113.70
21	N	436	ASP	N-CA-CB	5.93	121.28	110.60
22	S	475	TYR	CB-CG-CD2	-5.93	117.44	121.00
26	U	154	PHE	CB-CG-CD1	-5.93	116.65	120.80
8	h	183	ARG	NE-CZ-NH1	-5.93	117.34	120.30
10	3	142	ALA	CB-CA-C	5.93	118.99	110.10
21	N	398	ARG	NE-CZ-NH1	5.93	123.26	120.30
9	2	175	LEU	CA-CB-CG	5.92	128.92	115.30
25	R	383	ARG	NE-CZ-NH2	-5.92	117.34	120.30
31	L	69	ARG	NE-CZ-NH1	-5.92	117.34	120.30
33	J	339	ARG	NE-CZ-NH1	5.92	123.26	120.30
8	h	19	ASP	CA-C-N	5.92	128.05	116.20
1	a	73	PHE	CB-CG-CD2	-5.92	116.66	120.80
23	P	168	TYR	CG-CD2-CE2	-5.92	116.56	121.30
33	J	248	ASP	CB-CG-OD2	-5.92	112.97	118.30
25	R	187	VAL	CA-CB-CG1	5.92	119.77	110.90
31	L	109	MET	CA-CB-CG	5.92	123.36	113.30
7	g	139	GLY	O-C-N	-5.91	113.15	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	h	195	LEU	N-CA-CB	5.91	122.22	110.40
8	h	38	ARG	NE-CZ-NH1	5.91	123.25	120.30
14	7	109	TYR	N-CA-CB	5.91	121.23	110.60
32	M	329	ARG	CD-NE-CZ	5.91	131.87	123.60
12	l	256	THR	CA-CB-CG2	-5.90	104.14	112.40
20	Z	550	PHE	CB-CG-CD1	5.90	124.93	120.80
32	M	373	ASP	CB-CG-OD1	5.90	123.61	118.30
9	2	37	PHE	CB-CG-CD2	-5.90	116.67	120.80
9	i	232	TYR	CG-CD2-CE2	5.90	126.02	121.30
31	L	91	THR	CA-CB-CG2	-5.90	104.14	112.40
24	Q	84	TYR	CZ-CE2-CD2	-5.90	114.49	119.80
24	Q	177	VAL	CA-CB-CG2	-5.90	102.06	110.90
24	Q	373	VAL	CA-CB-CG2	-5.90	102.06	110.90
20	Z	253	VAL	N-CA-C	-5.89	95.09	111.00
21	N	282	TYR	CB-CG-CD1	-5.89	117.46	121.00
21	N	651	PHE	CG-CD2-CE2	5.89	127.28	120.80
33	J	279	LEU	CB-CG-CD1	5.89	121.02	111.00
7	g	93	ARG	NE-CZ-NH1	5.89	123.24	120.30
21	N	575	ALA	N-CA-CB	5.89	118.34	110.10
9	i	45	ALA	N-CA-CB	5.88	118.33	110.10
33	J	368	TYR	CB-CG-CD2	5.88	124.53	121.00
13	6	208	ASP	CB-CG-OD2	-5.88	113.01	118.30
23	P	170	SER	O-C-N	-5.88	113.30	122.70
10	3	125	ASP	CB-CG-OD2	5.88	123.59	118.30
9	2	211	LYS	CA-CB-CG	5.87	126.32	113.40
19	Y	37	ASP	CB-CG-OD1	5.87	123.59	118.30
24	Q	214	THR	O-C-N	5.87	132.09	122.70
29	I	54	ARG	NE-CZ-NH1	-5.87	117.36	120.30
29	I	346	ARG	NE-CZ-NH2	-5.87	117.37	120.30
14	7	149	VAL	N-CA-C	-5.87	95.16	111.00
14	7	183	MET	CA-CB-CG	5.87	123.27	113.30
22	S	244	ASN	CB-CA-C	-5.86	98.67	110.40
12	l	253	TYR	CB-CG-CD1	-5.86	117.48	121.00
20	Z	736	LEU	N-CA-CB	-5.86	98.68	110.40
14	7	221	ASP	CB-CG-OD1	5.86	123.58	118.30
18	X	85	ARG	CD-NE-CZ	-5.86	115.40	123.60
8	h	185	VAL	CA-CB-CG2	-5.86	102.12	110.90
27	O	166	ARG	NH1-CZ-NH2	-5.85	112.96	119.40
4	d	56	ASP	CB-CG-OD2	5.85	123.57	118.30
9	i	148	THR	CA-CB-OG1	5.85	121.28	109.00
24	Q	6	SER	N-CA-CB	5.85	119.27	110.50
29	I	292	TYR	CB-CG-CD1	-5.85	117.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	101	ARG	NE-CZ-NH2	-5.85	117.38	120.30
21	N	584	ARG	CG-CD-NE	-5.85	99.52	111.80
25	R	62	TYR	CZ-CE2-CD2	-5.85	114.54	119.80
13	6	196	PHE	CB-CG-CD2	-5.85	116.71	120.80
2	b	23	TYR	CZ-CE2-CD2	-5.84	114.54	119.80
5	e	51	GLU	N-CA-C	-5.84	95.22	111.00
10	j	125	ASP	CB-CG-OD2	-5.84	113.04	118.30
11	k	23	ARG	NE-CZ-NH2	5.84	123.22	120.30
33	J	210	PHE	CB-CG-CD1	5.84	124.89	120.80
11	k	11	ASP	CB-CG-OD2	-5.84	113.04	118.30
13	6	132	SER	N-CA-CB	5.84	119.26	110.50
24	Q	397	LEU	N-CA-C	-5.84	95.23	111.00
14	7	159	PHE	CB-CG-CD2	5.84	124.89	120.80
28	H	73	ASP	CB-CG-OD1	5.84	123.55	118.30
28	H	45	TYR	CB-CG-CD1	-5.83	117.50	121.00
14	n	240	THR	CA-CB-CG2	-5.83	104.24	112.40
13	6	53	ASP	CB-CG-OD2	5.83	123.55	118.30
21	N	198	THR	CA-CB-CG2	-5.83	104.24	112.40
24	Q	389	VAL	CG1-CB-CG2	5.83	120.23	110.90
29	I	61	ARG	NH1-CZ-NH2	-5.83	112.99	119.40
12	l	210	PHE	CB-CG-CD1	5.83	124.88	120.80
30	K	377	SER	CB-CA-C	-5.83	99.03	110.10
31	L	132	ARG	NE-CZ-NH1	5.83	123.21	120.30
33	J	296	ARG	NE-CZ-NH1	-5.83	117.39	120.30
27	O	142	ASP	CB-CG-OD2	5.83	123.54	118.30
29	I	306	MET	CG-SD-CE	-5.83	90.88	100.20
30	K	169	VAL	CA-CB-CG2	-5.83	102.16	110.90
33	J	222	TYR	CG-CD2-CE2	-5.83	116.64	121.30
24	Q	287	THR	N-CA-CB	5.82	121.37	110.30
21	N	902	VAL	CA-CB-CG2	-5.82	102.17	110.90
10	3	69	TYR	CZ-CE2-CD2	5.82	125.04	119.80
7	g	219	CYS	N-CA-CB	5.82	121.07	110.60
10	j	147	PHE	CB-CG-CD2	5.82	124.87	120.80
18	X	75	TRP	CH2-CZ2-CE2	5.82	123.22	117.40
14	7	74	ARG	NE-CZ-NH2	-5.82	117.39	120.30
25	R	328	PHE	CB-CG-CD2	5.82	124.87	120.80
27	O	361	ASP	CB-CG-OD1	-5.82	113.07	118.30
28	H	204	PRO	N-CA-C	-5.82	96.98	112.10
3	c	6	TYR	CG-CD1-CE1	-5.81	116.65	121.30
32	M	198	VAL	CB-CA-C	-5.81	100.35	111.40
11	4	67	TYR	CA-CB-CG	-5.81	102.36	113.40
20	Z	786	SER	N-CA-CB	-5.81	101.79	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	f	171	TYR	CB-CG-CD1	5.80	124.48	121.00
9	i	215	TYR	CG-CD2-CE2	-5.80	116.66	121.30
8	1	202	TYR	CB-CG-CD2	-5.80	117.52	121.00
29	I	181	TYR	CG-CD2-CE2	5.80	125.94	121.30
7	g	169	ARG	NE-CZ-NH1	5.80	123.20	120.30
12	l	163	TYR	CG-CD1-CE1	5.80	125.94	121.30
17	T	245	TYR	N-CA-CB	5.80	121.04	110.60
12	5	287	GLY	N-CA-C	-5.80	98.61	113.10
22	S	461	PHE	CB-CG-CD1	5.80	124.86	120.80
28	H	290	MET	CA-CB-CG	5.79	123.15	113.30
14	n	165	LEU	CB-CG-CD2	5.79	120.84	111.00
23	P	213	TYR	CB-CG-CD2	-5.79	117.53	121.00
31	L	347	VAL	CA-CB-CG2	-5.79	102.21	110.90
5	e	8	TYR	CB-CG-CD1	-5.79	117.53	121.00
9	i	226	GLU	N-CA-CB	5.78	121.01	110.60
20	Z	254	PRO	CA-C-N	-5.78	104.48	117.20
22	S	23	LYS	N-CA-CB	5.78	121.00	110.60
24	Q	434	TYR	CZ-CE2-CD2	5.78	125.00	119.80
25	R	207	ARG	NE-CZ-NH2	-5.78	117.41	120.30
30	K	196	ASP	CB-CG-OD1	-5.78	113.10	118.30
29	I	280	PHE	CB-CG-CD1	5.78	124.84	120.80
23	P	359	ARG	CD-NE-CZ	-5.77	115.52	123.60
5	e	41	ALA	N-CA-CB	5.77	118.18	110.10
12	l	196	ARG	NE-CZ-NH1	-5.77	117.41	120.30
20	Z	248	TYR	CB-CA-C	-5.77	98.85	110.40
21	N	213	PHE	CB-CG-CD2	5.77	124.84	120.80
19	Y	69	VAL	CA-CB-CG2	-5.77	102.24	110.90
30	K	336	ARG	NE-CZ-NH2	5.77	123.19	120.30
4	d	179	TYR	CG-CD2-CE2	-5.77	116.69	121.30
8	1	120	TYR	CB-CG-CD1	5.77	124.46	121.00
7	g	160	TYR	CG-CD1-CE1	-5.77	116.69	121.30
21	N	781	ALA	CB-CA-C	-5.76	101.45	110.10
24	Q	377	LEU	CB-CG-CD1	-5.76	101.20	111.00
16	V	108	TYR	CG-CD1-CE1	-5.76	116.69	121.30
28	H	197	MET	CG-SD-CE	-5.76	90.98	100.20
11	k	117	TYR	CG-CD1-CE1	5.76	125.91	121.30
27	O	189	TYR	CB-CG-CD2	-5.76	117.54	121.00
20	Z	735	GLU	CB-CA-C	-5.76	98.88	110.40
20	Z	729	GLU	N-CA-C	5.76	126.54	111.00
7	g	66	LYS	N-CA-CB	5.75	120.95	110.60
12	5	212	TYR	N-CA-CB	5.75	120.95	110.60
28	H	440	GLU	N-CA-CB	5.75	120.95	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	85	PHE	CB-CG-CD1	-5.75	116.78	120.80
24	Q	409	TYR	CB-CG-CD1	5.75	124.45	121.00
8	h	33	ALA	N-CA-CB	5.74	118.14	110.10
16	V	179	LEU	CB-CG-CD1	5.74	120.77	111.00
23	P	300	VAL	CA-CB-CG1	5.74	119.52	110.90
6	f	209	ASP	CB-CG-OD1	5.74	123.47	118.30
7	g	197	ALA	N-CA-CB	5.74	118.14	110.10
7	g	230	PHE	CB-CG-CD1	5.74	124.82	120.80
15	W	7	VAL	CA-CB-CG1	-5.74	102.29	110.90
20	Z	513	ALA	N-CA-CB	5.74	118.13	110.10
30	K	140	HIS	N-CA-CB	5.73	120.92	110.60
1	a	120	ARG	NE-CZ-NH1	5.72	123.16	120.30
16	V	142	ASP	CB-CG-OD1	-5.72	113.15	118.30
30	K	145	ALA	CB-CA-C	-5.72	101.51	110.10
1	a	120	ARG	NE-CZ-NH2	-5.72	117.44	120.30
28	H	288	ALA	N-CA-CB	5.72	118.11	110.10
33	J	260	GLY	C-N-CA	5.72	136.00	121.70
10	j	98	ARG	NE-CZ-NH2	-5.72	117.44	120.30
31	L	157	ARG	NE-CZ-NH1	5.71	123.16	120.30
2	b	161	ALA	CB-CA-C	-5.71	101.53	110.10
10	j	100	PHE	CB-CG-CD1	-5.71	116.80	120.80
9	2	48	ARG	NE-CZ-NH2	5.71	123.15	120.30
20	Z	264	PHE	CB-CG-CD1	5.71	124.80	120.80
15	W	25	ARG	CD-NE-CZ	-5.71	115.61	123.60
14	n	184	ALA	C-N-CA	5.70	135.96	121.70
32	M	126	THR	N-CA-CB	5.70	121.14	110.30
2	b	101	TYR	CZ-CE2-CD2	-5.70	114.67	119.80
2	b	179	TRP	CA-CB-CG	5.70	124.53	113.70
14	n	119	ALA	CB-CA-C	-5.70	101.55	110.10
9	2	193	TRP	CB-CG-CD1	5.70	134.41	127.00
6	f	222	PHE	CB-CG-CD1	-5.70	116.81	120.80
22	S	373	LYS	O-C-N	5.70	131.82	122.70
25	R	328	PHE	CB-CG-CD1	-5.70	116.81	120.80
32	M	176	PRO	O-C-N	5.70	131.82	122.70
3	c	5	ARG	NE-CZ-NH2	-5.70	117.45	120.30
11	k	195	PHE	CB-CG-CD1	5.70	124.79	120.80
25	R	256	THR	CA-CB-CG2	-5.70	104.42	112.40
10	3	179	ALA	CB-CA-C	5.69	118.64	110.10
12	l	230	TYR	CG-CD1-CE1	-5.69	116.75	121.30
24	Q	332	ARG	NH1-CZ-NH2	-5.69	113.14	119.40
10	3	46	TYR	CB-CG-CD2	-5.69	117.59	121.00
21	N	762	ARG	NH1-CZ-NH2	-5.69	113.14	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	234	SER	N-CA-CB	5.69	119.03	110.50
12	5	172	MET	CA-CB-CG	5.68	122.96	113.30
9	2	122	HIS	CA-CB-CG	-5.68	103.94	113.60
30	K	258	PHE	CB-CG-CD1	5.68	124.78	120.80
27	O	38	TRP	CH2-CZ2-CE2	5.68	123.08	117.40
12	5	119	THR	CA-CB-CG2	-5.68	104.45	112.40
28	H	438	ALA	CB-CA-C	-5.68	101.58	110.10
30	K	342	SER	N-CA-CB	5.68	119.02	110.50
31	L	320	GLN	C-N-CA	5.68	135.89	121.70
10	j	172	LEU	CB-CG-CD1	5.67	120.65	111.00
16	V	251	TYR	CG-CD2-CE2	-5.67	116.76	121.30
21	N	333	SER	N-CA-CB	5.67	119.01	110.50
30	K	374	ARG	NE-CZ-NH2	-5.67	117.46	120.30
32	M	166	ARG	NE-CZ-NH2	5.67	123.14	120.30
18	X	85	ARG	NE-CZ-NH2	-5.67	117.46	120.30
7	g	142	ASP	CB-CG-OD2	-5.67	113.20	118.30
12	l	195	THR	CA-CB-OG1	5.67	120.90	109.00
1	A	128	TYR	CB-CG-CD1	5.67	124.40	121.00
14	7	34	THR	CA-CB-CG2	5.67	120.33	112.40
13	m	134	ASP	CB-CG-OD1	-5.67	113.20	118.30
20	Z	728	LYS	CA-C-N	5.67	129.66	117.20
33	J	78	ILE	N-CA-C	-5.67	95.70	111.00
33	J	361	VAL	CB-CA-C	-5.67	100.64	111.40
29	I	374	ASP	CB-CG-OD1	-5.66	113.20	118.30
9	2	217	ARG	CD-NE-CZ	-5.66	115.67	123.60
16	V	284	ALA	CB-CA-C	-5.66	101.61	110.10
23	P	208	PHE	CB-CG-CD2	5.66	124.76	120.80
21	N	123	PHE	CD1-CG-CD2	-5.66	110.94	118.30
27	O	216	ASP	CB-CG-OD1	-5.66	113.21	118.30
30	K	262	ARG	NE-CZ-NH1	5.66	123.13	120.30
12	l	219	TYR	CB-CG-CD1	5.66	124.39	121.00
8	1	61	THR	CA-CB-CG2	-5.66	104.48	112.40
8	1	79	TYR	CB-CG-CD2	-5.65	117.61	121.00
15	W	153	LEU	CB-CG-CD2	5.65	120.61	111.00
21	N	109	TYR	CD1-CE1-CZ	-5.65	114.71	119.80
26	U	146	ASP	N-CA-CB	5.65	120.77	110.60
30	K	308	GLN	N-CA-CB	5.65	120.77	110.60
22	S	195	ALA	CB-CA-C	5.65	118.57	110.10
23	P	240	TYR	CB-CG-CD1	-5.65	117.61	121.00
9	2	195	ASP	CB-CG-OD1	5.64	123.38	118.30
30	K	106	ASN	N-CA-CB	5.64	120.76	110.60
28	H	145	TYR	CZ-CE2-CD2	-5.64	114.72	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	e	132	ARG	NE-CZ-NH2	-5.64	117.48	120.30
12	l	94	ARG	NE-CZ-NH1	-5.63	117.48	120.30
12	5	165	TYR	CB-CG-CD2	-5.63	117.62	121.00
23	P	168	TYR	CB-CG-CD2	-5.63	117.62	121.00
23	P	223	LEU	N-CA-CB	5.63	121.67	110.40
28	H	234	ARG	NE-CZ-NH2	-5.63	117.48	120.30
6	f	179	PHE	CB-CG-CD1	-5.63	116.86	120.80
16	V	68	VAL	O-C-N	-5.63	113.69	122.70
5	e	228	PHE	CB-CG-CD2	5.63	124.74	120.80
12	5	133	TRP	CG-CD2-CE3	-5.63	128.84	133.90
29	I	264	CYS	CB-CA-C	-5.63	99.14	110.40
14	7	141	ASN	N-CA-C	-5.63	95.81	111.00
32	M	386	PHE	CB-CG-CD2	-5.63	116.86	120.80
11	k	116	LEU	CB-CG-CD2	-5.62	101.44	111.00
16	V	95	LEU	CB-CG-CD2	5.62	120.56	111.00
6	f	68	GLU	OE1-CD-OE2	-5.62	116.56	123.30
17	T	169	GLN	CG-CD-OE1	-5.62	110.36	121.60
5	e	182	GLU	CG-CD-OE2	-5.62	107.06	118.30
15	W	15	TYR	CG-CD2-CE2	-5.62	116.81	121.30
25	R	228	ALA	N-CA-CB	5.62	117.96	110.10
29	I	121	THR	CA-CB-CG2	5.62	120.26	112.40
9	i	240	ALA	CB-CA-C	-5.62	101.67	110.10
27	O	91	ASP	CB-CG-OD2	-5.62	113.25	118.30
13	m	215	VAL	N-CA-C	-5.61	95.85	111.00
21	N	839	ARG	CG-CD-NE	-5.61	100.01	111.80
24	Q	434	TYR	CG-CD2-CE2	-5.61	116.81	121.30
28	H	429	PHE	CB-CG-CD1	5.61	124.73	120.80
14	n	133	MET	CG-SD-CE	-5.61	91.22	100.20
23	P	381	SER	N-CA-CB	5.61	118.92	110.50
28	H	299	ARG	NE-CZ-NH2	5.61	123.10	120.30
15	W	37	PHE	CB-CG-CD2	-5.61	116.88	120.80
24	Q	65	TYR	CD1-CE1-CZ	-5.60	114.76	119.80
32	M	346	LYS	N-CA-C	-5.60	95.87	111.00
25	R	187	VAL	CA-CB-CG2	-5.60	102.50	110.90
25	R	342	LEU	CB-CG-CD2	5.60	120.52	111.00
7	g	220	SER	N-CA-CB	5.60	118.90	110.50
7	g	59	LEU	CB-CA-C	-5.60	99.56	110.20
28	H	305	ILE	N-CA-C	-5.60	95.89	111.00
30	K	171	TYR	CB-CG-CD1	-5.60	117.64	121.00
26	U	123	VAL	CA-CB-CG1	-5.60	102.51	110.90
26	U	78	GLU	CG-CD-OE1	5.59	129.49	118.30
8	1	38	ARG	NE-CZ-NH1	5.59	123.10	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	c	42	ASP	CB-CG-OD1	5.59	123.33	118.30
14	7	128	TYR	CB-CG-CD2	5.59	124.35	121.00
23	P	402	PHE	CB-CG-CD1	-5.59	116.89	120.80
27	O	373	TRP	CG-CD2-CE3	-5.59	128.87	133.90
28	H	49	LEU	CB-CG-CD1	5.59	120.50	111.00
17	T	266	TYR	CB-CG-CD2	-5.59	117.65	121.00
6	f	6	TYR	CG-CD2-CE2	-5.59	116.83	121.30
12	l	183	GLU	CB-CG-CD	-5.59	99.12	114.20
24	Q	291	TYR	CB-CG-CD2	5.59	124.35	121.00
29	I	119	ILE	N-CA-C	-5.59	95.92	111.00
13	m	10	PHE	CB-CG-CD1	5.58	124.71	120.80
4	d	201	GLU	OE1-CD-OE2	5.58	130.00	123.30
16	V	117	TRP	CG-CD2-CE3	-5.58	128.88	133.90
21	N	610	SER	N-CA-CB	5.58	118.87	110.50
21	N	765	ASP	CB-CG-OD2	-5.58	113.28	118.30
25	R	233	ASP	N-CA-CB	5.58	120.65	110.60
33	J	320	SER	CB-CA-C	5.58	120.70	110.10
16	V	175	SER	N-CA-CB	5.58	118.87	110.50
12	l	82	ARG	NH1-CZ-NH2	5.58	125.54	119.40
24	Q	279	LYS	N-CA-CB	5.58	120.64	110.60
10	j	199	TYR	O-C-N	5.58	131.62	122.70
11	4	138	PHE	CB-CG-CD1	5.58	124.70	120.80
14	7	240	THR	N-CA-C	-5.58	95.94	111.00
31	L	267	PHE	CB-CG-CD1	-5.58	116.90	120.80
6	f	157	TYR	CZ-CE2-CD2	-5.57	114.78	119.80
14	n	245	LEU	CB-CG-CD2	5.57	120.47	111.00
6	F	13	PHE	C-N-CA	5.57	135.64	121.70
11	4	98	TYR	CZ-CE2-CD2	5.57	124.82	119.80
21	N	677	ASP	CB-CG-OD1	-5.57	113.29	118.30
25	R	331	ARG	NE-CZ-NH1	5.57	123.08	120.30
7	g	116	LEU	CB-CA-C	-5.57	99.62	110.20
21	N	57	ASP	CB-CG-OD1	5.57	123.31	118.30
1	a	222	ASP	CB-CG-OD2	-5.57	113.29	118.30
25	R	24	TYR	CG-CD2-CE2	-5.57	116.85	121.30
2	b	82	TYR	CZ-CE2-CD2	5.56	124.81	119.80
2	b	140	ASP	CB-CG-OD1	5.56	123.31	118.30
18	X	97	TYR	CB-CG-CD1	-5.56	117.66	121.00
11	k	138	PHE	CB-CG-CD2	-5.56	116.91	120.80
8	1	14	ALA	N-CA-CB	5.56	117.89	110.10
30	K	245	LYS	CB-CA-C	-5.56	99.28	110.40
9	i	216	LEU	CB-CA-C	5.56	120.76	110.20
11	k	95	ARG	NE-CZ-NH1	-5.56	117.52	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
12	l	245	TYR	CB-CG-CD1	5.56	124.33	121.00
16	V	67	ASP	CB-CG-OD2	-5.56	113.30	118.30
29	I	265	ARG	NE-CZ-NH2	-5.56	117.52	120.30
23	P	103	TYR	CG-CD2-CE2	-5.55	116.86	121.30
30	K	350	ARG	NE-CZ-NH1	5.55	123.08	120.30
33	J	200	ARG	NE-CZ-NH1	5.55	123.08	120.30
2	b	95	THR	CA-CB-CG2	-5.55	104.63	112.40
11	4	16	ALA	N-CA-CB	5.55	117.87	110.10
12	5	192	SER	N-CA-C	5.55	125.99	111.00
27	O	130	ASP	N-CA-CB	5.55	120.59	110.60
27	O	228	TYR	CA-CB-CG	-5.55	102.85	113.40
14	7	252	TRP	CZ3-CH2-CZ2	-5.55	114.94	121.60
16	V	190	HIS	CA-CB-CG	5.55	123.03	113.60
24	Q	277	ASP	CB-CG-OD1	-5.55	113.31	118.30
12	l	196	ARG	NE-CZ-NH2	5.55	123.07	120.30
11	4	73	TYR	CB-CG-CD2	5.55	124.33	121.00
15	W	109	ARG	NH1-CZ-NH2	-5.55	113.30	119.40
22	S	288	THR	CA-CB-CG2	-5.54	104.64	112.40
27	O	51	ASP	CB-CG-OD2	-5.54	113.31	118.30
29	I	129	TYR	CD1-CE1-CZ	5.54	124.79	119.80
31	L	266	MET	CA-CB-CG	5.54	122.72	113.30
22	S	406	ASP	CB-CG-OD2	-5.54	113.31	118.30
31	L	254	LYS	CA-CB-CG	5.54	125.58	113.40
8	1	79	TYR	CB-CG-CD1	5.54	124.32	121.00
13	6	162	VAL	CA-CB-CG2	-5.54	102.60	110.90
19	Y	32	ASP	CB-CG-OD2	5.54	123.28	118.30
25	R	213	TYR	CG-CD2-CE2	-5.54	116.87	121.30
6	f	209	ASP	CB-CG-OD2	-5.53	113.32	118.30
15	W	37	PHE	CD1-CE1-CZ	-5.53	113.46	120.10
8	h	47	HIS	N-CA-CB	5.53	120.55	110.60
17	T	15	PHE	CB-CG-CD1	-5.53	116.93	120.80
22	S	143	GLN	N-CA-CB	5.53	120.55	110.60
22	S	352	VAL	CA-CB-CG1	5.53	119.19	110.90
24	Q	85	MET	CA-CB-CG	5.53	122.70	113.30
25	R	238	PHE	CB-CG-CD2	-5.53	116.93	120.80
10	3	130	ILE	CA-CB-CG2	-5.53	99.84	110.90
19	Y	83	ARG	NH1-CZ-NH2	-5.53	113.32	119.40
23	P	228	SER	N-CA-CB	-5.53	102.21	110.50
11	k	59	TYR	CG-CD1-CE1	-5.53	116.88	121.30
10	3	17	GLY	N-CA-C	-5.53	99.28	113.10
12	5	175	MET	N-CA-CB	5.53	120.55	110.60
14	7	80	ASP	CB-CG-OD2	5.53	123.27	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	95	ASP	CB-CG-OD2	-5.52	113.33	118.30
2	b	130	PHE	CB-CG-CD2	5.52	124.67	120.80
21	N	528	ARG	N-CA-CB	5.52	120.54	110.60
21	N	706	MET	CA-CB-CG	5.52	122.69	113.30
27	O	352	TRP	CE3-CZ3-CH2	5.52	127.27	121.20
29	I	256	TYR	CG-CD1-CE1	-5.52	116.88	121.30
13	m	47	TYR	CB-CG-CD1	5.52	124.31	121.00
10	3	164	PHE	CB-CG-CD2	-5.52	116.94	120.80
2	B	23	TYR	CB-CG-CD2	-5.52	117.69	121.00
12	5	227	ASP	CB-CG-OD2	-5.52	113.33	118.30
24	Q	229	ASP	CB-CG-OD2	-5.52	113.33	118.30
2	b	207	ASP	CB-CG-OD1	5.52	123.26	118.30
13	6	36	ARG	NE-CZ-NH2	5.52	123.06	120.30
28	H	140	ASP	O-C-N	5.52	131.53	122.70
21	N	814	ALA	CB-CA-C	-5.51	101.83	110.10
23	P	311	TRP	CG-CD2-CE3	-5.51	128.94	133.90
9	i	252	ILE	CA-C-O	5.51	131.67	120.10
21	N	742	TRP	CB-CG-CD2	-5.51	119.44	126.60
30	K	408	GLU	OE1-CD-OE2	5.51	129.91	123.30
31	L	331	ASP	CB-CG-OD2	-5.51	113.34	118.30
25	R	146	ASP	CB-CG-OD1	5.50	123.25	118.30
14	n	170	TYR	CB-CG-CD2	5.50	124.30	121.00
16	V	57	PHE	CB-CG-CD1	5.50	124.65	120.80
16	V	140	VAL	CB-CA-C	-5.50	100.95	111.40
8	h	111	TYR	CB-CG-CD2	-5.50	117.70	121.00
12	l	272	PHE	CB-CG-CD1	-5.50	116.95	120.80
7	G	132	PHE	CB-CG-CD1	5.50	124.65	120.80
14	7	120	LEU	CB-CG-CD2	5.50	120.35	111.00
14	7	190	LYS	C-N-CA	5.50	135.44	121.70
21	N	451	GLY	O-C-N	5.50	131.50	122.70
23	P	257	TRP	CA-CB-CG	5.50	124.14	113.70
31	L	267	PHE	CB-CG-CD2	5.50	124.65	120.80
8	h	70	TYR	CB-CG-CD2	-5.49	117.70	121.00
12	5	186	THR	CA-CB-CG2	-5.49	104.71	112.40
13	6	213	LEU	N-CA-CB	5.49	121.38	110.40
21	N	148	SER	N-CA-CB	5.49	118.74	110.50
33	J	2	THR	CA-CB-CG2	-5.49	104.71	112.40
10	3	198	ARG	NE-CZ-NH2	5.49	123.04	120.30
26	U	14	VAL	CB-CA-C	-5.49	100.98	111.40
26	U	15	LEU	CB-CA-C	-5.49	99.78	110.20
14	n	161	ARG	NE-CZ-NH1	5.48	123.04	120.30
13	6	214	ILE	CA-CB-CG1	-5.48	100.59	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	H	166	THR	CA-CB-CG2	-5.48	104.73	112.40
4	d	129	PHE	CG-CD1-CE1	5.48	126.83	120.80
21	N	138	GLU	CB-CA-C	-5.48	99.44	110.40
13	6	198	SER	N-CA-CB	5.48	118.72	110.50
27	O	98	TYR	CB-CG-CD1	-5.48	117.71	121.00
8	h	60	ASP	CB-CA-C	-5.47	99.46	110.40
33	J	317	PRO	N-CD-CG	5.47	111.41	103.20
15	W	79	THR	N-CA-CB	5.47	120.69	110.30
21	N	548	ARG	C-N-CA	5.47	135.37	121.70
16	V	181	ASN	N-CA-CB	5.47	120.44	110.60
10	3	32	GLN	N-CA-CB	5.47	120.44	110.60
2	b	111	VAL	CA-CB-CG2	-5.46	102.70	110.90
25	R	392	ARG	NE-CZ-NH1	-5.46	117.57	120.30
12	5	179	TYR	CB-CG-CD2	-5.46	117.72	121.00
10	j	40	PHE	CB-CG-CD2	5.46	124.62	120.80
33	J	238	ARG	NH1-CZ-NH2	-5.46	113.39	119.40
8	h	44	THR	CA-CB-CG2	-5.46	104.76	112.40
21	N	355	TRP	CG-CD2-CE3	-5.46	128.99	133.90
23	P	83	SER	N-CA-CB	5.46	118.69	110.50
28	H	400	ARG	NE-CZ-NH1	5.46	123.03	120.30
28	H	448	ASP	CB-CG-OD2	-5.46	113.39	118.30
2	b	14	PRO	N-CA-CB	5.45	109.84	103.30
19	Y	83	ARG	N-CA-CB	5.45	120.41	110.60
11	k	153	THR	N-CA-C	-5.45	96.28	111.00
31	L	374	PHE	CB-CG-CD2	-5.45	116.98	120.80
32	M	291	PHE	CB-CG-CD2	5.45	124.61	120.80
14	7	223	ARG	NE-CZ-NH1	5.45	123.02	120.30
20	Z	946	THR	N-CA-C	-5.45	96.29	111.00
31	L	264	ARG	NE-CZ-NH1	5.45	123.03	120.30
30	K	135	MET	CA-CB-CG	5.45	122.56	113.30
14	7	162	TYR	CB-CG-CD1	-5.44	117.73	121.00
21	N	494	LYS	CA-C-O	-5.44	108.67	120.10
22	S	314	ASN	CB-CA-C	-5.44	99.51	110.40
24	Q	408	THR	CA-CB-CG2	-5.44	104.78	112.40
25	R	321	TYR	CG-CD2-CE2	5.44	125.65	121.30
30	K	141	ARG	NH1-CZ-NH2	-5.44	113.41	119.40
33	J	153	LEU	N-CA-CB	5.44	121.29	110.40
16	V	98	THR	CA-CB-CG2	-5.44	104.78	112.40
5	e	156	PHE	CB-CG-CD2	5.44	124.61	120.80
5	E	15	PHE	C-N-CA	5.44	135.30	121.70
22	S	253	PHE	CB-CG-CD2	5.44	124.61	120.80
11	k	141	PHE	CB-CG-CD2	5.44	124.61	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	m	24	ALA	N-CA-CB	5.44	117.71	110.10
13	m	142	GLU	N-CA-CB	5.44	120.39	110.60
12	5	255	VAL	CA-CB-CG2	-5.44	102.75	110.90
9	i	230	LYS	N-CA-CB	5.43	120.38	110.60
10	j	143	SER	N-CA-CB	5.43	118.65	110.50
27	O	92	PHE	CB-CG-CD2	-5.43	117.00	120.80
23	P	267	PHE	CB-CG-CD1	5.43	124.60	120.80
23	P	395	ARG	NE-CZ-NH1	5.43	123.01	120.30
26	U	53	ALA	CB-CA-C	-5.43	101.96	110.10
30	K	310	THR	CA-CB-CG2	-5.43	104.80	112.40
2	b	101	TYR	CG-CD2-CE2	5.42	125.64	121.30
10	j	127	ILE	C-N-CA	5.42	133.69	122.30
9	2	203	ASP	CB-CG-OD2	-5.42	113.42	118.30
1	a	205	PHE	CB-CG-CD2	5.42	124.59	120.80
8	h	61	THR	CA-CB-CG2	-5.42	104.81	112.40
30	K	294	ARG	NH1-CZ-NH2	5.42	125.36	119.40
31	L	267	PHE	CD1-CE1-CZ	5.42	126.60	120.10
27	O	249	ASP	CB-CG-OD1	5.42	123.17	118.30
32	M	44	PHE	N-CA-CB	5.42	120.35	110.60
32	M	45	ARG	NE-CZ-NH1	5.42	123.01	120.30
5	e	132	ARG	NE-CZ-NH1	5.42	123.01	120.30
28	H	415	THR	CA-CB-CG2	-5.42	104.82	112.40
23	P	325	ASP	N-CA-CB	5.41	120.35	110.60
24	Q	277	ASP	CB-CG-OD2	5.41	123.17	118.30
4	d	108	TYR	CB-CG-CD2	5.41	124.25	121.00
13	6	134	ASP	CB-CG-OD2	-5.41	113.43	118.30
25	R	251	THR	CA-CB-CG2	-5.41	104.82	112.40
32	M	339	ARG	CA-CB-CG	5.41	125.30	113.40
8	1	195	LEU	O-C-N	-5.41	114.05	122.70
21	N	741	TYR	CB-CG-CD2	-5.41	117.75	121.00
32	M	153	TYR	CB-CG-CD2	5.41	124.25	121.00
11	k	101	ASN	CA-CB-CG	-5.41	101.51	113.40
25	R	324	ARG	NE-CZ-NH2	-5.41	117.60	120.30
31	L	187	THR	C-N-CA	5.41	135.21	121.70
5	e	165	TYR	CB-CG-CD1	5.40	124.24	121.00
22	S	338	MET	CG-SD-CE	-5.40	91.56	100.20
9	2	193	TRP	CB-CG-CD2	-5.40	119.58	126.60
9	i	180	ALA	CB-CA-C	-5.39	102.01	110.10
14	n	110	ASP	CB-CG-OD2	-5.39	113.44	118.30
26	U	219	LEU	CB-CG-CD2	5.39	120.17	111.00
13	m	13	TYR	CG-CD2-CE2	-5.39	116.99	121.30
17	T	244	ASP	CB-CG-OD2	5.39	123.15	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
25	R	363	PHE	CB-CG-CD1	-5.39	117.03	120.80
31	L	376	PHE	CB-CG-CD1	-5.39	117.03	120.80
2	b	18	LEU	N-CA-CB	5.39	121.18	110.40
7	g	165	THR	N-CA-C	-5.39	96.44	111.00
31	L	78	ARG	NH1-CZ-NH2	5.39	125.33	119.40
6	f	203	ASP	CB-CG-OD2	5.39	123.15	118.30
9	i	81	THR	CA-CB-CG2	-5.39	104.85	112.40
31	L	111	GLU	OE1-CD-OE2	-5.39	116.83	123.30
10	j	172	LEU	N-CA-CB	5.39	121.18	110.40
9	2	247	VAL	N-CA-C	-5.39	96.45	111.00
21	N	570	ARG	NE-CZ-NH1	-5.39	117.61	120.30
21	N	863	SER	N-CA-CB	5.39	118.58	110.50
22	S	335	GLN	CB-CA-C	-5.39	99.62	110.40
3	c	179	ASP	CB-CG-OD2	5.39	123.15	118.30
13	m	164	PHE	CB-CG-CD2	-5.39	117.03	120.80
16	V	185	ILE	N-CA-C	-5.39	96.46	111.00
2	b	101	TYR	CB-CG-CD2	5.38	124.23	121.00
6	F	24	TYR	CB-CG-CD2	-5.38	117.77	121.00
29	I	120	VAL	CA-CB-CG2	5.38	118.97	110.90
5	e	93	ARG	NE-CZ-NH2	5.38	122.99	120.30
20	Z	738	TYR	CA-CB-CG	5.38	123.63	113.40
7	g	26	TYR	CG-CD1-CE1	-5.38	116.99	121.30
24	Q	210	CYS	CA-CB-SG	-5.38	104.31	114.00
24	Q	251	THR	CA-CB-CG2	-5.38	104.87	112.40
28	H	121	ASN	N-CA-CB	5.38	120.29	110.60
31	L	89	ASP	CB-CG-OD2	-5.38	113.46	118.30
13	6	221	ARG	NE-CZ-NH1	5.38	122.99	120.30
30	K	207	ARG	NE-CZ-NH2	5.38	122.99	120.30
1	a	153	SER	CB-CA-C	-5.38	99.88	110.10
7	g	157	TYR	CD1-CG-CD2	-5.38	111.99	117.90
31	L	62	ARG	N-CA-CB	5.38	120.28	110.60
31	L	145	ARG	N-CA-CB	5.38	120.28	110.60
32	M	308	LEU	CB-CG-CD1	5.38	120.14	111.00
3	c	5	ARG	NE-CZ-NH1	5.38	122.99	120.30
5	e	169	ALA	N-CA-CB	5.38	117.62	110.10
1	a	118	ALA	N-CA-CB	5.37	117.62	110.10
17	T	118	ASN	CB-CA-C	-5.37	99.65	110.40
18	X	17	TYR	CB-CG-CD2	5.37	124.22	121.00
22	S	42	SER	CB-CA-C	-5.37	99.89	110.10
28	H	124	ASN	C-N-CA	5.37	135.13	121.70
8	h	60	ASP	CB-CG-OD2	-5.37	113.47	118.30
7	g	135	SER	O-C-N	5.37	131.29	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	I	408	ARG	CA-CB-CG	5.37	125.21	113.40
24	Q	48	ASP	C-N-CA	5.37	135.11	121.70
13	m	132	SER	N-CA-CB	5.36	118.55	110.50
14	7	254	PHE	CG-CD2-CE2	-5.36	114.90	120.80
7	g	201	TYR	CB-CG-CD1	5.36	124.22	121.00
22	S	76	PHE	CB-CG-CD1	5.36	124.55	120.80
26	U	121	LEU	CB-CG-CD1	5.36	120.11	111.00
13	6	90	LYS	N-CA-C	-5.36	96.53	111.00
21	N	820	GLU	OE1-CD-OE2	5.36	129.73	123.30
13	6	41	TYR	CG-CD2-CE2	-5.36	117.02	121.30
18	X	93	SER	N-CA-CB	5.36	118.54	110.50
20	Z	550	PHE	CB-CG-CD2	-5.36	117.05	120.80
20	Z	767	TYR	CB-CG-CD1	5.36	124.22	121.00
14	n	207	GLU	CB-CA-C	-5.36	99.69	110.40
11	k	128	LEU	N-CA-CB	5.35	121.11	110.40
31	L	401	PHE	CB-CG-CD2	-5.35	117.05	120.80
10	3	199	TYR	CB-CG-CD2	-5.35	117.79	121.00
21	N	526	TYR	CG-CD2-CE2	5.35	125.58	121.30
25	R	70	TYR	CB-CG-CD1	5.35	124.21	121.00
29	I	350	PHE	CB-CG-CD2	5.35	124.55	120.80
7	G	26	TYR	CB-CG-CD1	5.35	124.21	121.00
15	W	38	GLN	O-C-N	-5.35	114.14	122.70
17	T	197	TYR	CB-CG-CD2	-5.35	117.79	121.00
29	I	159	VAL	CB-CA-C	5.35	121.56	111.40
30	K	289	ASP	CB-CG-OD2	5.35	123.11	118.30
26	U	137	TYR	CB-CG-CD1	5.35	124.21	121.00
25	R	116	LYS	O-C-N	-5.34	114.15	122.70
11	k	190	ARG	NE-CZ-NH1	5.34	122.97	120.30
33	J	311	ASP	CB-CG-OD2	-5.34	113.50	118.30
13	m	182	TYR	CB-CG-CD1	-5.34	117.80	121.00
16	V	238	LEU	CB-CG-CD2	5.34	120.08	111.00
27	O	306	ARG	NE-CZ-NH2	-5.34	117.63	120.30
11	k	183	ILE	CA-CB-CG2	-5.34	100.23	110.90
23	P	303	PHE	CB-CG-CD1	5.34	124.54	120.80
25	R	361	VAL	CG1-CB-CG2	5.34	119.44	110.90
27	O	119	SER	N-CA-CB	5.34	118.50	110.50
27	O	369	ARG	NH1-CZ-NH2	5.34	125.27	119.40
31	L	354	GLU	OE1-CD-OE2	5.33	129.70	123.30
8	h	184	MET	CG-SD-CE	-5.33	91.67	100.20
10	3	68	ARG	NE-CZ-NH2	-5.33	117.63	120.30
10	j	63	LEU	CB-CG-CD1	5.33	120.06	111.00
21	N	69	TYR	CB-CG-CD1	-5.33	117.80	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	j	137	ILE	N-CA-C	-5.33	96.61	111.00
9	2	175	LEU	CB-CA-C	-5.33	100.07	110.20
21	N	839	ARG	NE-CZ-NH2	-5.33	117.64	120.30
1	a	133	TYR	CG-CD1-CE1	-5.33	117.04	121.30
24	Q	238	TYR	CG-CD2-CE2	5.33	125.56	121.30
28	H	118	ASP	CB-CG-OD1	5.33	123.09	118.30
3	c	187	ASP	CB-CG-OD2	5.33	123.09	118.30
18	X	75	TRP	CD2-CE2-CZ2	-5.33	115.91	122.30
25	R	318	PRO	O-C-N	5.33	131.22	122.70
32	M	344	ASP	CB-CG-OD1	-5.33	113.51	118.30
13	m	82	TRP	CD2-CE2-CZ2	-5.32	115.91	122.30
24	Q	298	ALA	N-CA-CB	5.32	117.55	110.10
30	K	340	PHE	CD1-CG-CD2	5.32	125.22	118.30
21	N	489	MET	CG-SD-CE	-5.32	91.69	100.20
7	g	119	TYR	CB-CG-CD1	-5.32	117.81	121.00
16	V	60	ASP	CB-CG-OD1	-5.32	113.51	118.30
23	P	179	PHE	CB-CG-CD2	-5.32	117.08	120.80
6	f	214	ALA	CB-CA-C	-5.32	102.12	110.10
20	Z	251	ALA	N-CA-C	5.32	125.36	111.00
29	I	148	LEU	CB-CG-CD2	5.32	120.04	111.00
31	L	255	TYR	CG-CD2-CE2	-5.32	117.05	121.30
6	f	221	PRO	N-CD-CG	5.32	111.17	103.20
8	h	56	GLY	N-CA-C	-5.32	99.81	113.10
21	N	355	TRP	CE2-CD2-CE3	5.32	125.08	118.70
19	Y	86	ARG	N-CA-CB	5.31	120.17	110.60
22	S	475	TYR	N-CA-CB	5.31	120.17	110.60
2	b	81	ASP	CB-CG-OD2	5.31	123.08	118.30
25	R	387	ILE	CA-CB-CG1	5.31	121.09	111.00
31	L	292	SER	CB-CA-C	-5.31	100.01	110.10
15	W	174	VAL	N-CA-C	-5.31	96.66	111.00
2	b	78	MET	C-N-CA	5.31	133.45	122.30
9	2	148	THR	O-C-N	5.31	131.19	122.70
27	O	203	THR	N-CA-CB	5.31	120.38	110.30
13	6	224	PHE	N-CA-C	-5.31	96.67	111.00
32	M	255	TYR	CZ-CE2-CD2	5.31	124.58	119.80
13	6	25	GLY	N-CA-C	-5.30	99.84	113.10
17	T	253	GLU	O-C-N	5.30	131.19	122.70
12	l	191	ASP	CB-CG-OD1	5.30	123.07	118.30
25	R	318	PRO	N-CD-CG	5.30	111.16	103.20
3	c	42	ASP	CB-CG-OD2	-5.30	113.53	118.30
18	X	62	ASP	CB-CG-OD1	-5.30	113.53	118.30
28	H	97	LEU	N-CA-C	-5.30	96.68	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
14	n	220	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
9	2	119	TYR	CB-CG-CD1	-5.30	117.82	121.00
9	2	193	TRP	CD1-NE1-CE2	-5.30	104.23	109.00
15	W	182	TYR	CG-CD2-CE2	-5.30	117.06	121.30
24	Q	278	VAL	CG1-CB-CG2	-5.30	102.42	110.90
24	Q	340	ASP	CB-CG-OD1	5.30	123.07	118.30
26	U	21	HIS	O-C-N	-5.30	114.22	122.70
31	L	161	ARG	NH1-CZ-NH2	5.30	125.23	119.40
33	J	57	PHE	CB-CG-CD2	5.30	124.51	120.80
27	O	183	ASN	O-C-N	-5.30	114.23	122.70
29	I	407	ARG	NE-CZ-NH1	5.30	122.95	120.30
22	S	488	GLN	C-N-CA	5.29	134.93	121.70
16	V	35	LEU	C-N-CA	5.29	134.93	121.70
23	P	103	TYR	CB-CG-CD2	-5.29	117.83	121.00
2	b	150	VAL	CA-CB-CG2	-5.29	102.97	110.90
8	1	120	TYR	CG-CD2-CE2	-5.29	117.07	121.30
24	Q	252	HIS	CA-CB-CG	5.29	122.59	113.60
27	O	33	TYR	CB-CG-CD2	-5.29	117.83	121.00
7	g	236	LEU	CB-CG-CD1	5.28	119.98	111.00
13	m	106	TYR	CB-CG-CD2	-5.28	117.83	121.00
21	N	659	ALA	CB-CA-C	-5.28	102.18	110.10
1	a	218	PHE	CB-CG-CD2	-5.28	117.10	120.80
11	k	171	ARG	NE-CZ-NH1	-5.28	117.66	120.30
33	J	51	LEU	CB-CG-CD2	5.28	119.98	111.00
16	V	153	ILE	N-CA-C	-5.28	96.75	111.00
16	V	241	THR	CA-CB-CG2	-5.28	105.01	112.40
23	P	156	ALA	N-CA-CB	5.28	117.49	110.10
32	M	171	GLU	C-N-CA	5.28	134.89	121.70
22	S	44	THR	N-CA-CB	5.28	120.32	110.30
14	7	252	TRP	CH2-CZ2-CE2	5.27	122.67	117.40
1	a	133	TYR	CB-CG-CD1	5.27	124.16	121.00
23	P	359	ARG	NE-CZ-NH2	-5.27	117.66	120.30
31	L	243	PHE	CB-CG-CD2	5.27	124.49	120.80
31	L	401	PHE	CG-CD1-CE1	-5.27	115.00	120.80
16	V	37	MET	N-CA-CB	5.27	120.09	110.60
18	X	97	TYR	N-CA-CB	5.27	120.09	110.60
22	S	462	ASP	CB-CG-OD1	5.27	123.04	118.30
15	W	128	LEU	N-CA-CB	5.27	120.94	110.40
25	R	120	LEU	O-C-N	-5.27	114.27	122.70
15	W	33	VAL	CA-CB-CG1	5.27	118.80	110.90
14	n	126	PHE	CG-CD1-CE1	5.26	126.59	120.80
29	I	408	ARG	NE-CZ-NH2	-5.26	117.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	4	194	ASP	CB-CA-C	-5.26	99.88	110.40
13	6	13	TYR	CB-CG-CD1	-5.26	117.84	121.00
13	6	62	ALA	N-CA-C	-5.26	96.79	111.00
27	O	174	THR	N-CA-CB	5.26	120.30	110.30
5	e	78	MET	CG-SD-CE	-5.26	91.78	100.20
22	S	108	ALA	O-C-N	-5.26	114.28	122.70
1	a	112	MET	N-CA-CB	-5.26	101.14	110.60
13	m	155	MET	CG-SD-CE	5.26	108.61	100.20
30	K	336	ARG	CA-CB-CG	5.26	124.97	113.40
18	X	14	VAL	CG1-CB-CG2	5.25	119.31	110.90
31	L	415	LEU	CB-CG-CD2	5.25	119.93	111.00
32	M	299	ARG	NH1-CZ-NH2	-5.25	113.62	119.40
10	3	31	SER	N-CA-CB	5.25	118.38	110.50
29	I	316	PHE	CG-CD2-CE2	-5.25	115.03	120.80
14	7	139	LYS	N-CA-CB	5.25	120.05	110.60
26	U	41	ALA	N-CA-CB	5.25	117.45	110.10
26	U	166	ALA	CB-CA-C	-5.25	102.23	110.10
22	S	110	LEU	N-CA-C	-5.25	96.84	111.00
33	J	7	SER	N-CA-CB	5.25	118.37	110.50
6	f	78	ALA	CA-C-O	-5.24	109.09	120.10
22	S	54	TRP	CB-CG-CD2	-5.24	119.78	126.60
25	R	252	TYR	CB-CG-CD2	-5.24	117.85	121.00
25	R	304	TYR	CB-CG-CD2	-5.24	117.85	121.00
25	R	408	ASP	CB-CG-OD2	-5.24	113.58	118.30
6	f	179	PHE	CB-CG-CD2	5.24	124.47	120.80
17	T	102	LYS	N-CA-CB	-5.24	101.16	110.60
22	S	339	GLN	N-CA-CB	5.24	120.03	110.60
21	N	146	LYS	N-CA-CB	5.24	120.03	110.60
31	L	254	LYS	C-N-CA	5.24	134.80	121.70
22	S	459	GLN	N-CA-CB	-5.24	101.17	110.60
23	P	10	ASP	CB-CG-OD1	-5.24	113.59	118.30
28	H	341	ASP	CB-CG-OD2	-5.24	113.58	118.30
30	K	180	GLN	CG-CD-OE1	-5.24	111.12	121.60
7	g	126	TYR	O-C-N	-5.24	114.32	122.70
3	c	128	LEU	N-CA-CB	5.24	120.87	110.40
9	i	171	TRP	CG-CD2-CE3	-5.23	129.19	133.90
18	X	102	GLN	N-CA-C	-5.23	96.87	111.00
3	c	34	THR	CA-CB-CG2	-5.23	105.08	112.40
12	5	196	ARG	CG-CD-NE	-5.23	100.81	111.80
14	n	135	GLN	CB-CA-C	-5.23	99.94	110.40
28	H	326	ASP	CA-CB-CG	-5.23	101.89	113.40
10	3	11	ILE	O-C-N	-5.23	114.33	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Q	146	TYR	CB-CG-CD2	-5.23	117.86	121.00
3	c	16	GLU	CB-CA-C	-5.22	99.95	110.40
29	I	343	ARG	NE-CZ-NH1	5.22	122.91	120.30
2	b	36	GLY	N-CA-C	-5.22	100.05	113.10
28	H	348	ASN	N-CA-CB	5.22	120.00	110.60
20	Z	213	LYS	CA-CB-CG	5.22	124.88	113.40
31	L	434	TYR	CG-CD1-CE1	-5.22	117.12	121.30
6	f	50	LYS	CB-CA-C	-5.22	99.96	110.40
27	O	375	ASP	CB-CG-OD1	-5.22	113.60	118.30
29	I	128	TYR	CG-CD1-CE1	5.22	125.47	121.30
30	K	268	ILE	N-CA-C	-5.22	96.91	111.00
4	d	123	SER	O-C-N	-5.21	114.33	123.20
32	M	267	PHE	CG-CD2-CE2	-5.21	115.06	120.80
33	J	339	ARG	NE-CZ-NH2	-5.21	117.69	120.30
24	Q	20	TYR	CD1-CE1-CZ	-5.21	115.11	119.80
6	f	168	ALA	CB-CA-C	-5.21	102.28	110.10
11	4	37	GLN	N-CA-CB	5.21	119.98	110.60
21	N	582	ASP	CB-CG-OD1	-5.21	113.61	118.30
24	Q	239	PHE	CB-CG-CD1	-5.21	117.15	120.80
33	J	234	PHE	CG-CD1-CE1	-5.21	115.07	120.80
8	h	120	TYR	N-CA-CB	5.21	119.97	110.60
11	k	2	ASP	CB-CG-OD1	5.21	122.99	118.30
10	3	22	ALA	CB-CA-C	-5.21	102.29	110.10
15	W	62	LEU	N-CA-CB	5.21	120.81	110.40
23	P	78	GLN	N-CA-CB	5.21	119.97	110.60
5	e	150	ASP	CB-CG-OD2	5.21	122.99	118.30
14	n	126	PHE	CB-CG-CD2	-5.21	117.16	120.80
21	N	564	ASN	N-CA-CB	5.21	119.97	110.60
23	P	417	HIS	CA-CB-CG	5.21	122.45	113.60
1	a	234	PHE	CG-CD1-CE1	5.21	126.53	120.80
21	N	814	ALA	N-CA-CB	5.21	117.39	110.10
21	N	55	PHE	CB-CG-CD1	5.20	124.44	120.80
28	H	408	SER	N-CA-CB	5.20	118.31	110.50
22	S	205	ASN	CA-CB-CG	-5.20	101.96	113.40
27	O	266	PHE	CB-CG-CD2	5.20	124.44	120.80
9	2	215	TYR	CB-CG-CD2	5.20	124.12	121.00
15	W	73	LEU	CB-CG-CD2	-5.20	102.16	111.00
28	H	95	HIS	CA-CB-CG	5.20	122.44	113.60
28	H	184	GLU	N-CA-C	-5.20	96.96	111.00
13	m	229	ARG	NE-CZ-NH2	-5.20	117.70	120.30
21	N	923	MET	CG-SD-CE	-5.20	91.89	100.20
5	e	22	PHE	N-CA-CB	5.20	119.95	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	j	80	ARG	NE-CZ-NH1	5.20	122.90	120.30
11	k	56	PHE	CB-CA-C	-5.20	100.01	110.40
28	H	442	ASP	CB-CG-OD1	5.20	122.98	118.30
18	X	11	ARG	NE-CZ-NH1	5.19	122.90	120.30
4	d	105	THR	CA-CB-CG2	-5.19	105.13	112.40
8	h	120	TYR	CG-CD2-CE2	-5.19	117.15	121.30
14	n	74	ARG	NE-CZ-NH2	-5.19	117.70	120.30
16	V	217	HIS	N-CA-CB	5.19	119.95	110.60
17	T	151	TRP	CH2-CZ2-CE2	5.19	122.59	117.40
21	N	552	ALA	CB-CA-C	-5.19	102.31	110.10
27	O	142	ASP	O-C-N	-5.19	114.39	122.70
28	H	142	ASP	CB-CG-OD1	-5.19	113.63	118.30
30	K	117	SER	N-CA-CB	5.19	118.29	110.50
27	O	371	VAL	CA-CB-CG2	-5.19	103.12	110.90
32	M	235	CYS	CB-CA-C	-5.19	100.03	110.40
16	V	69	PHE	CB-CA-C	5.18	120.77	110.40
28	H	235	PHE	CB-CG-CD1	5.18	124.43	120.80
13	m	153	LEU	CB-CG-CD2	-5.18	102.19	111.00
9	2	211	LYS	N-CA-CB	5.18	119.93	110.60
14	7	119	ALA	CB-CA-C	-5.18	102.33	110.10
31	L	216	LYS	CB-CA-C	-5.18	100.03	110.40
16	V	83	VAL	CA-CB-CG2	5.18	118.67	110.90
13	6	164	PHE	CA-CB-CG	-5.18	101.47	113.90
5	e	9	ASP	CB-CG-OD2	5.18	122.96	118.30
9	i	171	TRP	N-CA-C	5.18	124.97	111.00
14	7	49	TYR	CB-CG-CD2	5.18	124.11	121.00
32	M	396	VAL	CA-CB-CG1	5.18	118.67	110.90
1	a	166	TYR	CG-CD2-CE2	-5.17	117.16	121.30
23	P	113	ASN	CA-CB-CG	-5.17	102.01	113.40
31	L	342	ARG	NE-CZ-NH1	5.17	122.89	120.30
13	m	47	TYR	CZ-CE2-CD2	-5.17	115.14	119.80
17	T	245	TYR	CB-CA-C	-5.17	100.05	110.40
13	m	155	MET	CA-CB-CG	5.17	122.09	113.30
21	N	469	VAL	CA-CB-CG1	-5.17	103.14	110.90
24	Q	286	TYR	CB-CG-CD1	5.17	124.10	121.00
27	O	241	THR	CA-CB-CG2	-5.17	105.16	112.40
3	c	180	TYR	CD1-CE1-CZ	5.17	124.45	119.80
25	R	301	TYR	CG-CD2-CE2	-5.17	117.16	121.30
7	g	234	ASP	CB-CG-OD1	-5.17	113.65	118.30
12	l	210	PHE	CB-CG-CD2	-5.17	117.18	120.80
13	m	223	GLU	N-CA-CB	5.17	119.90	110.60
19	Y	7	ALA	CB-CA-C	-5.17	102.35	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
13	6	225	TYR	CB-CG-CD1	-5.17	117.90	121.00
23	P	47	ARG	NE-CZ-NH2	-5.17	117.72	120.30
24	Q	328	ASP	CB-CG-OD1	-5.17	113.65	118.30
28	H	148	ASN	CA-CB-CG	-5.17	102.03	113.40
27	O	272	VAL	CA-CB-CG2	-5.17	103.15	110.90
25	R	286	LEU	CB-CG-CD1	5.16	119.78	111.00
10	3	87	PHE	CB-CG-CD2	-5.16	117.19	120.80
25	R	357	PHE	CB-CG-CD2	-5.16	117.19	120.80
27	O	214	ALA	CB-CA-C	5.16	117.84	110.10
28	H	372	ASP	CB-CG-OD1	5.16	122.94	118.30
29	I	181	TYR	CD1-CG-CD2	-5.16	112.22	117.90
12	5	219	TYR	CB-CG-CD2	-5.16	117.91	121.00
30	K	58	TYR	N-CA-CB	5.16	119.88	110.60
31	L	89	ASP	CB-CG-OD1	5.16	122.94	118.30
33	J	83	LYS	N-CA-C	-5.16	97.07	111.00
21	N	559	TYR	CE1-CZ-CE2	5.16	128.05	119.80
23	P	73	ASP	CB-CG-OD2	-5.16	113.66	118.30
26	U	210	TYR	CD1-CE1-CZ	-5.16	115.16	119.80
28	H	112	SER	N-CA-CB	5.16	118.23	110.50
9	i	153	TYR	N-CA-CB	5.15	119.87	110.60
12	l	183	GLU	OE1-CD-OE2	-5.15	117.12	123.30
14	7	221	ASP	CB-CG-OD2	-5.15	113.66	118.30
15	W	35	PHE	CB-CG-CD1	-5.15	117.19	120.80
21	N	713	VAL	CA-CB-CG1	-5.15	103.18	110.90
29	I	139	GLU	CA-CB-CG	5.15	124.73	113.40
31	L	144	VAL	CA-CB-CG1	5.15	118.62	110.90
4	d	179	TYR	CB-CG-CD2	-5.15	117.91	121.00
23	P	197	THR	O-C-N	-5.15	114.47	122.70
24	Q	244	GLU	O-C-N	5.15	130.93	122.70
10	j	67	PHE	CB-CG-CD2	-5.14	117.20	120.80
13	m	145	ARG	NE-CZ-NH2	5.14	122.87	120.30
22	S	440	ASP	N-CA-CB	5.14	119.86	110.60
25	R	353	MET	CG-SD-CE	-5.14	91.97	100.20
7	g	185	GLU	CA-CB-CG	5.14	124.71	113.40
23	P	329	PHE	CB-CA-C	-5.14	100.11	110.40
30	K	192	LEU	CB-CG-CD1	5.14	119.74	111.00
23	P	311	TRP	CA-C-N	5.14	131.49	117.10
5	e	35	SER	N-CA-CB	5.14	118.21	110.50
12	5	188	TYR	N-CA-C	-5.14	97.12	111.00
6	f	7	ASP	CB-CG-OD2	5.14	122.92	118.30
7	g	48	PHE	CA-CB-CG	-5.14	101.58	113.90
10	j	72	ASN	CB-CA-C	5.14	120.67	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	S	449	LEU	N-CA-CB	5.14	120.67	110.40
32	M	320	ARG	NE-CZ-NH1	-5.14	117.73	120.30
12	l	250	VAL	CA-CB-CG2	5.13	118.60	110.90
12	5	202	PHE	N-CA-CB	5.13	119.84	110.60
28	H	208	TYR	CG-CD1-CE1	-5.13	117.19	121.30
12	l	195	THR	CA-CB-CG2	-5.13	105.21	112.40
11	4	190	ARG	O-C-N	5.13	130.91	122.70
21	N	438	ASP	CB-CG-OD1	-5.13	113.68	118.30
14	n	35	GLN	C-N-CA	5.13	134.53	121.70
15	W	47	ASN	CB-CG-OD1	5.13	131.86	121.60
25	R	70	TYR	CZ-CE2-CD2	5.13	124.42	119.80
8	1	75	TYR	CB-CG-CD2	-5.13	117.92	121.00
11	4	13	VAL	CG1-CB-CG2	5.13	119.11	110.90
16	V	226	LYS	N-CA-CB	5.13	119.83	110.60
28	H	377	PHE	N-CA-CB	5.13	119.83	110.60
10	j	154	TYR	CB-CG-CD1	-5.13	117.92	121.00
20	Z	729	GLU	C-N-CA	5.13	134.52	121.70
20	Z	825	ALA	N-CA-CB	5.13	117.28	110.10
27	O	38	TRP	CD2-CE2-CZ2	-5.13	116.15	122.30
12	5	206	SER	N-CA-CB	5.13	118.19	110.50
19	Y	58	ASN	N-CA-CB	5.13	119.83	110.60
21	N	319	SER	N-CA-CB	5.13	118.19	110.50
27	O	312	ASP	N-CA-CB	5.13	119.83	110.60
29	I	137	ASP	CB-CG-OD1	-5.13	113.69	118.30
19	Y	61	GLU	OE1-CD-OE2	5.12	129.45	123.30
14	7	42	THR	N-CA-CB	5.12	120.04	110.30
15	W	17	ARG	CD-NE-CZ	5.12	130.77	123.60
17	T	78	PHE	CB-CG-CD1	5.12	124.39	120.80
18	X	36	LYS	CB-CG-CD	5.12	124.92	111.60
1	a	190	LYS	N-CA-CB	5.12	119.82	110.60
16	V	181	ASN	CB-CG-OD1	-5.12	111.36	121.60
26	U	246	GLU	CB-CG-CD	-5.12	100.37	114.20
27	O	380	LEU	CB-CG-CD1	5.12	119.71	111.00
28	H	155	PHE	CB-CG-CD2	5.12	124.38	120.80
30	K	330	ARG	NE-CZ-NH2	-5.12	117.74	120.30
30	K	104	ASP	N-CA-C	-5.12	97.19	111.00
7	g	192	ALA	CB-CA-C	-5.12	102.43	110.10
31	L	137	ARG	NE-CZ-NH2	-5.12	117.74	120.30
3	c	44	ILE	N-CA-CB	5.11	122.56	110.80
6	f	225	TYR	CD1-CE1-CZ	-5.11	115.20	119.80
11	k	8	ARG	NE-CZ-NH1	-5.11	117.74	120.30
28	H	234	ARG	CB-CA-C	-5.11	100.18	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	4	42	THR	N-CA-C	-5.11	97.20	111.00
11	4	81	SER	O-C-N	-5.11	114.52	122.70
21	N	485	MET	CG-SD-CE	-5.11	92.02	100.20
28	H	118	ASP	N-CA-CB	5.11	119.80	110.60
9	i	104	ARG	CG-CD-NE	-5.11	101.07	111.80
13	m	52	PHE	CB-CG-CD1	-5.11	117.22	120.80
16	V	156	PHE	CB-CG-CD1	-5.11	117.22	120.80
21	N	316	LYS	CB-CA-C	-5.11	100.19	110.40
22	S	122	ASN	CA-CB-CG	-5.11	102.16	113.40
22	S	317	HIS	CA-CB-CG	5.11	122.28	113.60
1	a	51	THR	N-CA-C	-5.11	97.21	111.00
23	P	311	TRP	CE2-CD2-CG	5.11	111.39	107.30
2	b	28	VAL	CG1-CB-CG2	5.10	119.06	110.90
9	i	205	CYS	N-CA-CB	5.10	119.79	110.60
8	1	70	TYR	CG-CD2-CE2	5.10	125.38	121.30
10	3	38	ASN	N-CA-C	-5.10	97.22	111.00
13	6	218	ASP	CB-CG-OD2	-5.10	113.71	118.30
33	J	249	GLU	N-CA-CB	5.10	119.78	110.60
3	c	47	ALA	CB-CA-C	5.10	117.75	110.10
3	c	80	LEU	CB-CG-CD1	5.10	119.67	111.00
14	7	63	TYR	CB-CG-CD1	-5.10	117.94	121.00
21	N	436	ASP	CB-CA-C	-5.10	100.20	110.40
24	Q	127	ARG	NH1-CZ-NH2	5.10	125.01	119.40
28	H	386	ALA	N-CA-CB	5.10	117.24	110.10
32	M	153	TYR	CB-CG-CD1	-5.10	117.94	121.00
21	N	759	ILE	CA-CB-CG2	-5.10	100.71	110.90
28	H	274	VAL	N-CA-C	-5.10	97.24	111.00
33	J	388	LYS	CB-CG-CD	5.10	124.85	111.60
5	e	15	PHE	C-N-CA	5.09	134.43	121.70
32	M	312	LEU	CB-CG-CD2	-5.09	102.34	111.00
9	i	56	ALA	CB-CA-C	-5.09	102.46	110.10
29	I	380	LEU	N-CA-CB	5.09	120.58	110.40
1	a	105	ARG	CD-NE-CZ	-5.09	116.48	123.60
21	N	183	VAL	CA-CB-CG2	-5.09	103.27	110.90
29	I	345	ASP	CB-CA-C	5.09	120.57	110.40
33	J	213	VAL	N-CA-C	-5.09	97.27	111.00
27	O	62	TYR	N-CA-CB	5.08	119.75	110.60
8	h	91	PHE	CB-CA-C	-5.08	100.23	110.40
12	l	92	ASP	CB-CG-OD1	5.08	122.88	118.30
12	l	120	MET	CG-SD-CE	-5.08	92.06	100.20
25	R	313	ALA	N-CA-CB	5.08	117.22	110.10
30	K	399	ARG	NE-CZ-NH2	5.08	122.84	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
32	M	366	ARG	NE-CZ-NH2	-5.08	117.76	120.30
13	6	173	ASN	N-CA-CB	5.08	119.75	110.60
14	7	128	TYR	O-C-N	5.08	130.83	122.70
15	W	118	ILE	CA-CB-CG1	5.08	120.65	111.00
30	K	393	ARG	NH1-CZ-NH2	5.08	124.99	119.40
33	J	68	PRO	N-CD-CG	5.08	110.82	103.20
16	V	71	MET	CG-SD-CE	5.08	108.33	100.20
23	P	311	TRP	CD1-CG-CD2	-5.08	102.24	106.30
16	V	65	VAL	CA-CB-CG2	-5.08	103.29	110.90
21	N	362	TRP	CH2-CZ2-CE2	5.08	122.48	117.40
22	S	179	ILE	CB-CA-C	-5.08	101.45	111.60
8	1	52	CYS	N-CA-CB	5.07	119.73	110.60
11	4	38	LEU	CB-CG-CD2	5.07	119.63	111.00
21	N	614	ASN	CB-CG-OD1	5.07	131.75	121.60
22	S	186	TYR	N-CA-CB	5.07	119.73	110.60
23	P	271	SER	N-CA-CB	5.07	118.11	110.50
25	R	339	ALA	CB-CA-C	-5.07	102.49	110.10
6	f	23	GLU	CB-CA-C	-5.07	100.26	110.40
10	j	96	TYR	CZ-CE2-CD2	5.07	124.36	119.80
14	n	244	ASN	N-CA-CB	5.07	119.73	110.60
18	X	125	MET	CG-SD-CE	-5.07	92.09	100.20
25	R	321	TYR	CD1-CE1-CZ	5.07	124.36	119.80
27	O	81	TYR	CG-CD1-CE1	-5.07	117.24	121.30
11	k	96	ARG	NE-CZ-NH1	5.07	122.83	120.30
24	Q	405	GLN	N-CA-CB	5.07	119.72	110.60
14	n	58	ASP	CB-CG-OD1	5.07	122.86	118.30
9	2	118	LYS	CA-CB-CG	5.07	124.54	113.40
28	H	400	ARG	N-CA-CB	5.07	119.72	110.60
29	I	75	PHE	CB-CG-CD2	-5.07	117.25	120.80
4	d	179	TYR	N-CA-C	-5.06	97.33	111.00
29	I	156	ILE	CB-CA-C	-5.06	101.47	111.60
21	N	53	ASP	CB-CG-OD2	5.06	122.86	118.30
21	N	774	ASN	N-CA-CB	5.06	119.71	110.60
25	R	310	GLU	N-CA-CB	5.06	119.71	110.60
26	U	110	PHE	CB-CG-CD2	5.06	124.34	120.80
8	h	153	GLU	C-N-CA	5.06	134.34	121.70
14	7	174	THR	CA-CB-OG1	5.06	119.62	109.00
25	R	186	TYR	CB-CG-CD1	5.06	124.03	121.00
27	O	185	PHE	CB-CG-CD2	-5.06	117.26	120.80
29	I	137	ASP	N-CA-CB	5.06	119.70	110.60
32	M	281	ASP	N-CA-CB	5.06	119.70	110.60
4	d	159	TRP	CB-CG-CD2	5.06	133.17	126.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
11	k	185	ASP	CB-CG-OD2	5.06	122.85	118.30
10	3	36	VAL	CA-CB-CG1	5.06	118.48	110.90
25	R	189	GLU	OE1-CD-OE2	5.06	129.37	123.30
18	X	9	LYS	CB-CA-C	-5.05	100.29	110.40
31	L	146	VAL	CA-CB-CG1	-5.05	103.32	110.90
20	Z	738	TYR	CZ-CE2-CD2	5.05	124.35	119.80
24	Q	130	ARG	NE-CZ-NH1	5.05	122.83	120.30
8	h	14	ALA	N-CA-C	-5.05	97.36	111.00
13	m	40	ASP	N-CA-CB	5.05	119.69	110.60
31	L	309	LEU	CB-CG-CD2	5.05	119.58	111.00
6	f	128	TYR	C-N-CA	5.05	132.90	122.30
29	I	319	ARG	NE-CZ-NH2	-5.05	117.78	120.30
33	J	244	ILE	CA-CB-CG1	-5.05	101.41	111.00
6	f	130	VAL	C-N-CA	5.04	132.90	122.30
8	h	129	HIS	N-CA-C	-5.04	97.38	111.00
22	S	475	TYR	CZ-CE2-CD2	5.04	124.34	119.80
30	K	334	LEU	N-CA-CB	5.04	120.49	110.40
5	E	26	TYR	CB-CG-CD2	-5.04	117.97	121.00
12	5	103	SER	N-CA-CB	5.04	118.06	110.50
17	T	29	PRO	N-CD-CG	5.04	110.76	103.20
24	Q	434	TYR	CG-CD1-CE1	5.04	125.33	121.30
21	N	861	TYR	CZ-CE2-CD2	5.04	124.34	119.80
23	P	322	LEU	CB-CA-C	-5.04	100.62	110.20
6	f	6	TYR	N-CA-CB	5.04	119.67	110.60
15	W	174	VAL	CG1-CB-CG2	5.04	118.96	110.90
22	S	210	LEU	CB-CG-CD1	5.04	119.56	111.00
12	l	168	ALA	N-CA-CB	-5.04	103.05	110.10
21	N	96	GLN	O-C-N	5.04	130.76	122.70
27	O	130	ASP	CB-CG-OD1	-5.04	113.77	118.30
7	g	157	TYR	CD1-CE1-CZ	5.03	124.33	119.80
3	c	237	ASP	CB-CG-OD1	-5.03	113.77	118.30
11	4	174	MET	CG-SD-CE	-5.03	92.15	100.20
23	P	95	TYR	CB-CG-CD1	-5.03	117.98	121.00
30	K	388	GLN	CA-CB-CG	5.03	124.47	113.40
4	d	138	PHE	CZ-CE2-CD2	5.03	126.14	120.10
21	N	150	LEU	CB-CG-CD2	5.03	119.55	111.00
27	O	26	PHE	CB-CG-CD2	-5.03	117.28	120.80
8	h	72	LEU	CB-CG-CD1	-5.03	102.45	111.00
12	l	219	TYR	CA-CB-CG	-5.03	103.85	113.40
16	V	111	HIS	CA-CB-CG	5.03	122.15	113.60
16	V	257	GLU	N-CA-C	-5.03	97.43	111.00
18	X	90	VAL	N-CA-C	-5.03	97.43	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	L	428	LEU	O-C-N	-5.03	114.66	122.70
32	M	145	LEU	N-CA-CB	5.03	120.45	110.40
14	n	144	TRP	CB-CG-CD1	5.02	133.53	127.00
9	2	252	ILE	N-CA-C	-5.02	97.44	111.00
32	M	33	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
25	R	231	LEU	CB-CG-CD2	5.02	119.54	111.00
21	N	432	GLY	N-CA-C	-5.02	100.55	113.10
9	i	247	VAL	CA-CB-CG2	-5.02	103.37	110.90
18	X	113	GLU	C-N-CA	5.02	134.25	121.70
20	Z	767	TYR	CB-CG-CD2	-5.02	117.99	121.00
23	P	326	ASP	CA-CB-CG	-5.02	102.36	113.40
28	H	179	SER	CB-CA-C	-5.02	100.57	110.10
30	K	196	ASP	CB-CG-OD2	5.02	122.81	118.30
32	M	57	VAL	CA-CB-CG1	5.02	118.42	110.90
12	5	162	VAL	CA-CB-CG1	-5.02	103.38	110.90
27	O	73	ILE	N-CA-C	-5.02	97.46	111.00
32	M	284	ASP	CB-CG-OD1	5.02	122.81	118.30
2	b	225	THR	N-CA-CB	5.01	119.83	110.30
4	d	34	VAL	N-CA-C	-5.01	97.46	111.00
27	O	62	TYR	CB-CG-CD2	-5.01	117.99	121.00
3	c	99	LEU	CB-CG-CD1	5.01	119.52	111.00
7	g	65	VAL	CG1-CB-CG2	5.01	118.92	110.90
17	T	50	ILE	O-C-N	-5.01	114.68	122.70
21	N	397	SER	N-CA-CB	5.01	118.02	110.50
21	N	806	THR	CA-CB-CG2	-5.01	105.38	112.40
26	U	81	LYS	N-CA-CB	5.01	119.62	110.60
12	l	188	TYR	CB-CG-CD2	5.01	124.01	121.00
11	4	23	ARG	NH1-CZ-NH2	5.01	124.91	119.40
16	V	296	LEU	CB-CG-CD1	5.01	119.52	111.00
24	Q	18	LYS	N-CA-CB	5.01	119.61	110.60
32	M	381	ARG	NH1-CZ-NH2	5.01	124.91	119.40
11	k	132	ALA	N-CA-CB	5.01	117.11	110.10
9	2	65	ARG	NE-CZ-NH1	-5.01	117.80	120.30
16	V	251	TYR	CD1-CE1-CZ	-5.01	115.29	119.80
29	I	230	THR	O-C-N	-5.00	114.69	122.70
8	1	34	TYR	CG-CD2-CE2	-5.00	117.30	121.30
14	7	205	VAL	CA-CB-CG1	5.00	118.40	110.90
28	H	53	GLU	CB-CA-C	-5.00	100.40	110.40

There are no chirality outliers.

All (351) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
8	1	104	ALA	Peptide
8	1	111	TYR	Sidechain
8	1	120	TYR	Sidechain
8	1	133	TYR	Sidechain
8	1	194	ARG	Sidechain
8	1	202	TYR	Sidechain
9	2	153	TYR	Sidechain
9	2	215	TYR	Sidechain
9	2	232	TYR	Sidechain
9	2	236	ARG	Sidechain
10	3	103	TYR	Sidechain
10	3	46	TYR	Sidechain
10	3	74	TYR	Sidechain
10	3	96	TYR	Sidechain
11	4	133	HIS	Sidechain
11	4	135	TYR	Sidechain
11	4	149	ARG	Sidechain
11	4	59	TYR	Sidechain
11	4	73	TYR	Sidechain
11	4	96	ARG	Sidechain
12	5	139	ARG	Sidechain
12	5	144	ARG	Sidechain
12	5	148	ARG	Sidechain
12	5	179	TYR	Sidechain
12	5	189	TYR	Sidechain
12	5	212	TYR	Sidechain
13	6	103	HIS	Sidechain
13	6	139	TYR	Sidechain
13	6	157	PHE	Sidechain
13	6	168	TYR	Sidechain
13	6	221	ARG	Sidechain
13	6	229	ARG	Sidechain,Peptide
13	6	36	ARG	Sidechain
13	6	83	TYR	Sidechain
14	7	128	TYR	Sidechain
14	7	162	TYR	Sidechain
14	7	219	TYR	Sidechain
14	7	261	TYR	Sidechain
14	7	63	TYR	Sidechain
4	D	90	ARG	Sidechain
6	F	18	ARG	Peptide
7	G	13	SER	Peptide
7	G	21	ASN	Peptide

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Mol	Chain	Res	Type	Group
28	H	173	ARG	Sidechain
28	H	181	TYR	Sidechain
28	H	266	ARG	Sidechain
28	H	271	PHE	Sidechain
28	H	292	ARG	Sidechain
28	H	318	ARG	Sidechain
28	H	319	PHE	Sidechain
28	H	344	ASP	Peptide
28	H	385	ARG	Sidechain
28	H	409	ARG	Sidechain
28	H	454	TYR	Sidechain
28	H	62	ARG	Sidechain
28	H	72	SER	Peptide
29	I	127	ASP	Peptide
29	I	135	PHE	Sidechain
29	I	208	TYR	Sidechain
29	I	223	GLY	Peptide
29	I	228	GLY	Mainchain
29	I	265	ARG	Sidechain
29	I	346	ARG	Sidechain
29	I	424	MET	Peptide
29	I	54	ARG	Sidechain
33	J	116	ARG	Sidechain
33	J	211	ILE	Mainchain
33	J	228	ARG	Sidechain
33	J	274	GLU	Peptide
33	J	296	ARG	Sidechain
33	J	309	ARG	Sidechain
33	J	339	ARG	Sidechain
33	J	344	ARG	Sidechain
33	J	368	TYR	Sidechain
33	J	373	ARG	Sidechain
33	J	374	ARG	Sidechain
33	J	56	ARG	Sidechain
33	J	63	ARG	Sidechain
33	J	71	TYR	Sidechain
33	J	94	TYR	Sidechain
30	K	118	TYR	Sidechain
30	K	128	ARG	Sidechain
30	K	167	PRO	Mainchain,Peptide
30	K	174	VAL	Peptide
30	K	176	GLY	Peptide

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Mol	Chain	Res	Type	Group
30	K	218	GLY	Mainchain
30	K	236	ARG	Peptide
30	K	246	TYR	Sidechain
30	K	258	PHE	Sidechain
30	K	259	ARG	Sidechain
30	K	262	ARG	Sidechain
30	K	303	MET	Peptide
30	K	311	ASN	Peptide
30	K	329	LEU	Peptide
30	K	400	TYR	Sidechain
30	K	411	TYR	Sidechain
30	K	58	TYR	Sidechain
30	K	77	ARG	Sidechain
31	L	132	ARG	Sidechain
31	L	137	ARG	Sidechain
31	L	168	TYR	Sidechain
31	L	185	GLY	Mainchain
31	L	194	ARG	Sidechain
31	L	255	TYR	Sidechain
31	L	261	ARG	Sidechain
31	L	269	TYR	Sidechain
31	L	289	ARG	Sidechain
31	L	290	ARG	Sidechain
31	L	321	THR	Peptide
31	L	341	GLY	Peptide
31	L	342	ARG	Peptide
31	L	345	ARG	Sidechain
31	L	350	PRO	Peptide
31	L	392	ARG	Sidechain
31	L	401	PHE	Sidechain
31	L	69	ARG	Sidechain
32	M	166	ARG	Sidechain
32	M	203	ARG	Sidechain
32	M	290	ARG	Sidechain
32	M	311	GLN	Mainchain
32	M	320	ARG	Sidechain
32	M	321	VAL	Peptide
32	M	329	ARG	Sidechain
32	M	339	ARG	Sidechain
32	M	342	ARG	Sidechain,Mainchain
32	M	364	HIS	Sidechain
32	M	425	ARG	Peptide

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Mol	Chain	Res	Type	Group
32	M	50	ARG	Sidechain
21	N	109	TYR	Sidechain
21	N	282	TYR	Sidechain
21	N	299	TYR	Sidechain
21	N	329	HIS	Sidechain
21	N	389	TYR	Sidechain
21	N	394	ARG	Sidechain
21	N	421	ASP	Sidechain
21	N	471	TYR	Sidechain
21	N	515	ARG	Sidechain
21	N	528	ARG	Sidechain
21	N	549	TYR	Sidechain
21	N	593	PHE	Sidechain
21	N	597	ARG	Sidechain
21	N	69	TYR	Sidechain
21	N	762	ARG	Sidechain
21	N	776	TYR	Sidechain
21	N	786	ARG	Sidechain
21	N	788	TYR	Sidechain
21	N	81	TYR	Sidechain
21	N	836	GLU	Peptide
21	N	861	TYR	Sidechain
21	N	866	TYR	Sidechain
21	N	88	ARG	Sidechain
21	N	921	ARG	Sidechain
27	O	115	ARG	Sidechain
27	O	137	TYR	Sidechain
27	O	181	PHE	Sidechain
27	O	189	TYR	Sidechain
27	O	58	ARG	Sidechain
27	O	62	TYR	Sidechain
27	O	69	PHE	Sidechain
27	O	70	TYR	Sidechain
27	O	92	PHE	Sidechain
23	P	110	LEU	Peptide
23	P	13	TYR	Sidechain
23	P	131	PHE	Sidechain
23	P	220	TYR	Sidechain
23	P	232	ARG	Sidechain
23	P	240	TYR	Sidechain
23	P	245	TYR	Sidechain
23	P	267	PHE	Sidechain

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Mol	Chain	Res	Type	Group
23	P	273	TYR	Sidechain
23	P	344	ARG	Sidechain
23	P	351	ARG	Sidechain
23	P	356	TYR	Sidechain
23	P	386	GLN	Peptide
23	P	390	TYR	Sidechain
23	P	402	PHE	Sidechain
23	P	95	TYR	Sidechain
24	Q	116	PHE	Sidechain
24	Q	127	ARG	Sidechain
24	Q	13	ARG	Sidechain
24	Q	146	TYR	Sidechain
24	Q	151	TYR	Sidechain
24	Q	20	TYR	Sidechain
24	Q	255	TYR	Sidechain
24	Q	291	TYR	Sidechain
24	Q	294	ARG	Sidechain
24	Q	306	TYR	Sidechain
24	Q	334	HIS	Sidechain
24	Q	409	TYR	Sidechain
24	Q	75	ARG	Sidechain
25	R	20	ARG	Sidechain
25	R	214	TYR	Sidechain
25	R	252	TYR	Sidechain
25	R	263	ARG	Sidechain
25	R	297	TYR	Sidechain
25	R	334	ARG	Sidechain
25	R	338	TYR	Sidechain
25	R	400	TYR	Sidechain
25	R	43	ARG	Sidechain
25	R	70	TYR	Peptide
25	R	81	HIS	Sidechain
22	S	111	ARG	Sidechain
22	S	186	TYR	Sidechain
22	S	196	ARG	Sidechain
22	S	25	TYR	Sidechain
22	S	273	PHE	Sidechain
22	S	333	PHE	Sidechain
22	S	345	TYR	Sidechain
22	S	346	TYR	Sidechain
22	S	382	ARG	Sidechain
22	S	425	ARG	Sidechain

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Mol	Chain	Res	Type	Group
22	S	442	PHE	Sidechain
22	S	475	TYR	Sidechain
22	S	480	ARG	Sidechain
22	S	51	ARG	Sidechain
22	S	52	TYR	Sidechain
22	S	55	ARG	Sidechain
22	S	82	TYR	Sidechain
22	S	95	PHE	Sidechain
17	T	177	PHE	Sidechain
17	T	20	TYR	Sidechain
17	T	211	PHE	Sidechain
17	T	234	TYR	Sidechain
17	T	251	HIS	Peptide
17	T	72	THR	Peptide
17	T	75	PHE	Sidechain
17	T	81	TYR	Sidechain
17	T	91	SER	Peptide
17	T	96	LEU	Peptide
26	U	176	ARG	Sidechain
26	U	189	ARG	Sidechain
26	U	277	TYR	Sidechain
26	U	283	ARG	Sidechain
26	U	32	ARG	Sidechain
26	U	72	TYR	Sidechain
16	V	110	SER	Peptide
16	V	230	TYR	Sidechain
16	V	251	TYR	Sidechain
16	V	273	ARG	Sidechain
16	V	28	TYR	Sidechain
16	V	42	ARG	Sidechain
15	W	101	ARG	Sidechain
15	W	109	ARG	Sidechain
15	W	179	ARG	Sidechain
15	W	182	TYR	Sidechain
15	W	23	ARG	Sidechain
15	W	25	ARG	Sidechain
15	W	37	PHE	Sidechain
18	X	27	ILE	Peptide
18	X	51	ARG	Sidechain
19	Y	86	ARG	Sidechain
20	Z	210	TYR	Sidechain
20	Z	248	TYR	Sidechain

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Mol	Chain	Res	Type	Group
20	Z	254	PRO	Mainchain
20	Z	269	TYR	Sidechain
20	Z	726	GLU	Mainchain
20	Z	727	GLU	Peptide
20	Z	728	LYS	Mainchain,Peptide
20	Z	738	TYR	Sidechain
1	a	105	ARG	Sidechain
1	a	128	TYR	Sidechain
1	a	131	ARG	Sidechain
1	a	143	PHE	Sidechain
1	a	155	TYR	Sidechain
1	a	166	TYR	Sidechain
1	a	218	PHE	Sidechain
1	a	30	TYR	Sidechain
1	a	46	ARG	Sidechain
2	b	234	ARG	Sidechain
2	b	97	TYR	Sidechain
2	b	99	ARG	Sidechain
3	c	13	PHE	Sidechain
3	c	137	TYR	Sidechain
3	c	143	ARG	Sidechain
3	c	144	TYR	Sidechain
3	c	4	ARG	Sidechain
4	d	11	PHE	Sidechain
4	d	127	ARG	Sidechain
4	d	197	ARG	Sidechain
4	d	22	TYR	Sidechain
4	d	254	HIS	Sidechain
5	e	132	ARG	Sidechain
5	e	167	TYR	Sidechain
5	e	231	TYR	Sidechain
6	f	123	TYR	Sidechain
6	f	164	ARG	Sidechain
6	f	18	ARG	Peptide
6	f	225	TYR	Sidechain
6	f	233	TYR	Sidechain
6	f	94	TYR	Sidechain
7	g	115	ARG	Sidechain
7	g	126	TYR	Sidechain
7	g	13	SER	Peptide
7	g	130	ARG	Sidechain
7	g	138	PHE	Sidechain

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Mol	Chain	Res	Type	Group
7	g	190	ARG	Sidechain
7	g	21	ASN	Peptide
7	g	230	PHE	Sidechain
7	g	242	PHE	Sidechain
7	g	78	TYR	Sidechain
7	g	8	TYR	Sidechain
7	g	86	ARG	Sidechain
8	h	111	TYR	Sidechain
8	h	133	TYR	Sidechain
8	h	146	TYR	Sidechain
8	h	34	TYR	Sidechain
8	h	38	ARG	Sidechain
8	h	70	TYR	Sidechain
8	h	75	TYR	Sidechain
8	h	96	TYR	Sidechain
9	i	117	PHE	Sidechain
9	i	153	TYR	Sidechain
9	i	217	ARG	Sidechain
9	i	234	PHE	Sidechain
9	i	236	ARG	Sidechain
9	i	98	TYR	Sidechain
10	j	103	TYR	Sidechain
10	j	124	PHE	Sidechain
10	j	154	TYR	Sidechain
10	j	199	TYR	Sidechain
11	k	130	TYR	Sidechain
11	k	190	ARG	Sidechain
11	k	59	TYR	Sidechain
11	k	67	TYR	Sidechain
12	l	165	TYR	Sidechain
12	l	179	TYR	Sidechain
12	l	189	TYR	Sidechain
12	l	245	TYR	Sidechain
12	l	262	TYR	Sidechain
13	m	114	TYR	Sidechain
13	m	13	TYR	Sidechain
13	m	131	TYR	Sidechain
13	m	168	TYR	Sidechain
13	m	193	ARG	Sidechain
13	m	41	TYR	Sidechain
14	n	117	GLU	Peptide
14	n	124	TYR	Sidechain

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Mol	Chain	Res	Type	Group
14	n	128	TYR	Sidechain
14	n	134	TYR	Sidechain
14	n	136	ARG	Sidechain
14	n	170	TYR	Sidechain
14	n	189	ARG	Sidechain
14	n	194	ARG	Sidechain
14	n	218	TYR	Sidechain
14	n	219	TYR	Sidechain
14	n	63	TYR	Sidechain
14	n	98	ARG	Sidechain

5.2 Too-close contacts (i)

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

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
1	A	239/241 (99%)	223 (93%)	16 (7%)	0	100	100
1	a	239/241 (99%)	226 (95%)	11 (5%)	2 (1%)	19	60
2	B	247/249 (99%)	232 (94%)	15 (6%)	0	100	100
2	b	247/249 (99%)	231 (94%)	14 (6%)	2 (1%)	19	60
3	C	242/244 (99%)	232 (96%)	10 (4%)	0	100	100
3	c	242/244 (99%)	230 (95%)	12 (5%)	0	100	100
4	D	235/251 (94%)	222 (94%)	13 (6%)	0	100	100
4	d	249/251 (99%)	229 (92%)	14 (6%)	6 (2%)	6	35
5	E	242/244 (99%)	225 (93%)	11 (4%)	6 (2%)	5	34
5	e	242/244 (99%)	222 (92%)	17 (7%)	3 (1%)	13	50
6	F	229/231 (99%)	219 (96%)	9 (4%)	1 (0%)	34	72

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	f	229/231 (99%)	211 (92%)	13 (6%)	5 (2%)	6	37
7	G	240/242 (99%)	229 (95%)	11 (5%)	0	100	100
7	g	240/242 (99%)	229 (95%)	10 (4%)	1 (0%)	34	72
8	1	194/196 (99%)	185 (95%)	8 (4%)	1 (0%)	29	69
8	h	194/196 (99%)	177 (91%)	12 (6%)	5 (3%)	5	33
9	2	224/226 (99%)	215 (96%)	7 (3%)	2 (1%)	17	56
9	i	224/226 (99%)	206 (92%)	15 (7%)	3 (1%)	12	48
10	3	202/204 (99%)	187 (93%)	14 (7%)	1 (0%)	29	69
10	j	202/204 (99%)	185 (92%)	11 (5%)	6 (3%)	4	30
11	4	193/195 (99%)	183 (95%)	7 (4%)	3 (2%)	9	44
11	k	193/195 (99%)	176 (91%)	13 (7%)	4 (2%)	7	37
12	5	210/212 (99%)	197 (94%)	12 (6%)	1 (0%)	29	69
12	l	210/212 (99%)	195 (93%)	15 (7%)	0	100	100
13	6	220/222 (99%)	204 (93%)	12 (6%)	4 (2%)	8	41
13	m	220/222 (99%)	207 (94%)	10 (4%)	3 (1%)	11	46
14	7	227/232 (98%)	205 (90%)	18 (8%)	4 (2%)	8	41
14	n	230/232 (99%)	214 (93%)	14 (6%)	2 (1%)	17	56
15	W	195/197 (99%)	178 (91%)	11 (6%)	6 (3%)	4	30
16	V	287/289 (99%)	260 (91%)	20 (7%)	7 (2%)	6	35
17	T	264/266 (99%)	248 (94%)	14 (5%)	2 (1%)	19	60
18	X	125/127 (98%)	105 (84%)	15 (12%)	5 (4%)	3	25
19	Y	87/89 (98%)	72 (83%)	10 (12%)	5 (6%)	1	19
20	Z	902/970 (93%)	820 (91%)	59 (6%)	23 (2%)	5	34
21	N	920/922 (100%)	865 (94%)	41 (4%)	14 (2%)	10	46
22	S	473/475 (100%)	445 (94%)	19 (4%)	9 (2%)	8	39
23	P	438/440 (100%)	415 (95%)	16 (4%)	7 (2%)	9	44
24	Q	432/434 (100%)	394 (91%)	26 (6%)	12 (3%)	5	32
25	R	403/405 (100%)	388 (96%)	10 (2%)	5 (1%)	13	50
26	U	302/304 (99%)	288 (95%)	13 (4%)	1 (0%)	41	76
27	O	386/388 (100%)	371 (96%)	10 (3%)	5 (1%)	12	48
28	H	415/417 (100%)	364 (88%)	39 (9%)	12 (3%)	4	31

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
29	I	379/385 (98%)	353 (93%)	18 (5%)	8 (2%)	7	37
30	K	392/394 (100%)	353 (90%)	28 (7%)	11 (3%)	5	32
31	L	384/388 (99%)	360 (94%)	18 (5%)	6 (2%)	9	44
32	M	419/421 (100%)	376 (90%)	30 (7%)	13 (3%)	4	30
33	J	403/405 (100%)	362 (90%)	22 (6%)	19 (5%)	2	23
All	All	13911/14094 (99%)	12913 (93%)	763 (6%)	235 (2%)	13	43

All (235) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	d	31	THR
4	d	50	SER
6	f	14	SER
5	E	16	SER
13	6	27	ASP
13	6	138	SER
15	W	190	ILE
16	V	171	ARG
16	V	217	HIS
17	T	97	SER
19	Y	3	THR
20	Z	24	THR
20	Z	85	VAL
20	Z	728	LYS
20	Z	870	ALA
21	N	17	GLN
21	N	175	ASP
21	N	832	HIS
21	N	863	SER
22	S	47	THR
22	S	84	ASP
24	Q	68	MET
24	Q	384	LYS
24	Q	387	TYR
25	R	73	ASN
25	R	280	ILE
28	H	141	GLU
29	I	86	GLU
29	I	290	LYS
29	I	317	ASP

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Mol	Chain	Res	Type
30	K	219	LYS
30	K	284	ALA
31	L	101	ILE
31	L	290	ARG
31	L	343	LEU
32	M	172	VAL
32	M	322	LYS
32	M	339	ARG
32	M	343	LEU
33	J	212	ARG
4	d	205	THR
9	i	175	LEU
10	j	7	ILE
10	j	40	PHE
11	k	73	TYR
13	m	27	ASP
6	F	14	SER
15	W	179	ARG
18	X	21	SER
18	X	29	VAL
18	X	106	SER
20	Z	82	MET
20	Z	255	LEU
21	N	612	SER
21	N	742	TRP
21	N	790	GLU
22	S	108	ALA
23	P	273	TYR
24	Q	149	LYS
25	R	182	ASN
28	H	112	SER
28	H	343	PHE
28	H	348	ASN
29	I	115	ASP
29	I	126	PRO
29	I	173	MET
29	I	229	LYS
30	K	104	ASP
30	K	160	VAL
31	L	177	GLU
31	L	292	SER
31	L	322	LYS

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Mol	Chain	Res	Type
32	M	344	ASP
33	J	4	ALA
33	J	69	GLY
33	J	72	VAL
33	J	119	SER
33	J	261	SER
33	J	285	SER
2	b	41	ASN
5	e	53	ARG
6	f	58	SER
6	f	203	ASP
8	h	49	LYS
9	i	212	ASP
9	i	223	ASN
10	j	56	LEU
11	k	4	ILE
5	E	126	GLY
5	E	128	SER
5	E	169	ALA
9	2	60	CYS
10	3	157	ASN
11	4	150	PRO
14	7	60	LEU
14	7	173	PRO
15	W	149	GLN
15	W	166	GLU
19	Y	49	ILE
19	Y	55	THR
20	Z	611	THR
20	Z	825	ALA
20	Z	887	GLY
20	Z	926	ASN
20	Z	940	GLY
21	N	87	ASP
21	N	123	PHE
21	N	393	SER
22	S	97	THR
22	S	172	ASN
23	P	109	SER
23	P	328	ALA
27	O	71	ASP
27	O	204	SER

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Mol	Chain	Res	Type
28	H	94	GLU
28	H	181	TYR
30	K	167	PRO
30	K	206	PRO
30	K	334	LEU
32	M	296	SER
33	J	82	LYS
33	J	180	ALA
33	J	281	GLY
4	d	40	ASN
5	e	16	SER
5	e	126	GLY
8	h	101	ASN
8	h	154	ASN
10	j	8	ASN
11	k	176	PHE
13	m	208	ASP
14	n	249	ASN
9	2	174	ASP
11	4	11	ASP
12	5	93	SER
14	7	80	ASP
19	Y	32	ASP
20	Z	142	ASP
20	Z	205	LEU
20	Z	233	LEU
20	Z	578	GLY
20	Z	947	GLY
21	N	842	ASN
21	N	861	TYR
22	S	448	LEU
22	S	450	ASN
23	P	3	ARG
23	P	68	SER
24	Q	46	VAL
24	Q	67	THR
24	Q	110	SER
24	Q	170	ASP
24	Q	230	LYS
26	U	42	ASN
28	H	124	ASN
28	H	139	ASP

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Mol	Chain	Res	Type
29	I	134	SER
30	K	308	GLN
30	K	327	ALA
32	M	223	PRO
33	J	228	ARG
33	J	252	SER
2	b	17	LYS
4	d	217	PRO
6	f	205	SER
8	h	138	SER
10	j	157	ASN
11	k	11	ASP
14	n	35	GLN
13	6	48	GLU
14	7	43	SER
15	W	180	LEU
16	V	175	SER
16	V	262	THR
18	X	55	LYS
19	Y	31	GLU
20	Z	25	PRO
20	Z	65	GLU
20	Z	463	HIS
20	Z	557	GLU
20	Z	789	GLN
21	N	397	SER
23	P	89	LEU
24	Q	48	ASP
24	Q	289	GLU
24	Q	309	ARG
25	R	72	VAL
25	R	125	GLU
27	O	70	TYR
27	O	120	LYS
28	H	152	ILE
28	H	203	LYS
28	H	282	LYS
32	M	105	ASN
32	M	151	ASP
32	M	179	THR
32	M	230	LEU
33	J	141	LYS

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Mol	Chain	Res	Type
33	J	213	VAL
33	J	221	LYS
33	J	251	ASP
33	J	280	ASP
33	J	287	ASN
33	J	341	ILE
1	a	60	PRO
1	a	75	ILE
5	E	13	SER
5	E	53	ARG
13	6	40	ASP
16	V	185	ILE
17	T	171	ILE
18	X	39	GLU
20	Z	802	ASP
22	S	44	THR
22	S	113	SER
27	O	56	PRO
32	M	215	PRO
6	f	11	VAL
13	m	12	PRO
11	4	9	VAL
15	W	117	PRO
16	V	72	PRO
21	N	744	PRO
16	V	46	PRO
23	P	130	ILE
32	M	91	ILE
7	g	131	PRO
8	h	32	GLY
20	Z	886	VAL
28	H	314	VAL
30	K	415	VAL
4	d	102	ASP
10	j	102	PRO
8	1	123	PRO
30	K	274	VAL

5.3.2 Protein sidechains (i)

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

entries.

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	206/206 (100%)	204 (99%)	2 (1%)	76	86
1	a	206/206 (100%)	201 (98%)	5 (2%)	49	69
2	B	208/208 (100%)	205 (99%)	3 (1%)	67	81
2	b	208/208 (100%)	203 (98%)	5 (2%)	49	69
3	C	203/203 (100%)	202 (100%)	1 (0%)	88	93
3	c	203/203 (100%)	199 (98%)	4 (2%)	55	73
4	D	210/224 (94%)	207 (99%)	3 (1%)	67	81
4	d	224/224 (100%)	217 (97%)	7 (3%)	40	62
5	E	200/200 (100%)	196 (98%)	4 (2%)	55	73
5	e	200/200 (100%)	192 (96%)	8 (4%)	31	56
6	F	190/190 (100%)	188 (99%)	2 (1%)	73	85
6	f	190/190 (100%)	181 (95%)	9 (5%)	26	52
7	G	200/200 (100%)	196 (98%)	4 (2%)	55	73
7	g	200/200 (100%)	189 (94%)	11 (6%)	21	48
8	1	162/162 (100%)	157 (97%)	5 (3%)	40	62
8	h	162/162 (100%)	159 (98%)	3 (2%)	57	75
9	2	185/185 (100%)	180 (97%)	5 (3%)	44	65
9	i	185/185 (100%)	178 (96%)	7 (4%)	33	57
10	3	172/172 (100%)	168 (98%)	4 (2%)	50	70
10	j	172/172 (100%)	168 (98%)	4 (2%)	50	70
11	4	173/173 (100%)	168 (97%)	5 (3%)	42	64
11	k	173/173 (100%)	170 (98%)	3 (2%)	60	78
12	5	169/169 (100%)	166 (98%)	3 (2%)	59	77
12	l	169/169 (100%)	161 (95%)	8 (5%)	26	52
13	6	185/185 (100%)	182 (98%)	3 (2%)	62	79
13	m	185/185 (100%)	178 (96%)	7 (4%)	33	57
14	7	195/198 (98%)	186 (95%)	9 (5%)	27	53
14	n	198/198 (100%)	188 (95%)	10 (5%)	24	50
15	W	171/171 (100%)	165 (96%)	6 (4%)	36	60

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	V	253/253 (100%)	249 (98%)	4 (2%)	62	79
17	T	249/249 (100%)	243 (98%)	6 (2%)	49	69
18	X	116/116 (100%)	112 (97%)	4 (3%)	37	60
19	Y	81/81 (100%)	78 (96%)	3 (4%)	34	58
20	Z	773/828 (93%)	746 (96%)	27 (4%)	36	60
21	N	776/776 (100%)	758 (98%)	18 (2%)	50	70
22	S	447/447 (100%)	433 (97%)	14 (3%)	40	62
23	P	412/412 (100%)	405 (98%)	7 (2%)	60	78
24	Q	391/391 (100%)	380 (97%)	11 (3%)	43	65
25	R	356/356 (100%)	350 (98%)	6 (2%)	60	78
26	U	277/277 (100%)	268 (97%)	9 (3%)	39	61
27	O	363/363 (100%)	348 (96%)	15 (4%)	30	55
28	H	352/352 (100%)	343 (97%)	9 (3%)	46	67
29	I	342/342 (100%)	329 (96%)	13 (4%)	33	57
30	K	346/346 (100%)	329 (95%)	17 (5%)	25	51
31	L	332/332 (100%)	321 (97%)	11 (3%)	38	61
32	M	364/364 (100%)	357 (98%)	7 (2%)	57	75
33	J	352/352 (100%)	339 (96%)	13 (4%)	34	58
All	All	12086/12158 (99%)	11742 (97%)	344 (3%)	46	65

All (344) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	a	45	VAL
1	a	78	THR
1	a	95	LEU
1	a	104	PHE
1	a	175	GLN
2	b	84	VAL
2	b	97	TYR
2	b	119	GLN
2	b	128	ARG
2	b	217	GLU
3	c	11	THR
3	c	54	SER
3	c	141	ASP

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Mol	Chain	Res	Type
3	c	213	PHE
4	d	6	ARG
4	d	11	PHE
4	d	119	ARG
4	d	126	VAL
4	d	158	SER
4	d	187	THR
4	d	243	GLN
5	e	36	THR
5	e	47	VAL
5	e	71	ASP
5	e	121	LEU
5	e	142	LEU
5	e	188	HIS
5	e	214	GLU
5	e	225	GLN
6	f	7	ASP
6	f	23	GLU
6	f	67	ASP
6	f	72	LEU
6	f	74	LEU
6	f	80	ASP
6	f	92	CYS
6	f	117	GLN
6	f	226	ASP
7	g	9	ASP
7	g	15	PHE
7	g	46	VAL
7	g	69	VAL
7	g	109	ILE
7	g	129	VAL
7	g	185	GLU
7	g	202	LEU
7	g	212	PHE
7	g	218	TRP
7	g	220	SER
8	h	112	ASP
8	h	188	THR
8	h	199	PRO
9	i	80	ASP
9	i	97	LEU
9	i	109	LEU

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Mol	Chain	Res	Type
9	i	148	THR
9	i	193	TRP
9	i	206	VAL
9	i	212	ASP
10	j	61	THR
10	j	156	PRO
10	j	172	LEU
10	j	183	TRP
11	k	93	ARG
11	k	141	PHE
11	k	180	ILE
12	l	79	LEU
12	l	139	ARG
12	l	166	LYS
12	l	171	SER
12	l	174	THR
12	l	179	TYR
12	l	186	THR
12	l	215	LEU
13	m	34	ASP
13	m	109	ARG
13	m	115	VAL
13	m	125	ASP
13	m	167	GLN
13	m	201	GLU
13	m	217	LYS
14	n	36	GLN
14	n	55	ILE
14	n	137	ARG
14	n	165	LEU
14	n	189	ARG
14	n	190	LYS
14	n	220	ARG
14	n	223	ARG
14	n	241	PHE
14	n	258	ILE
1	A	139	VAL
1	A	175	GLN
2	B	119	GLN
2	B	128	ARG
2	B	174	PHE
3	C	152	ASN

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Mol	Chain	Res	Type
4	D	6	ARG
4	D	11	PHE
4	D	70	HIS
5	E	22	PHE
5	E	68	VAL
5	E	136	ARG
5	E	214	GLU
6	F	74	LEU
6	F	117	GLN
7	G	121	GLN
7	G	185	GLU
7	G	212	PHE
7	G	218	TRP
8	1	66	ASP
8	1	124	LEU
8	1	135	ILE
8	1	144	TYR
8	1	199	PRO
9	2	88	ILE
9	2	147	SER
9	2	233	LYS
9	2	236	ARG
9	2	251	ASP
10	3	51	LEU
10	3	144	ASP
10	3	147	PHE
10	3	166	THR
11	4	32	ASP
11	4	40	PRO
11	4	72	ASP
11	4	78	GLN
11	4	186	LYS
12	5	179	TYR
12	5	193	ASP
12	5	195	THR
13	6	20	ILE
13	6	39	THR
13	6	61	SER
14	7	34	THR
14	7	39	VAL
14	7	53	VAL
14	7	115	ASP

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Mol	Chain	Res	Type
14	7	131	THR
14	7	194	ARG
14	7	214	MET
14	7	230	LEU
14	7	241	PHE
15	W	69	PHE
15	W	103	ASN
15	W	155	ASP
15	W	187	SER
15	W	191	ILE
15	W	194	GLU
16	V	58	VAL
16	V	60	ASP
16	V	135	ARG
16	V	189	ILE
17	T	46	ILE
17	T	78	PHE
17	T	109	TYR
17	T	150	ARG
17	T	224	ARG
17	T	238	GLN
18	X	11	ARG
18	X	14	VAL
18	X	36	LYS
18	X	78	ILE
19	Y	3	THR
19	Y	33	ASP
19	Y	66	ASP
20	Z	27	LYS
20	Z	64	TYR
20	Z	103	TYR
20	Z	156	HIS
20	Z	171	LYS
20	Z	222	ASP
20	Z	236	PHE
20	Z	255	LEU
20	Z	402	ASP
20	Z	411	LYS
20	Z	548	ASP
20	Z	557	GLU
20	Z	563	VAL
20	Z	566	LEU

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Mol	Chain	Res	Type
20	Z	613	ASP
20	Z	624	LEU
20	Z	728	LYS
20	Z	729	GLU
20	Z	734	ASP
20	Z	748	LEU
20	Z	756	MET
20	Z	767	TYR
20	Z	842	GLN
20	Z	850	LEU
20	Z	874	ASN
20	Z	927	VAL
20	Z	951	GLN
21	N	60	MET
21	N	71	ASN
21	N	79	VAL
21	N	104	LYS
21	N	175	ASP
21	N	282	TYR
21	N	496	GLU
21	N	534	ASP
21	N	566	SER
21	N	666	GLN
21	N	765	ASP
21	N	823	PRO
21	N	829	LYS
21	N	839	ARG
21	N	840	GLU
21	N	871	MET
21	N	873	ARG
21	N	900	ASN
22	S	72	GLU
22	S	89	LYS
22	S	93	LEU
22	S	101	LYS
22	S	145	PHE
22	S	169	CYS
22	S	226	ASP
22	S	232	MET
22	S	326	ASP
22	S	339	GLN
22	S	405	ARG

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Mol	Chain	Res	Type
22	S	428	ARG
22	S	455	GLU
22	S	488	GLN
23	P	75	LEU
23	P	224	LEU
23	P	309	MET
23	P	370	ASP
23	P	396	PRO
23	P	435	LYS
23	P	439	MET
24	Q	64	LEU
24	Q	66	VAL
24	Q	79	PRO
24	Q	91	SER
24	Q	109	ASP
24	Q	170	ASP
24	Q	214	THR
24	Q	323	LYS
24	Q	384	LYS
24	Q	385	ILE
24	Q	389	VAL
25	R	146	ASP
25	R	162	ILE
25	R	199	GLU
25	R	243	LEU
25	R	333	MET
25	R	337	VAL
26	U	13	LEU
26	U	28	LYS
26	U	70	HIS
26	U	125	VAL
26	U	130	VAL
26	U	212	ASP
26	U	223	HIS
26	U	224	THR
26	U	268	LYS
27	O	47	LYS
27	O	58	ARG
27	O	88	ASP
27	O	117	ASN
27	O	173	SER
27	O	198	THR

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Mol	Chain	Res	Type
27	O	207	LEU
27	O	258	LEU
27	O	312	ASP
27	O	320	PRO
27	O	329	MET
27	O	348	VAL
27	O	350	ILE
27	O	355	PRO
27	O	393	VAL
28	H	44	PRO
28	H	82	TRP
28	H	178	ARG
28	H	197	MET
28	H	217	GLN
28	H	219	GLU
28	H	267	THR
28	H	307	PHE
28	H	360	THR
29	I	66	LYS
29	I	68	HIS
29	I	85	PHE
29	I	112	ILE
29	I	120	VAL
29	I	171	MET
29	I	181	TYR
29	I	192	GLN
29	I	352	ASN
29	I	354	ASP
29	I	393	GLN
29	I	416	PHE
29	I	424	MET
30	K	51	LEU
30	K	67	TYR
30	K	121	ARG
30	K	135	MET
30	K	161	MET
30	K	183	GLU
30	K	206	PRO
30	K	234	PHE
30	K	236	ARG
30	K	267	SER
30	K	313	LYS

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Mol	Chain	Res	Type
30	K	320	ARG
30	K	379	SER
30	K	387	MET
30	K	401	VAL
30	K	404	GLN
30	K	406	ASP
31	L	63	LYS
31	L	135	VAL
31	L	137	ARG
31	L	148	LEU
31	L	199	LEU
31	L	261	ARG
31	L	284	ASP
31	L	312	MET
31	L	333	LEU
31	L	386	PHE
31	L	415	LEU
32	M	18	LEU
32	M	38	ASP
32	M	64	ASP
32	M	146	VAL
32	M	172	VAL
32	M	377	GLN
32	M	426	LYS
33	J	2	THR
33	J	22	TYR
33	J	32	LEU
33	J	48	ARG
33	J	53	ASP
33	J	172	GLU
33	J	228	ARG
33	J	289	LYS
33	J	309	ARG
33	J	338	THR
33	J	344	ARG
33	J	373	ARG
33	J	388	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (120) such sidechains are listed below:

Mol	Chain	Res	Type
1	a	209	HIS

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Mol	Chain	Res	Type
1	a	251	GLN
2	b	94	HIS
2	b	119	GLN
2	b	139	HIS
3	c	31	HIS
4	d	96	HIS
4	d	117	GLN
5	e	73	HIS
5	e	91	HIS
6	f	117	GLN
7	g	33	ASN
7	g	87	HIS
8	h	47	HIS
8	h	150	ASN
9	i	189	GLN
10	j	72	ASN
10	j	173	ASN
11	k	65	GLN
11	k	86	GLN
11	k	101	ASN
11	k	112	ASN
12	l	160	ASN
13	m	78	ASN
13	m	103	HIS
13	m	167	GLN
14	n	111	ASN
3	C	31	HIS
6	F	21	GLN
6	F	117	GLN
7	G	204	HIS
7	G	248	ASN
8	1	101	ASN
8	1	154	ASN
9	2	248	ASN
10	3	173	ASN
11	4	63	ASN
11	4	99	GLN
11	4	133	HIS
11	4	146	HIS
12	5	241	HIS
12	5	251	ASN
13	6	11	ASN

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Mol	Chain	Res	Type
13	6	44	ASN
13	6	63	ASN
13	6	84	HIS
13	6	160	ASN
13	6	203	HIS
14	7	35	GLN
15	W	77	HIS
15	W	103	ASN
16	V	190	HIS
16	V	217	HIS
16	V	291	ASN
17	T	37	ASN
17	T	53	ASN
17	T	117	ASN
17	T	123	HIS
17	T	204	ASN
19	Y	9	GLN
19	Y	11	GLN
20	Z	15	GLN
20	Z	214	HIS
20	Z	235	GLN
20	Z	622	HIS
20	Z	823	ASN
20	Z	829	GLN
20	Z	926	ASN
21	N	29	ASN
21	N	361	ASN
21	N	430	ASN
21	N	613	HIS
21	N	690	HIS
21	N	738	GLN
21	N	870	ASN
21	N	900	ASN
22	S	139	HIS
22	S	417	GLN
23	P	76	ASN
23	P	98	GLN
23	P	242	GLN
23	P	263	HIS
23	P	278	ASN
23	P	348	HIS
23	P	425	HIS

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Mol	Chain	Res	Type
23	P	431	HIS
24	Q	21	ASN
24	Q	372	GLN
25	R	96	GLN
25	R	136	ASN
25	R	325	HIS
25	R	397	ASN
25	R	406	GLN
26	U	30	ASN
26	U	70	HIS
26	U	127	GLN
26	U	156	HIS
26	U	193	GLN
26	U	256	ASN
26	U	280	ASN
27	O	256	ASN
27	O	345	ASN
28	H	80	HIS
28	H	128	ASN
29	I	150	HIS
29	I	204	HIS
29	I	365	HIS
30	K	142	HIS
30	K	244	HIS
31	L	67	HIS
31	L	189	GLN
31	L	311	GLN
32	M	56	ASN
32	M	189	GLN
32	M	405	ASN
33	J	15	HIS
33	J	47	GLN
33	J	89	GLN
33	J	123	HIS
33	J	331	HIS

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)

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

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
36	ATP	L	501	35	26,33,33	1.30	3 (11%)	31,52,52	1.61	5 (16%)
36	ATP	J	501	35	26,33,33	1.21	3 (11%)	31,52,52	1.91	6 (19%)
36	ATP	I	501	35	26,33,33	1.37	3 (11%)	31,52,52	1.61	6 (19%)
36	ATP	K	501	35	26,33,33	1.37	3 (11%)	31,52,52	1.61	6 (19%)
34	ADP	H	501	35	24,29,29	1.27	3 (12%)	29,45,45	2.41	6 (20%)
34	ADP	M	501	35	24,29,29	2.00	6 (25%)	29,45,45	2.33	6 (20%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
36	ATP	L	501	35	-	5/18/38/38	0/3/3/3
36	ATP	J	501	35	-	4/18/38/38	0/3/3/3
36	ATP	I	501	35	-	5/18/38/38	0/3/3/3
36	ATP	K	501	35	-	4/18/38/38	0/3/3/3
34	ADP	H	501	35	-	4/12/32/32	0/3/3/3
34	ADP	M	501	35	-	4/12/32/32	0/3/3/3

All (21) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
34	M	501	ADP	C4-N3	-5.43	1.28	1.35
34	M	501	ADP	O4'-C4'	4.85	1.55	1.45
36	L	501	ATP	C2-N3	4.26	1.39	1.32
36	K	501	ATP	C2-N3	4.26	1.39	1.32
36	I	501	ATP	C2-N3	4.25	1.38	1.32
36	J	501	ATP	C2-N3	3.60	1.37	1.32
34	M	501	ADP	C2-N3	3.42	1.37	1.32
34	H	501	ADP	C2'-C3'	-3.17	1.44	1.53
34	H	501	ADP	C2'-C1'	3.01	1.58	1.53
36	J	501	ATP	C8-N7	-2.98	1.29	1.34
34	M	501	ADP	C8-N7	-2.59	1.30	1.34
36	J	501	ATP	C2-N1	-2.51	1.29	1.33
36	K	501	ATP	C5-C4	-2.48	1.34	1.40
36	L	501	ATP	C5-C4	-2.47	1.34	1.40
36	I	501	ATP	C5-C4	-2.45	1.34	1.40
36	I	501	ATP	C8-N7	-2.31	1.30	1.34
36	K	501	ATP	C8-N7	-2.27	1.30	1.34
36	L	501	ATP	C8-N7	-2.27	1.30	1.34
34	H	501	ADP	C8-N7	-2.25	1.30	1.34
34	M	501	ADP	C5-C4	-2.10	1.35	1.40
34	M	501	ADP	PB-O2B	-2.02	1.47	1.54

All (35) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
34	M	501	ADP	PA-O3A-PB	10.20	167.84	132.83
34	H	501	ADP	PA-O3A-PB	8.49	161.96	132.83
36	J	501	ATP	PB-O3B-PG	5.53	151.80	132.83
36	J	501	ATP	PA-O3A-PB	5.00	149.97	132.83
34	H	501	ADP	N3-C2-N1	4.95	136.41	128.68
36	L	501	ATP	PA-O3A-PB	4.88	149.58	132.83
36	K	501	ATP	PA-O3A-PB	4.86	149.51	132.83
36	I	501	ATP	PA-O3A-PB	4.85	149.46	132.83
34	H	501	ADP	N6-C6-N1	4.43	127.77	118.57
34	H	501	ADP	C5-C6-N6	-4.12	114.09	120.35
34	M	501	ADP	N6-C6-N1	4.07	127.03	118.57
36	L	501	ATP	N6-C6-N1	3.99	126.85	118.57
36	I	501	ATP	N6-C6-N1	3.97	126.81	118.57
36	K	501	ATP	N6-C6-N1	3.95	126.78	118.57
36	J	501	ATP	N3-C2-N1	3.90	134.78	128.68
34	H	501	ADP	C2-N1-C6	-3.86	112.15	118.75
36	J	501	ATP	N6-C6-N1	3.84	126.55	118.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
36	I	501	ATP	PB-O3B-PG	2.74	142.23	132.83
36	L	501	ATP	PB-O3B-PG	2.74	142.22	132.83
34	M	501	ADP	C5-C6-N1	-2.74	114.15	120.35
36	K	501	ATP	PB-O3B-PG	2.73	142.21	132.83
36	L	501	ATP	C5-C6-N6	-2.34	116.80	120.35
36	K	501	ATP	C5-C6-N6	-2.30	116.86	120.35
36	I	501	ATP	C5-C6-N6	-2.29	116.87	120.35
36	I	501	ATP	O3G-PG-O2G	2.26	116.27	107.64
36	K	501	ATP	O3G-PG-O2G	2.24	116.22	107.64
34	M	501	ADP	C3'-C2'-C1'	2.24	104.35	100.98
34	M	501	ADP	O3B-PB-O2B	2.23	116.16	107.64
34	H	501	ADP	O2B-PB-O3A	2.22	112.07	104.64
36	K	501	ATP	C2-N1-C6	-2.18	115.03	118.75
36	L	501	ATP	C2-N1-C6	-2.15	115.07	118.75
36	I	501	ATP	C2-N1-C6	-2.13	115.10	118.75
36	J	501	ATP	C5-C6-N6	-2.11	117.14	120.35
34	M	501	ADP	C5'-C4'-C3'	2.04	122.82	115.18
36	J	501	ATP	O3G-PG-O2G	2.02	115.35	107.64

There are no chirality outliers.

All (26) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
34	H	501	ADP	C5'-O5'-PA-O2A
34	H	501	ADP	C5'-O5'-PA-O3A
34	M	501	ADP	C5'-O5'-PA-O1A
36	I	501	ATP	PB-O3B-PG-O2G
36	K	501	ATP	PB-O3B-PG-O2G
36	L	501	ATP	PB-O3B-PG-O2G
36	L	501	ATP	PB-O3B-PG-O3G
36	J	501	ATP	PB-O3B-PG-O2G
36	J	501	ATP	C5'-O5'-PA-O1A
36	J	501	ATP	C5'-O5'-PA-O2A
34	M	501	ADP	C5'-O5'-PA-O3A
34	M	501	ADP	C5'-O5'-PA-O2A
36	I	501	ATP	O4'-C4'-C5'-O5'
36	K	501	ATP	O4'-C4'-C5'-O5'
36	L	501	ATP	O4'-C4'-C5'-O5'
36	I	501	ATP	PG-O3B-PB-O2B
36	I	501	ATP	C3'-C4'-C5'-O5'
36	K	501	ATP	C3'-C4'-C5'-O5'
36	L	501	ATP	C3'-C4'-C5'-O5'

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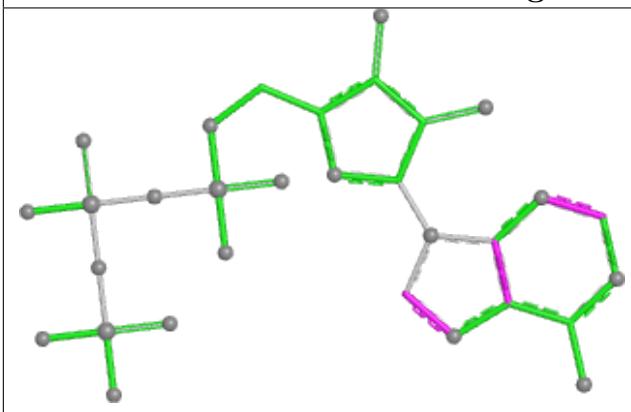
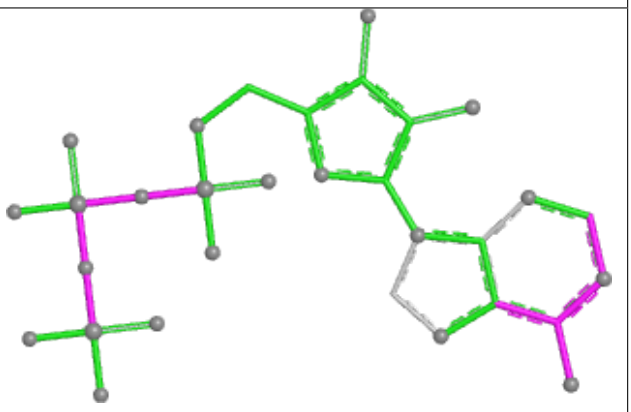
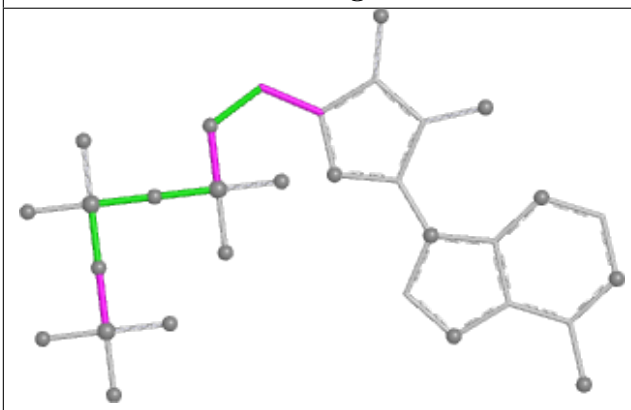
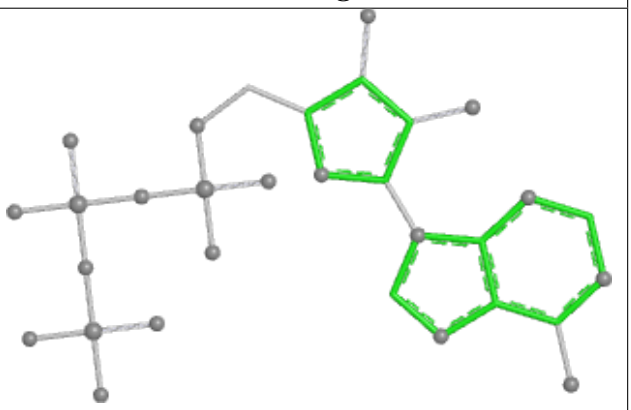
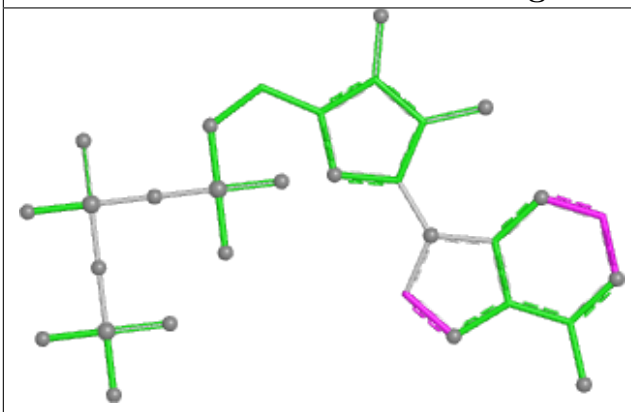
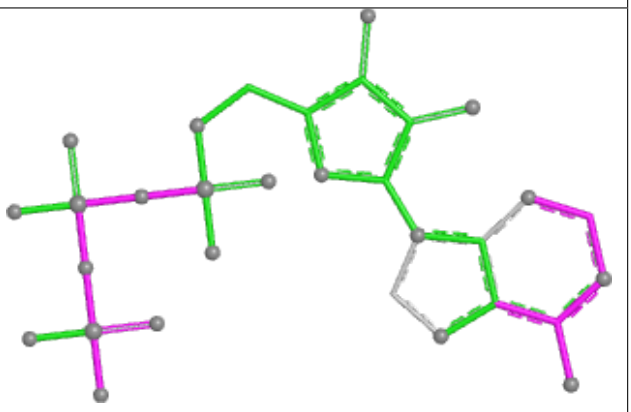
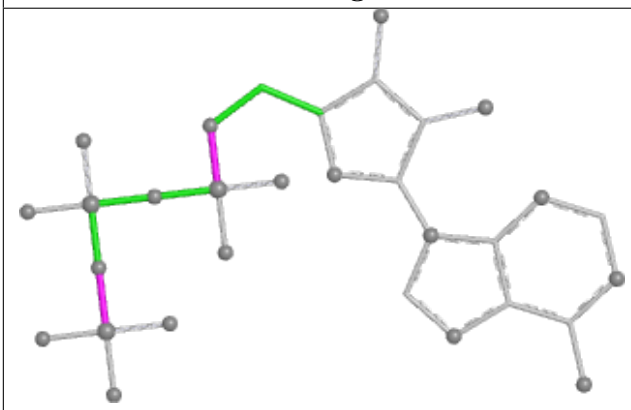
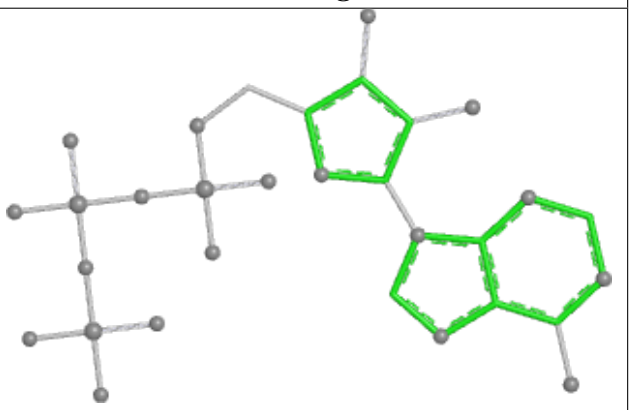
Mol	Chain	Res	Type	Atoms
36	I	501	ATP	C5'-O5'-PA-O3A
36	K	501	ATP	C5'-O5'-PA-O3A
36	L	501	ATP	C5'-O5'-PA-O3A
36	J	501	ATP	C5'-O5'-PA-O3A
34	M	501	ADP	C4'-C5'-O5'-PA
34	H	501	ADP	PB-O3A-PA-O1A
34	H	501	ADP	PB-O3A-PA-O2A

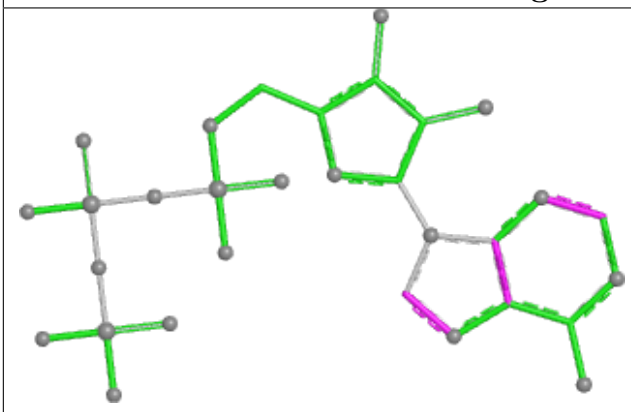
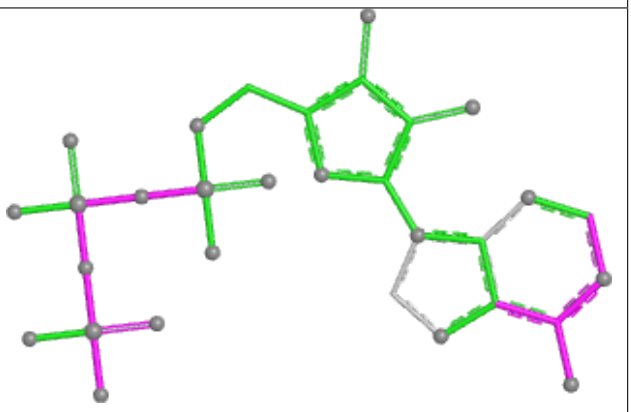
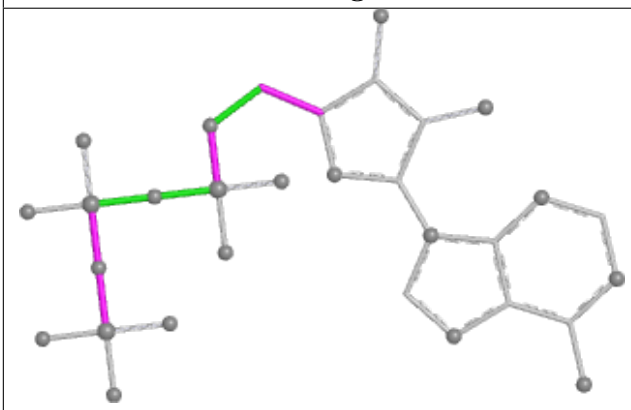
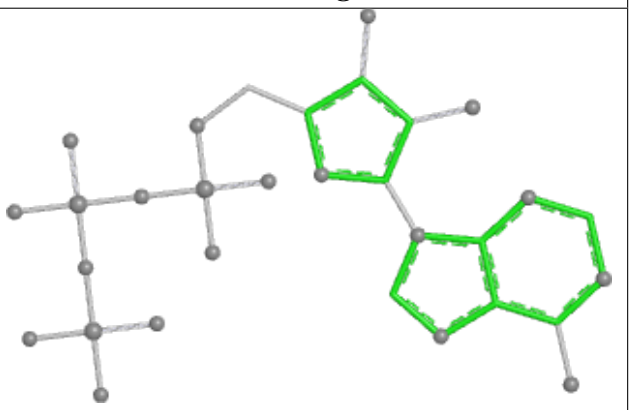
There are no ring outliers.

No monomer is involved in short contacts.

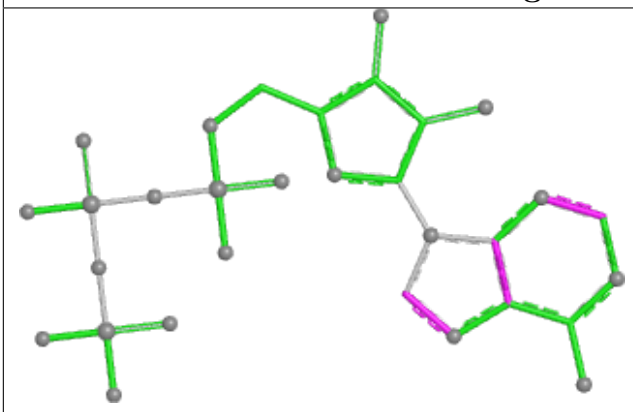
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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

Ligand ATP L 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

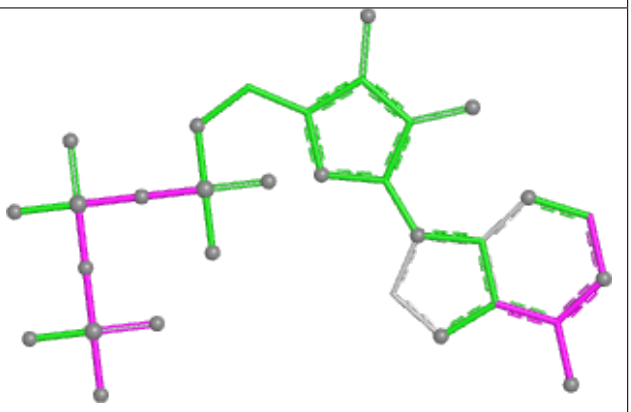
Ligand ATP J 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand ATP I 501	
 Bond lengths	 Bond angles
 Torsions	 Rings

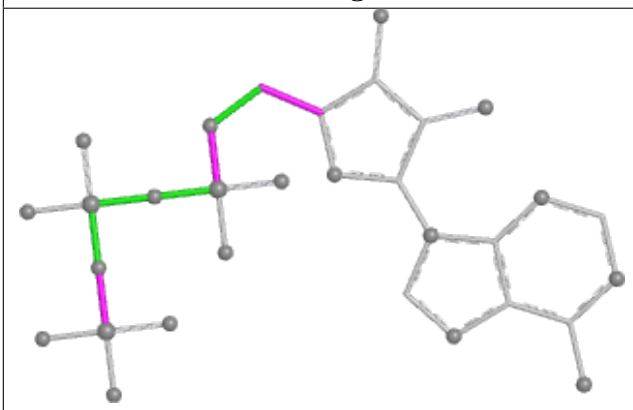
Ligand ATP K 501



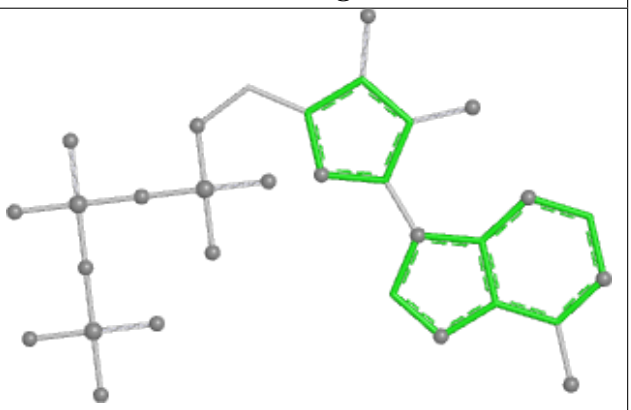
Bond lengths



Bond angles

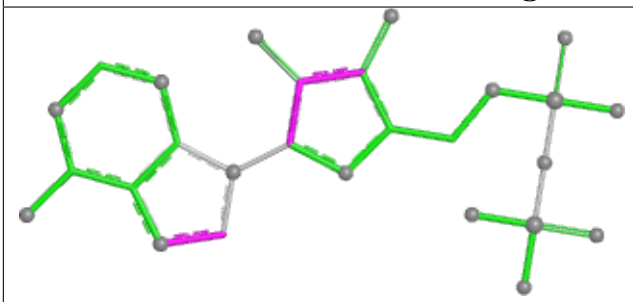


Torsions

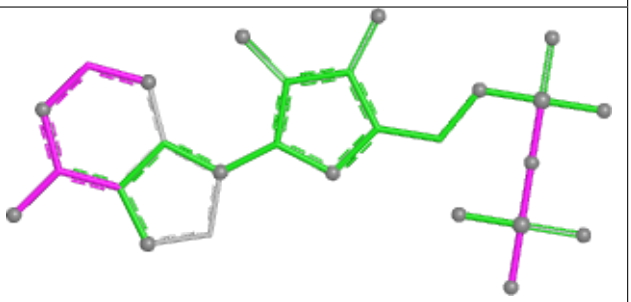


Rings

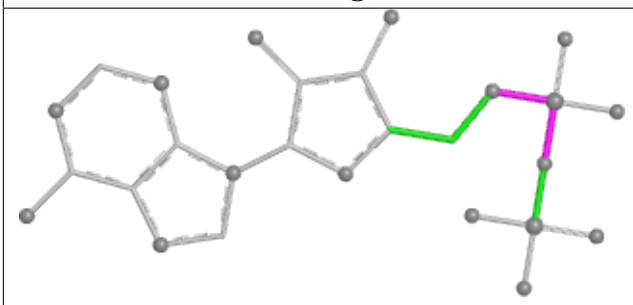
Ligand ADP H 501



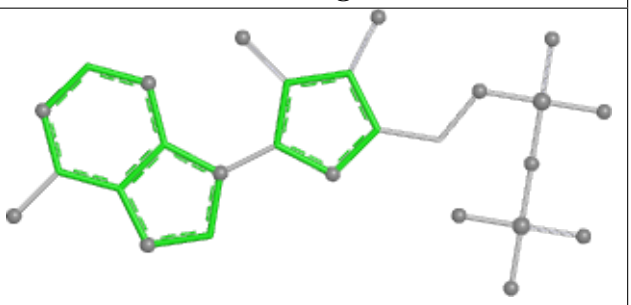
Bond lengths



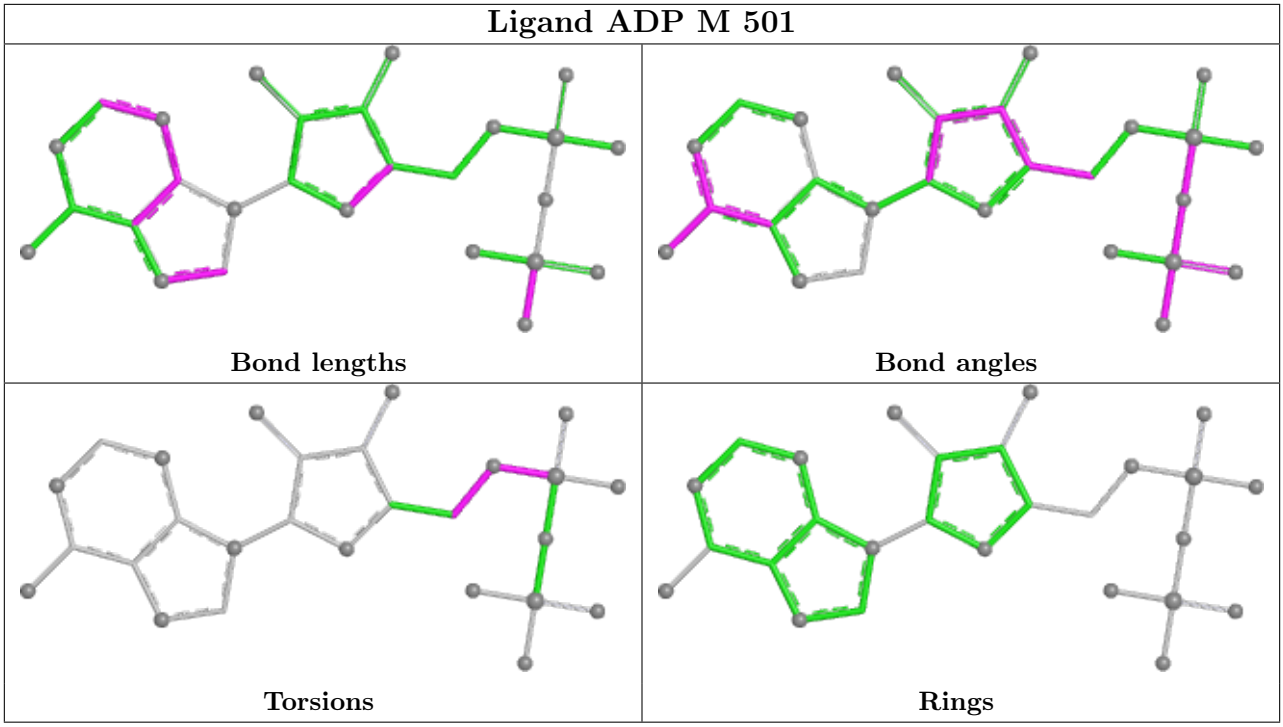
Bond angles



Torsions



Rings



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
29	I	2
32	M	2
33	J	2
31	L	1
30	K	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	L	180:PHE	C	181:ASP	N	2.67
1	I	183:ASP	C	184:ILE	N	2.58
1	I	186:GLY	C	187:LEU	N	2.56
1	M	338:LEU	C	339:ARG	N	1.69
1	J	212:ARG	C	213:VAL	N	1.68
1	M	342:ARG	C	343:LEU	N	1.18

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Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	K	220:THR	C	221:MET	N	0.91
1	J	211:ILE	C	212:ARG	N	0.52

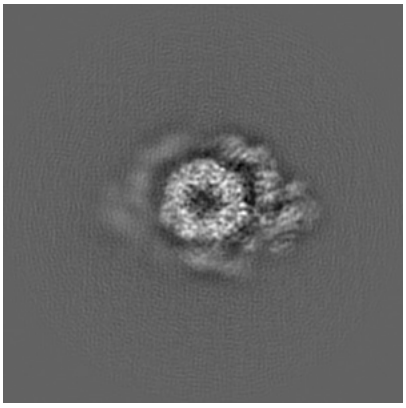
6 Map visualisation (i)

This section contains visualisations of the EMDB entry EMD-4321. These allow visual inspection of the internal detail of the map and identification of artifacts.

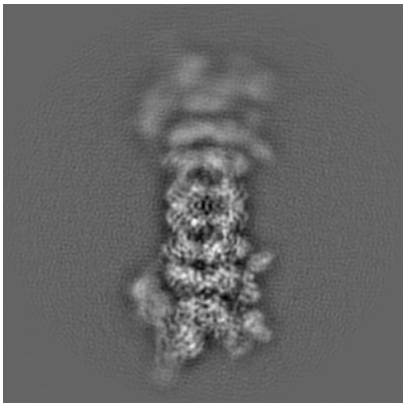
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections (i)

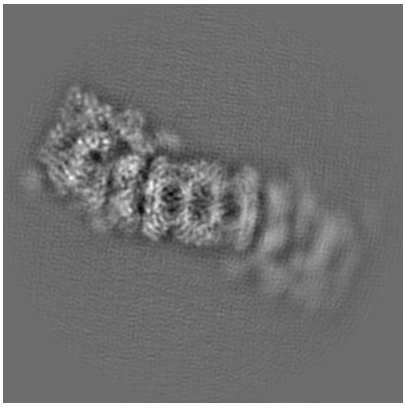
6.1.1 Primary map



X



Y

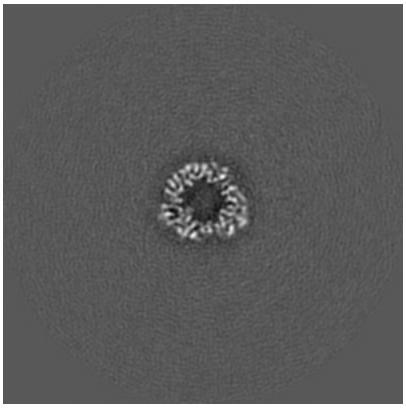


Z

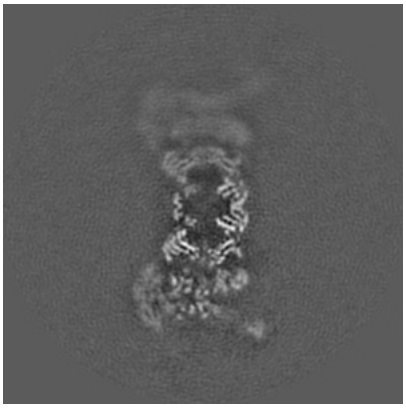
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

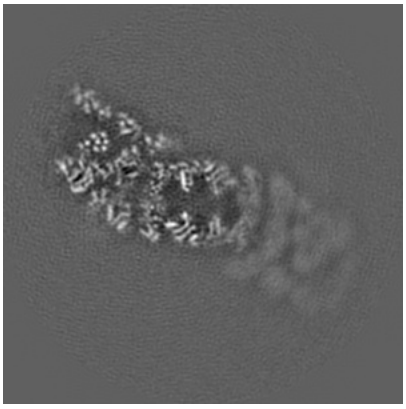
6.2.1 Primary map



X Index: 192



Y Index: 192

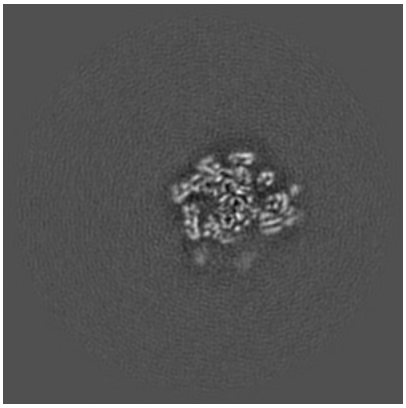


Z Index: 192

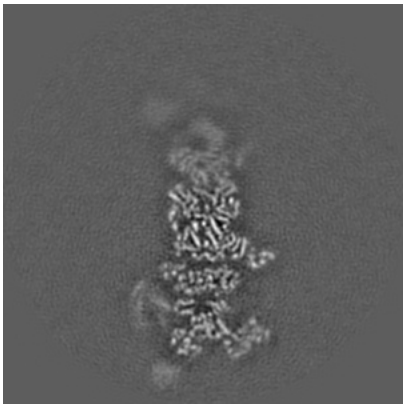
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

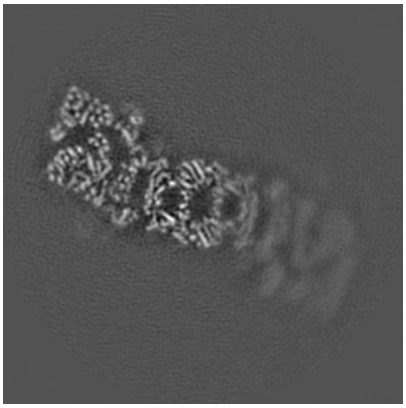
6.3.1 Primary map



X Index: 122



Y Index: 213



Z Index: 182

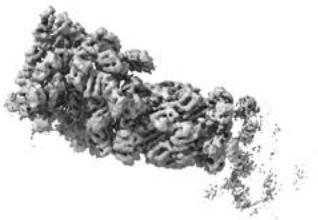
The images above show the largest variance slices of the map in three orthogonal directions.

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

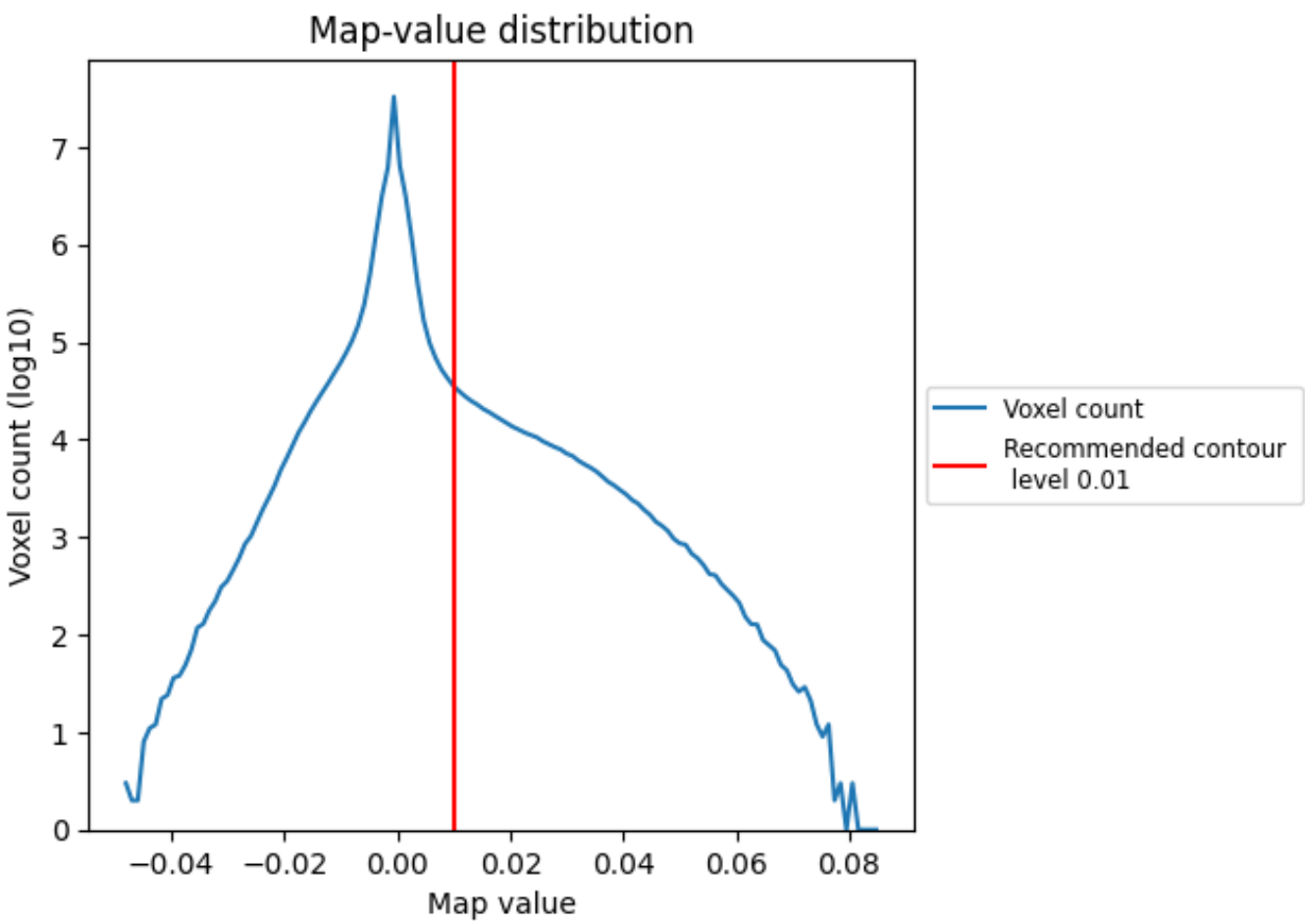
6.5 Mask visualisation (i)

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

7 Map analysis (i)

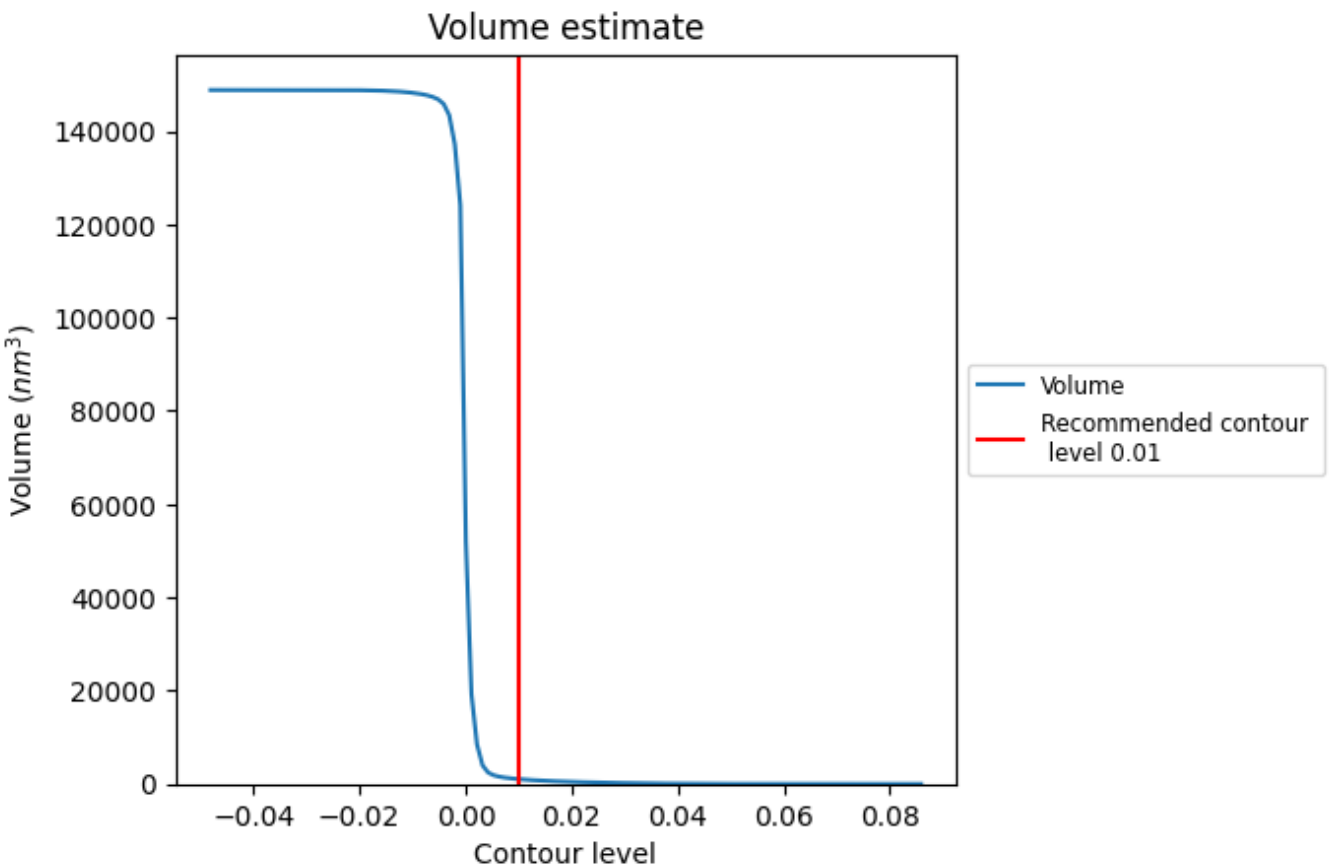
This section contains the results of statistical analysis of the map.

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.

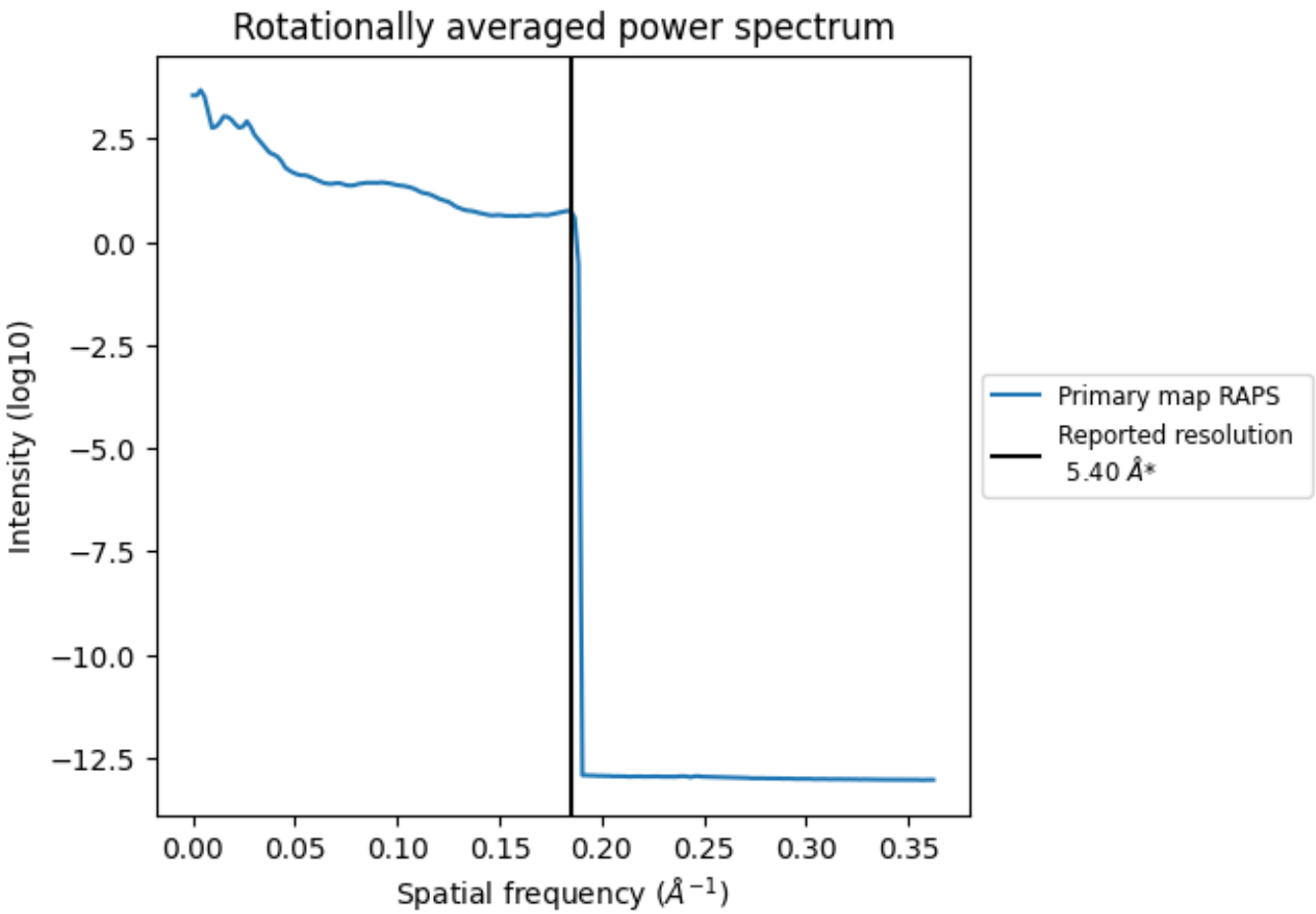
7.2 Volume estimate (i)



The volume at the recommended contour level is 1039 nm^3; this corresponds to an approximate mass of 938 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 0.185 Å^{-1}

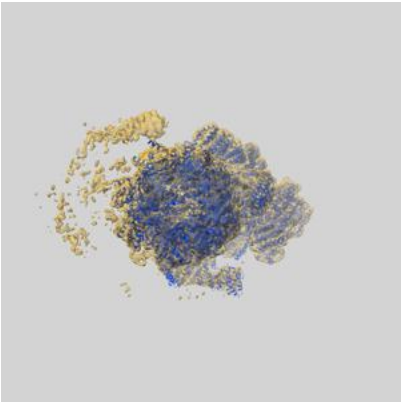
8 Fourier-Shell correlation (i)

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

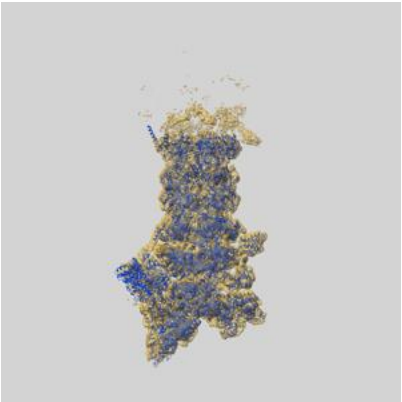
9 Map-model fit (i)

This section contains information regarding the fit between EMDB map EMD-4321 and PDB model 6FVV. Per-residue inclusion information can be found in section 3 on page 13.

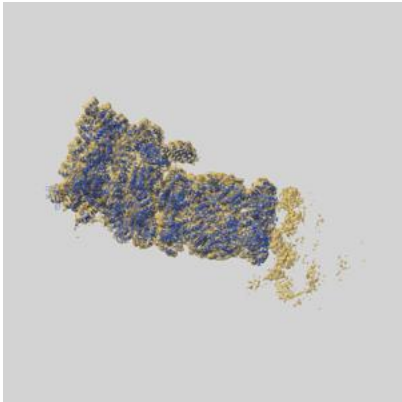
9.1 Map-model overlay (i)



X



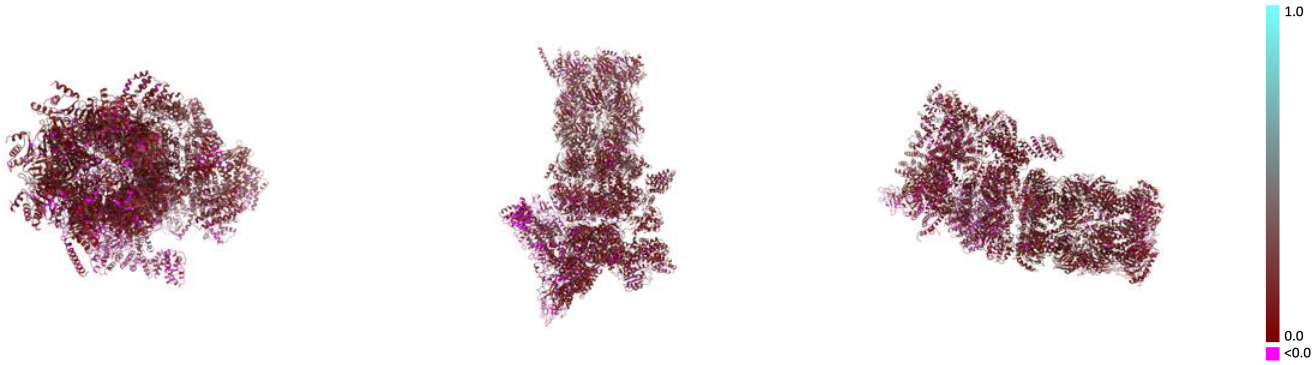
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 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.

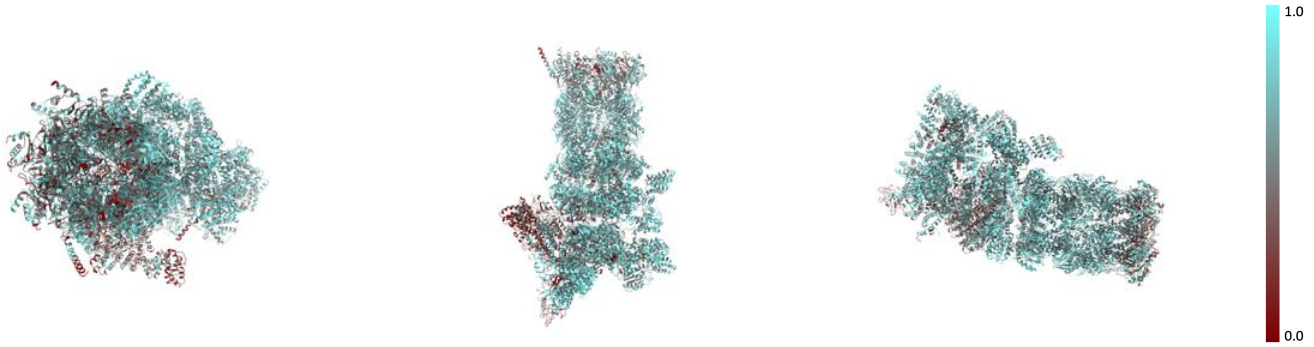
9.2 Q-score mapped to coordinate model (i)



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.

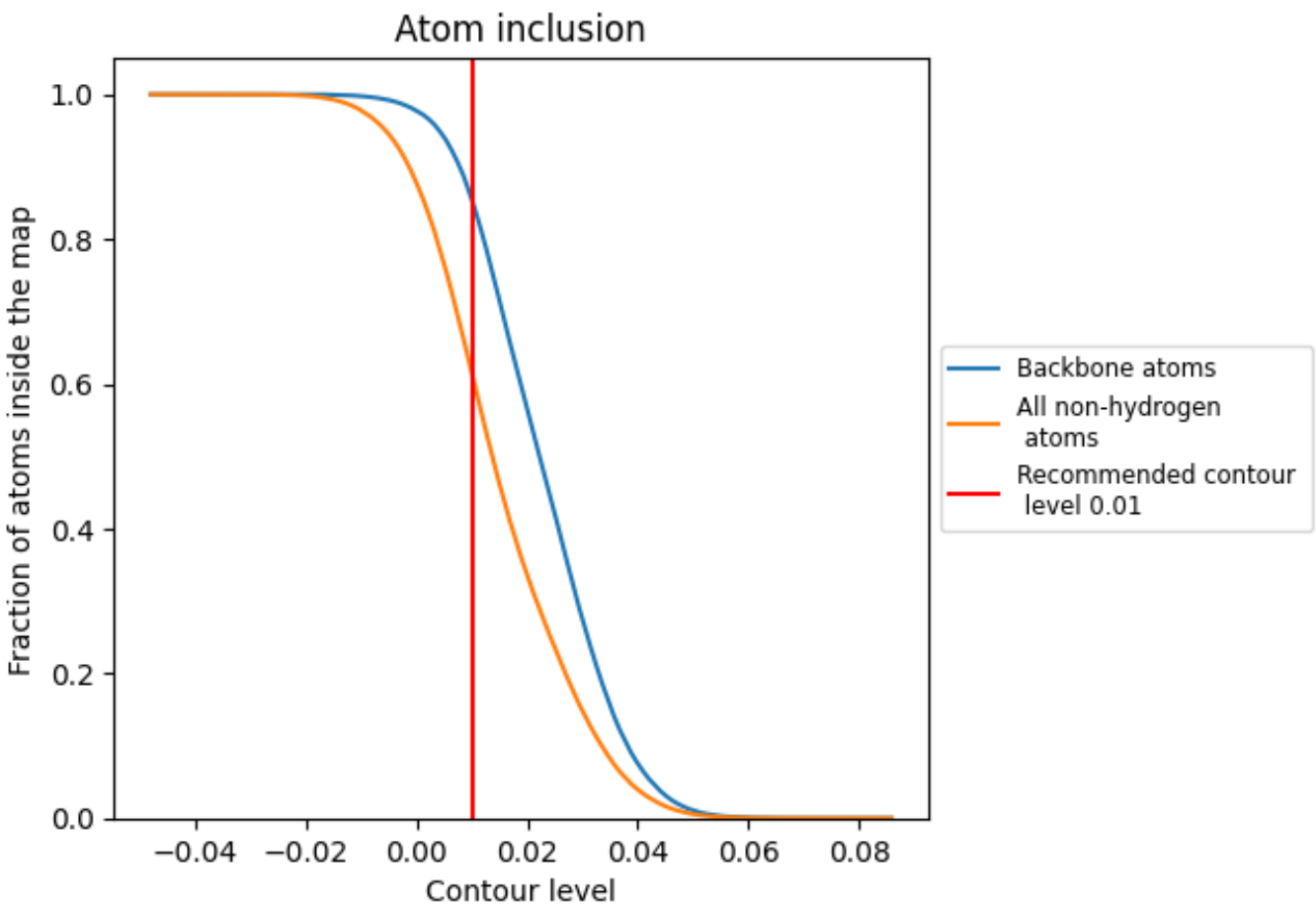
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 85% of all backbone atoms, 61% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6137	0.1490
1	0.7305	0.1860
2	0.7209	0.1970
3	0.6851	0.1880
4	0.7142	0.1830
5	0.7396	0.1850
6	0.7096	0.1840
7	0.7228	0.1830
A	0.7003	0.1800
B	0.6814	0.1950
C	0.6883	0.1850
D	0.7001	0.1870
E	0.6742	0.1750
F	0.7096	0.1830
G	0.7101	0.1820
H	0.5848	0.1240
I	0.5764	0.1380
J	0.5794	0.1250
K	0.5986	0.1410
L	0.6451	0.1490
M	0.5988	0.1300
N	0.6509	0.1540
O	0.6891	0.1520
P	0.7388	0.1520
Q	0.6927	0.1450
R	0.6898	0.1450
S	0.6218	0.1380
T	0.6385	0.1340
U	0.6133	0.1490
V	0.6502	0.1610
W	0.6015	0.1360
X	0.2613	0.0510
Y	0.4136	0.0670
Z	0.3348	0.0590
a	0.5005	0.1460

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Chain	Atom inclusion	Q-score
b	0.4422	0.1550
c	0.4705	0.1370
d	0.4515	0.1300
e	0.4498	0.1420
f	0.5227	0.1570
g	0.5167	0.1430
h	0.6954	0.1650
i	0.6779	0.1790
j	0.6600	0.1750
k	0.6763	0.1760
l	0.6874	0.1680
m	0.6527	0.1690
n	0.6639	0.1710