Full wwPDB EM Validation Report ⓘ

Oct 5, 2023 – 12:44 PM EDT

PDB ID	:	8TJ5
EMDB ID	:	EMD-41300
Title	:	Inner spoke ring of the yeast NPC
Authors	:	Akey, C.W.; Echeverria, I.; Ouch, C.; Fernandez-Martinez, J.; Rout, M.P.
Deposited on	:	2023-07-20
Resolution	:	6.60 Å(reported)
Based on initial model	:	.

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

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

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

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

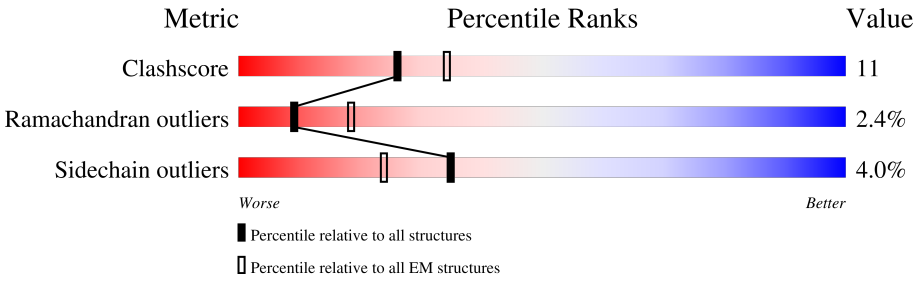
EMDB validation analysis	:	0.0.1.dev50
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.35.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 6.60 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)
Clashscore	158937	4297
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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

Mol	Chain	Length	Quality of chain
1	3	37	8% 35% 8% 57%
1	4	37	5% 35% 8% 57%
1	7	37	19% 24% 54%
1	8	37	19% 24% 54%
1	a	37	16% 22% 78%
1	b	37	32% 95% 5%
1	c	37	22% 46% 54%
1	d	37	11% 59% 41%

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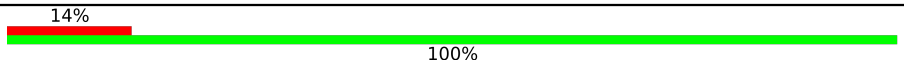
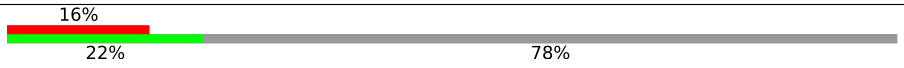
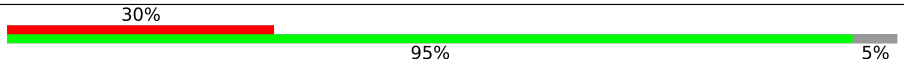
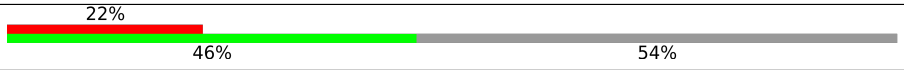
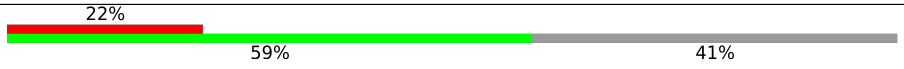
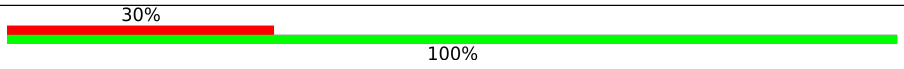
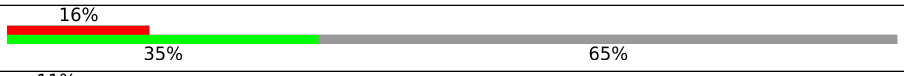
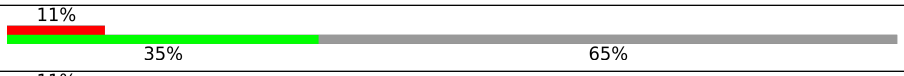
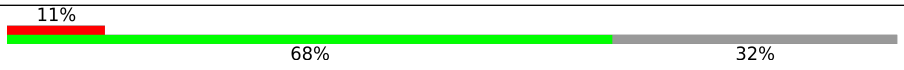
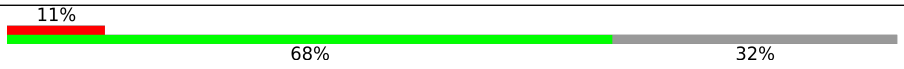
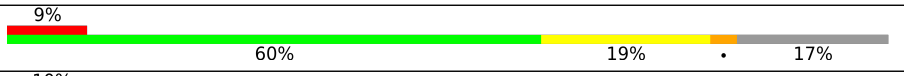
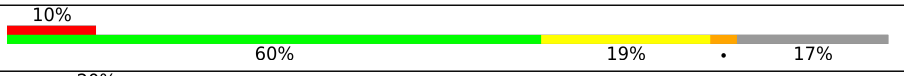
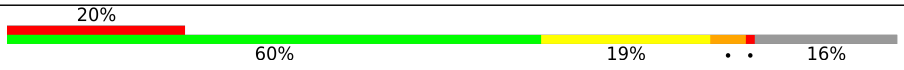
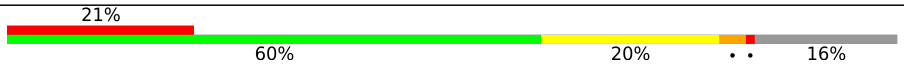
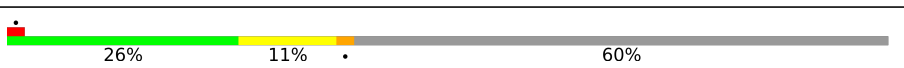
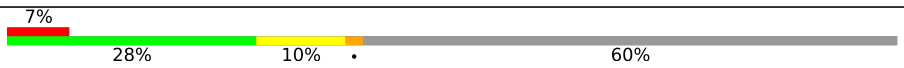
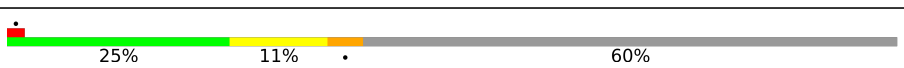
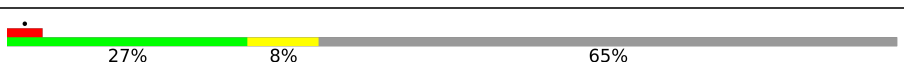
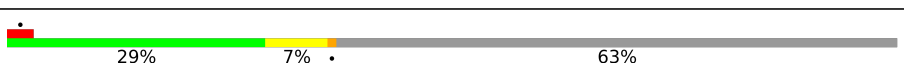
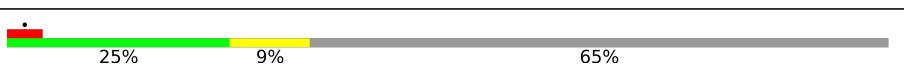
Mol	Chain	Length	Quality of chain
1	e	37	
1	f	37	
1	g	37	
1	h	37	
1	i	37	
1	j	37	
1	k	37	
1	l	37	
1	m	37	
1	n	37	
2	0	1502	
2	Y	1502	
3	1	1391	
3	Z	1391	
4	A	823	
4	D	823	
4	G	823	
4	J	823	
5	B	541	
5	E	541	
5	H	541	
5	K	541	
6	C	472	
6	F	472	
6	I	472	

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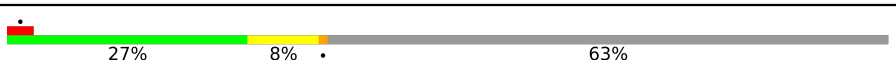
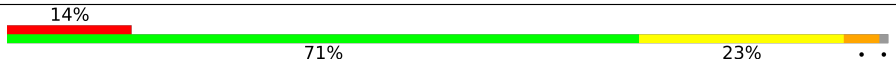
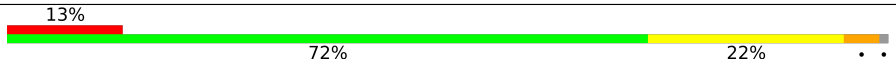
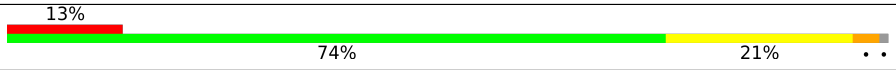
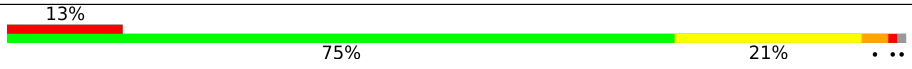
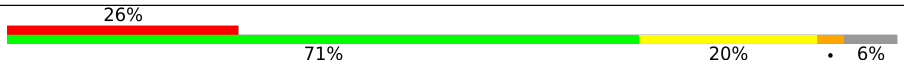
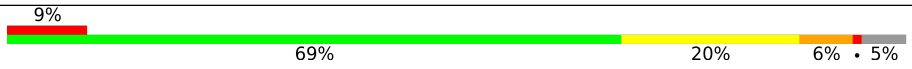
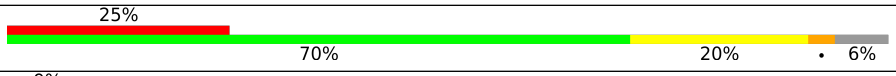
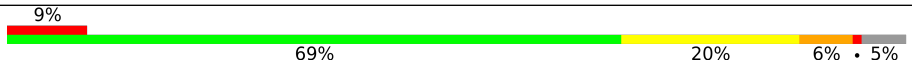
Mol	Chain	Length	Quality of chain
6	L	472	
7	M	1683	
7	O	1683	
8	N	1655	
8	P	1655	
9	Q	839	
9	R	839	
9	S	839	
9	T	839	
10	U	475	
10	W	475	
11	V	528	
11	X	528	

2 Entry composition (i)

There are 11 unique types of molecules in this entry. The entry contains 138272 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 Spoke connector.

Mol	Chain	Residues	Atoms				AltConf	Trace
1	7	17	Total	C	N	O	0	0
			85	51	17	17		
1	3	16	Total	C	N	O	0	0
			80	48	16	16		
1	8	17	Total	C	N	O	0	0
			85	51	17	17		
1	4	16	Total	C	N	O	0	0
			80	48	16	16		
1	a	8	Total	C	N	O	0	0
			40	24	8	8		
1	b	35	Total	C	N	O	0	0
			175	105	35	35		
1	k	13	Total	C	N	O	0	0
			65	39	13	13		
1	c	17	Total	C	N	O	0	0
			85	51	17	17		
1	m	25	Total	C	N	O	0	0
			125	75	25	25		
1	d	22	Total	C	N	O	0	0
			110	66	22	22		
1	e	37	Total	C	N	O	0	0
			185	111	37	37		
1	f	8	Total	C	N	O	0	0
			40	24	8	8		
1	g	35	Total	C	N	O	0	0
			175	105	35	35		
1	l	13	Total	C	N	O	0	0
			65	39	13	13		
1	h	17	Total	C	N	O	0	0
			85	51	17	17		
1	n	25	Total	C	N	O	0	0
			125	75	25	25		
1	j	37	Total	C	N	O	0	0
			185	111	37	37		

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Mol	Chain	Residues	Atoms				AltConf	Trace
1	i	22	Total 110	C 66	N 22	O 22	0	0

- Molecule 2 is a protein called Nucleoporin NUP170.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	Y	1246	Total 10015	C 6434	N 1644	O 1901	S 36	0	0
2	0	1246	Total 10015	C 6434	N 1644	O 1901	S 36	0	0

- Molecule 3 is a protein called Nucleoporin NUP157.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	Z	1164	Total 9319	C 5964	N 1544	O 1778	S 33	0	0
3	1	1164	Total 9319	C 5964	N 1544	O 1778	S 33	0	0

- Molecule 4 is a protein called Nucleoporin NSP1.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	163	Total 1315	C 814	N 220	O 280	S 1	0	0
4	D	169	Total 1345	C 832	N 226	O 286	S 1	0	0
4	G	163	Total 1315	C 814	N 220	O 280	S 1	0	0
4	J	169	Total 1347	C 833	N 226	O 287	S 1	0	0

- Molecule 5 is a protein called Nucleoporin NUP57.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	217	Total 1771	C 1115	N 317	O 336	S 3	0	0
5	E	217	Total 1771	C 1115	N 317	O 336	S 3	0	0
5	H	217	Total 1771	C 1115	N 317	O 336	S 3	0	0
5	K	217	Total 1771	C 1115	N 317	O 336	S 3	0	0

- Molecule 6 is a protein called Nucleoporin NUP49/NSP49.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	166	Total	C	N	O	S	0	0
			1347	863	217	265	2		
6	F	173	Total	C	N	O	S	0	0
			1381	883	224	272	2		
6	I	166	Total	C	N	O	S	0	0
			1347	863	217	265	2		
6	L	173	Total	C	N	O	S	0	0
			1381	883	224	272	2		

- Molecule 7 is a protein called Nucleoporin NUP192.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	M	1659	Total	C	N	O	S	0	0
			13334	8597	2155	2542	40		
7	O	1659	Total	C	N	O	S	0	0
			13334	8597	2155	2542	40		

- Molecule 8 is a protein called Nucleoporin NUP188.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	N	1640	Total	C	N	O	S	0	0
			13181	8518	2115	2519	29		
8	P	1641	Total	C	N	O	S	0	0
			13190	8524	2117	2520	29		

- Molecule 9 is a protein called Nucleoporin NIC96.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	Q	791	Total	C	N	O	S	0	0
			5961	3768	1032	1144	17		
9	R	800	Total	C	N	O	S	0	0
			5983	3783	1037	1146	17		
9	S	791	Total	C	N	O	S	0	0
			5961	3768	1032	1144	17		
9	T	801	Total	C	N	O	S	0	0
			5988	3786	1038	1147	17		

- Molecule 10 is a protein called Nucleoporin NUP53.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	U	94	Total	C	N	O	S	0	0
			745	486	120	137	2		
10	W	94	Total	C	N	O	S	0	0
			745	486	120	137	2		

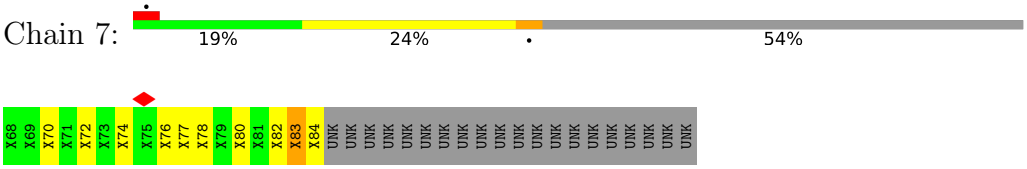
- Molecule 11 is a protein called Nucleoporin 59.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	V	90	Total	C	N	O	S	0	0
			710	459	117	131	3		
11	X	90	Total	C	N	O	S	0	0
			710	459	117	131	3		

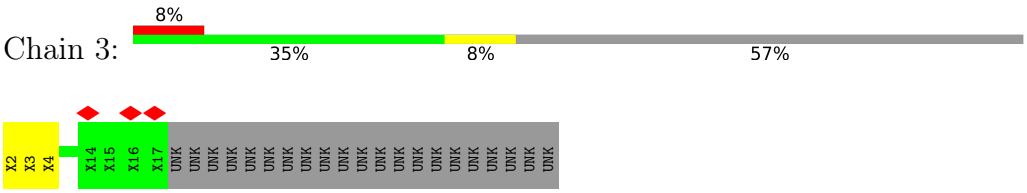
3 Residue-property plots (i)

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.

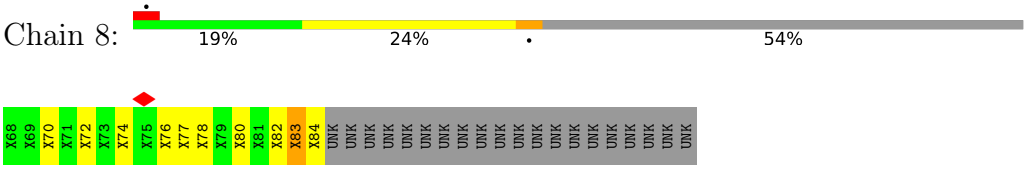
- Molecule 1: Spoke connector



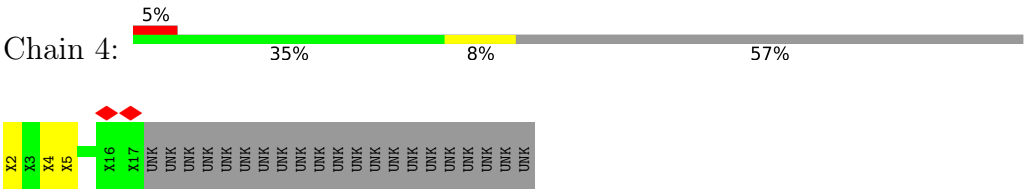
- Molecule 1: Spoke connector



- Molecule 1: Spoke connector



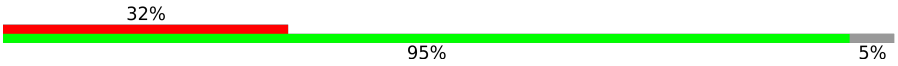
- Molecule 1: Spoke connector

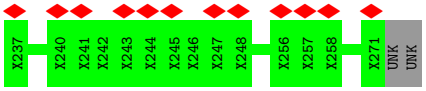


- Molecule 1: Spoke connector

• Molecule 1: Spoke connector

Chain b:



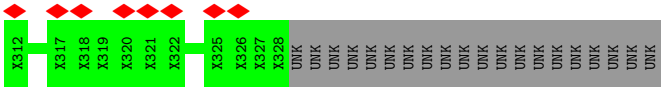


• Molecule 1: Spoke connector

Chain k:

• Molecule 1: Spoke connector

Chain c:



• Molecule 1: Spoke connector

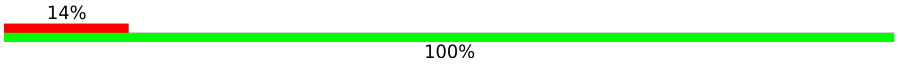
Chain m:

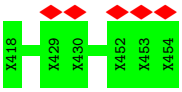
• Molecule 1: Spoke connector

Chain d:

• Molecule 1: Spoke connector

Chain e:



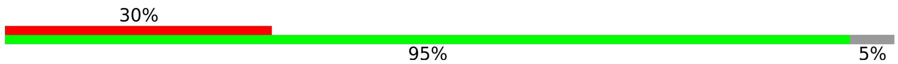


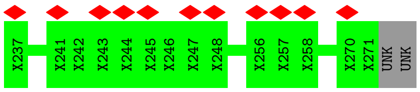
• Molecule 1: Spoke connector

Chain f:

• Molecule 1: Spoke connector

Chain g:





• Molecule 1: Spoke connector

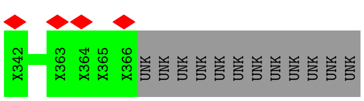
Chain l:

• Molecule 1: Spoke connector

Chain h:

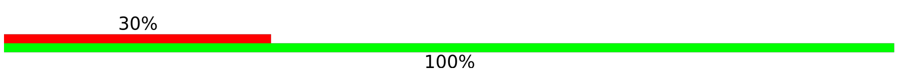
• Molecule 1: Spoke connector

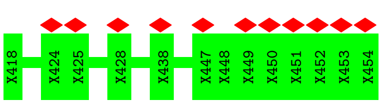
Chain n:



• Molecule 1: Spoke connector

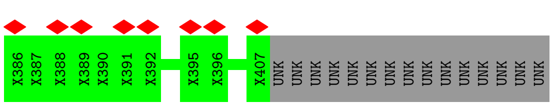
Chain j:





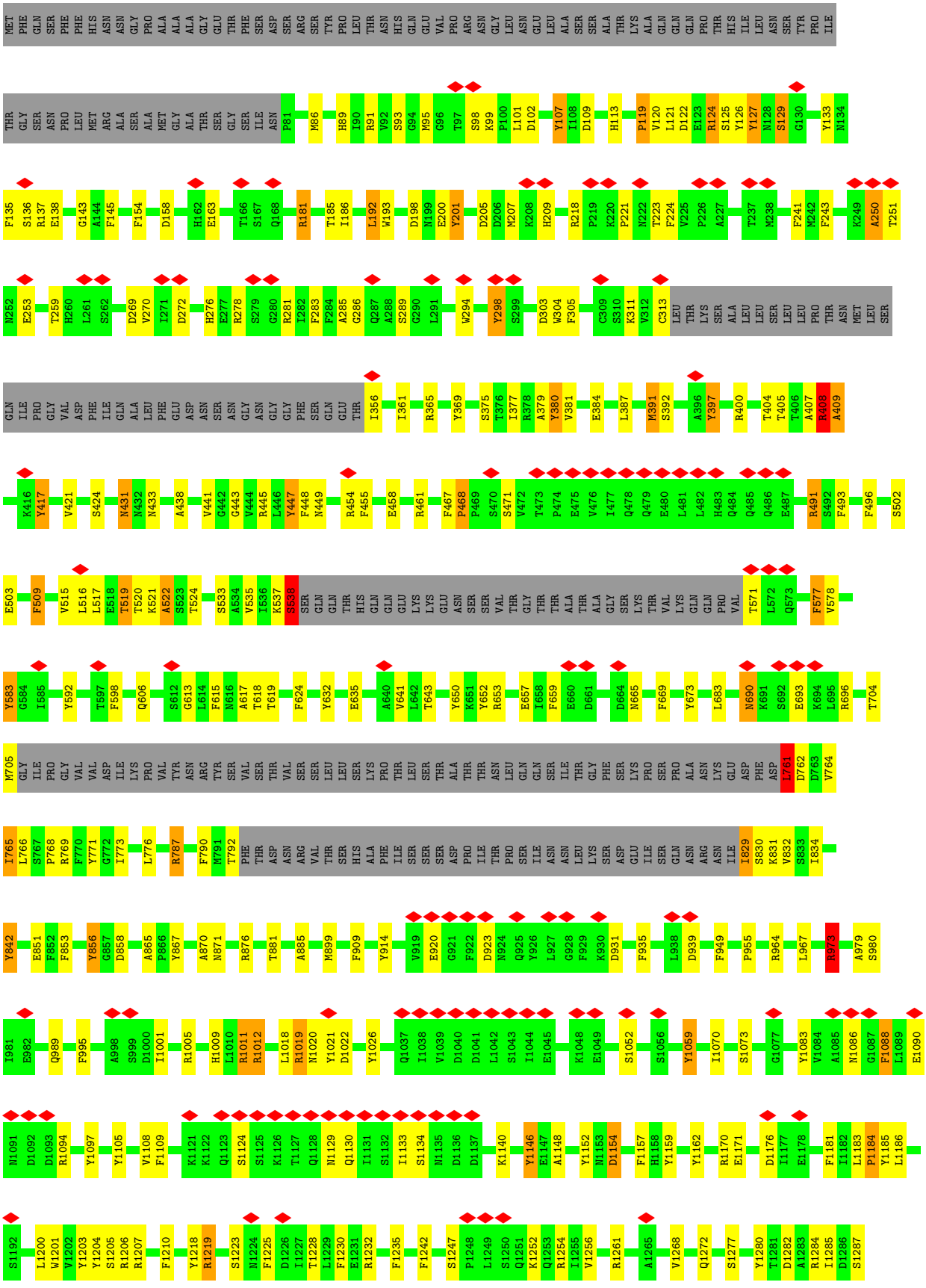
• Molecule 1: Spoke connector

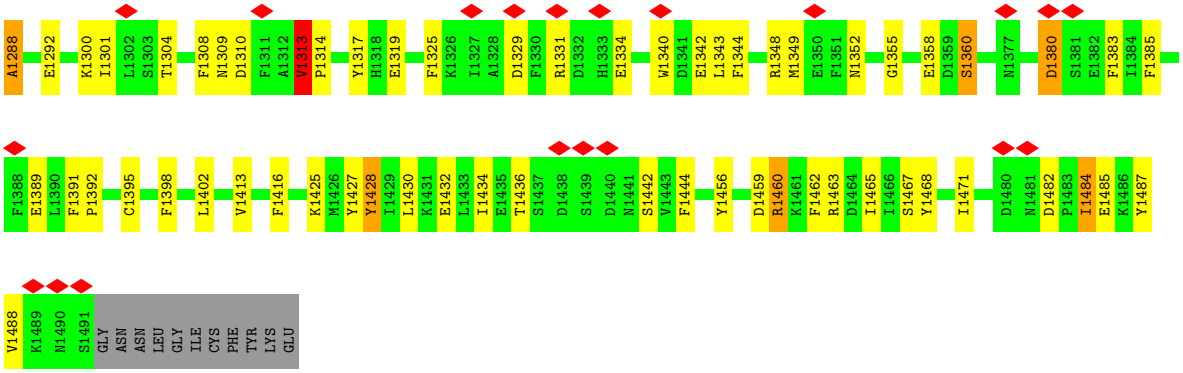
Chain i:



• Molecule 2: Nucleoporin NUP170

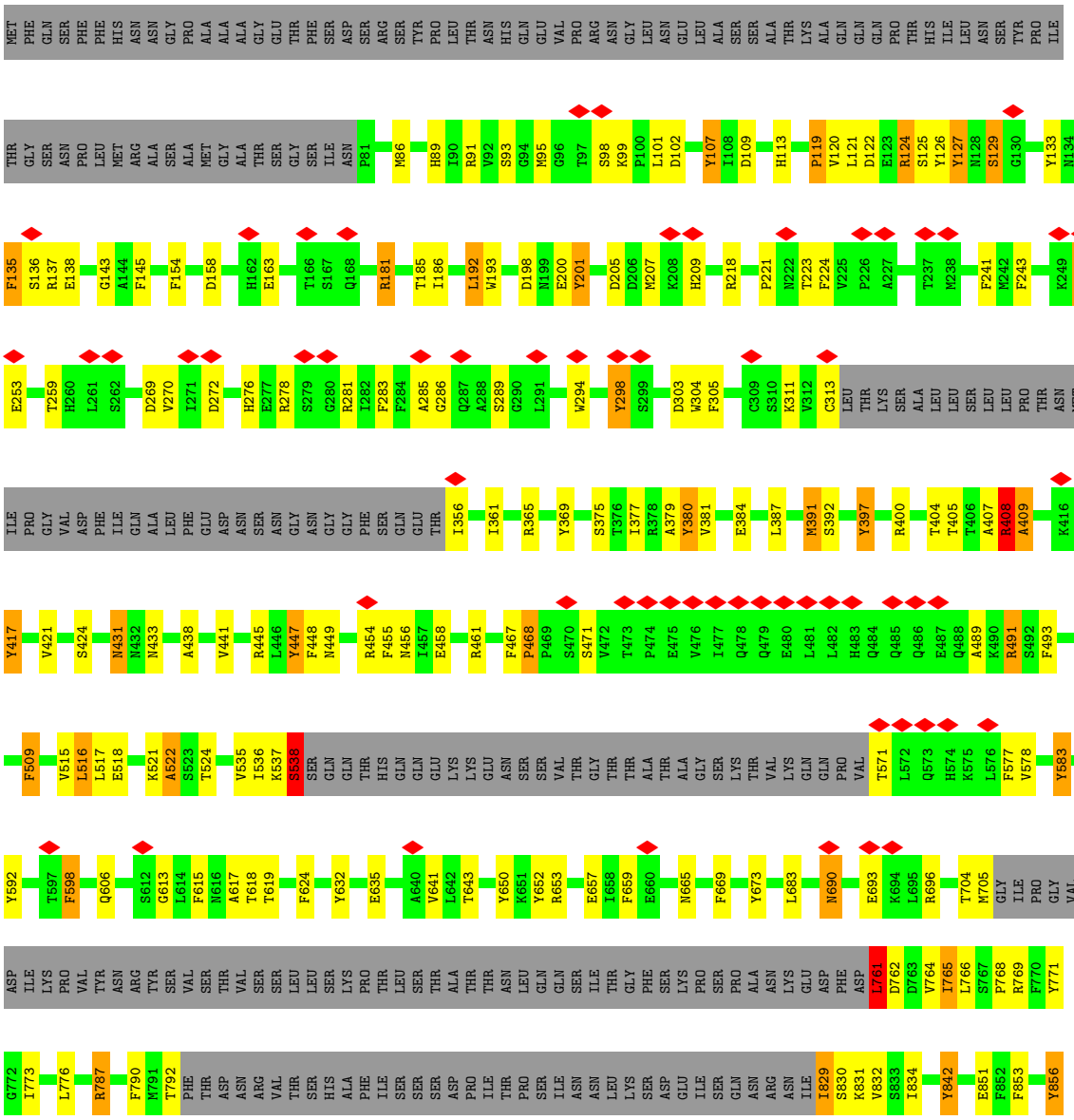
Chain Y:

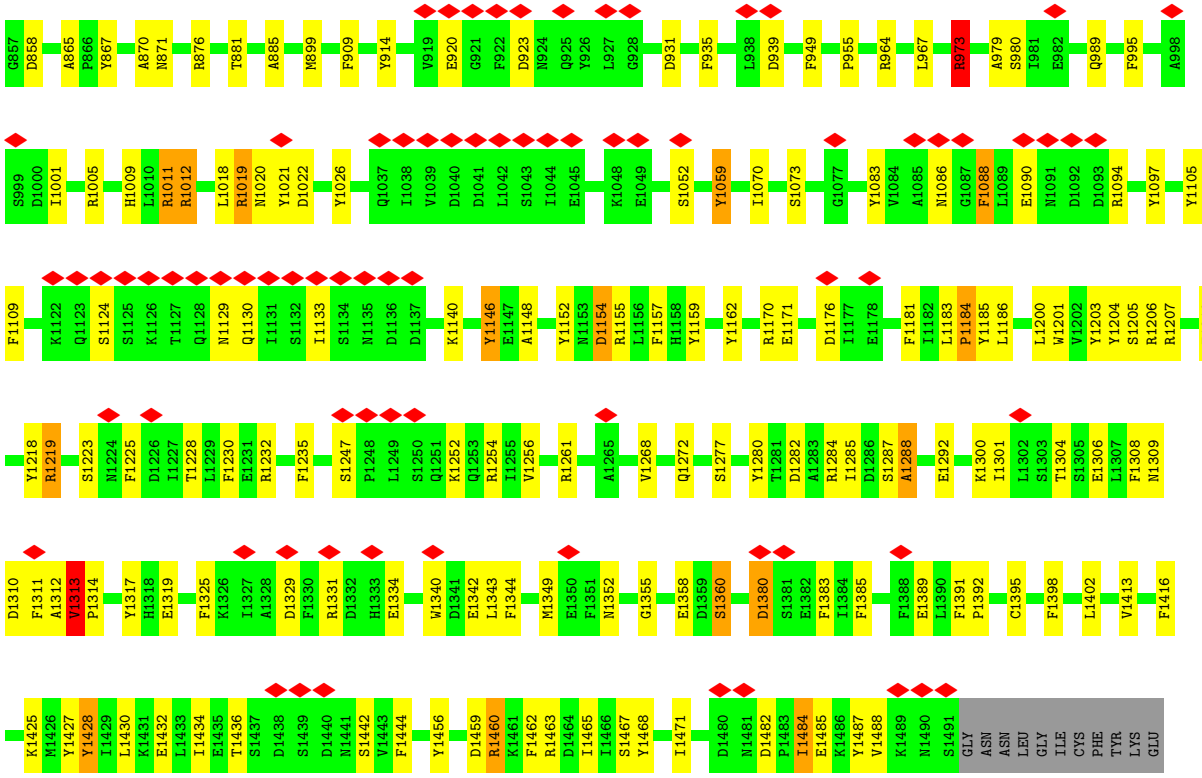




• Molecule 2: Nucleoporin NUP170

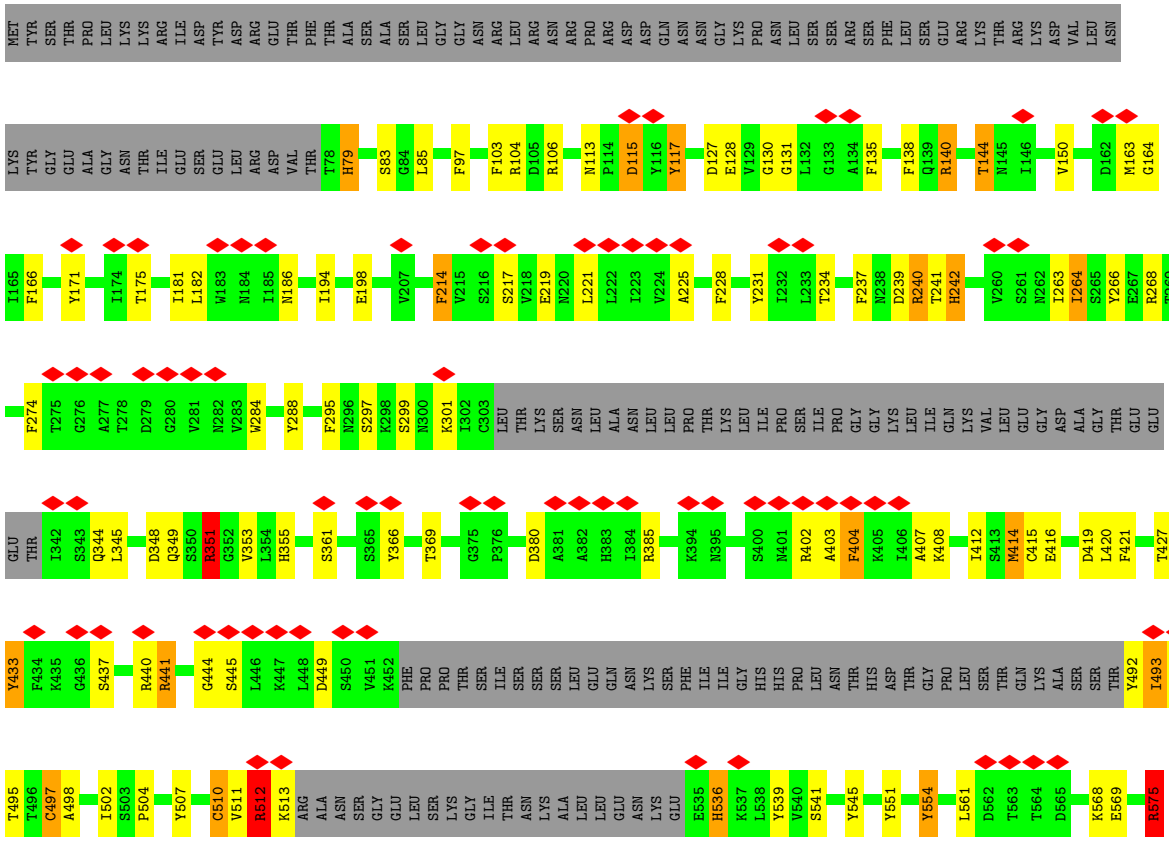
Chain 0:

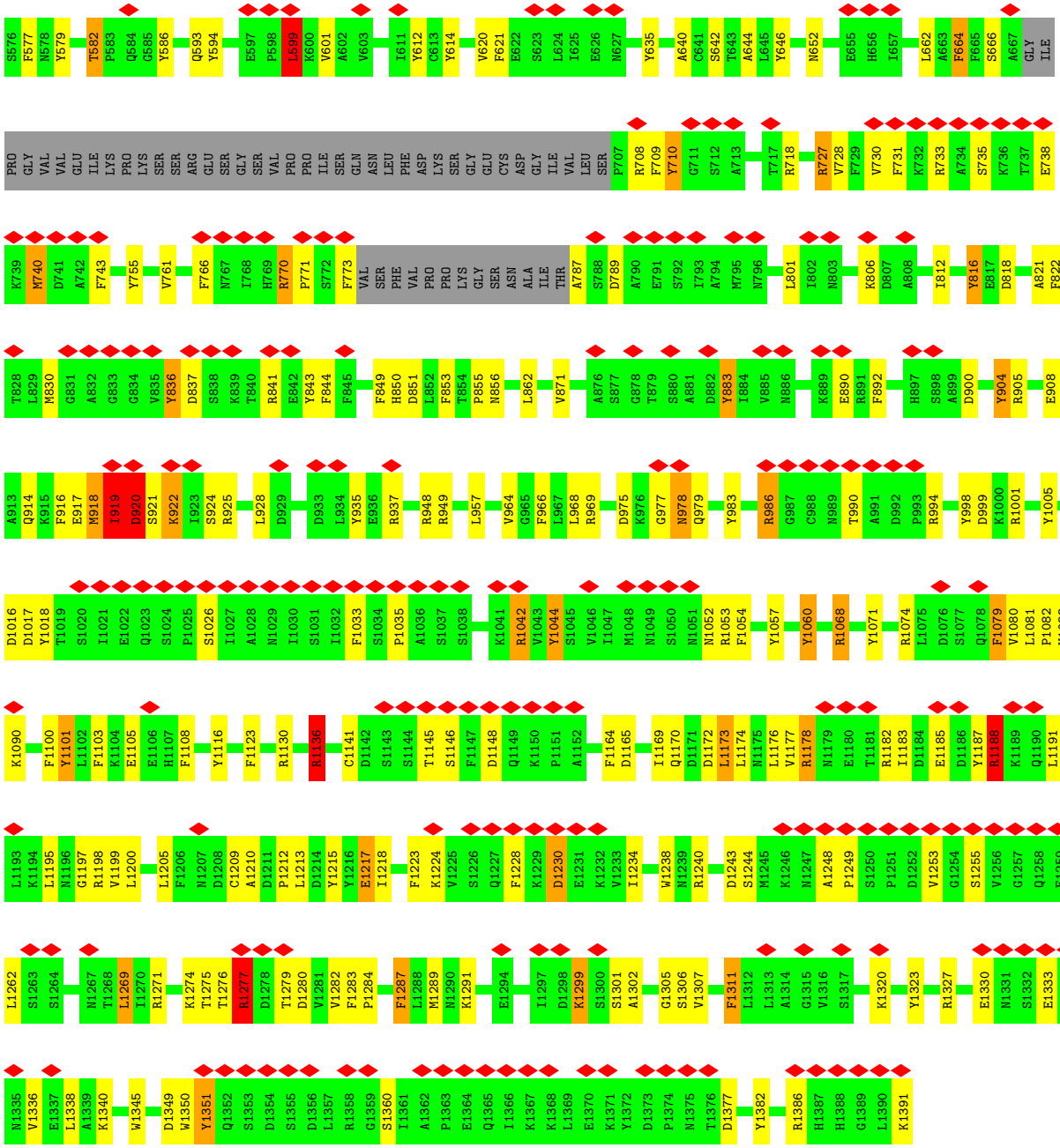




• Molecule 3: Nucleoporin NUP157

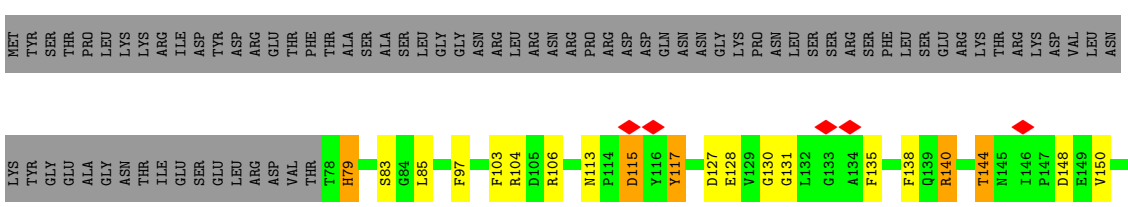
Chain Z:

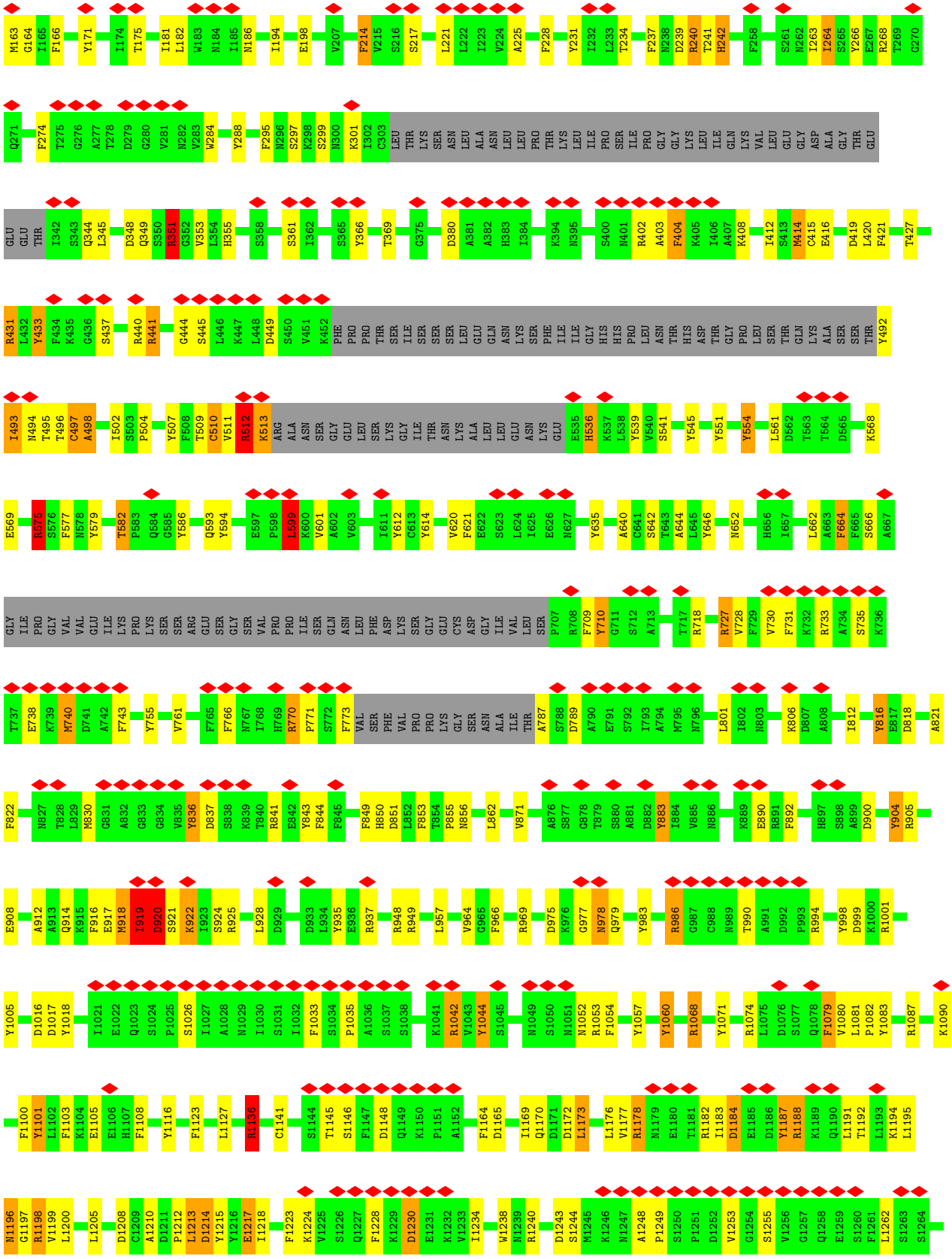


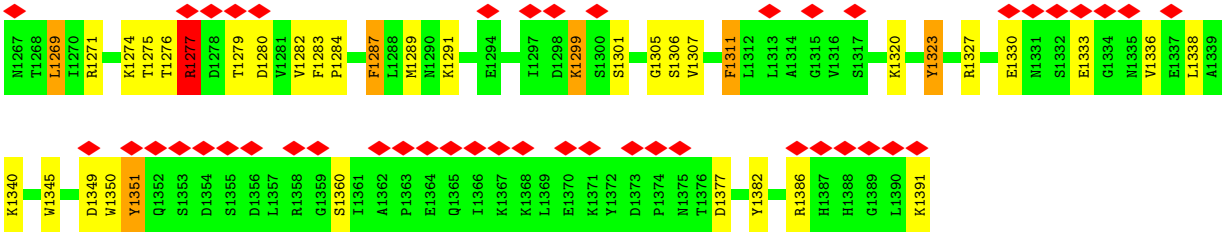


• Molecule 3: Nucleoporin NUP157

Chain 1:

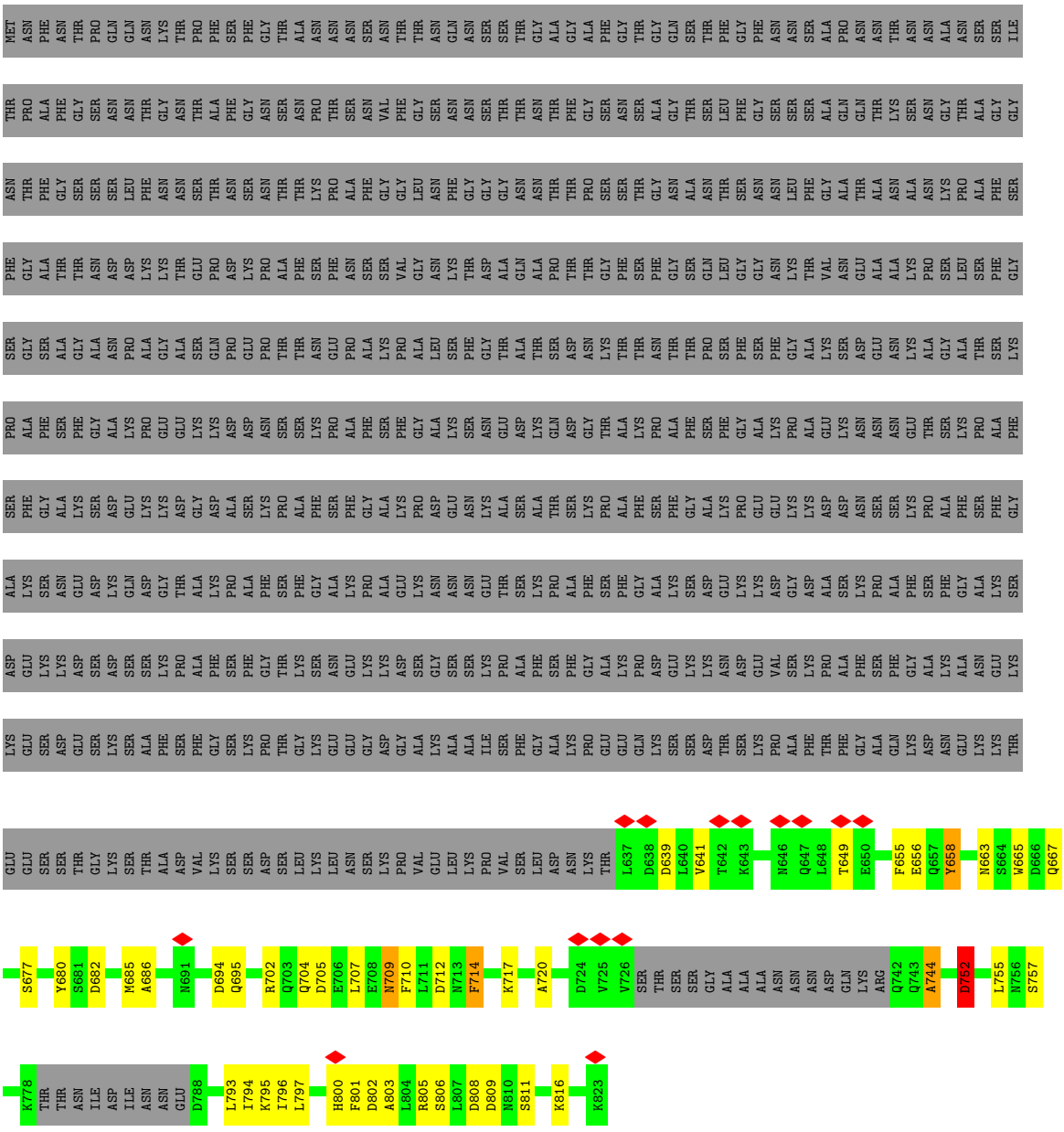



M163 G164 I165 F166 Y171 I174 T175 I181 L182 W183 N184 I185 N186 I194 E198 V207 F214 V215 S216 S217 L221 L222 I223 V224 A225 F228 Y231 I232 L233 T234 F237 N238 D239 R240 T241 H242 F258 S261 N262 I263 I264 S265 Y266 E267 R268 T269 G270
Q271 F274 T275 G276 A277 T278 D279 G280 V281 N282 V283 W284 Y288 F295 W296 S297 K298 S299 N300 K301 I302 C303 LEU THR LYS SER ASN LEU ALA ASN LEU LEU PRO THR LYS LEU ILE PRO SER ILE PRO GLY GLY LYS LEU ILE GLN LYS VAL LEU GLU GLY ASP ALA GLY THR GLU
GLU GLU THR I342 S343 Q344 L345 D348 Q349 S350 R351 G352 V353 L354 H355 S358 S361 I362 S365 Y366 T369 G375 D380 A381 A382 H383 I384 K394 N395 S400 N401 R402 A403 F404 K405 I406 A407 K408 I412 S413 M414 C415 E416 D419 L420 F421 T427
R431 L432 Y433 F434 K435 G436 S437 R440 R441 G444 S445 L446 K447 L448 D449 S450 V451 K452 PHE PRO PRO PRO THR SER ILE SER SER SER SER LEU GLU GLN ASN LYS SER PHE ILE ILE GLY HIS HIS PRO LEU ASN THR HIS ASP THR GLY PRO LEU SER THR GLN LYS ALA SER SER THR Y492
I493 N494 T495 T496 C497 A498 I502 S503 P504 Y507 F508 T509 C510 V511 R512 K513 ARG ALA ASN SER GLY GLU LEU SER LYS GLY ILE THR ASN LYS ALA LEU LEU GLU ASN LYS SER GLU E535 H536 K537 L538 Y539 V540 S541 Y545 Y551 Y554 L561 D562 T563 T564 D565 K568
E569 R575 S576 F577 N578 Y579 T582 P583 Q584 G585 Y586 Q593 Y594 E597 P598 L599 K600 V601 A602 V603 I611 Y612 C613 Y614 V620 F621 E622 S623 L624 I625 E626 N627 Y635 A640 C641 S642 T643 A644 L645 Y646 N652 H656 I657 L662 A663 F664 F665 S666 A667
GLY ILE PRO GLY VAL VAL GLU ILE LYS PRO LYS SER SER ARG GLU SER GLY SER GLY VAL PRO PRO ILE SER GLN ASN LEU LEU PHE ASP VAL LYS SER GLY GLU CYS ASP GLY ILE VAL LEU SER P707 R708 F709 Y710 G711 S712 A713 T717 R718 R727 V728 F729 V730 F731 K732 R733 A734 S735 K736
T737 E738 K739 M740 D741 A742 F743 Y755 V761 F765 F766 N767 I768 H769 R770 P771 S772 F773 VAL SER PHE VAL PRO PRO LYS GLY SER ASN ALA ILE THR A787 S788 D789 A790 E791 S792 I793 A794 M795 N796 L801 I802 N803 K806 D807 A808 I812 Y816 E817 D818 A821
F822 M827 T828 L829 M830 G831 A832 G833 G834 V835 Y836 D837 S838 K839 T840 R841 E842 Y843 F844 F845 F849 H850 D851 L852 F853 T854 P855 N856 L862 V871 A876 S877 G878 T879 S880 A881 D882 Y883 I884 V885 N886 K889 E890 R891 F892 H897 S898 A899 D900 Y904 R905
E908 A912 A913 Q914 K915 F916 E917 M918 I919 D920 S921 K922 I923 S924 R925 L928 D929 D933 L934 Y935 E936 R937 R948 R949 L957 V964 G965 F966 R969 D975 K976 G977 N978 Q979 Y983 R986 G987 C988 N989 T990 A991 D992 P993 R994 Y998 D999 K1000 R1001
Y1005 D1016 D1017 Y1018 I1021 E1022 Q1023 S1024 P1025 S1026 I1027 A1028 N1029 I1030 S1031 I1032 F1033 S1034 P1035 A1036 S1037 S1038 K1041 R1042 Y1043 Y1044 S1045 N1049 S1050 N1051 N1052 R1053 F1054 Y1057 Y1060 R1068 Y1071 R1074 L1075 D1076 S1077 Q1078 F1079 V1080 L1081 P1082 Y1083 R1087 K1090
F1100 Y1101 L1102 F1103 K1104 E1105 E1106 H1107 F1108 Y1116 F1123 L1127 R1136 C1141 S1144 T1145 S1146 F1147 D1148 Q1149 K1150 P1151 A1152 F1164 D1165 I1169 Q1170 D1171 D1172 L1173 L1176 V1177 R1178 N1179 E1180 T1181 R1182 I1183 D1184 E1185 D1186 Y1187 R1188 K1189 Q1190 L1191 T1192 L1193 K1194 L1195
N1196 G1197 R1198 V1199 L1200 L1205 D1208 C1209 A1210 D1211 P1212 L1213 D1214 Y1215 Y1216 E1217 I1218 F1223 K1224 V1225 S1226 Q1227 F1228 K1229 D1230 E1231 K1232 V1233 I1234 W1238 N1239 R1240 D1243 S1244 M1245 K1246 N1247 A1248 P1249 S1250 P1251 D1252 V1253 G1254 S1255 V1256 G1257 Q1258 E1259 S1260 F1261 L1262 S1263 S1264



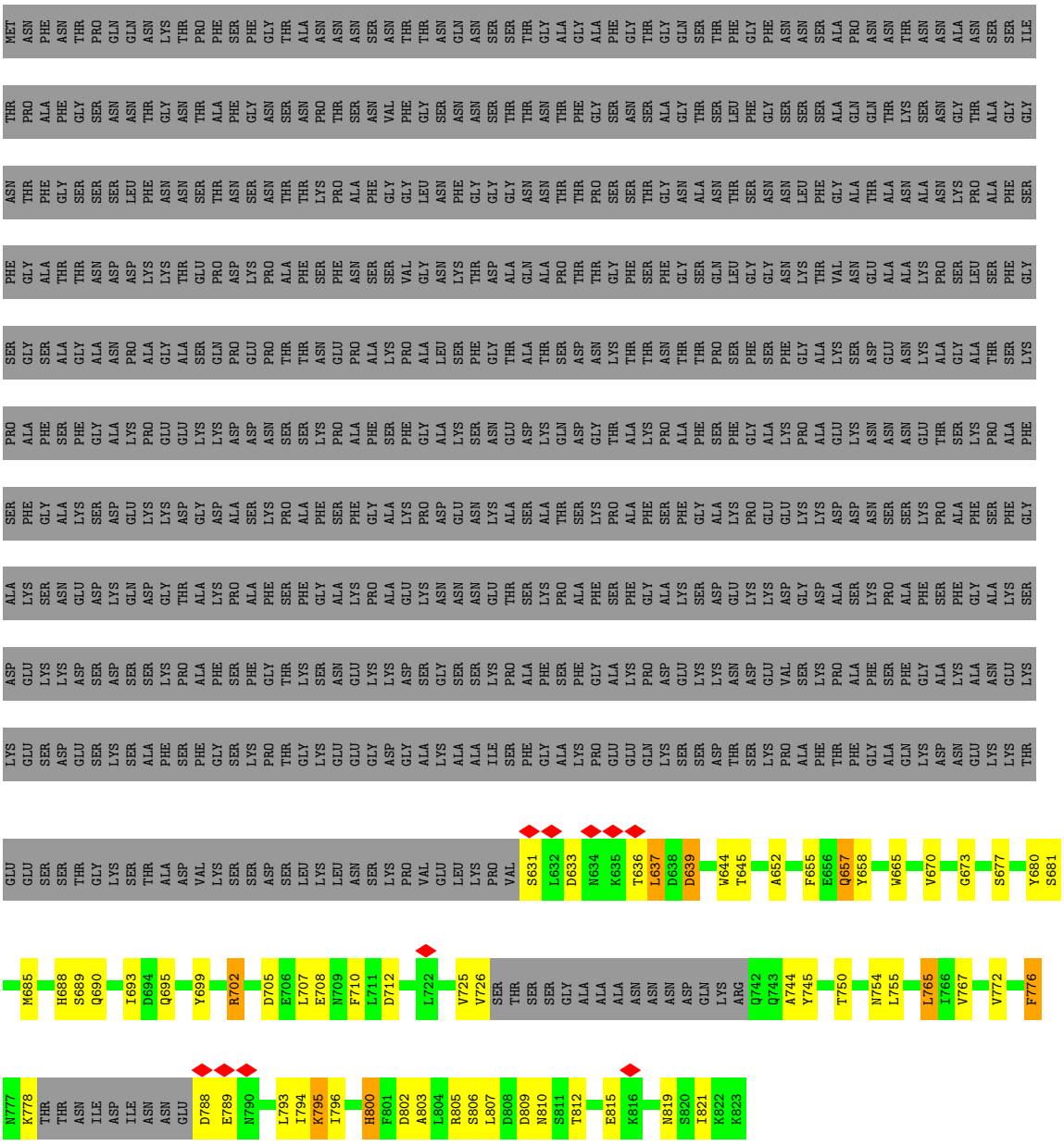
• Molecule 4: Nucleoporin NSP1

Chain A:



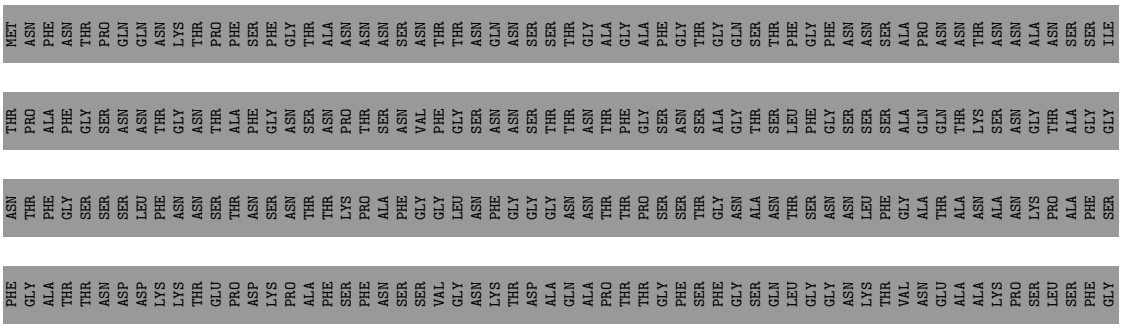
• Molecule 4: Nucleoporin NSP1

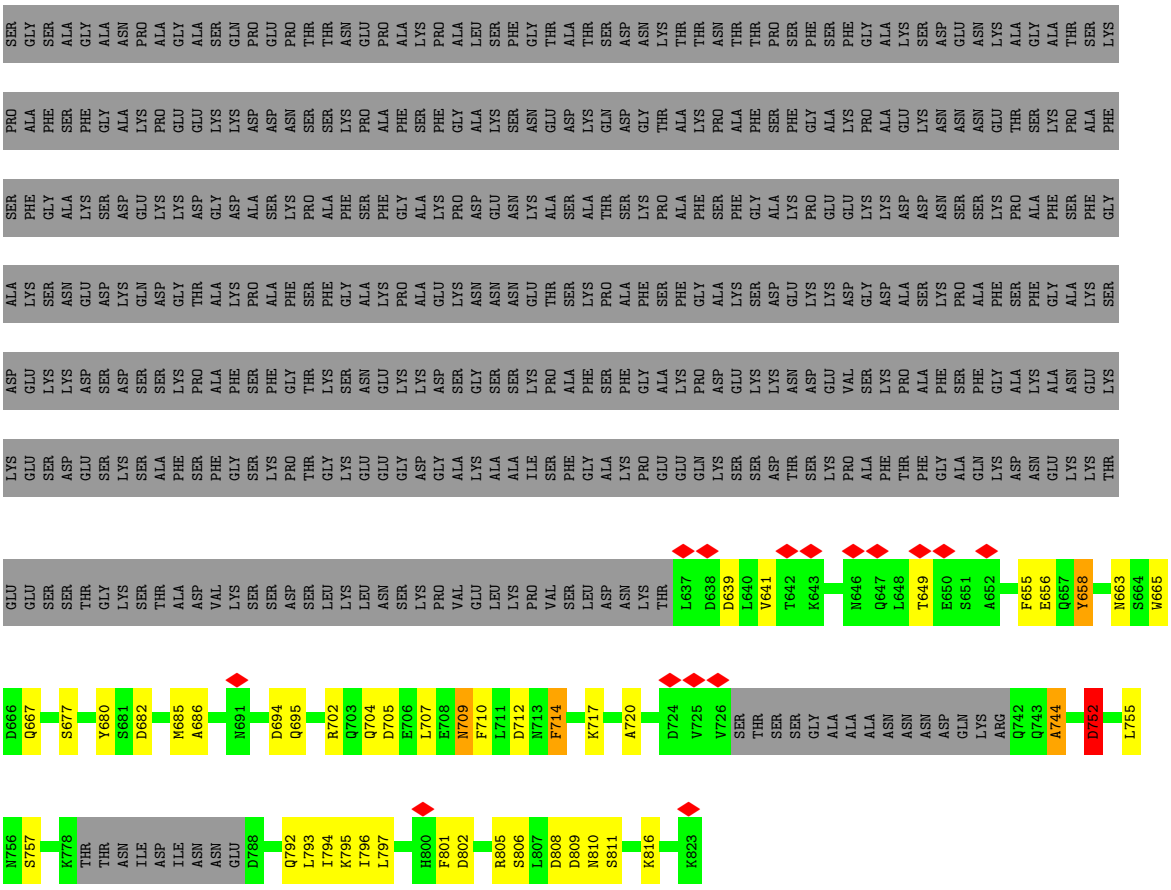
Chain D:



• Molecule 4: Nucleoporin NSP1

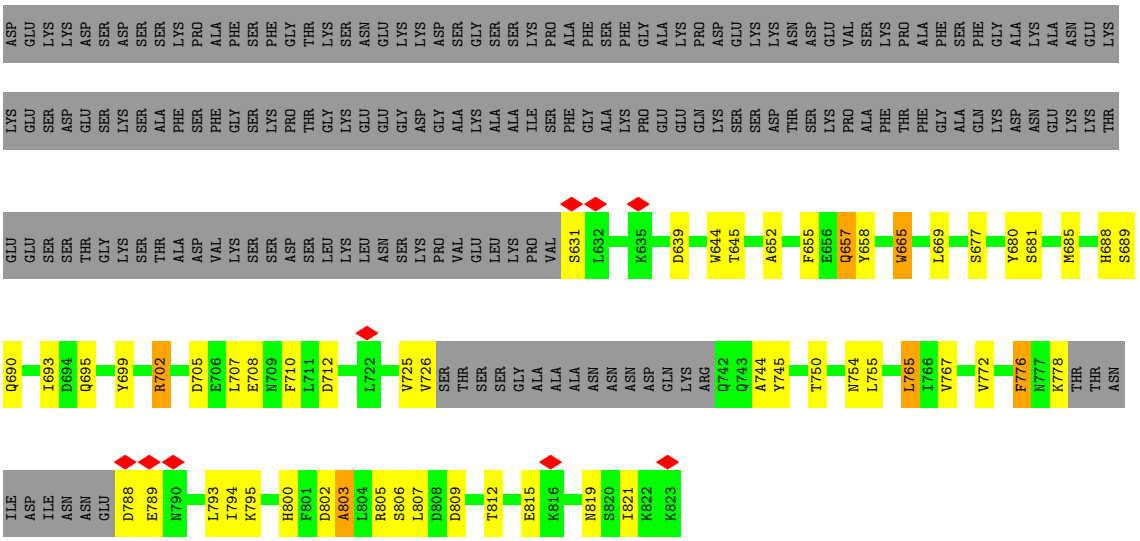
Chain G:





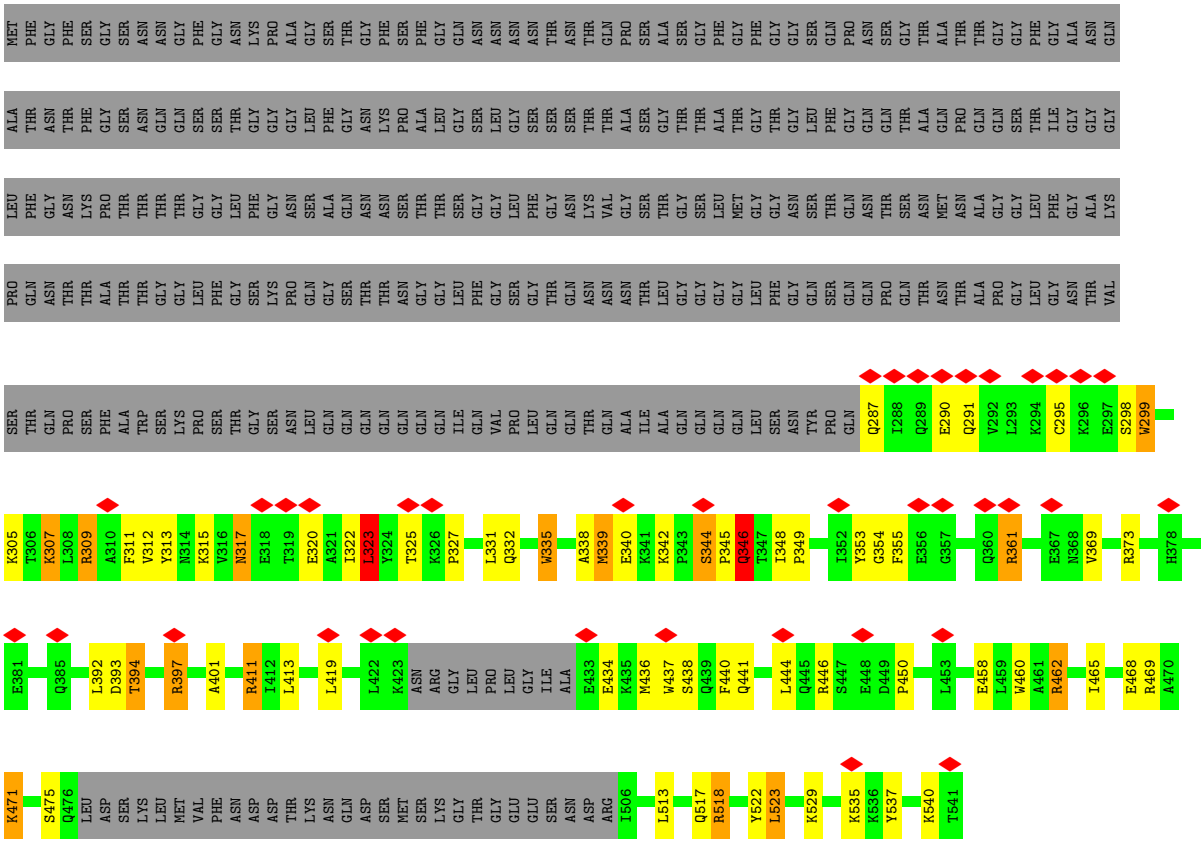
- Molecule 4: Nucleoporin NSP1

Chain J:



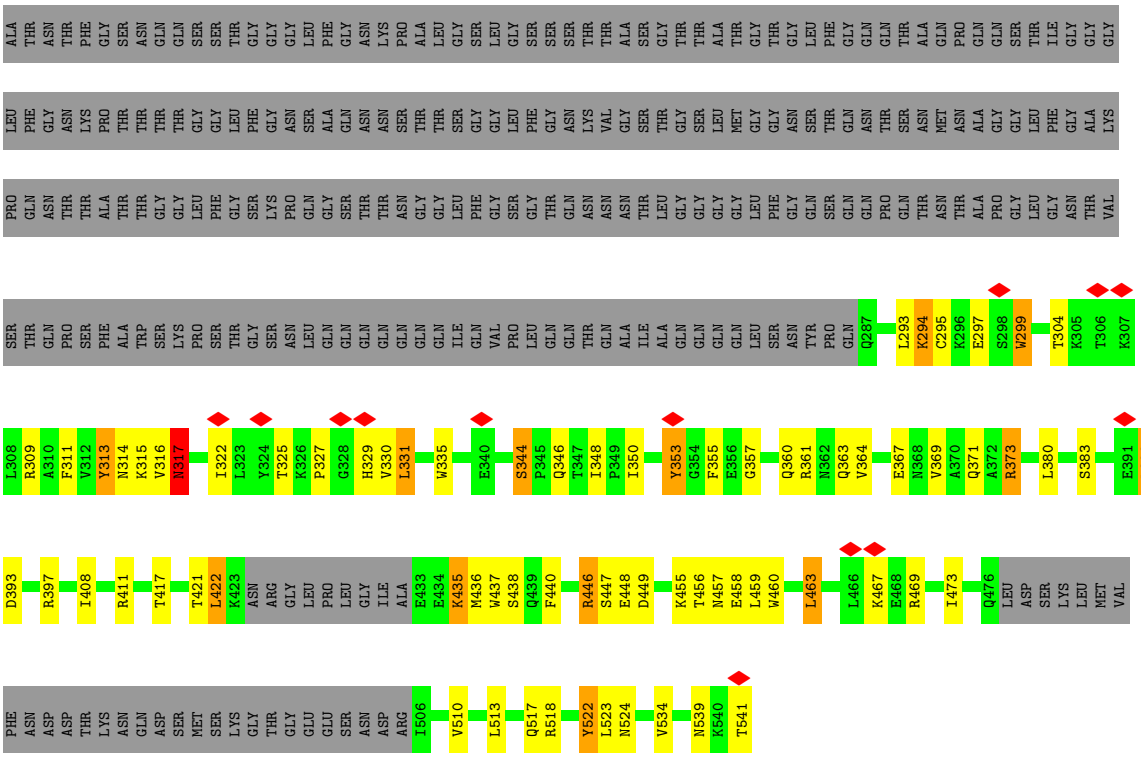
• Molecule 5: Nucleoporin NUP57

Chain B:



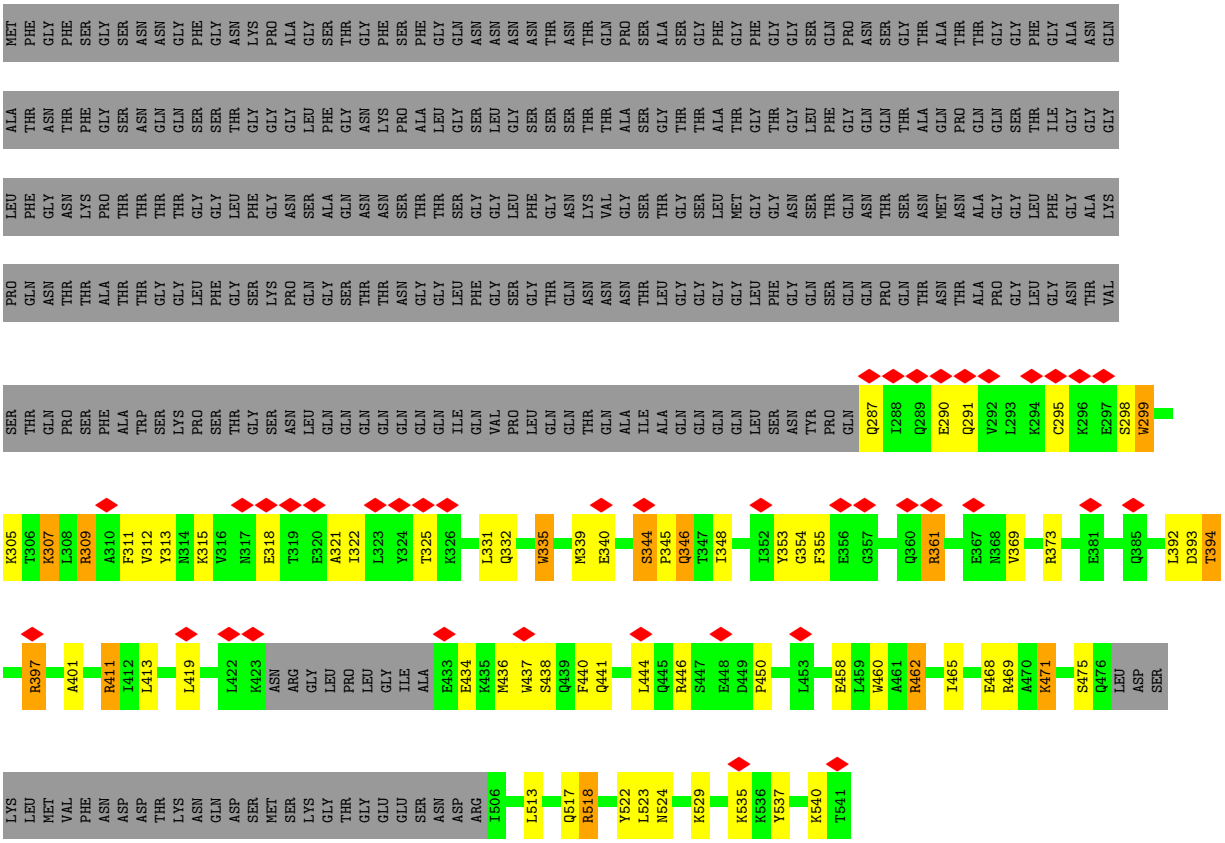
• Molecule 5: Nucleoporin NUP57

Chain E:



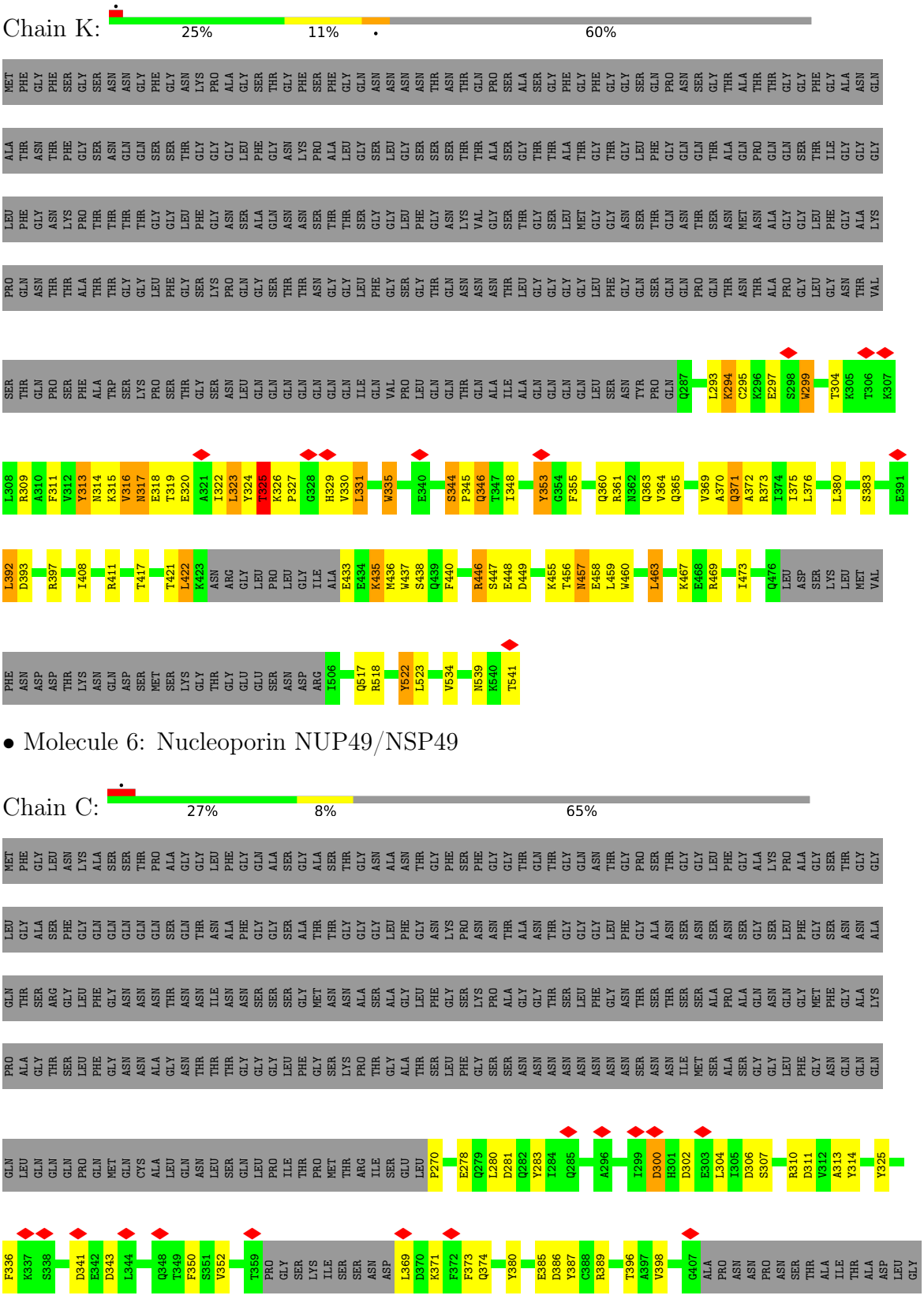
• Molecule 5: Nucleoporin NUP57

Chain H:



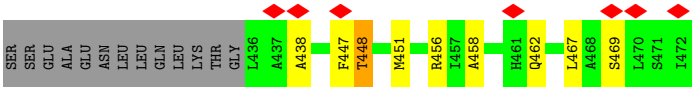
• Molecule 5: Nucleoporin NUP57

Chain K:



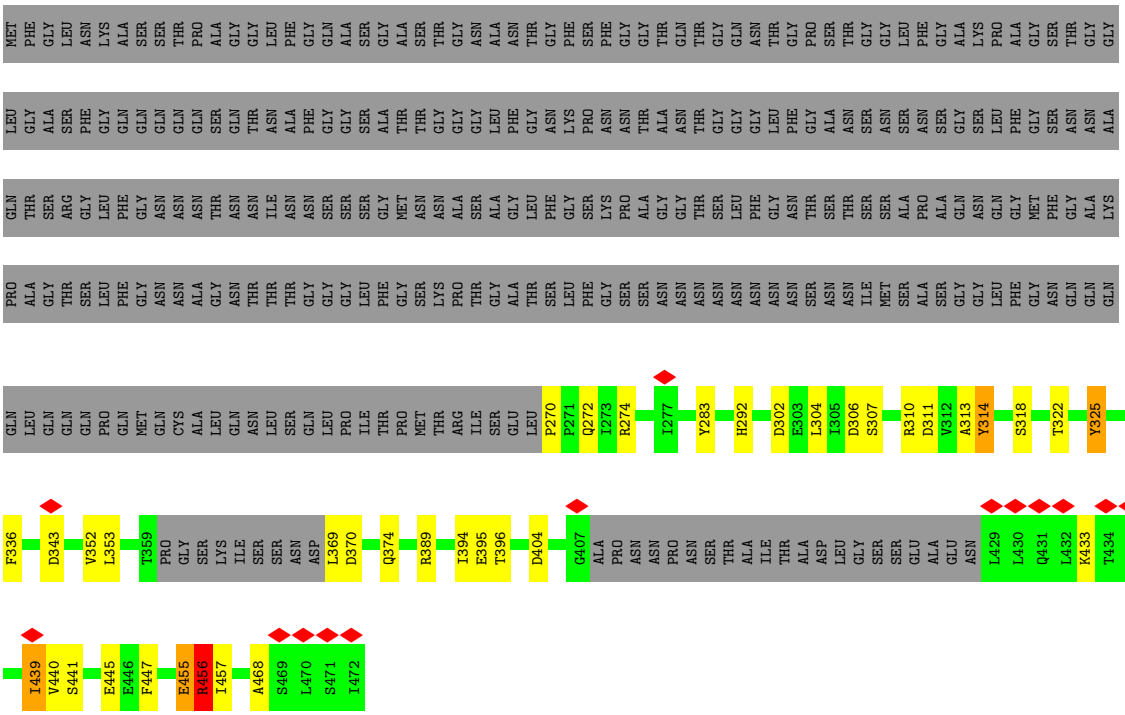
• Molecule 6: Nucleoporin NUP49/NSP49

Chain C:



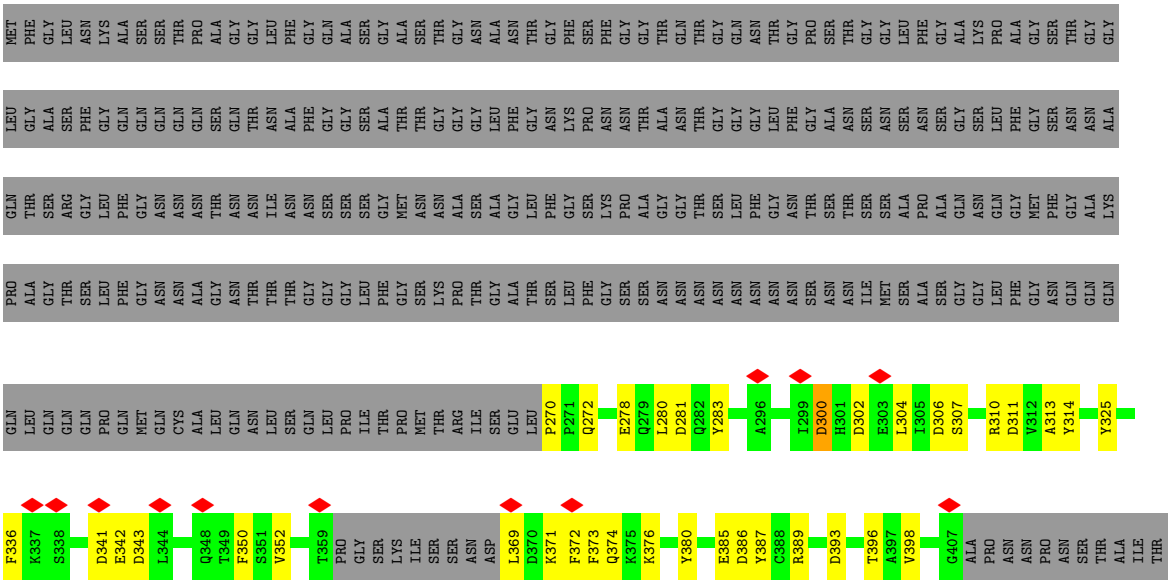
• Molecule 6: Nucleoporin NUP49/NSP49

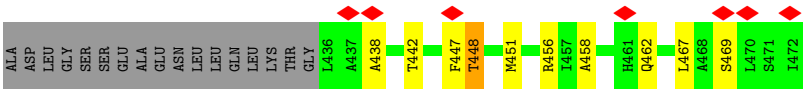
Chain F:



• Molecule 6: Nucleoporin NUP49/NSP49

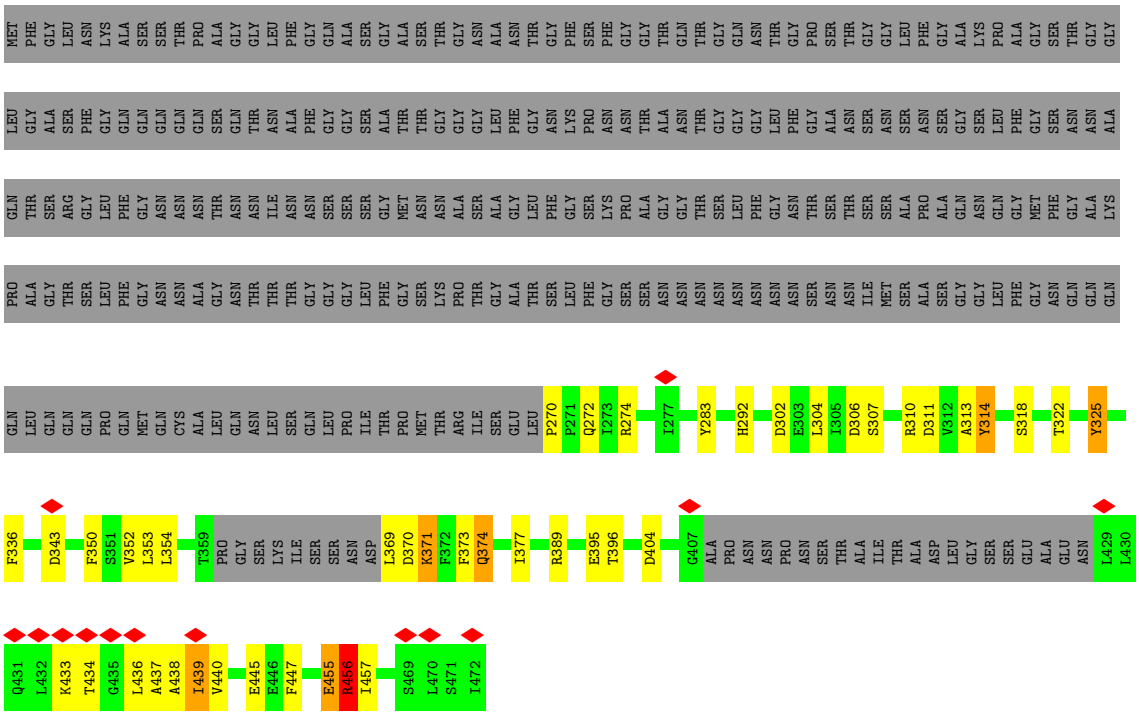
Chain I:





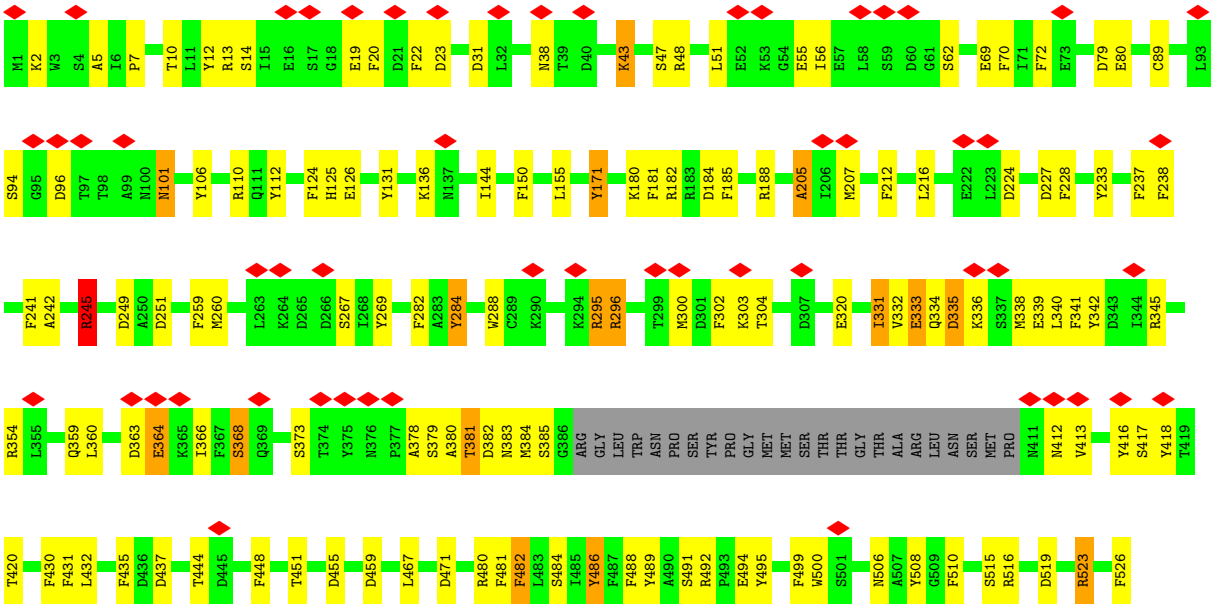
• Molecule 6: Nucleoporin NUP49/NSP49

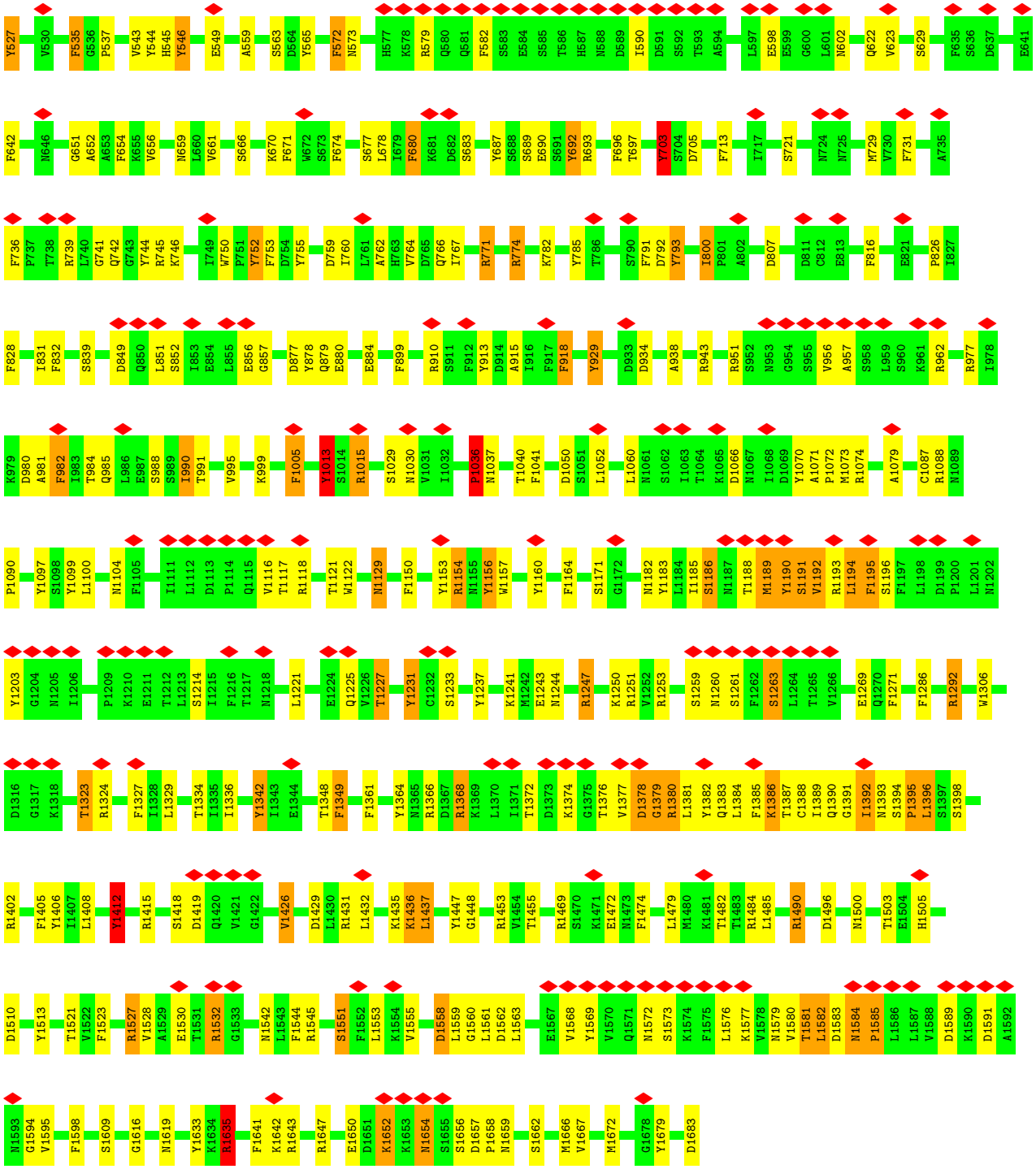
Chain L:



• Molecule 7: Nucleoporin NUP192

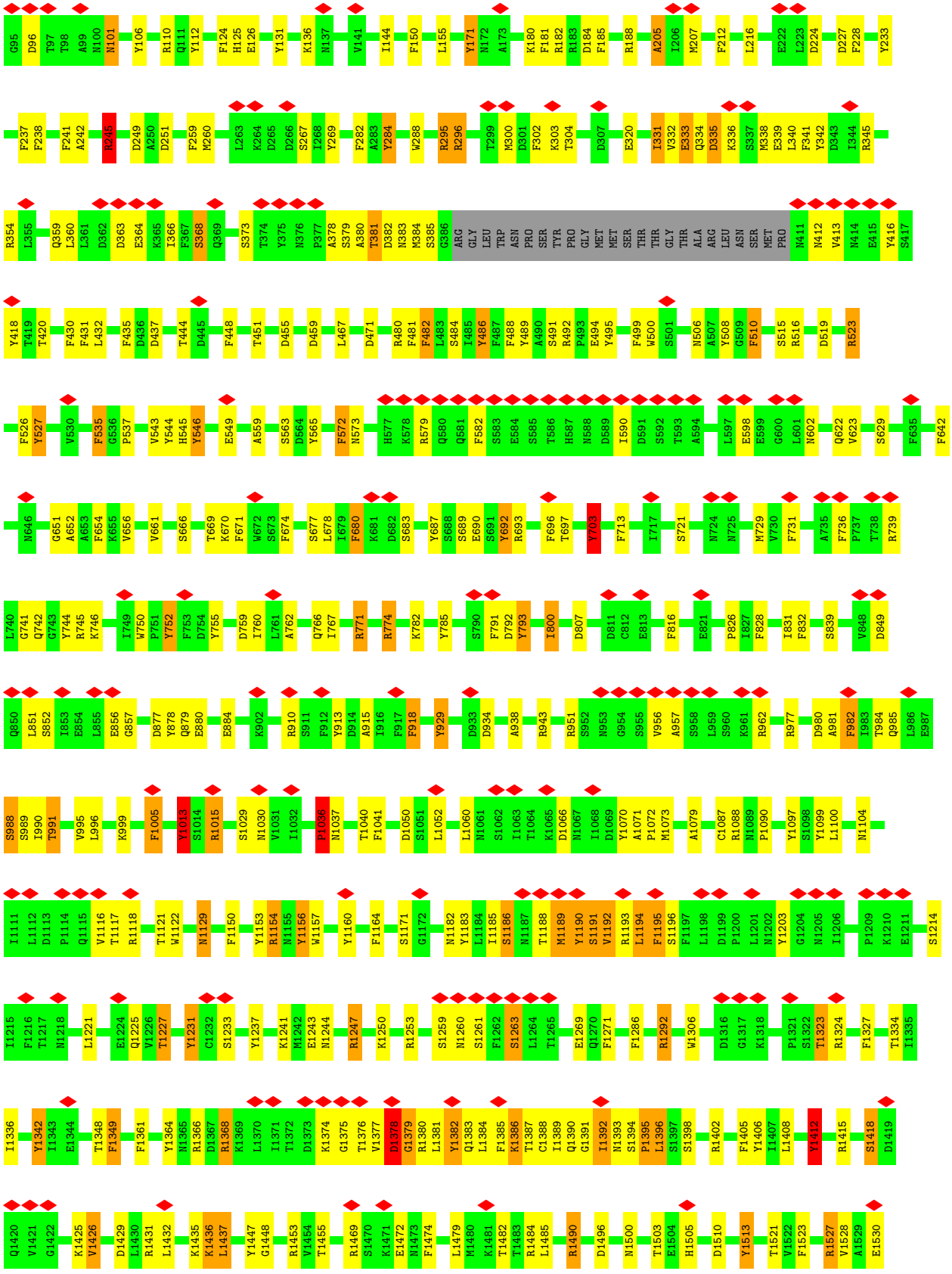
Chain M:





• Molecule 7: Nucleoporin NUP192

Chain O: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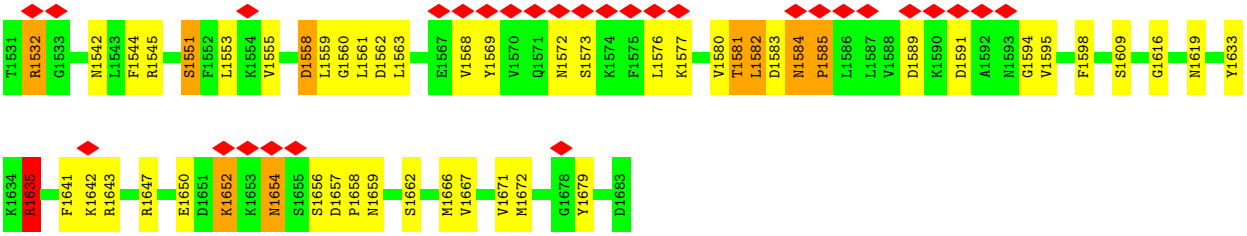
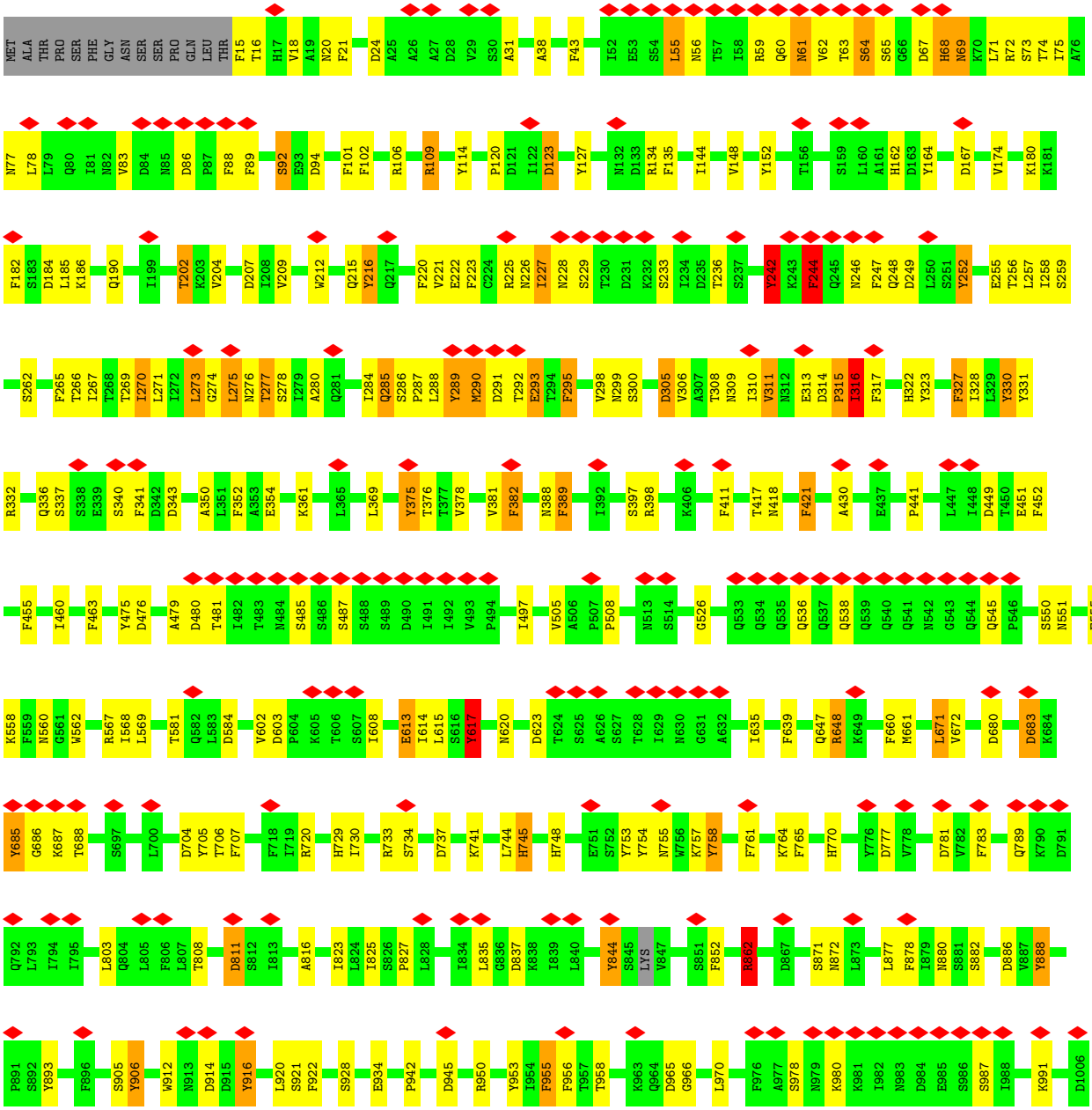
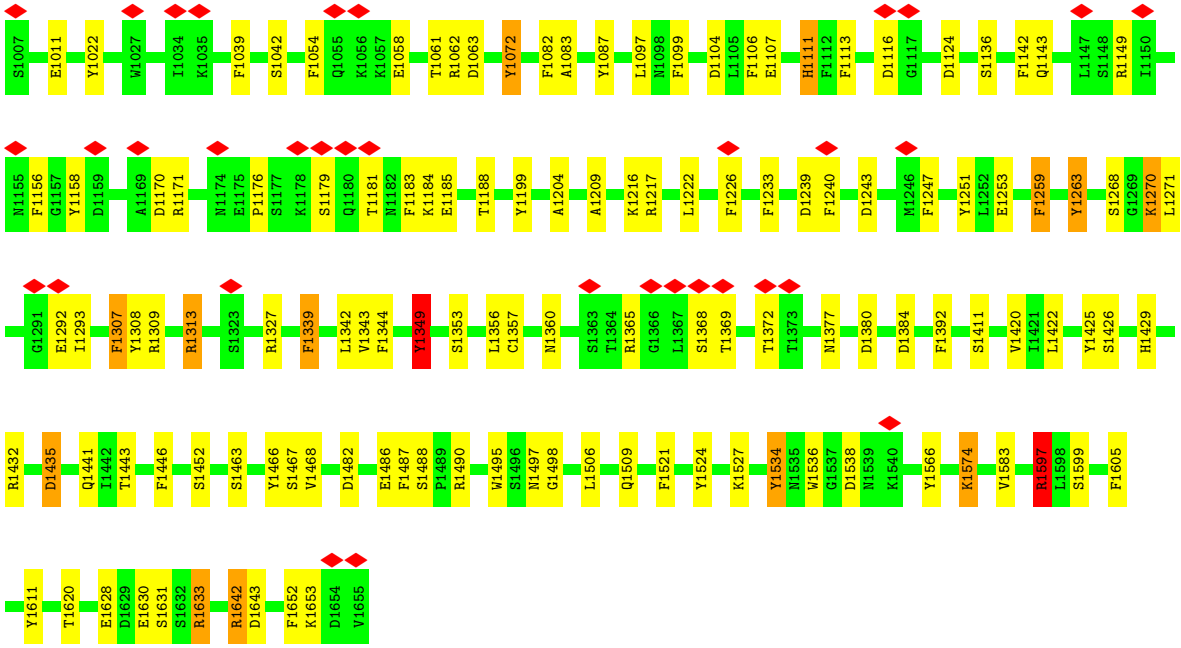
F237 F238 F241 A242 R245 D249 A250 D251 F259 M260 L263 K264 D265 D266 S267 I268 Y269 F282 A283 Y284 W288 R295 R296 T299 M300 D301 F302 K303 T304 D307 E320 I331 V332 E333 Q334 D335 K336 S337 M338 E339 L340 F341 Y342 D343 I344 R345
R354 L355 Q359 L360 L361 D362 D363 E364 K365 I366 F367 S368 Q369 S373 T374 Y375 N376 P377 A378 S379 A380 T381 D382 N383 M384 S385 G386 ARG GLY LEU TRP ASN PRO SER TYR PRO GLY MET MET SER THR THR GLY THR ALA ARG LEU ASN SER MET PRO N411 N412 V413 N414 E415 Y416 S417
Y418 T419 T420 F430 F431 L432 F435 D436 D437 T444 D445 F448 T451 D455 D459 L467 D471 R480 F481 F482 L483 S484 I485 Y486 F487 F488 Y489 A490 S491 R492 P493 E494 Y495 F499 W500 S501 N506 A507 Y508 G509 F510 S515 R516 D519 R523
F526 Y527 V530 F535 G536 P537 V543 Y544 H545 Y546 E549 A559 S563 D564 Y565 F572 N573 H577 K578 R579 Q580 Q581 F582 S583 E584 S585 T586 H587 N588 D589 I590 D591 S592 T593 A594 L597 E598 E599 G600 L601 N602 Q622 V623 S629 F635 F642
N646 G651 A652 A653 F654 K655 V656 V661 S666 T669 K670 F671 W672 S673 F674 S677 L678 I679 F680 K681 D682 S683 Y687 S688 S689 E690 S691 Y692 R693 F696 T697 Y703 F713 T717 S721 N724 N725 M729 V730 F731 A735 F736 P737 T738 R739
L740 G741 Q742 G743 Y744 R745 K746 I749 W750 P751 Y752 F753 D754 Y755 D759 I760 L761 A762 Q766 I767 R771 R774 K782 Y785 S790 F791 D792 Y793 I800 D807 D811 C812 E813 F816 E821 P826 I827 F828 I831 F832 S839 V848 D849
Q850 L851 S852 I853 E854 L855 E856 G857 D877 Y878 Q879 E880 E884 K902 R910 S911 F912 Y913 D914 A915 I916 F917 F918 Y929 D933 D934 A938 R943 R951 S952 N953 G954 S955 V956 A957 S958 L959 S960 K961 R962 R977 D980 A981 F982 I983 T984 Q985 L986 E987
S988 S989 I990 T991 V995 L996 K999 F1005 Y1013 S1014 R1015 S1029 N1030 V1031 I1032 P1036 N1037 T1040 F1041 D1050 S1051 L1052 L1060 N1061 S1062 I1063 T1064 K1065 D1066 N1067 I1068 D1069 Y1070 A1071 P1072 M1073 A1079 C1087 R1088 N1089 P1090 Y1097 S1098 Y1099 L1100 N1104
I1111 L1112 D1113 P1114 Q1115 V1116 T1117 R1118 T1121 W1122 N1129 F1150 Y1153 R1154 N1155 Y1156 W1157 Y1160 F1164 S1171 G1172 N1182 Y1183 L1184 I1185 S1186 N1187 T1188 M1189 Y1190 S1191 V1192 R1193 L1194 F1195 S1196 F1197 L1198 D1199 P1200 L1201 N1202 Y1203 G1204 N1205 I1206 P1209 K1210 E1211 S1214
I1215 F1216 T1217 N1218 L1221 E1224 Q1225 V1226 T1227 Y1231 C1232 S1233 Y1237 K1241 M1242 E1243 N1244 R1247 K1250 R1253 S1259 N1260 S1261 F1262 S1263 L1264 T1265 E1269 Q1270 F1271 F1286 R1292 W1306 D1316 G1317 K1318 P1321 S1322 T1323 R1324 F1327 T1334 I1335
I1336 Y1342 I1343 E1344 T1348 F1349 F1361 Y1364 N1365 R1366 D1367 R1368 K1369 L1370 I1371 T1372 D1373 K1374 G1375 T1376 V1377 D1378 G1379 R1380 L1381 Y1382 Q1383 L1384 F1385 K1386 T1387 C1388 I1389 Q1390 G1391 I1392 N1393 S1394 P1395 L1396 S1397 S1398 R1402 F1405 Y1406 I1407 L1408 Y1412 R1415 S1418 D1419
Q1420 V1421 G1422 K1425 V1426 D1429 L1430 R1431 L1432 K1435 K1436 L1437 Y1447 G1448 R1453 V1454 T1455 R1469 S1470 K1471 E1472 N1473 F1474 L1479 M1480 K1481 T1482 T1483 R1484 L1485 R1490 D1496 N1500 T1503 E1504 H1505 D1510 Y1513 T1521 V1522 F1523 R1527 V1528 A1529 E1530



• Molecule 8: Nucleoporin NUP188

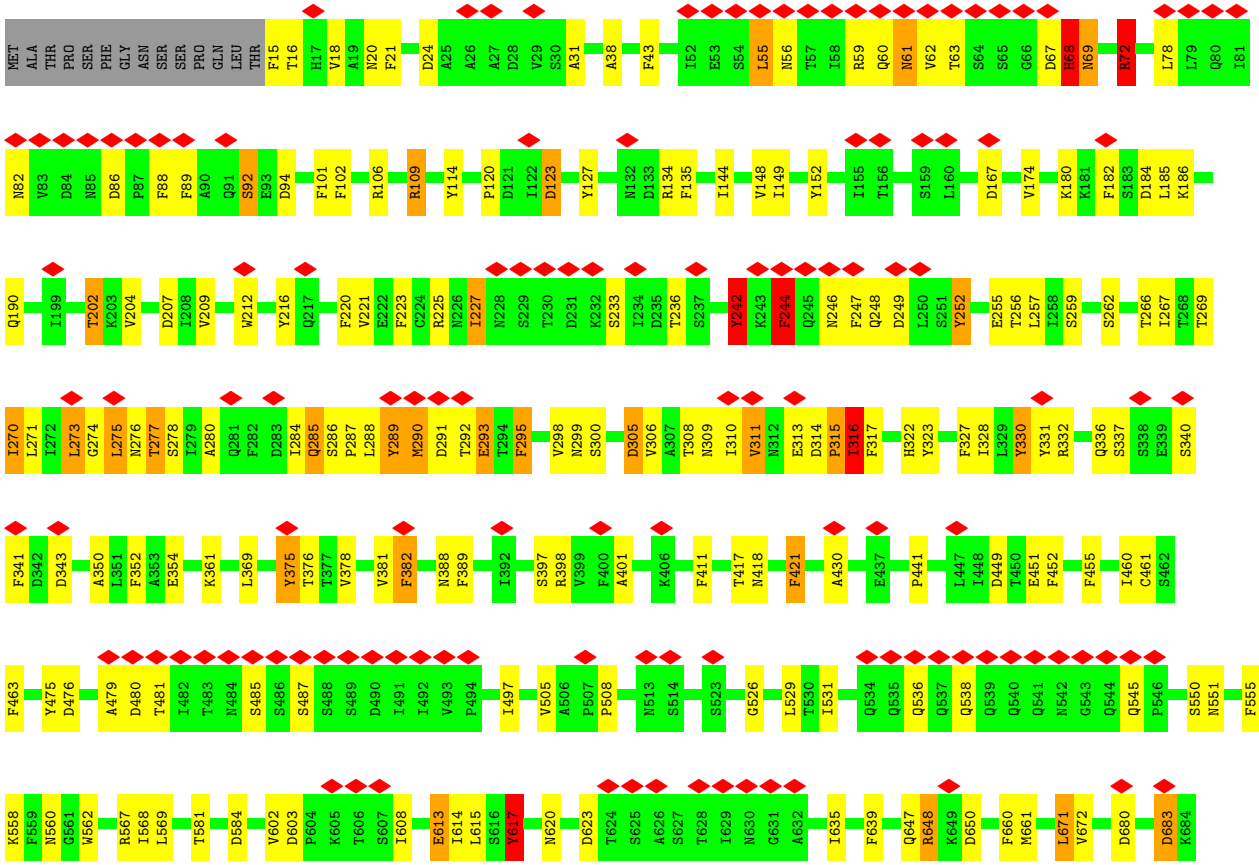
Chain N:

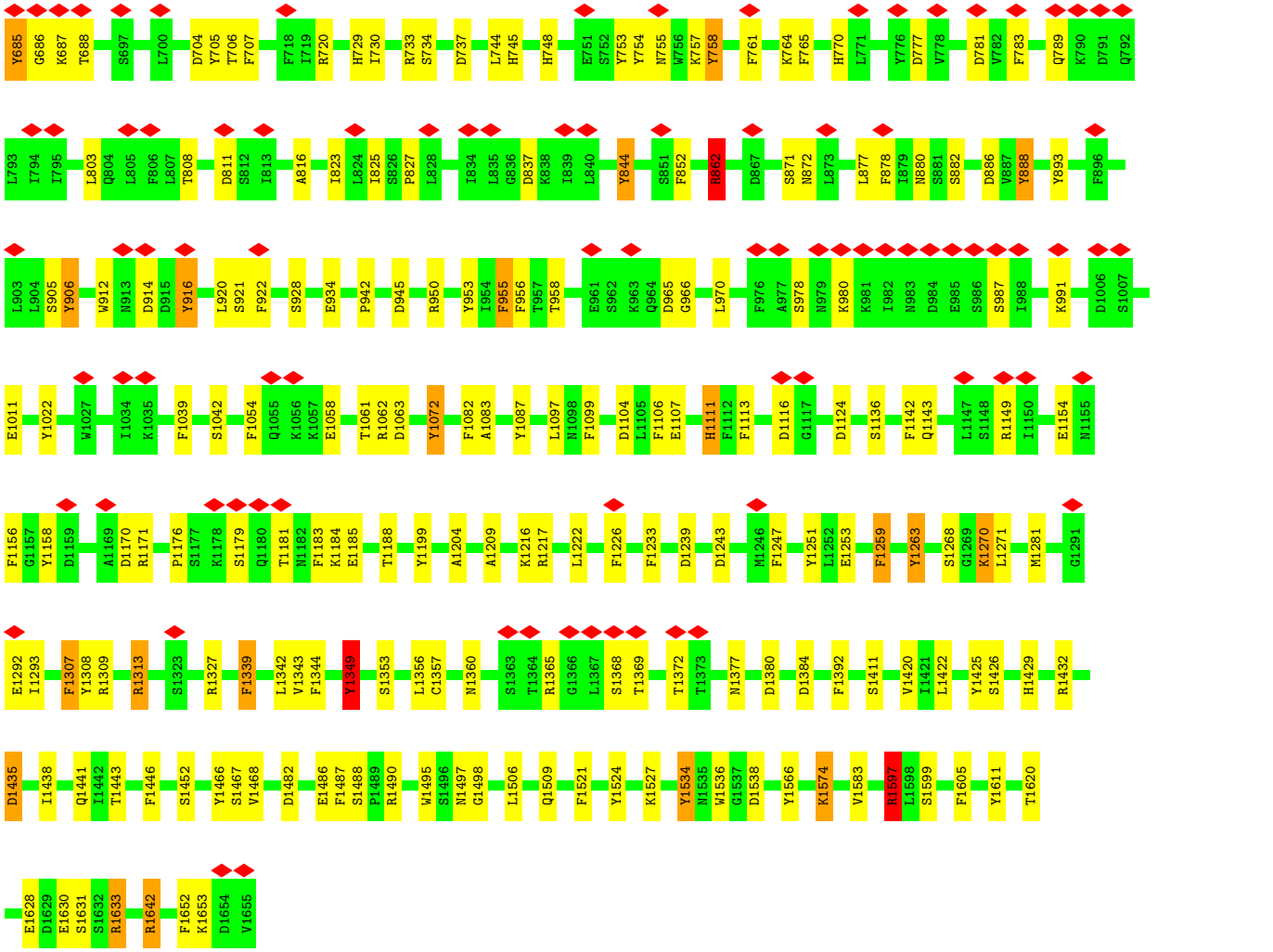




• Molecule 8: Nucleoporin NUP188

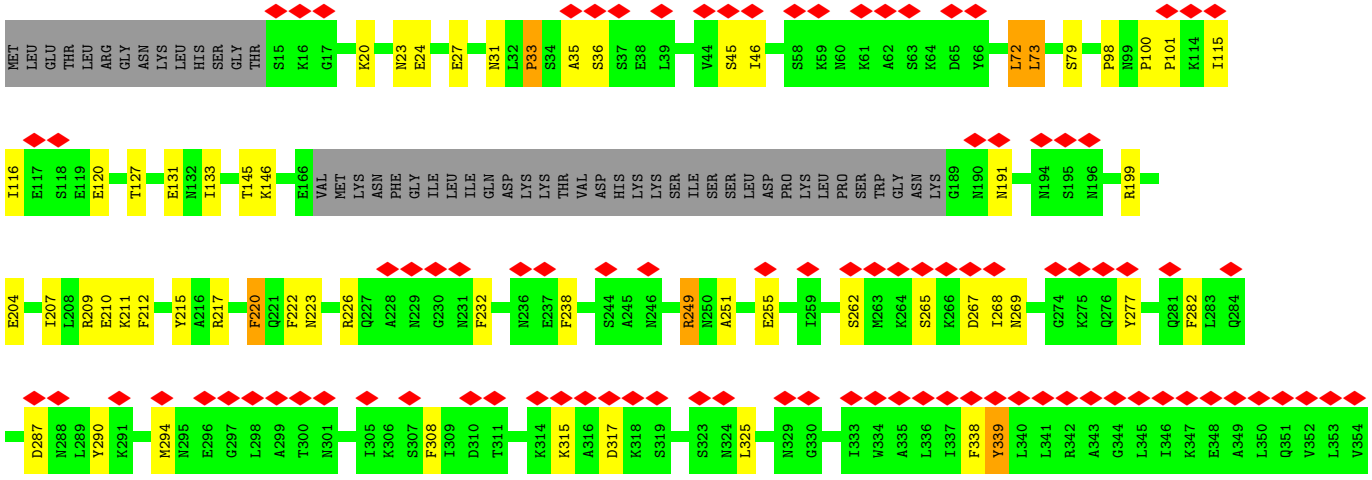
Chain P:

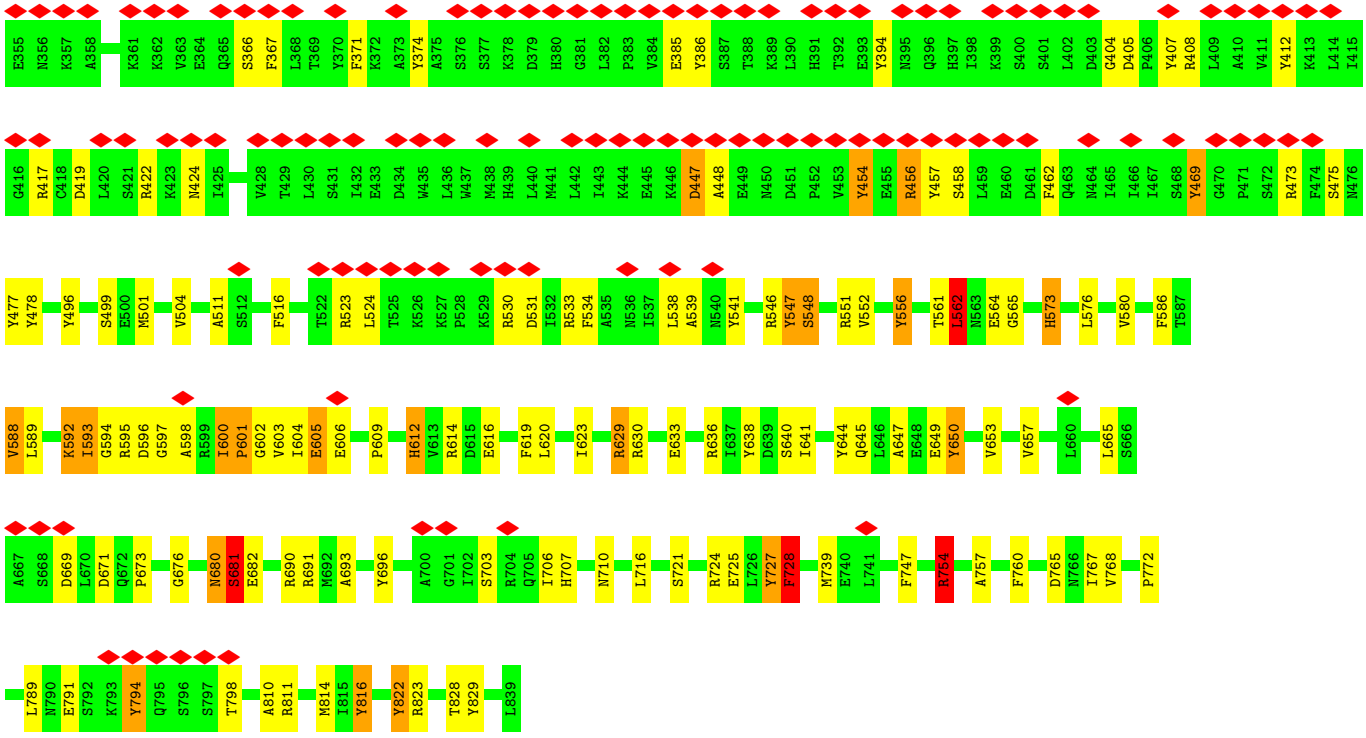




• Molecule 9: Nucleoporin NIC96

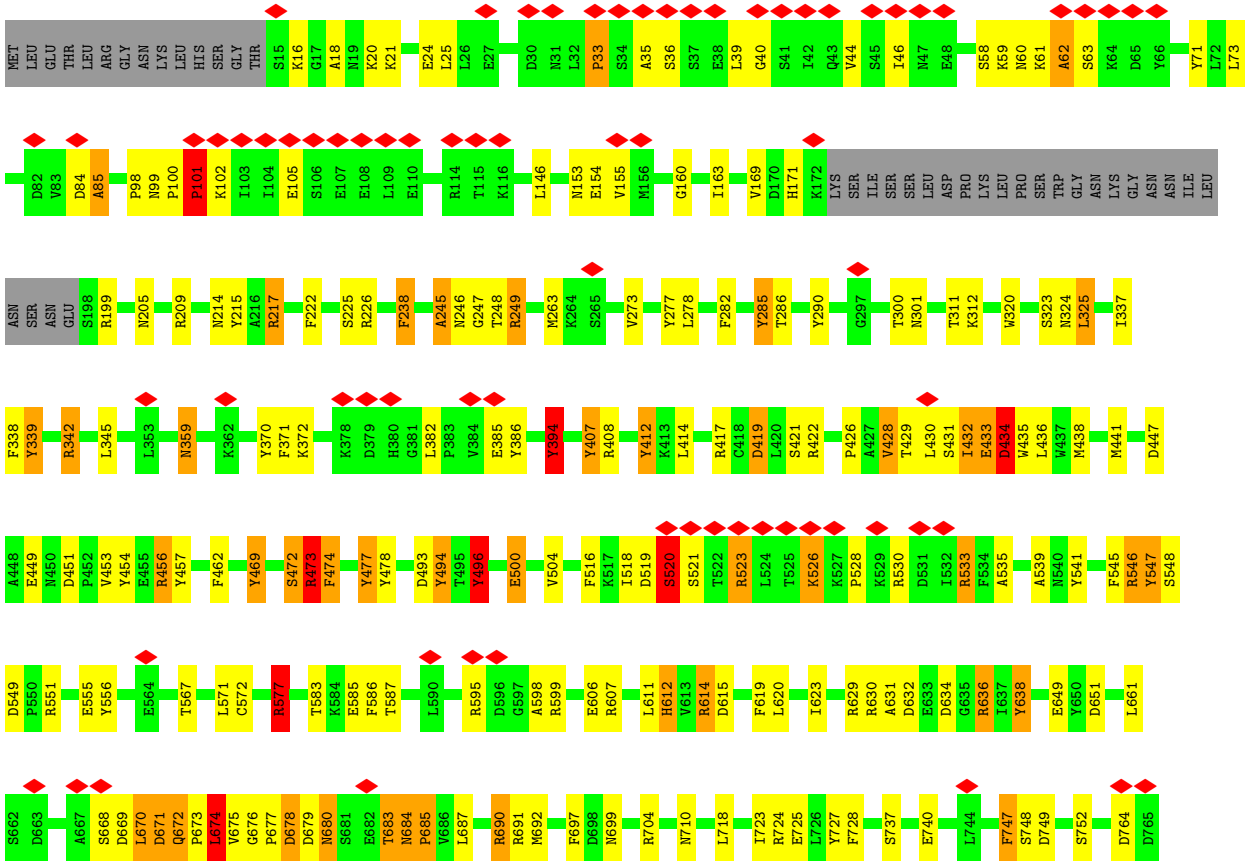
Chain Q:

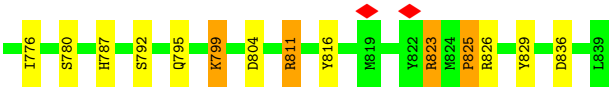




• Molecule 9: Nucleoporin NIC96

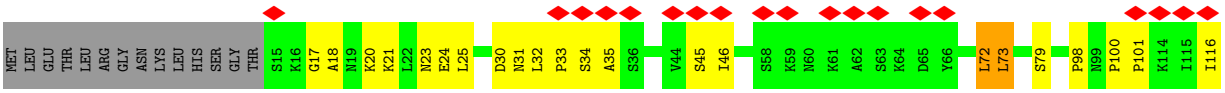
Chain R:

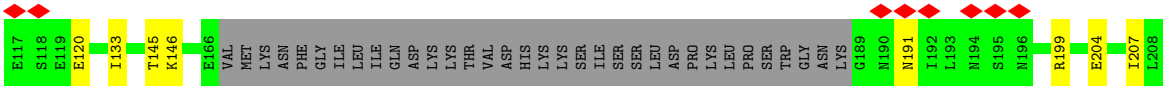


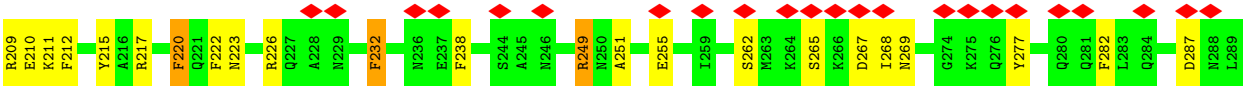


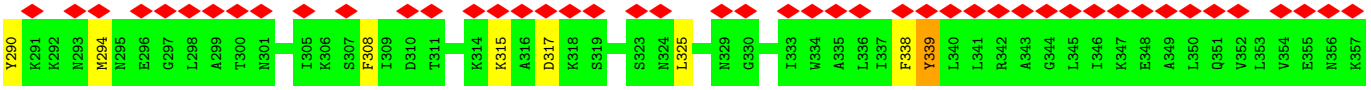
• Molecule 9: Nucleoporin NIC96

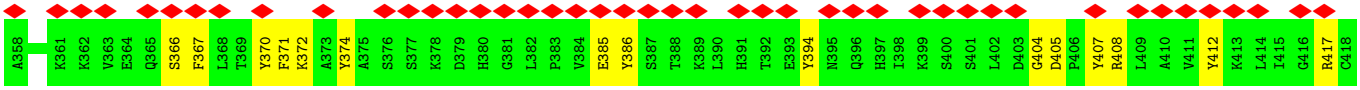
Chain S:

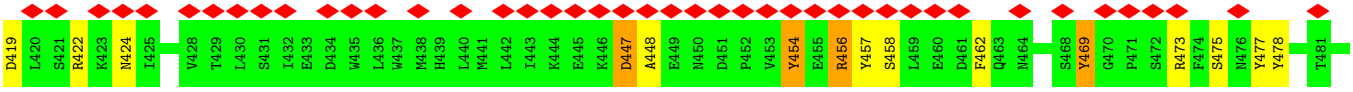


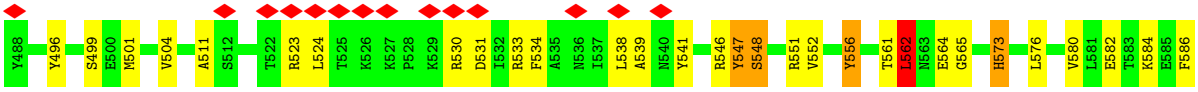


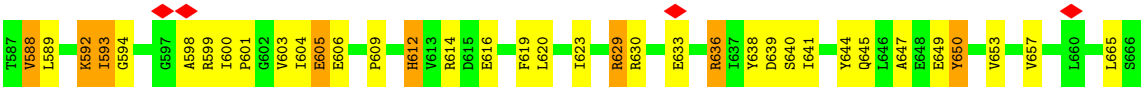


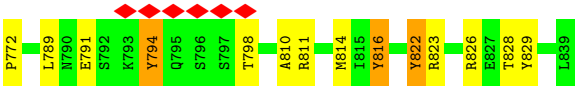






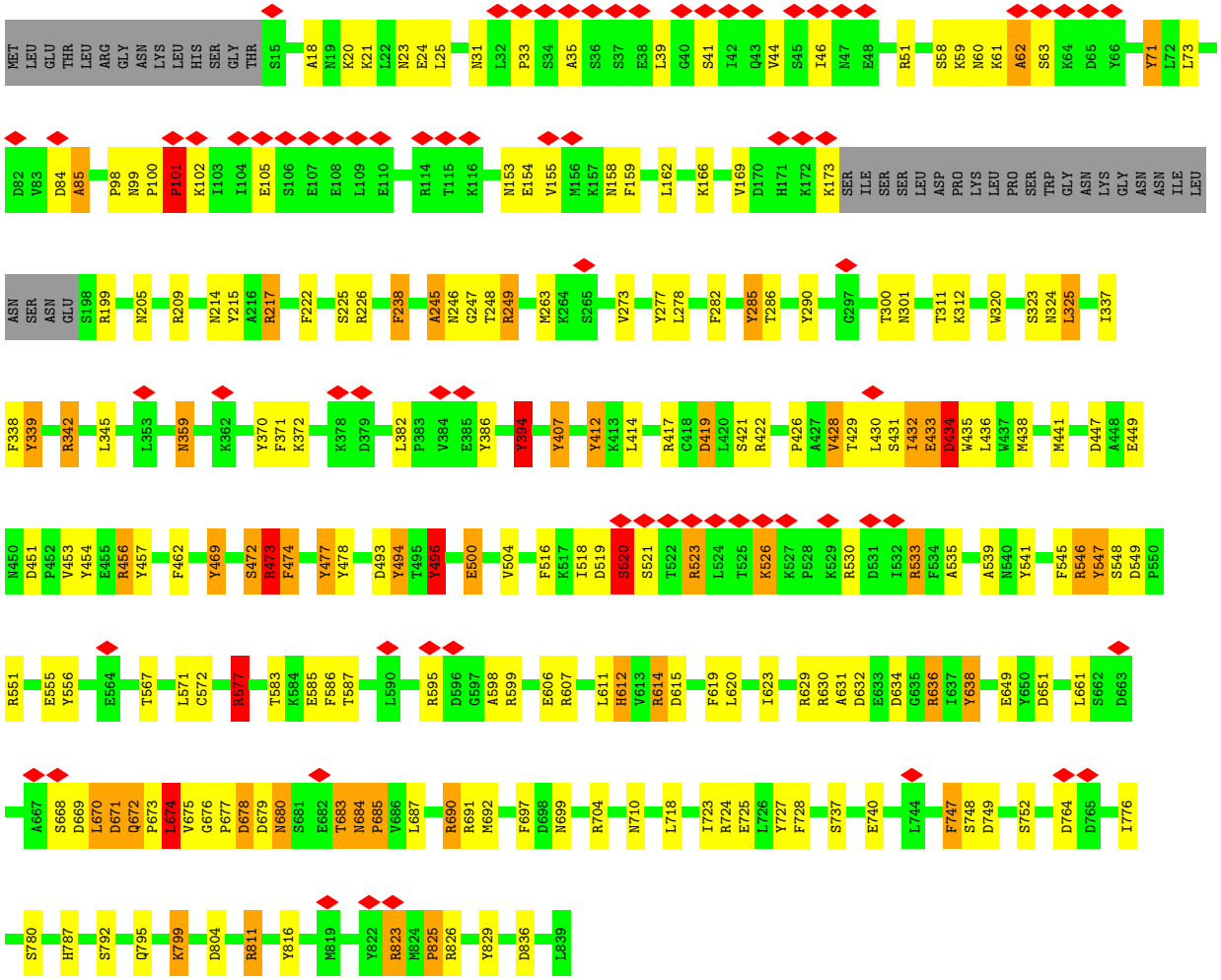






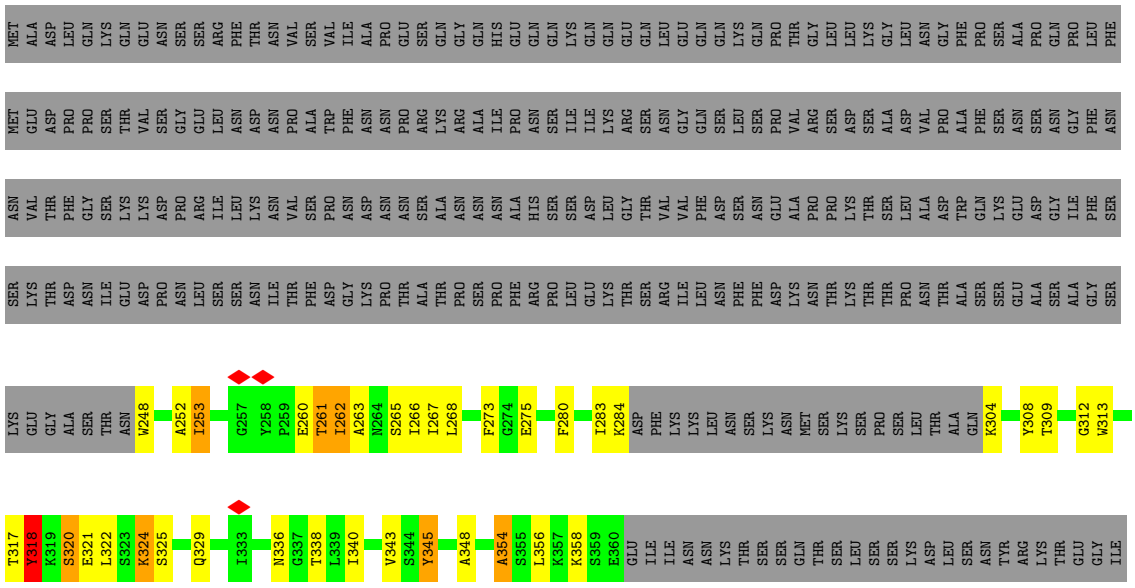
• Molecule 9: Nucleoporin NIC96

Chain T:



• Molecule 10: Nucleoporin NUP53

Chain U:



PHE GLU LYS ALA LYS ALA LYS ALA VAL THR SER LYS VAL ARG ASN ALA GLU PHE LYS VAL SER LYS ASN SER THR SER PHE LYS ASN PRO ARG ARG LEU GLU ILE LYS ASP GLY ARG SER LEU PHE LEU ARG ASN ARG GLY LYS ILE HIS SER GLY VAL LEU SER SER ILE GLU SER ASP

LEU LYS LYS ARG GLU GLN ALA SER LYS SER LYS LYS SER TRP LEU ASN ARG LEU ASN ASN TRP LEU PHE GLY TRP ASN ASP LEU

- Molecule 10: Nucleoporin NUP53

Chain W: 12% 6% 80%

MET ALA ASP LEU GLN LYS GLN GLU ASN SER SER ARG PHE THR ASN VAL SER VAL ILE ALA PRO GLU SER GLN GLY GLN HIS GLU GLN GLN LYS GLN GLN GLU GLN LEU GLU GLN GLN LYS GLN PRO THR GLY LEU LEU LYS GLY LEU ASN GLY PHE PRO SER ALA PRO GLN PRO LEU PHE

MET GLU ASP PRO PRO SER THR VAL SER GLY GLU LEU ASN ASP ASN PRO ALA TRP PHE ASN ASN PRO ARG LYS ARG ALA ILE PRO ASN SER ILE ILE LYS ARG SER ASN GLY GLN SER LEU SER PRO VAL ARG SER ASP SER ALA ASP VAL PRO ALA PHE SER ASN SER ASN GLY PHE ASN

ASN VAL THR PHE GLY SER LYS LYS ASP PRO ARG ILE LEU LYS ASN VAL SER PRO ASN ASP ASN ASN SER ALA ASN ASN ASN ALA HIS SER SER ASP LEU GLY THR VAL VAL PHE ASP SER ASN GLU ALA PRO PRO LYS THR SER LEU ALA ASP TRP GLN LYS GLU ASP GLY ILE PHE SER

SER LYS THR ASP ASN ILE GLU ASP PRO ASN LEU SER SER ASN ILE THR PHE ASP GLY LYS PRO THR ALA THR PRO SER PRO PHE ARG PRO LEU GLU LYS THR SER ARG ILE LEU ASN PHE PHE ASP LYS ASN THR LYS THR THR PRO ASN THR ALA SER SER GLU ALA SER ALA GLY SER

LYS GLU GLY ALA SER THR ASN W248 A252 I253 G257 Y258 P259 E260 T261 I262 A263 I266 A271 N272 F273 G274 E275 I276 F280 R281 V282 I283 K284 ASP PHE LYS LYS LEU ASN SER LYS ASN MET SER LYS SER PRO SER LEU THR ALA GLN K304 Y308 T309 G312 W313

T317 Y318 K319 S320 E321 L322 S323 K324 S325 E330 I333 N336 G337 T338 L339 I340 V343 S344 Y345 A348 A354 S355 L356 K357 K358 S359 E360 GLU ILE ILE ASN ASN LYS THR SER SER GLN THR SER LEU SER SER LYS ASP LEU SER ASN TYR ARG LYS THR GLU GLY

ILE PHE GLU LYS ALA LYS ALA LYS ALA VAL THR SER LYS VAL ARG ASN ALA GLU PHE LYS VAL SER LYS ASN SER THR SER PHE LYS ASN PRO ARG ARG LEU GLU ILE LYS ASP GLY ARG SER LEU PHE LEU ARG ASN ARG GLY LYS ILE HIS SER GLY VAL LEU SER SER ILE GLU SER

ASP LEU LYS LYS ARG GLU GLN ALA SER LYS SER LYS LYS SER TRP LEU ASN ARG LEU ASN ASN TRP LEU PHE GLY TRP ASN ASP LEU

- Molecule 11: Nucleoporin 59

Chain V: 8% 6% 83%

MET PHE GLY ILE ARG SER GLY ASN ASN ASN GLY GLY PHE THR ASN LEU THR SER GLN ALA PRO GLN THR THR GLN MET PHE GLN SER GLN SER GLN LEU GLN PRO GLN PRO GLN PRO GLN PRO GLN GLN GLN GLN GLN HIS LEU GLN PHE ASN GLY SER SER ASP ALA SER SER LEU ARG

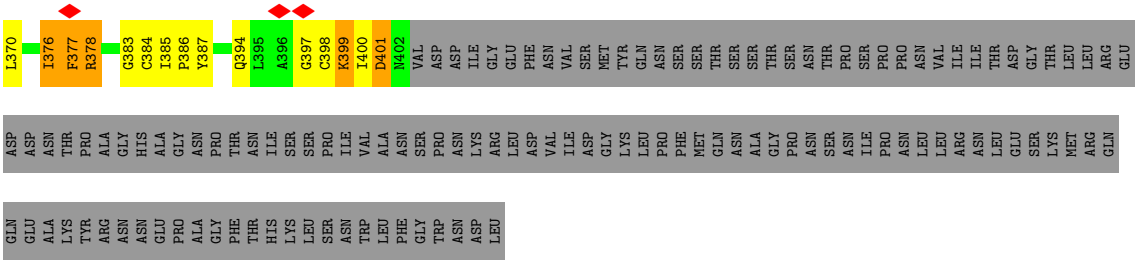
PHE GLY ASN SER LEU SER ASN THR VAL ASN ALA ASN ASN TYR SER SER ASN ILE GLY ASN ASN SER ILE ASN ASN ASN ASN ILE LYS ASN GLY THR ASN ASN ILE SER GLN HIS GLY GLN GLY ASN ASN PRO SER TRP VAL ASN ASN PRO LYS LYS ARG PHE THR PRO HIS THR VAL ILE

ARG ARG LYS THR THR LYS GLN ASN SER SER SER ASP ILE ASN GLN ASN ASP ASP SER SER SER MET ASN ALA THR MET ARG ASN PHE SER LYS GLN ASN GLN ASP SER LYS HIS ASN GLU ARG ASN LYS SER ALA ALA ASN ASN ASP ILE ASN SER LEU LEU SER ASN PHE ASN ASP ILE

PRO PRO SER VAL THR LEU GLN ASP TRP GLN ARG GLU ASP GLU PHE GLY SER ILE PRO SER LEU THR THR GLN PHE VAL THR ASP LYS TYR THR ALA LYS LYS THR ASN ARG SER ALA TYR ASP SER LYS ASN THR PRO ASN VAL PHE ASP LYS ASP SER TYR VAL ARG ILE ALA ASN ILE

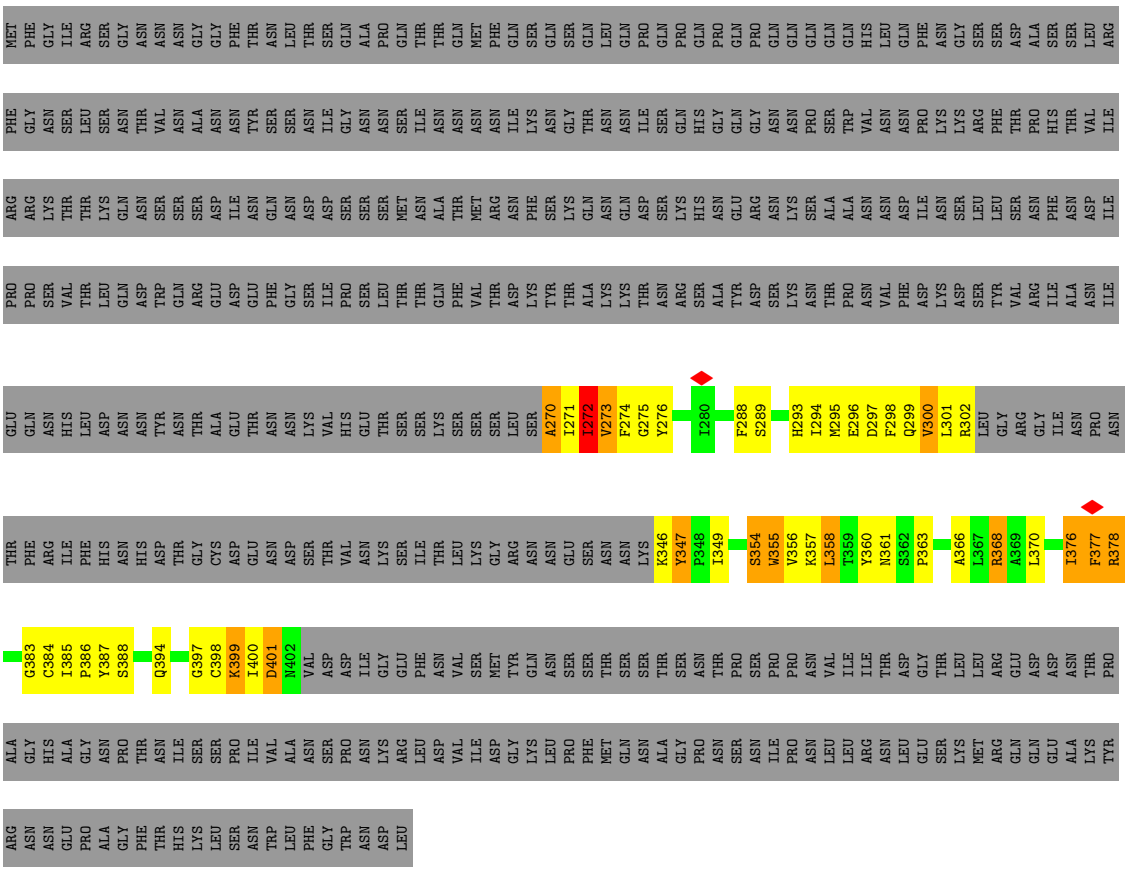
GLU GLN ASN HIS LEU ASP ASN ASN TYR ASN THR ALA GLU THR ASN ASN LYS VAL HIS GLU THR SER SER LYS SER SER SER LEU SER A270 I271 I272 V273 F274 G275 Y276 I280 S281 N282 I285 E286 H287 F288 S289 H293 I294 M295 E296 D297 F298 Q299 V300 L301 R302 LEU GLY ARG

GLY ILE ASN PRO ASN THR PHE ARG ILE PHE HIS ASN HIS ASP THR GLY CYS ASP GLU ASN ASP SER THR VAL ASN LYS SER ILE THR LEU LYS GLY ARG ASN ASN GLU SER ASN ASN LYS K346 Y347 P348 I349 S354 W355 V356 K357 L358 T359 Y360 N361 S362 P363 A366 L367 R368 A369



• Molecule 11: Nucleoporin 59

Chain X: 8% 6% • 83%



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	208392	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION; CTF correction applied in RELION during the alignment and reconstruction	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	40	Depositor
Minimum defocus (nm)	1500	Depositor
Maximum defocus (nm)	3500	Depositor
Magnification	37651	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	5.816	Depositor
Minimum map value	-1.894	Depositor
Average map value	0.011	Depositor
Map value standard deviation	0.095	Depositor
Recommended contour level	0.65	Depositor
Map size (Å)	1276.8, 1276.8, 1276.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.66, 2.66, 2.66	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
2	0	1.68	62/10219 (0.6%)	1.92	243/13825 (1.8%)
2	Y	1.68	61/10219 (0.6%)	1.92	243/13825 (1.8%)
3	1	1.70	68/9504 (0.7%)	1.99	274/12863 (2.1%)
3	Z	1.70	73/9504 (0.8%)	1.98	267/12863 (2.1%)
4	A	1.59	8/1328 (0.6%)	1.86	34/1791 (1.9%)
4	D	1.68	7/1358 (0.5%)	1.84	35/1833 (1.9%)
4	G	1.59	8/1328 (0.6%)	1.86	34/1791 (1.9%)
4	J	1.67	7/1360 (0.5%)	1.83	34/1836 (1.9%)
5	B	1.89	15/1793 (0.8%)	1.92	40/2411 (1.7%)
5	E	1.61	10/1793 (0.6%)	1.82	36/2411 (1.5%)
5	H	1.67	14/1793 (0.8%)	1.83	36/2411 (1.5%)
5	K	1.58	10/1793 (0.6%)	1.80	33/2411 (1.4%)
6	C	1.55	8/1364 (0.6%)	1.80	28/1837 (1.5%)
6	F	1.55	5/1398 (0.4%)	1.84	26/1884 (1.4%)
6	I	1.54	9/1364 (0.7%)	1.79	30/1837 (1.6%)
6	L	1.55	5/1398 (0.4%)	1.85	26/1884 (1.4%)
7	M	1.67	111/13592 (0.8%)	1.89	284/18408 (1.5%)
7	O	1.67	107/13592 (0.8%)	1.89	278/18408 (1.5%)
8	N	1.94	78/13423 (0.6%)	1.85	278/18194 (1.5%)
8	P	1.95	76/13433 (0.6%)	1.86	281/18208 (1.5%)
9	Q	1.67	45/6050 (0.7%)	1.87	133/8208 (1.6%)
9	R	1.63	49/6073 (0.8%)	1.80	113/8244 (1.4%)
9	S	1.67	47/6050 (0.8%)	1.87	138/8208 (1.7%)
9	T	1.63	47/6078 (0.8%)	1.80	111/8251 (1.3%)
10	U	1.42	3/761 (0.4%)	1.67	10/1027 (1.0%)
10	W	1.37	2/761 (0.3%)	1.64	10/1027 (1.0%)
11	V	1.50	6/727 (0.8%)	1.80	18/982 (1.8%)
11	X	1.50	7/727 (1.0%)	1.80	18/982 (1.8%)
All	All	1.72	948/138783 (0.7%)	1.88	3091/187860 (1.6%)

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	7	0	1
1	8	0	1
2	0	0	34
2	Y	0	35
3	1	0	37
3	Z	0	37
4	A	0	1
4	D	0	1
4	G	0	1
4	J	0	1
5	B	0	3
5	E	0	3
5	H	0	3
5	K	0	2
6	C	0	2
6	F	0	1
6	I	0	2
6	L	0	1
7	M	0	44
7	O	0	45
8	N	0	26
8	P	0	27
9	Q	0	16
9	R	0	17
9	S	0	17
9	T	0	17
10	U	0	2
10	W	0	1
11	V	0	1
11	X	0	1
All	All	0	380

All (948) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	613	GLU	CG-CD	99.91	3.01	1.51
8	N	613	GLU	CG-CD	99.88	3.01	1.51
5	B	323	LEU	CB-CG	37.01	2.59	1.52
8	N	617	TYR	CG-CD2	34.45	1.83	1.39
8	P	617	TYR	CG-CD2	34.40	1.83	1.39
8	P	617	TYR	CG-CD1	33.86	1.83	1.39
8	N	617	TYR	CG-CD1	33.84	1.83	1.39
8	P	617	TYR	CE2-CZ	32.46	1.80	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	617	TYR	CE2-CZ	32.30	1.80	1.38
8	P	617	TYR	CE1-CZ	31.46	1.79	1.38
8	N	617	TYR	CE1-CZ	31.45	1.79	1.38
8	P	617	TYR	CD1-CE1	24.42	1.75	1.39
8	N	617	TYR	CD1-CE1	24.34	1.75	1.39
8	N	617	TYR	CD2-CE2	22.16	1.72	1.39
8	P	617	TYR	CD2-CE2	22.03	1.72	1.39
3	Z	431	ARG	CZ-NH2	9.64	1.45	1.33
3	1	431	ARG	CZ-NH2	9.57	1.45	1.33
4	D	644	TRP	NE1-CE2	-9.21	1.25	1.37
4	J	644	TRP	NE1-CE2	-9.21	1.25	1.37
8	P	1268	SER	CA-CB	8.26	1.65	1.52
7	M	752	TYR	CE2-CZ	8.22	1.49	1.38
8	N	1268	SER	CA-CB	8.20	1.65	1.52
7	O	752	TYR	CE2-CZ	8.19	1.49	1.38
3	1	231	TYR	CZ-OH	8.10	1.51	1.37
3	Z	231	TYR	CZ-OH	8.10	1.51	1.37
4	J	677	SER	CA-CB	8.08	1.65	1.52
4	D	677	SER	CA-CB	8.05	1.65	1.52
7	M	1013	TYR	CG-CD1	8.05	1.49	1.39
7	O	1013	TYR	CG-CD1	8.01	1.49	1.39
3	1	1311	PHE	CG-CD1	7.99	1.50	1.38
3	Z	1311	PHE	CG-CD1	7.99	1.50	1.38
7	M	22	PHE	CE2-CZ	7.94	1.52	1.37
8	P	905	SER	CA-CB	7.94	1.64	1.52
7	O	22	PHE	CE2-CZ	7.87	1.52	1.37
2	0	286	GLY	N-CA	-7.82	1.34	1.46
2	Y	286	GLY	N-CA	-7.82	1.34	1.46
8	N	905	SER	CA-CB	7.79	1.64	1.52
7	O	1551	SER	CA-CB	7.77	1.64	1.52
2	0	1152	TYR	CG-CD1	7.74	1.49	1.39
7	M	1551	SER	CA-CB	7.70	1.64	1.52
9	Q	794	TYR	CE1-CZ	7.69	1.48	1.38
9	S	794	TYR	CE1-CZ	7.69	1.48	1.38
2	Y	1152	TYR	CG-CD1	7.67	1.49	1.39
3	1	843	TYR	CG-CD2	7.66	1.49	1.39
3	Z	843	TYR	CG-CD2	7.63	1.49	1.39
8	N	1426	SER	CA-CB	7.57	1.64	1.52
8	P	1426	SER	CA-CB	7.44	1.64	1.52
3	Z	735	SER	CA-CB	7.41	1.64	1.52
3	1	735	SER	CA-CB	7.40	1.64	1.52
7	M	1647	ARG	CZ-NH1	7.39	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	1647	ARG	CZ-NH1	7.37	1.42	1.33
2	Y	447	TYR	CB-CG	7.35	1.62	1.51
2	0	447	TYR	CB-CG	7.33	1.62	1.51
9	S	255	GLU	CG-CD	7.32	1.62	1.51
9	Q	255	GLU	CG-CD	7.28	1.62	1.51
9	Q	265	SER	CA-CB	7.24	1.63	1.52
9	Q	533	ARG	CD-NE	7.21	1.58	1.46
9	S	265	SER	CA-CB	7.21	1.63	1.52
3	Z	299	SER	CA-CB	7.20	1.63	1.52
6	I	447	PHE	CG-CD1	7.20	1.49	1.38
8	N	1087	TYR	CB-CG	7.18	1.62	1.51
3	1	299	SER	CA-CB	7.18	1.63	1.52
5	H	475	SER	CA-CB	7.18	1.63	1.52
6	C	447	PHE	CG-CD1	7.17	1.49	1.38
9	R	371	PHE	CG-CD1	7.15	1.49	1.38
9	S	533	ARG	CD-NE	7.15	1.58	1.46
9	T	371	PHE	CG-CD1	7.15	1.49	1.38
5	B	475	SER	CA-CB	7.12	1.63	1.52
9	S	412	TYR	CE1-CZ	7.11	1.47	1.38
3	Z	855	PRO	N-CA	-7.11	1.35	1.47
8	P	1087	TYR	CB-CG	7.08	1.62	1.51
7	M	1237	TYR	CE2-CZ	7.08	1.47	1.38
8	N	1597	ARG	CZ-NH1	7.07	1.42	1.33
3	1	855	PRO	N-CA	-7.07	1.35	1.47
8	P	1597	ARG	CZ-NH1	7.06	1.42	1.33
2	Y	136	SER	CA-CB	7.05	1.63	1.52
9	S	614	ARG	CD-NE	7.04	1.58	1.46
7	O	1237	TYR	CE2-CZ	7.04	1.47	1.38
9	Q	412	TYR	CE1-CZ	7.03	1.47	1.38
7	M	1261	SER	CB-OG	7.01	1.51	1.42
9	S	217	ARG	CZ-NH1	7.01	1.42	1.33
7	M	499	PHE	CB-CG	7.00	1.63	1.51
7	O	499	PHE	CB-CG	7.00	1.63	1.51
8	P	783	PHE	CG-CD2	7.00	1.49	1.38
9	T	607	ARG	CZ-NH2	6.99	1.42	1.33
2	Y	392	SER	CB-OG	6.97	1.51	1.42
9	R	607	ARG	CZ-NH2	6.97	1.42	1.33
8	N	783	PHE	CG-CD2	6.97	1.49	1.38
9	S	417	ARG	CZ-NH2	6.96	1.42	1.33
7	O	1261	SER	CB-OG	6.96	1.51	1.42
2	0	136	SER	CA-CB	6.96	1.63	1.52
9	Q	217	ARG	CZ-NH1	6.94	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	392	SER	CB-OG	6.94	1.51	1.42
2	0	93	SER	CB-OG	-6.94	1.33	1.42
2	Y	93	SER	CB-OG	-6.93	1.33	1.42
9	R	530	ARG	CZ-NH1	6.91	1.42	1.33
5	K	447	SER	CA-CB	6.91	1.63	1.52
9	R	541	TYR	CG-CD2	6.90	1.48	1.39
9	Q	614	ARG	CD-NE	6.89	1.58	1.46
9	S	565	GLY	CA-C	-6.89	1.40	1.51
9	T	530	ARG	CZ-NH1	6.89	1.42	1.33
9	T	748	SER	CA-CB	6.87	1.63	1.52
9	T	541	TYR	CG-CD2	6.87	1.48	1.39
5	E	447	SER	CA-CB	6.85	1.63	1.52
8	P	720	ARG	CZ-NH2	6.85	1.42	1.33
9	Q	417	ARG	CZ-NH2	6.84	1.42	1.33
9	Q	565	GLY	CA-C	-6.84	1.41	1.51
9	R	370	TYR	CG-CD2	6.84	1.48	1.39
10	W	312	GLY	CA-C	-6.83	1.41	1.51
10	U	312	GLY	CA-C	-6.83	1.41	1.51
7	O	448	PHE	CG-CD1	6.82	1.49	1.38
3	1	836	TYR	CE1-CZ	6.82	1.47	1.38
8	N	720	ARG	CZ-NH2	6.82	1.42	1.33
7	M	269	TYR	CG-CD2	6.80	1.48	1.39
3	1	416	GLU	CD-OE1	6.80	1.33	1.25
7	O	269	TYR	CG-CD2	6.80	1.48	1.39
9	T	370	TYR	CG-CD2	6.80	1.48	1.39
9	R	748	SER	CA-CB	6.79	1.63	1.52
7	M	112	TYR	CB-CG	6.79	1.61	1.51
7	M	448	PHE	CG-CD1	6.78	1.49	1.38
7	M	288	TRP	NE1-CE2	-6.76	1.28	1.37
8	P	1136	SER	CA-CB	6.76	1.63	1.52
8	P	1432	ARG	CZ-NH1	6.74	1.41	1.33
5	E	327	PRO	N-CD	-6.74	1.38	1.47
3	Z	416	GLU	CD-OE1	6.73	1.33	1.25
7	O	288	TRP	NE1-CE2	-6.73	1.28	1.37
8	P	1353	SER	CA-CB	6.72	1.63	1.52
7	M	1116	VAL	CB-CG1	6.72	1.67	1.52
9	S	290	TYR	CD2-CE2	6.72	1.49	1.39
7	O	112	TYR	CB-CG	6.72	1.61	1.51
2	Y	1073	SER	CA-CB	6.71	1.63	1.52
8	N	1136	SER	CA-CB	6.71	1.63	1.52
2	0	1073	SER	CA-CB	6.71	1.63	1.52
7	M	364	GLU	CG-CD	6.71	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	1566	TYR	CE1-CZ	6.71	1.47	1.38
7	O	364	GLU	CG-CD	6.71	1.62	1.51
7	O	1116	VAL	CB-CG1	6.70	1.67	1.52
9	T	238	PHE	CG-CD1	6.70	1.48	1.38
9	R	826	ARG	CZ-NH1	6.70	1.41	1.33
7	O	1029	SER	CA-CB	6.69	1.62	1.52
8	P	1566	TYR	CE1-CZ	6.69	1.47	1.38
7	M	1029	SER	CA-CB	6.69	1.62	1.52
9	R	829	TYR	CE2-CZ	6.68	1.47	1.38
2	Y	1204	TYR	CG-CD2	6.68	1.47	1.39
3	Z	836	TYR	CE1-CZ	6.67	1.47	1.38
5	K	327	PRO	N-CD	-6.67	1.38	1.47
9	T	829	TYR	CE2-CZ	6.66	1.47	1.38
8	N	1353	SER	CA-CB	6.66	1.62	1.52
9	R	238	PHE	CG-CD1	6.66	1.48	1.38
9	Q	290	TYR	CD2-CE2	6.65	1.49	1.39
4	D	699	TYR	CG-CD1	6.64	1.47	1.39
8	N	1432	ARG	CZ-NH1	6.64	1.41	1.33
4	J	699	TYR	CG-CD1	6.64	1.47	1.39
3	1	709	PHE	N-CA	-6.63	1.33	1.46
2	0	1204	TYR	CG-CD2	6.63	1.47	1.39
2	Y	964	ARG	NE-CZ	6.63	1.41	1.33
9	R	407	TYR	CE2-CZ	6.62	1.47	1.38
3	Z	709	PHE	N-CA	-6.61	1.33	1.46
7	M	1569	TYR	CG-CD1	6.61	1.47	1.39
9	R	585	GLU	CG-CD	-6.60	1.42	1.51
9	T	826	ARG	CZ-NH1	6.59	1.41	1.33
2	0	964	ARG	NE-CZ	6.59	1.41	1.33
2	0	1277	SER	CA-CB	6.58	1.62	1.52
8	N	1452	SER	CA-CB	6.57	1.62	1.52
9	Q	210	GLU	CD-OE2	6.57	1.32	1.25
2	Y	1277	SER	CA-CB	6.56	1.62	1.52
9	Q	477	TYR	CD2-CE2	6.56	1.49	1.39
7	O	1569	TYR	CG-CD1	6.55	1.47	1.39
9	T	407	TYR	CE2-CZ	6.54	1.47	1.38
9	S	404	GLY	CA-C	-6.53	1.41	1.51
2	Y	583	TYR	CG-CD1	6.53	1.47	1.39
9	S	210	GLU	CD-OE2	6.53	1.32	1.25
7	O	629	SER	CA-CB	6.52	1.62	1.52
8	P	1452	SER	CA-CB	6.52	1.62	1.52
9	S	477	TYR	CD2-CE2	6.52	1.49	1.39
3	Z	351	ARG	NE-CZ	6.52	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	T	585	GLU	CG-CD	-6.52	1.42	1.51
9	Q	404	GLY	CA-C	-6.51	1.41	1.51
3	Z	103	PHE	CG-CD1	6.50	1.48	1.38
2	0	200	GLU	CD-OE2	6.50	1.32	1.25
2	0	583	TYR	CG-CD1	6.49	1.47	1.39
7	M	629	SER	CA-CB	6.48	1.62	1.52
2	Y	1292	GLU	CG-CD	6.48	1.61	1.51
7	O	508	TYR	CD2-CE2	6.45	1.49	1.39
8	N	550	SER	CA-CB	6.44	1.62	1.52
2	0	397	TYR	CB-CG	-6.44	1.42	1.51
3	1	351	ARG	NE-CZ	6.44	1.41	1.33
2	Y	200	GLU	CD-OE2	6.44	1.32	1.25
7	M	508	TYR	CD2-CE2	6.44	1.49	1.39
2	Y	397	TYR	CB-CG	-6.44	1.42	1.51
4	D	805	ARG	NE-CZ	6.43	1.41	1.33
2	0	1292	GLU	CG-CD	6.43	1.61	1.51
2	Y	138	GLU	CD-OE1	6.43	1.32	1.25
3	1	103	PHE	CG-CD1	6.43	1.48	1.38
8	P	397	SER	CA-CB	6.41	1.62	1.52
8	N	950	ARG	NE-CZ	6.41	1.41	1.33
8	P	550	SER	CA-CB	6.40	1.62	1.52
4	J	805	ARG	NE-CZ	6.40	1.41	1.33
9	R	606	GLU	CG-CD	6.38	1.61	1.51
3	Z	164	GLY	CA-C	-6.38	1.41	1.51
3	1	164	GLY	CA-C	-6.36	1.41	1.51
7	O	1153	TYR	CB-CG	6.36	1.61	1.51
2	0	138	GLU	CD-OE1	6.36	1.32	1.25
2	Y	1206	ARG	C-N	6.36	1.48	1.34
8	N	397	SER	CA-CB	6.36	1.62	1.52
9	T	606	GLU	CG-CD	6.35	1.61	1.51
2	0	1383	PHE	CG-CD1	6.34	1.48	1.38
8	N	966	GLY	CA-C	-6.34	1.41	1.51
8	P	950	ARG	NE-CZ	6.33	1.41	1.33
7	M	1153	TYR	CB-CG	6.33	1.61	1.51
2	0	1360	SER	CA-CB	6.33	1.62	1.52
5	B	311	PHE	CG-CD1	6.33	1.48	1.38
8	N	298	VAL	CB-CG2	6.33	1.66	1.52
2	0	1206	ARG	C-N	6.31	1.48	1.34
3	Z	836	TYR	CE2-CZ	6.31	1.46	1.38
9	Q	534	PHE	CG-CD1	6.30	1.48	1.38
2	Y	1383	PHE	CG-CD1	6.30	1.48	1.38
9	S	534	PHE	CG-CD1	6.30	1.48	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	633	GLU	CD-OE2	-6.29	1.18	1.25
9	S	556	TYR	CG-CD2	6.29	1.47	1.39
3	1	1005	TYR	CD2-CE2	6.29	1.48	1.39
9	S	633	GLU	CD-OE2	-6.28	1.18	1.25
8	P	1490	ARG	NE-CZ	6.28	1.41	1.33
9	S	339	TYR	CZ-OH	6.28	1.48	1.37
9	Q	339	TYR	CZ-OH	6.27	1.48	1.37
2	Y	1360	SER	CA-CB	6.26	1.62	1.52
2	Y	1317	TYR	CE2-CZ	6.26	1.46	1.38
8	P	966	GLY	CA-C	-6.26	1.41	1.51
9	Q	556	TYR	CG-CD2	6.26	1.47	1.39
2	0	1317	TYR	CE2-CZ	6.26	1.46	1.38
8	P	298	VAL	CB-CG2	6.26	1.66	1.52
8	P	1466	TYR	CG-CD1	6.25	1.47	1.39
8	N	1466	TYR	CG-CD1	6.25	1.47	1.39
5	H	311	PHE	CG-CD1	6.25	1.48	1.38
7	M	89	CYS	CB-SG	6.25	1.92	1.82
7	O	89	CYS	CB-SG	6.24	1.92	1.82
3	1	1382	TYR	CG-CD1	6.23	1.47	1.39
3	Z	1005	TYR	CD2-CE2	6.23	1.48	1.39
3	1	836	TYR	CE2-CZ	6.22	1.46	1.38
3	Z	198	GLU	CD-OE2	6.22	1.32	1.25
2	0	1456	TYR	CE1-CZ	6.21	1.46	1.38
9	R	520	SER	CB-OG	6.21	1.50	1.42
5	B	537	TYR	CG-CD2	6.21	1.47	1.39
9	R	555	GLU	CG-CD	6.20	1.61	1.51
7	O	295	ARG	NE-CZ	6.20	1.41	1.33
7	M	431	PHE	CB-CG	6.20	1.61	1.51
3	Z	1382	TYR	CG-CD1	6.19	1.47	1.39
2	Y	1456	TYR	CE1-CZ	6.18	1.46	1.38
7	M	284	TYR	CG-CD2	6.18	1.47	1.39
8	N	1490	ARG	NE-CZ	6.18	1.41	1.33
5	H	537	TYR	CG-CD2	6.18	1.47	1.39
9	Q	693	ALA	CA-CB	6.17	1.65	1.52
5	H	438	SER	CA-CB	6.17	1.62	1.52
9	T	457	TYR	CE1-CZ	6.17	1.46	1.38
9	T	520	SER	CB-OG	6.16	1.50	1.42
2	0	1083	TYR	CG-CD2	6.16	1.47	1.39
3	Z	843	TYR	CE2-CZ	6.15	1.46	1.38
8	P	101	PHE	CG-CD1	6.15	1.48	1.38
3	1	198	GLU	CD-OE2	6.15	1.32	1.25
7	M	94	SER	CA-CB	6.15	1.62	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	1083	TYR	CG-CD2	6.14	1.47	1.39
7	O	259	PHE	CE2-CZ	6.14	1.49	1.37
7	M	259	PHE	CE2-CZ	6.14	1.49	1.37
7	O	94	SER	CA-CB	6.14	1.62	1.52
8	P	295	PHE	CG-CD2	6.13	1.48	1.38
5	H	522	TYR	CB-CG	6.12	1.60	1.51
7	O	431	PHE	CB-CG	6.12	1.61	1.51
9	S	693	ALA	CA-CB	6.12	1.65	1.52
9	T	555	GLU	CG-CD	6.12	1.61	1.51
8	N	295	PHE	CG-CD2	6.12	1.48	1.38
7	M	1233	SER	CA-CB	6.11	1.62	1.52
5	B	438	SER	CA-CB	6.09	1.62	1.52
7	M	1364	TYR	CE2-CZ	6.09	1.46	1.38
8	N	101	PHE	CG-CD1	6.09	1.47	1.38
3	1	843	TYR	CE2-CZ	6.08	1.46	1.38
8	P	882	SER	CA-CB	6.07	1.62	1.52
3	1	1103	PHE	CE1-CZ	6.07	1.48	1.37
7	O	1233	SER	CA-CB	6.07	1.62	1.52
9	S	681	SER	CA-CB	6.07	1.62	1.52
8	N	844	TYR	CE1-CZ	6.06	1.46	1.38
5	B	522	TYR	CB-CG	6.05	1.60	1.51
2	0	1460	ARG	CD-NE	6.05	1.56	1.46
8	P	844	TYR	CE1-CZ	6.05	1.46	1.38
7	M	579	ARG	NE-CZ	6.05	1.41	1.33
3	Z	1103	PHE	CE1-CZ	6.04	1.48	1.37
9	Q	681	SER	CA-CB	6.04	1.62	1.52
9	R	457	TYR	CE1-CZ	6.04	1.46	1.38
3	1	104	ARG	CD-NE	6.04	1.56	1.46
7	M	295	ARG	NE-CZ	6.04	1.40	1.33
4	A	801	PHE	CG-CD2	6.03	1.47	1.38
3	Z	104	ARG	CD-NE	6.03	1.56	1.46
7	O	284	TYR	CG-CD2	6.03	1.47	1.39
2	Y	1460	ARG	CD-NE	6.03	1.56	1.46
6	C	283	TYR	CB-CG	-6.01	1.42	1.51
6	I	283	TYR	CB-CG	-6.01	1.42	1.51
2	Y	1342	GLU	CB-CG	6.01	1.63	1.52
9	Q	212	PHE	CG-CD2	6.00	1.47	1.38
8	N	882	SER	CA-CB	6.00	1.61	1.52
3	1	1035	PRO	N-CD	-6.00	1.39	1.47
4	G	801	PHE	CG-CD2	5.99	1.47	1.38
4	G	811	SER	CA-CB	5.99	1.61	1.52
2	0	1342	GLU	CB-CG	5.99	1.63	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	1292	GLU	CG-CD	5.98	1.60	1.51
3	Z	1035	PRO	N-CD	-5.98	1.39	1.47
9	R	323	SER	CB-OG	5.98	1.50	1.42
7	M	368	SER	CA-CB	5.97	1.61	1.52
7	O	368	SER	CA-CB	5.97	1.61	1.52
5	H	450	PRO	N-CA	-5.97	1.37	1.47
7	O	1364	TYR	CE2-CZ	5.97	1.46	1.38
4	A	811	SER	CA-CB	5.96	1.61	1.52
9	R	780	SER	CA-CB	5.96	1.61	1.52
7	O	579	ARG	NE-CZ	5.95	1.40	1.33
7	O	750	TRP	CD2-CE3	-5.95	1.31	1.40
7	M	47	SER	CA-CB	5.94	1.61	1.52
9	R	548	SER	CA-CB	5.94	1.61	1.52
8	P	1042	SER	CA-CB	5.94	1.61	1.52
9	S	212	PHE	CG-CD2	5.94	1.47	1.38
7	O	55	GLU	CD-OE2	-5.94	1.19	1.25
9	R	285	TYR	CE2-CZ	5.93	1.46	1.38
6	L	318	SER	CA-CB	5.93	1.61	1.52
9	S	546	ARG	CD-NE	5.93	1.56	1.46
9	T	323	SER	CB-OG	5.93	1.50	1.42
9	R	478	TYR	CG-CD2	5.93	1.46	1.39
9	Q	546	ARG	CD-NE	5.92	1.56	1.46
7	O	482	PHE	CG-CD1	5.92	1.47	1.38
8	N	1292	GLU	CG-CD	5.92	1.60	1.51
3	1	727	ARG	NE-CZ	5.92	1.40	1.33
3	Z	731	PHE	N-CA	-5.92	1.34	1.46
7	O	47	SER	CA-CB	5.92	1.61	1.52
7	M	482	PHE	CG-CD1	5.91	1.47	1.38
5	E	437	TRP	CD1-NE1	-5.91	1.27	1.38
5	K	437	TRP	CD1-NE1	-5.91	1.27	1.38
9	T	780	SER	CA-CB	5.91	1.61	1.52
2	Y	1021	TYR	CZ-OH	5.90	1.47	1.37
7	O	1472	GLU	CD-OE1	5.90	1.32	1.25
9	S	829	TYR	CG-CD1	5.90	1.46	1.39
3	1	1351	TYR	CE1-CZ	5.90	1.46	1.38
3	1	731	PHE	N-CA	-5.89	1.34	1.46
6	I	302	ASP	CA-CB	5.89	1.67	1.53
7	M	1349	PHE	CE1-CZ	5.89	1.48	1.37
8	N	1042	SER	CA-CB	5.89	1.61	1.52
5	B	450	PRO	N-CA	-5.89	1.37	1.47
7	O	1292	ARG	CZ-NH1	5.89	1.40	1.33
3	Z	727	ARG	NE-CZ	5.88	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	0	1021	TYR	CZ-OH	5.88	1.47	1.37
3	Z	131	GLY	N-CA	-5.87	1.37	1.46
7	M	55	GLU	CD-OE2	-5.87	1.19	1.25
5	K	297	GLU	CB-CG	5.87	1.63	1.52
2	Y	1159	TYR	CG-CD2	5.87	1.46	1.39
7	O	1349	PHE	CE1-CZ	5.87	1.48	1.37
5	E	297	GLU	CB-CG	5.87	1.63	1.52
7	M	750	TRP	CD2-CE3	-5.87	1.31	1.40
9	T	548	SER	CA-CB	5.87	1.61	1.52
5	H	313	TYR	CE1-CZ	5.86	1.46	1.38
8	P	1307	PHE	CG-CD1	5.86	1.47	1.38
9	T	649	GLU	CD-OE2	5.86	1.32	1.25
3	Z	1351	TYR	CE1-CZ	5.86	1.46	1.38
3	Z	240	ARG	NE-CZ	5.86	1.40	1.33
3	1	131	GLY	N-CA	-5.86	1.37	1.46
2	0	1159	TYR	CG-CD2	5.86	1.46	1.39
9	S	690	ARG	CZ-NH1	5.85	1.40	1.33
8	P	953	TYR	CG-CD1	5.85	1.46	1.39
6	F	318	SER	CA-CB	5.85	1.61	1.52
2	0	1052	SER	CA-CB	5.85	1.61	1.52
7	M	1292	ARG	CZ-NH1	5.85	1.40	1.33
9	Q	829	TYR	CG-CD1	5.84	1.46	1.39
5	K	522	TYR	CZ-OH	5.84	1.47	1.37
6	C	302	ASP	CA-CB	5.84	1.66	1.53
8	P	1011	GLU	CD-OE1	5.84	1.32	1.25
9	T	285	TYR	CE2-CZ	5.83	1.46	1.38
8	N	1011	GLU	CD-OE1	5.83	1.32	1.25
9	T	478	TYR	CG-CD2	5.83	1.46	1.39
7	O	1654	ASN	CB-CG	5.83	1.64	1.51
9	S	573	HIS	CB-CG	5.83	1.60	1.50
7	M	1259	SER	CA-CB	5.82	1.61	1.52
8	N	1307	PHE	CG-CD1	5.82	1.47	1.38
9	R	649	GLU	CD-OE2	5.82	1.32	1.25
3	1	234	THR	N-CA	5.82	1.57	1.46
3	Z	234	THR	N-CA	5.81	1.57	1.46
2	0	1334	GLU	CD-OE1	-5.81	1.19	1.25
8	N	1217	ARG	CZ-NH2	5.81	1.40	1.33
7	O	1079	ALA	CA-CB	5.81	1.64	1.52
3	1	240	ARG	NE-CZ	5.81	1.40	1.33
3	1	421	PHE	CG-CD1	5.80	1.47	1.38
7	O	1259	SER	CA-CB	5.80	1.61	1.52
7	M	10	THR	N-CA	-5.80	1.34	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	573	HIS	CB-CG	5.80	1.60	1.50
2	Y	89	HIS	CA-CB	5.80	1.66	1.53
2	0	458	GLU	CA-CB	5.80	1.66	1.53
3	Z	1071	TYR	CA-CB	5.79	1.66	1.53
2	Y	375	SER	CA-CB	5.79	1.61	1.52
5	E	522	TYR	CZ-OH	5.79	1.47	1.37
2	0	375	SER	CA-CB	5.79	1.61	1.52
3	1	1071	TYR	CA-CB	5.79	1.66	1.53
7	M	1472	GLU	CD-OE1	5.79	1.32	1.25
7	M	1079	ALA	CA-CB	5.78	1.64	1.52
8	N	953	TYR	CG-CD1	5.78	1.46	1.39
2	Y	241	PHE	CE1-CZ	5.77	1.48	1.37
7	O	10	THR	N-CA	-5.77	1.34	1.46
2	Y	1052	SER	CA-CB	5.77	1.61	1.52
3	Z	421	PHE	CG-CD1	5.77	1.47	1.38
9	Q	690	ARG	CZ-NH1	5.77	1.40	1.33
2	0	89	HIS	CA-CB	5.77	1.66	1.53
9	R	199	ARG	NE-CZ	5.76	1.40	1.33
6	L	455	GLU	CD-OE2	-5.76	1.19	1.25
2	Y	458	GLU	CA-CB	5.75	1.66	1.53
7	O	1679	TYR	CG-CD2	5.75	1.46	1.39
2	Y	1319	GLU	CG-CD	5.75	1.60	1.51
7	M	1654	ASN	CB-CG	5.74	1.64	1.51
3	1	104	ARG	CZ-NH2	5.74	1.40	1.33
4	A	757	SER	CB-OG	-5.74	1.34	1.42
9	S	616	GLU	CD-OE2	5.74	1.31	1.25
6	C	380	TYR	CZ-OH	5.73	1.47	1.37
6	F	455	GLU	CD-OE2	-5.73	1.19	1.25
4	G	680	TYR	CE2-CZ	5.73	1.46	1.38
7	O	666	SER	CA-C	-5.73	1.38	1.52
3	Z	1141	CYS	CB-SG	5.72	1.92	1.82
9	T	199	ARG	NE-CZ	5.72	1.40	1.33
6	C	387	TYR	CG-CD2	5.72	1.46	1.39
6	I	380	TYR	CZ-OH	5.72	1.47	1.37
7	O	1036	PRO	N-CA	-5.72	1.37	1.47
7	M	1253	ARG	CZ-NH1	5.71	1.40	1.33
7	M	1679	TYR	CG-CD2	5.71	1.46	1.39
8	N	526	GLY	CA-C	-5.71	1.42	1.51
2	0	241	PHE	CE1-CZ	5.71	1.48	1.37
2	Y	1334	GLU	CD-OE1	-5.71	1.19	1.25
4	G	757	SER	CB-OG	-5.71	1.34	1.42
2	Y	1355	GLY	CA-C	-5.71	1.42	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	666	SER	CA-C	-5.71	1.38	1.52
10	W	275	GLU	CD-OE2	5.71	1.31	1.25
3	1	1141	CYS	CB-SG	5.71	1.92	1.82
8	N	1466	TYR	CB-CG	-5.70	1.43	1.51
7	M	721	SER	CA-CB	5.70	1.61	1.52
2	0	221	PRO	C-N	5.70	1.47	1.34
7	O	288	TRP	CA-C	-5.70	1.38	1.52
2	Y	221	PRO	C-N	5.70	1.47	1.34
8	N	1179	SER	CB-OG	5.70	1.49	1.42
6	I	387	TYR	CG-CD2	5.70	1.46	1.39
7	M	288	TRP	CA-C	-5.69	1.38	1.52
7	M	642	PHE	CA-CB	5.69	1.66	1.53
9	Q	823	ARG	CZ-NH1	5.69	1.40	1.33
4	A	680	TYR	CE2-CZ	5.68	1.46	1.38
7	M	1036	PRO	N-CA	-5.67	1.37	1.47
3	1	1330	GLU	CG-CD	5.67	1.60	1.51
8	P	1466	TYR	CB-CG	-5.67	1.43	1.51
5	B	313	TYR	CE1-CZ	5.67	1.46	1.38
7	O	642	PHE	CA-CB	5.67	1.66	1.53
3	Z	128	GLU	CD-OE2	5.67	1.31	1.25
7	M	1447	TYR	CD1-CE1	-5.67	1.30	1.39
10	U	275	GLU	CD-OE2	5.67	1.31	1.25
5	H	469	ARG	NE-CZ	5.66	1.40	1.33
4	J	708	GLU	CD-OE1	5.66	1.31	1.25
8	P	418	ASN	CB-CG	5.66	1.64	1.51
5	B	469	ARG	NE-CZ	5.66	1.40	1.33
7	O	1324	ARG	CD-NE	5.66	1.56	1.46
9	T	225	SER	CA-CB	5.65	1.61	1.52
9	R	556	TYR	CZ-OH	5.65	1.47	1.37
9	S	727	TYR	C-N	5.65	1.47	1.34
3	Z	104	ARG	CZ-NH2	5.65	1.40	1.33
3	Z	441	ARG	NE-CZ	5.64	1.40	1.33
8	N	418	ASN	CB-CG	5.64	1.64	1.51
8	P	1217	ARG	CZ-NH2	5.64	1.40	1.33
9	T	556	TYR	CZ-OH	5.64	1.47	1.37
11	X	270	ALA	N-CA	5.64	1.57	1.46
9	S	823	ARG	CZ-NH1	5.64	1.40	1.33
2	0	253	GLU	CD-OE1	5.64	1.31	1.25
9	Q	456	ARG	CD-NE	5.64	1.56	1.46
9	R	737	SER	CA-CB	5.64	1.61	1.52
8	P	1179	SER	CB-OG	5.64	1.49	1.42
9	S	456	ARG	CD-NE	5.63	1.56	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	Q	616	GLU	CD-OE2	5.63	1.31	1.25
7	O	1616	GLY	N-CA	-5.63	1.37	1.46
4	D	708	GLU	CD-OE1	5.63	1.31	1.25
9	Q	791	GLU	CB-CG	5.63	1.62	1.52
3	1	441	ARG	NE-CZ	5.63	1.40	1.33
7	O	1447	TYR	CD1-CE1	-5.62	1.30	1.39
5	H	290	GLU	N-CA	-5.62	1.35	1.46
8	P	734	SER	CA-CB	5.61	1.61	1.52
8	N	1185	GLU	CG-CD	5.61	1.60	1.51
7	O	296	ARG	CZ-NH1	5.61	1.40	1.33
7	M	1324	ARG	CD-NE	5.61	1.55	1.46
8	N	734	SER	CA-CB	5.61	1.61	1.52
9	Q	727	TYR	C-N	5.61	1.47	1.34
2	Y	973	ARG	CD-NE	5.61	1.55	1.46
3	Z	1178	ARG	CD-NE	5.61	1.55	1.46
7	O	1253	ARG	CZ-NH1	5.61	1.40	1.33
3	1	1178	ARG	CD-NE	5.60	1.55	1.46
9	S	791	GLU	CB-CG	5.60	1.62	1.52
2	0	1355	GLY	CA-C	-5.60	1.42	1.51
5	B	468	GLU	CB-CG	5.59	1.62	1.52
7	M	296	ARG	CZ-NH1	5.59	1.40	1.33
11	V	270	ALA	N-CA	5.59	1.57	1.46
3	1	664	PHE	CG-CD2	5.59	1.47	1.38
7	O	1609	SER	CA-CB	5.59	1.61	1.52
7	M	1616	GLY	N-CA	-5.58	1.37	1.46
3	1	948	ARG	CZ-NH1	5.58	1.40	1.33
5	H	468	GLU	CB-CG	5.58	1.62	1.52
7	O	721	SER	CA-CB	5.58	1.61	1.52
8	N	1253	GLU	CD-OE1	5.58	1.31	1.25
3	1	128	GLU	CD-OE2	5.58	1.31	1.25
3	Z	1330	GLU	CG-CD	5.58	1.60	1.51
2	0	1319	GLU	CG-CD	5.58	1.60	1.51
8	P	526	GLY	CA-C	-5.58	1.43	1.51
2	Y	253	GLU	CD-OE1	5.57	1.31	1.25
9	Q	547	TYR	CZ-OH	5.57	1.47	1.37
2	Y	491	ARG	NE-CZ	5.57	1.40	1.33
2	0	491	ARG	NE-CZ	5.57	1.40	1.33
8	P	330	TYR	CG-CD2	5.57	1.46	1.39
8	N	330	TYR	CG-CD2	5.56	1.46	1.39
8	P	1185	GLU	CG-CD	5.56	1.60	1.51
9	R	225	SER	CA-CB	5.55	1.61	1.52
2	0	1170	ARG	NE-CZ	5.54	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	1628	GLU	CB-CG	5.54	1.62	1.52
9	T	737	SER	CA-CB	5.54	1.61	1.52
3	Z	664	PHE	CG-CD2	5.54	1.47	1.38
3	Z	594	TYR	CG-CD1	5.54	1.46	1.39
2	Y	1432	GLU	CG-CD	5.54	1.60	1.51
3	Z	541	SER	N-CA	-5.54	1.35	1.46
3	Z	948	ARG	CZ-NH1	5.54	1.40	1.33
3	1	1217	GLU	CD-OE2	-5.53	1.19	1.25
2	0	1432	GLU	CG-CD	5.53	1.60	1.51
8	N	152	TYR	CE2-CZ	5.53	1.45	1.38
2	0	973	ARG	CD-NE	5.53	1.55	1.46
9	S	533	ARG	CZ-NH2	5.53	1.40	1.33
5	B	290	GLU	N-CA	-5.53	1.35	1.46
8	N	1628	GLU	CB-CG	5.53	1.62	1.52
3	Z	1217	GLU	CD-OE2	-5.52	1.19	1.25
3	Z	620	VAL	CB-CG2	5.52	1.64	1.52
8	P	685	TYR	CA-CB	5.52	1.66	1.53
8	N	551	ASN	N-CA	-5.51	1.35	1.46
2	0	851	GLU	CG-CD	5.51	1.60	1.51
3	1	541	SER	N-CA	-5.51	1.35	1.46
8	P	1253	GLU	CD-OE1	5.51	1.31	1.25
8	P	551	ASN	N-CA	-5.51	1.35	1.46
8	P	956	PHE	CE2-CZ	5.51	1.47	1.37
9	S	547	TYR	CZ-OH	5.50	1.47	1.37
2	Y	851	GLU	CG-CD	5.49	1.60	1.51
9	S	408	ARG	CZ-NH2	5.49	1.40	1.33
9	Q	533	ARG	CZ-NH2	5.49	1.40	1.33
3	1	594	TYR	CG-CD1	5.49	1.46	1.39
9	Q	408	ARG	CZ-NH2	5.49	1.40	1.33
2	Y	1170	ARG	NE-CZ	5.49	1.40	1.33
6	I	278	GLU	CG-CD	5.49	1.60	1.51
9	S	386	TYR	CE1-CZ	5.49	1.45	1.38
7	M	1171	SER	C-N	5.48	1.43	1.33
3	1	620	VAL	CB-CG2	5.48	1.64	1.52
6	C	278	GLU	CG-CD	5.48	1.60	1.51
7	M	1609	SER	CA-CB	5.48	1.61	1.52
8	N	1488	SER	CA-CB	5.48	1.61	1.52
9	R	752	SER	CA-CB	5.48	1.61	1.52
8	P	1058	GLU	CD-OE1	5.48	1.31	1.25
3	Z	1291	LYS	N-CA	-5.48	1.35	1.46
7	M	1530	GLU	CD-OE2	5.48	1.31	1.25
6	F	445	GLU	CG-CD	5.47	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	N	1142	PHE	CG-CD2	5.47	1.47	1.38
3	1	1291	LYS	N-CA	-5.47	1.35	1.46
8	N	685	TYR	CA-CB	5.47	1.66	1.53
7	O	839	SER	CA-CB	5.47	1.61	1.52
8	P	1467	SER	CA-CB	-5.47	1.44	1.52
7	O	1647	ARG	CD-NE	5.47	1.55	1.46
3	1	586	TYR	CG-CD2	5.46	1.46	1.39
8	N	956	PHE	CE2-CZ	5.46	1.47	1.37
7	M	1243	GLU	CG-CD	5.45	1.60	1.51
7	O	696	PHE	CE1-CZ	5.45	1.47	1.37
9	T	547	TYR	CD2-CE2	5.45	1.47	1.39
9	S	308	PHE	CG-CD1	5.45	1.47	1.38
2	Y	408	ARG	CZ-NH2	5.45	1.40	1.33
2	0	1389	GLU	CD-OE2	5.45	1.31	1.25
2	Y	995	PHE	CE1-CZ	5.45	1.47	1.37
9	T	533	ARG	CZ-NH2	5.45	1.40	1.33
3	1	1283	PHE	CG-CD2	5.45	1.47	1.38
7	M	839	SER	CA-CB	5.44	1.61	1.52
7	O	1171	SER	C-N	5.44	1.42	1.33
9	S	822	TYR	CZ-OH	5.44	1.47	1.37
8	P	152	TYR	CE2-CZ	5.44	1.45	1.38
8	N	888	TYR	CZ-OH	5.43	1.47	1.37
3	1	1087	ARG	CZ-NH2	5.43	1.40	1.33
7	O	1662	SER	CB-OG	-5.43	1.35	1.42
9	R	477	TYR	CE2-CZ	5.43	1.45	1.38
2	0	995	PHE	CE1-CZ	5.42	1.47	1.37
7	M	696	PHE	CE1-CZ	5.42	1.47	1.37
9	R	547	TYR	CD2-CE2	5.42	1.47	1.39
8	P	888	TYR	CZ-OH	5.42	1.47	1.37
8	N	1058	GLU	CD-OE1	5.42	1.31	1.25
9	Q	308	PHE	CG-CD1	5.42	1.46	1.38
9	T	612	HIS	CB-CG	5.42	1.59	1.50
9	S	367	PHE	CD2-CE2	5.41	1.50	1.39
9	R	533	ARG	CZ-NH2	5.41	1.40	1.33
7	M	828	PHE	CG-CD2	5.41	1.46	1.38
4	G	797	LEU	CA-CB	5.41	1.66	1.53
8	P	1488	SER	CA-CB	5.41	1.61	1.52
7	O	295	ARG	CZ-NH2	5.41	1.40	1.33
7	O	1530	GLU	CD-OE2	5.41	1.31	1.25
3	Z	1283	PHE	CG-CD2	5.41	1.46	1.38
7	M	1647	ARG	CD-NE	5.40	1.55	1.46
7	O	1243	GLU	CG-CD	5.40	1.60	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	1389	GLU	CD-OE2	5.40	1.31	1.25
3	Z	130	GLY	N-CA	-5.40	1.38	1.46
6	F	447	PHE	CB-CG	5.40	1.60	1.51
8	P	1142	PHE	CG-CD2	5.40	1.46	1.38
3	Z	586	TYR	CG-CD2	5.39	1.46	1.39
9	Q	367	PHE	CD2-CE2	5.39	1.50	1.39
8	N	1467	SER	CA-CB	-5.39	1.44	1.52
9	Q	822	TYR	CZ-OH	5.39	1.47	1.37
6	L	447	PHE	CB-CG	5.39	1.60	1.51
7	M	69	GLU	CG-CD	5.39	1.60	1.51
8	P	38	ALA	C-N	5.39	1.46	1.34
7	O	228	PHE	CG-CD1	5.39	1.46	1.38
4	A	797	LEU	CA-CB	5.38	1.66	1.53
9	T	752	SER	CA-CB	5.38	1.61	1.52
2	0	408	ARG	CZ-NH2	5.38	1.40	1.33
7	M	1662	SER	CB-OG	-5.38	1.35	1.42
7	O	828	PHE	CG-CD2	5.38	1.46	1.38
2	Y	1317	TYR	CG-CD1	5.37	1.46	1.39
11	V	360	TYR	CE1-CZ	5.37	1.45	1.38
2	0	669	PHE	CG-CD2	5.37	1.46	1.38
8	N	38	ALA	C-N	5.37	1.46	1.34
8	N	921	SER	CA-CB	5.37	1.60	1.52
9	R	612	HIS	CB-CG	5.37	1.59	1.50
5	K	411	ARG	CZ-NH2	5.37	1.40	1.33
8	P	921	SER	CA-CB	5.37	1.60	1.52
3	Z	935	TYR	CE1-CZ	5.36	1.45	1.38
9	R	226	ARG	CD-NE	5.36	1.55	1.46
3	Z	1087	ARG	CZ-NH2	5.36	1.40	1.33
7	O	1513	TYR	CG-CD1	5.36	1.46	1.39
6	L	445	GLU	CG-CD	5.35	1.59	1.51
8	N	451	GLU	CB-CG	5.35	1.62	1.52
7	M	791	PHE	CG-CD2	5.35	1.46	1.38
7	O	527	TYR	CE1-CZ	5.34	1.45	1.38
7	M	1650	GLU	CG-CD	5.34	1.59	1.51
7	O	69	GLU	CG-CD	5.34	1.59	1.51
3	1	130	GLY	N-CA	-5.34	1.38	1.46
11	X	276	TYR	CB-CG	5.34	1.59	1.51
11	X	360	TYR	CE1-CZ	5.34	1.45	1.38
9	Q	386	TYR	CE1-CZ	5.33	1.45	1.38
11	X	276	TYR	CE1-CZ	5.33	1.45	1.38
2	Y	224	PHE	CG-CD2	5.33	1.46	1.38
9	T	98	PRO	CA-CB	-5.33	1.42	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	V	276	TYR	CB-CG	5.33	1.59	1.51
9	Q	539	ALA	CA-CB	5.33	1.63	1.52
3	1	935	TYR	CE1-CZ	5.33	1.45	1.38
7	M	413	VAL	CB-CG2	5.32	1.64	1.52
9	S	539	ALA	CA-CB	5.32	1.63	1.52
5	E	448	GLU	CD-OE2	-5.32	1.19	1.25
7	M	295	ARG	CZ-NH2	5.32	1.40	1.33
5	E	411	ARG	CZ-NH2	5.32	1.40	1.33
7	O	549	GLU	CD-OE2	5.32	1.31	1.25
4	A	808	ASP	CG-OD1	5.32	1.37	1.25
7	M	1513	TYR	CG-CD1	5.32	1.46	1.39
2	0	224	PHE	CG-CD2	5.32	1.46	1.38
2	Y	1342	GLU	CD-OE1	5.31	1.31	1.25
7	M	692	TYR	CE1-CZ	5.31	1.45	1.38
7	O	692	TYR	CE1-CZ	5.31	1.45	1.38
9	T	595	ARG	CD-NE	5.31	1.55	1.46
9	R	595	ARG	CD-NE	5.31	1.55	1.46
7	O	420	THR	N-CA	-5.31	1.35	1.46
8	P	451	GLU	CB-CG	5.31	1.62	1.52
7	M	1160	TYR	CE1-CZ	5.30	1.45	1.38
7	O	884	GLU	CB-CG	5.30	1.62	1.52
9	R	98	PRO	CA-CB	-5.30	1.43	1.53
2	0	1317	TYR	CG-CD1	5.30	1.46	1.39
3	1	599	LEU	CA-CB	5.30	1.66	1.53
3	Z	599	LEU	CA-CB	5.30	1.66	1.53
6	L	283	TYR	CG-CD2	5.30	1.46	1.39
7	O	413	VAL	CB-CG2	5.30	1.64	1.52
9	S	338	PHE	CB-CG	5.29	1.60	1.51
7	O	1448	GLY	CA-C	-5.29	1.43	1.51
7	M	228	PHE	CG-CD1	5.29	1.46	1.38
7	O	1366	ARG	CA-CB	5.29	1.65	1.53
8	N	916	TYR	CZ-OH	5.28	1.46	1.37
2	0	380	TYR	CE1-CZ	5.28	1.45	1.38
9	T	214	ASN	CB-CG	5.28	1.63	1.51
3	Z	1164	PHE	CA-CB	5.28	1.65	1.53
9	R	222	PHE	CG-CD2	5.28	1.46	1.38
9	T	546	ARG	NE-CZ	5.28	1.40	1.33
7	O	791	PHE	CG-CD2	5.28	1.46	1.38
7	O	1650	GLU	CG-CD	5.28	1.59	1.51
7	M	598	GLU	CG-CD	5.27	1.59	1.51
9	T	477	TYR	CE2-CZ	5.27	1.45	1.38
9	Q	728	PHE	CG-CD2	5.27	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	G	808	ASP	CG-OD1	5.27	1.37	1.25
7	M	1366	ARG	CA-CB	5.27	1.65	1.53
6	F	283	TYR	CG-CD2	5.27	1.46	1.39
9	R	546	ARG	NE-CZ	5.26	1.39	1.33
3	1	1105	GLU	CB-CG	5.26	1.62	1.52
7	O	598	GLU	CG-CD	5.26	1.59	1.51
9	T	226	ARG	CD-NE	5.26	1.55	1.46
3	1	1164	PHE	CA-CB	5.26	1.65	1.53
7	M	782	LYS	CA-CB	5.26	1.65	1.53
7	M	1448	GLY	CA-C	-5.25	1.43	1.51
9	R	469	TYR	CE2-CZ	5.25	1.45	1.38
7	O	1426	VAL	CB-CG2	5.25	1.63	1.52
7	O	486	TYR	CE2-CZ	5.25	1.45	1.38
7	O	782	LYS	CA-CB	5.25	1.65	1.53
2	Y	669	PHE	CG-CD2	5.25	1.46	1.38
3	Z	593	GLN	CG-CD	5.24	1.63	1.51
8	P	888	TYR	CG-CD1	5.24	1.46	1.39
8	P	916	TYR	CZ-OH	5.24	1.46	1.37
8	N	204	VAL	N-CA	-5.23	1.35	1.46
8	N	1062	ARG	CZ-NH2	5.23	1.39	1.33
2	Y	380	TYR	CE1-CZ	5.23	1.45	1.38
9	T	691	ARG	NE-CZ	5.23	1.39	1.33
3	Z	1228	PHE	CE2-CZ	5.23	1.47	1.37
7	M	1426	VAL	CB-CG2	5.23	1.63	1.52
9	R	214	ASN	CB-CG	5.22	1.63	1.51
8	P	204	VAL	N-CA	-5.22	1.35	1.46
3	Z	710	TYR	CE2-CZ	5.22	1.45	1.38
8	P	43	PHE	CG-CD2	5.22	1.46	1.38
3	Z	284	TRP	CZ2-CH2	5.22	1.47	1.37
3	Z	948	ARG	NE-CZ	5.22	1.39	1.33
9	R	516	PHE	CB-CG	-5.22	1.42	1.51
7	M	420	THR	N-CA	-5.22	1.35	1.46
7	M	527	TYR	CE1-CZ	5.22	1.45	1.38
9	Q	338	PHE	CB-CG	5.22	1.60	1.51
9	T	222	PHE	CG-CD2	5.22	1.46	1.38
9	T	469	TYR	CE2-CZ	5.22	1.45	1.38
8	N	43	PHE	CG-CD2	5.21	1.46	1.38
3	Z	1336	VAL	C-N	5.21	1.46	1.34
9	Q	649	GLU	CD-OE1	5.21	1.31	1.25
7	M	884	GLU	CB-CG	5.21	1.62	1.52
5	H	437	TRP	CE2-CZ2	-5.21	1.30	1.39
2	Y	858	ASP	CB-CG	5.21	1.62	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	Y	914	TYR	CZ-OH	5.21	1.46	1.37
3	1	593	GLN	CG-CD	5.21	1.63	1.51
3	1	569	GLU	CG-CD	5.20	1.59	1.51
4	G	667	GLN	CA-CB	5.20	1.65	1.53
3	1	710	TYR	CE2-CZ	5.20	1.45	1.38
7	O	1090	PRO	N-CD	-5.20	1.40	1.47
5	E	383	SER	CA-CB	5.20	1.60	1.52
2	0	107	TYR	CZ-OH	5.20	1.46	1.37
3	1	1336	VAL	C-N	5.20	1.46	1.34
9	R	691	ARG	NE-CZ	5.20	1.39	1.33
3	1	1228	PHE	CE2-CZ	5.19	1.47	1.37
7	O	1253	ARG	CD-NE	5.19	1.55	1.46
8	P	1524	TYR	CB-CG	5.19	1.59	1.51
8	N	184	ASP	CB-CG	5.19	1.62	1.51
5	K	448	GLU	CD-OE2	-5.19	1.20	1.25
8	P	184	ASP	CB-CG	5.19	1.62	1.51
3	Z	569	GLU	CG-CD	5.19	1.59	1.51
8	N	1524	TYR	CB-CG	5.19	1.59	1.51
7	M	549	GLU	CD-OE2	5.18	1.31	1.25
3	Z	1105	GLU	CB-CG	5.18	1.61	1.52
5	B	354	GLY	N-CA	-5.18	1.38	1.46
7	M	1269	GLU	CD-OE1	5.18	1.31	1.25
5	H	353	TYR	CG-CD1	5.18	1.45	1.39
5	H	354	GLY	N-CA	-5.18	1.38	1.46
8	N	1467	SER	CB-OG	5.18	1.49	1.42
2	Y	107	TYR	CZ-OH	5.18	1.46	1.37
7	O	1160	TYR	CE1-CZ	5.18	1.45	1.38
7	M	1366	ARG	NE-CZ	5.17	1.39	1.33
9	S	548	SER	CA-CB	5.17	1.60	1.52
5	B	353	TYR	CG-CD1	5.17	1.45	1.39
2	0	1342	GLU	CD-OE1	5.17	1.31	1.25
7	O	523	ARG	NE-CZ	5.17	1.39	1.33
9	Q	548	SER	CA-CB	5.17	1.60	1.52
2	0	125	SER	CA-CB	5.17	1.60	1.52
11	V	276	TYR	CE1-CZ	5.17	1.45	1.38
7	O	1366	ARG	NE-CZ	5.17	1.39	1.33
11	X	347	TYR	CZ-OH	5.17	1.46	1.37
2	Y	1181	PHE	CG-CD1	5.16	1.46	1.38
7	M	1263	SER	CA-CB	5.16	1.60	1.52
8	N	888	TYR	CG-CD1	5.16	1.45	1.39
8	N	1259	PHE	CG-CD2	-5.16	1.31	1.38
7	O	832	PHE	CG-CD2	5.16	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	667	GLN	CA-CB	5.16	1.65	1.53
6	C	458	ALA	CA-CB	5.16	1.63	1.52
7	O	1469	ARG	CZ-NH2	5.16	1.39	1.33
7	O	416	TYR	CG-CD1	5.16	1.45	1.39
11	V	347	TYR	CZ-OH	5.16	1.46	1.37
3	Z	1382	TYR	CE1-CZ	5.16	1.45	1.38
2	0	657	GLU	CD-OE1	5.15	1.31	1.25
3	Z	402	ARG	CD-NE	5.15	1.55	1.46
2	0	1181	PHE	CG-CD1	5.15	1.46	1.38
7	M	342	TYR	CE1-CZ	5.15	1.45	1.38
7	M	510	PHE	CE1-CZ	5.15	1.47	1.37
2	0	762	ASP	CA-CB	5.15	1.65	1.53
2	0	914	TYR	CZ-OH	5.15	1.46	1.37
8	N	934	GLU	CD-OE1	5.15	1.31	1.25
9	S	644	TYR	CG-CD1	5.14	1.45	1.39
3	1	402	ARG	CD-NE	5.14	1.55	1.46
9	T	516	PHE	CB-CG	-5.14	1.42	1.51
7	M	486	TYR	CE2-CZ	5.14	1.45	1.38
7	M	1469	ARG	CZ-NH2	5.14	1.39	1.33
3	1	284	TRP	CZ2-CH2	5.14	1.47	1.37
5	B	437	TRP	CE2-CZ2	-5.14	1.31	1.39
8	N	733	ARG	CD-NE	5.14	1.55	1.46
3	1	1382	TYR	CE1-CZ	5.14	1.45	1.38
8	P	733	ARG	CD-NE	5.14	1.55	1.46
3	Z	440	ARG	CD-NE	5.13	1.55	1.46
9	S	728	PHE	CG-CD2	5.13	1.46	1.38
3	1	579	TYR	CG-CD1	5.13	1.45	1.39
6	I	469	SER	CB-OG	5.13	1.49	1.42
8	P	1062	ARG	CZ-NH2	5.13	1.39	1.33
8	P	1467	SER	CB-OG	5.13	1.49	1.42
7	M	1263	SER	N-CA	-5.13	1.36	1.46
7	M	482	PHE	CG-CD2	5.12	1.46	1.38
9	S	226	ARG	CZ-NH1	5.12	1.39	1.33
7	M	417	SER	CA-CB	5.12	1.60	1.52
7	M	651	GLY	CA-C	5.12	1.60	1.51
8	P	1259	PHE	CG-CD2	-5.12	1.31	1.38
9	Q	638	TYR	CG-CD1	5.12	1.45	1.39
2	0	858	ASP	CB-CG	5.12	1.62	1.51
4	A	663	ASN	CB-CG	5.11	1.62	1.51
7	O	510	PHE	CE1-CZ	5.11	1.47	1.37
7	O	1263	SER	N-CA	-5.11	1.36	1.46
2	Y	657	GLU	CD-OE1	5.11	1.31	1.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	M	880	GLU	CB-CG	5.11	1.61	1.52
7	O	342	TYR	CE1-CZ	5.11	1.45	1.38
8	P	375	TYR	CE1-CZ	5.11	1.45	1.38
2	Y	1205	SER	CA-CB	5.11	1.60	1.52
5	K	344	SER	CA-CB	5.11	1.60	1.52
3	Z	1108	PHE	CB-CG	5.11	1.60	1.51
5	E	446	ARG	NE-CZ	5.11	1.39	1.33
7	O	880	GLU	CB-CG	5.11	1.61	1.52
2	Y	397	TYR	CG-CD1	5.11	1.45	1.39
8	P	1599	SER	CA-CB	5.11	1.60	1.52
2	0	1021	TYR	CB-CG	-5.10	1.44	1.51
7	O	962	ARG	CZ-NH2	5.10	1.39	1.33
7	O	1269	GLU	CD-OE1	5.10	1.31	1.25
8	N	562	TRP	NE1-CE2	5.10	1.44	1.37
7	O	302	PHE	N-CA	-5.10	1.36	1.46
8	N	375	TYR	CE1-CZ	5.10	1.45	1.38
5	K	383	SER	CA-CB	5.10	1.60	1.52
7	M	302	PHE	N-CA	-5.10	1.36	1.46
7	M	416	TYR	CG-CD1	5.10	1.45	1.39
7	M	753	PHE	CG-CD2	5.10	1.46	1.38
7	M	1641	PHE	CE2-CZ	5.10	1.47	1.37
3	Z	806	LYS	CB-CG	5.09	1.66	1.52
9	S	649	GLU	CD-OE1	5.09	1.31	1.25
2	Y	1021	TYR	CB-CG	-5.09	1.44	1.51
7	M	523	ARG	NE-CZ	5.09	1.39	1.33
3	1	440	ARG	CD-NE	5.09	1.55	1.46
6	I	458	ALA	CA-CB	5.09	1.63	1.52
2	Y	1134	SER	CB-OG	5.09	1.48	1.42
7	M	489	TYR	CB-CG	5.09	1.59	1.51
8	N	1368	SER	CB-OG	5.09	1.48	1.42
7	O	546	TYR	CG-CD2	5.09	1.45	1.39
8	P	705	TYR	CG-CD1	5.09	1.45	1.39
6	C	469	SER	CB-OG	5.09	1.48	1.42
7	M	320	GLU	CB-CG	5.09	1.61	1.52
9	R	811	ARG	CZ-NH1	5.09	1.39	1.33
4	G	663	ASN	CB-CG	5.09	1.62	1.51
9	R	249	ARG	CD-NE	5.08	1.55	1.46
3	Z	1042	ARG	NE-CZ	5.08	1.39	1.33
8	N	1599	SER	CA-CB	5.08	1.60	1.52
3	1	1108	PHE	CB-CG	5.08	1.59	1.51
9	T	598	ALA	CA-CB	5.08	1.63	1.52
7	M	832	PHE	CG-CD2	5.08	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	P	934	GLU	CD-OE1	5.08	1.31	1.25
7	O	651	GLY	CA-C	5.08	1.59	1.51
9	T	215	TYR	CG-CD1	5.08	1.45	1.39
5	B	339	MET	CA-CB	5.08	1.65	1.53
7	M	1253	ARG	CD-NE	5.08	1.55	1.46
8	N	1463	SER	CA-CB	5.08	1.60	1.52
9	Q	226	ARG	CZ-NH1	5.08	1.39	1.33
5	H	339	MET	CA-CB	5.08	1.65	1.53
2	0	397	TYR	CG-CD1	5.08	1.45	1.39
2	0	1205	SER	CA-CB	5.08	1.60	1.52
8	N	1392	PHE	CE2-CZ	5.07	1.47	1.37
3	Z	966	PHE	CE1-CZ	5.07	1.47	1.37
7	O	785	TYR	CE2-CZ	5.07	1.45	1.38
9	T	599	ARG	CD-NE	5.07	1.55	1.46
8	N	1240	PHE	C-N	5.07	1.42	1.33
9	Q	644	TYR	CG-CD1	5.07	1.45	1.39
3	1	806	LYS	CB-CG	5.07	1.66	1.52
8	N	1251	TYR	CA-CB	5.07	1.65	1.53
9	R	277	TYR	CZ-OH	5.07	1.46	1.37
10	U	308	TYR	CG-CD2	5.07	1.45	1.39
3	Z	579	TYR	CG-CD1	5.07	1.45	1.39
2	0	1261	ARG	NE-CZ	5.06	1.39	1.33
3	1	966	PHE	CE1-CZ	5.06	1.47	1.37
7	M	546	TYR	CG-CD2	5.06	1.45	1.39
7	M	537	PRO	N-CA	-5.06	1.38	1.47
9	Q	366	SER	CB-OG	-5.06	1.35	1.42
3	1	241	THR	C-N	5.06	1.45	1.34
5	K	433	GLU	N-CA	5.06	1.56	1.46
7	O	537	PRO	N-CA	-5.06	1.38	1.47
7	O	1263	SER	CA-CB	5.06	1.60	1.52
4	J	789	GLU	CB-CG	5.06	1.61	1.52
7	M	19	GLU	CG-CD	5.05	1.59	1.51
9	R	528	PRO	N-CD	-5.05	1.40	1.47
7	O	188	ARG	CZ-NH1	5.05	1.39	1.33
7	O	1641	PHE	CE2-CZ	5.05	1.47	1.37
9	R	598	ALA	CA-CB	5.05	1.63	1.52
11	V	363	PRO	N-CD	-5.05	1.40	1.47
4	D	772	VAL	CB-CG2	5.05	1.63	1.52
4	D	789	GLU	CB-CG	5.05	1.61	1.52
7	M	980	ASP	CB-CG	5.05	1.62	1.51
4	J	772	VAL	CB-CG2	5.05	1.63	1.52
9	R	215	TYR	CG-CD1	5.05	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	O	489	TYR	CB-CG	5.05	1.59	1.51
2	Y	125	SER	CA-CB	5.05	1.60	1.52
2	0	650	TYR	CG-CD1	5.05	1.45	1.39
7	M	962	ARG	CZ-NH2	5.04	1.39	1.33
7	M	1097	TYR	CG-CD2	5.04	1.45	1.39
7	O	980	ASP	CB-CG	5.04	1.62	1.51
2	Y	762	ASP	CA-CB	5.04	1.65	1.53
8	N	705	TYR	CG-CD1	5.04	1.45	1.39
7	O	482	PHE	CG-CD2	5.04	1.46	1.38
9	T	277	TYR	CZ-OH	5.04	1.46	1.37
3	Z	513	LYS	C-O	5.04	1.32	1.23
8	P	1251	TYR	CA-CB	5.04	1.65	1.53
2	Y	278	ARG	CZ-NH1	5.04	1.39	1.33
7	O	1405	PHE	CG-CD2	5.04	1.46	1.38
8	P	562	TRP	NE1-CE2	5.04	1.44	1.37
9	T	811	ARG	CZ-NH1	5.04	1.39	1.33
7	M	69	GLU	CA-CB	5.03	1.65	1.53
7	M	785	TYR	CE2-CZ	5.03	1.45	1.38
7	O	320	GLU	CB-CG	5.03	1.61	1.52
8	P	1368	SER	CB-OG	5.03	1.48	1.42
5	E	344	SER	CA-CB	5.03	1.60	1.52
9	R	615	ASP	CB-CG	5.03	1.62	1.51
3	1	837	ASP	CB-CG	5.03	1.62	1.51
9	T	615	ASP	CB-CG	5.03	1.62	1.51
11	X	377	PHE	CG-CD2	5.03	1.46	1.38
9	S	638	TYR	CG-CD1	5.03	1.45	1.39
3	Z	708	ARG	CD-NE	5.03	1.54	1.46
7	M	1405	PHE	CG-CD2	5.03	1.46	1.38
3	Z	935	TYR	CG-CD1	5.02	1.45	1.39
3	1	1042	ARG	NE-CZ	5.02	1.39	1.33
7	M	703	TYR	CA-C	-5.02	1.39	1.52
2	0	1155	ARG	CD-NE	5.02	1.54	1.46
9	T	249	ARG	CD-NE	5.02	1.54	1.46
7	M	242	ALA	CA-CB	5.02	1.62	1.52
3	Z	1212	PRO	N-CD	-5.02	1.40	1.47
9	R	385	GLU	CB-CG	5.02	1.61	1.52
3	1	513	LYS	C-O	5.02	1.32	1.23
3	1	935	TYR	CG-CD1	5.02	1.45	1.39
7	O	703	TYR	CA-C	-5.02	1.40	1.52
2	Y	1348	ARG	CD-NE	5.02	1.54	1.46
8	P	401	ALA	CA-C	-5.02	1.40	1.52
9	S	366	SER	CB-OG	-5.02	1.35	1.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
11	X	363	PRO	N-CD	-5.01	1.40	1.47
9	R	599	ARG	CD-NE	5.01	1.54	1.46
3	Z	1136	ARG	CZ-NH2	5.01	1.39	1.33
8	P	1392	PHE	CE2-CZ	5.01	1.46	1.37
9	S	708	VAL	CB-CG2	5.01	1.63	1.52
3	Z	219	GLU	CG-CD	-5.01	1.44	1.51
9	S	826	ARG	CD-NE	5.01	1.54	1.46
9	R	408	ARG	NE-CZ	5.01	1.39	1.33
2	0	456	ASN	CA-C	-5.01	1.40	1.52
9	T	226	ARG	NE-CZ	5.01	1.39	1.33
3	Z	385	ARG	NE-CZ	5.00	1.39	1.33
3	Z	837	ASP	CB-CG	5.00	1.62	1.51
8	N	888	TYR	CG-CD2	5.00	1.45	1.39
6	I	272	GLN	CG-CD	5.00	1.62	1.51
7	M	1090	PRO	N-CD	-5.00	1.40	1.47
7	O	242	ALA	CA-CB	5.00	1.62	1.52

All (3091) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	323	LEU	CA-CB-CG	23.92	170.32	115.30
9	Q	533	ARG	NE-CZ-NH2	-21.58	109.51	120.30
9	S	533	ARG	NE-CZ-NH2	-21.53	109.53	120.30
9	Q	533	ARG	NE-CZ-NH1	20.88	130.74	120.30
9	S	533	ARG	NE-CZ-NH1	20.78	130.69	120.30
2	0	124	ARG	NE-CZ-NH1	20.29	130.44	120.30
2	Y	124	ARG	NE-CZ-NH1	20.20	130.40	120.30
3	Z	841	ARG	NE-CZ-NH2	-19.76	110.42	120.30
7	O	1484	ARG	NE-CZ-NH1	19.76	130.18	120.30
3	1	841	ARG	NE-CZ-NH2	-19.74	110.43	120.30
7	M	1484	ARG	NE-CZ-NH1	19.62	130.11	120.30
9	Q	629	ARG	NE-CZ-NH1	18.78	129.69	120.30
9	S	629	ARG	NE-CZ-NH1	18.72	129.66	120.30
8	N	1062	ARG	NE-CZ-NH2	-18.53	111.03	120.30
8	P	1062	ARG	NE-CZ-NH2	-18.46	111.07	120.30
5	K	411	ARG	NE-CZ-NH1	18.09	129.34	120.30
5	E	411	ARG	NE-CZ-NH1	18.03	129.31	120.30
7	O	1154	ARG	NE-CZ-NH1	17.80	129.20	120.30
7	M	1154	ARG	NE-CZ-NH1	17.76	129.18	120.30
9	S	408	ARG	NE-CZ-NH1	17.74	129.17	120.30
9	Q	408	ARG	NE-CZ-NH1	17.67	129.13	120.30
2	0	1185	TYR	CB-CG-CD1	-17.60	110.44	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	1185	TYR	CB-CG-CD1	-17.57	110.45	121.00
8	N	68	HIS	N-CA-CB	17.57	142.22	110.60
9	R	422	ARG	NE-CZ-NH1	17.17	128.89	120.30
9	T	422	ARG	NE-CZ-NH1	17.09	128.84	120.30
8	P	68	HIS	N-CA-CB	17.06	141.32	110.60
6	I	325	TYR	CB-CG-CD2	-16.45	111.13	121.00
7	M	1643	ARG	NE-CZ-NH2	-16.41	112.09	120.30
7	O	1643	ARG	NE-CZ-NH2	-16.37	112.12	120.30
6	C	325	TYR	CB-CG-CD2	-16.35	111.19	121.00
9	S	456	ARG	NE-CZ-NH2	-16.21	112.20	120.30
9	Q	456	ARG	NE-CZ-NH2	-16.18	112.21	120.30
5	H	411	ARG	NE-CZ-NH1	16.00	128.30	120.30
5	B	411	ARG	NE-CZ-NH1	15.99	128.30	120.30
7	M	1569	TYR	CB-CG-CD1	15.91	130.55	121.00
7	O	1569	TYR	CB-CG-CD1	15.91	130.55	121.00
3	1	1005	TYR	CB-CG-CD2	-15.86	111.49	121.00
8	N	1062	ARG	NE-CZ-NH1	15.80	128.20	120.30
8	P	1062	ARG	NE-CZ-NH1	15.80	128.20	120.30
3	Z	1005	TYR	CB-CG-CD2	-15.78	111.53	121.00
7	O	1545	ARG	NE-CZ-NH1	15.74	128.17	120.30
3	Z	969	ARG	NE-CZ-NH2	15.64	128.12	120.30
3	Z	1187	TYR	CB-CG-CD1	15.62	130.38	121.00
7	M	1545	ARG	NE-CZ-NH1	15.61	128.10	120.30
3	1	969	ARG	NE-CZ-NH2	15.60	128.10	120.30
3	1	1187	TYR	CB-CG-CD1	15.57	130.34	121.00
3	Z	1382	TYR	CB-CG-CD1	-15.48	111.71	121.00
3	1	1382	TYR	CB-CG-CD1	-15.43	111.75	121.00
3	1	1005	TYR	CB-CG-CD1	15.26	130.16	121.00
3	Z	1005	TYR	CB-CG-CD1	15.18	130.11	121.00
5	B	323	LEU	CB-CG-CD2	15.16	136.78	111.00
3	1	1087	ARG	NE-CZ-NH2	-15.10	112.75	120.30
3	Z	1087	ARG	NE-CZ-NH2	-15.02	112.79	120.30
7	M	106	TYR	CB-CG-CD2	-14.97	112.02	121.00
7	O	106	TYR	CB-CG-CD2	-14.83	112.10	121.00
3	1	1087	ARG	NE-CZ-NH1	14.81	127.71	120.30
9	S	456	ARG	NE-CZ-NH1	14.78	127.69	120.30
3	Z	1351	TYR	CB-CG-CD2	-14.70	112.18	121.00
9	Q	456	ARG	NE-CZ-NH1	14.70	127.65	120.30
3	1	1351	TYR	CB-CG-CD2	-14.65	112.21	121.00
7	O	112	TYR	CB-CG-CD1	-14.63	112.22	121.00
7	M	112	TYR	CB-CG-CD1	-14.62	112.23	121.00
3	Z	1087	ARG	NE-CZ-NH1	14.60	127.60	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1	1001	ARG	NE-CZ-NH2	-14.50	113.05	120.30
3	Z	1001	ARG	NE-CZ-NH2	-14.43	113.09	120.30
3	1	351	ARG	NE-CZ-NH1	14.36	127.48	120.30
7	M	482	PHE	CB-CG-CD1	14.33	130.83	120.80
7	M	680	PHE	CB-CG-CD2	-14.17	110.88	120.80
8	P	844	TYR	CB-CG-CD1	-14.17	112.50	121.00
7	O	482	PHE	CB-CG-CD1	14.16	130.71	120.80
8	N	844	TYR	CB-CG-CD1	-14.16	112.51	121.00
7	O	680	PHE	CB-CG-CD2	-14.09	110.94	120.80
3	Z	351	ARG	NE-CZ-NH1	14.08	127.34	120.30
8	P	109	ARG	NE-CZ-NH1	13.98	127.29	120.30
7	M	785	TYR	CB-CG-CD1	-13.91	112.66	121.00
7	O	785	TYR	CB-CG-CD1	-13.84	112.70	121.00
8	N	1158	TYR	CB-CG-CD1	-13.75	112.75	121.00
8	P	1158	TYR	CB-CG-CD1	-13.69	112.79	121.00
8	N	109	ARG	NE-CZ-NH1	13.57	127.08	120.30
3	1	1277	ARG	NE-CZ-NH2	13.55	127.08	120.30
3	1	994	ARG	NE-CZ-NH1	13.53	127.06	120.30
3	Z	1277	ARG	NE-CZ-NH2	13.51	127.05	120.30
3	1	766	PHE	CB-CG-CD1	13.50	130.25	120.80
2	0	1416	PHE	CB-CG-CD1	-13.48	111.36	120.80
3	Z	766	PHE	CB-CG-CD1	13.47	130.23	120.80
3	Z	994	ARG	NE-CZ-NH1	13.44	127.02	120.30
2	Y	1416	PHE	CB-CG-CD1	-13.30	111.49	120.80
8	N	1365	ARG	NE-CZ-NH1	13.20	126.90	120.30
2	0	615	PHE	CB-CG-CD1	13.18	130.03	120.80
8	P	1365	ARG	NE-CZ-NH1	13.17	126.88	120.30
2	Y	615	PHE	CB-CG-CD1	13.16	130.01	120.80
6	F	274	ARG	NE-CZ-NH2	13.12	126.86	120.30
8	P	733	ARG	NE-CZ-NH2	-13.09	113.76	120.30
9	S	551	ARG	NE-CZ-NH2	-12.99	113.81	120.30
8	N	1309	ARG	NE-CZ-NH2	-12.98	113.81	120.30
8	N	733	ARG	NE-CZ-NH2	-12.98	113.81	120.30
9	Q	551	ARG	NE-CZ-NH2	-12.97	113.81	120.30
6	F	389	ARG	NE-CZ-NH1	-12.95	113.82	120.30
6	L	389	ARG	NE-CZ-NH1	-12.93	113.84	120.30
7	O	1088	ARG	NE-CZ-NH1	12.92	126.76	120.30
6	L	274	ARG	NE-CZ-NH2	12.92	126.76	120.30
9	Q	629	ARG	NE-CZ-NH2	-12.90	113.85	120.30
8	P	1309	ARG	NE-CZ-NH2	-12.88	113.86	120.30
6	C	325	TYR	CB-CG-CD1	12.88	128.73	121.00
9	Q	277	TYR	CB-CG-CD1	-12.87	113.28	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	S	277	TYR	CB-CG-CD1	-12.87	113.28	121.00
6	I	325	TYR	CB-CG-CD1	12.86	128.72	121.00
2	0	1012	ARG	NE-CZ-NH2	12.85	126.72	120.30
7	M	1088	ARG	NE-CZ-NH1	12.85	126.72	120.30
9	S	422	ARG	NE-CZ-NH2	-12.81	113.89	120.30
9	S	629	ARG	NE-CZ-NH2	-12.81	113.90	120.30
2	Y	1325	PHE	CB-CG-CD1	12.79	129.75	120.80
9	S	473	ARG	NE-CZ-NH1	12.78	126.69	120.30
9	Q	422	ARG	NE-CZ-NH2	-12.74	113.93	120.30
2	Y	1012	ARG	NE-CZ-NH2	12.72	126.66	120.30
9	Q	473	ARG	NE-CZ-NH1	12.72	126.66	120.30
2	0	1325	PHE	CB-CG-CD1	12.69	129.68	120.80
7	O	228	PHE	CB-CG-CD1	-12.68	111.92	120.80
7	M	228	PHE	CB-CG-CD1	-12.67	111.93	120.80
7	M	1545	ARG	NE-CZ-NH2	-12.64	113.98	120.30
3	Z	614	TYR	CB-CG-CD2	12.63	128.58	121.00
9	R	547	TYR	CB-CG-CD1	-12.61	113.43	121.00
7	M	13	ARG	NE-CZ-NH2	-12.60	114.00	120.30
9	T	547	TYR	CB-CG-CD1	-12.58	113.45	121.00
2	0	1460	ARG	NE-CZ-NH1	12.53	126.56	120.30
3	1	614	TYR	CB-CG-CD2	12.49	128.49	121.00
2	Y	1460	ARG	NE-CZ-NH1	12.45	126.52	120.30
7	O	13	ARG	NE-CZ-NH2	-12.44	114.08	120.30
8	N	216	TYR	CB-CG-CD2	-12.38	113.57	121.00
7	O	1545	ARG	NE-CZ-NH2	-12.34	114.13	120.30
2	0	632	TYR	CB-CG-CD2	12.31	128.38	121.00
6	F	314	TYR	CB-CG-CD1	12.29	128.38	121.00
2	Y	615	PHE	CB-CG-CD2	-12.27	112.21	120.80
2	0	615	PHE	CB-CG-CD2	-12.25	112.22	120.80
3	1	621	PHE	CB-CG-CD1	-12.25	112.22	120.80
8	N	950	ARG	NE-CZ-NH2	-12.23	114.18	120.30
7	M	713	PHE	CB-CG-CD2	12.21	129.35	120.80
8	P	216	TYR	CB-CG-CD2	-12.19	113.69	121.00
7	O	713	PHE	CB-CG-CD2	12.17	129.32	120.80
6	L	314	TYR	CB-CG-CD1	12.16	128.30	121.00
8	P	950	ARG	NE-CZ-NH2	-12.12	114.24	120.30
2	Y	632	TYR	CB-CG-CD2	12.10	128.26	121.00
3	Z	621	PHE	CB-CG-CD1	-12.09	112.34	120.80
10	U	308	TYR	CB-CG-CD2	-12.06	113.76	121.00
6	L	325	TYR	CB-CG-CD2	-12.03	113.78	121.00
7	O	212	PHE	CB-CG-CD2	-12.03	112.38	120.80
10	W	308	TYR	CB-CG-CD2	-12.02	113.79	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	1185	TYR	CB-CG-CD2	12.01	128.21	121.00
7	M	1013	TYR	CB-CG-CD2	-11.99	113.81	121.00
7	M	212	PHE	CB-CG-CD2	-11.98	112.42	120.80
7	O	1013	TYR	CB-CG-CD2	-11.97	113.82	121.00
3	1	614	TYR	CB-CG-CD1	-11.96	113.82	121.00
2	Y	949	PHE	CB-CG-CD2	11.94	129.16	120.80
3	Z	614	TYR	CB-CG-CD1	-11.94	113.84	121.00
6	F	325	TYR	CB-CG-CD2	-11.90	113.86	121.00
2	0	949	PHE	CB-CG-CD2	11.87	129.11	120.80
2	0	1185	TYR	CB-CG-CD2	11.84	128.11	121.00
9	R	697	PHE	CB-CG-CD1	11.84	129.09	120.80
9	T	607	ARG	NE-CZ-NH2	-11.82	114.39	120.30
7	O	832	PHE	CB-CG-CD1	11.81	129.06	120.80
9	T	697	PHE	CB-CG-CD1	11.78	129.05	120.80
8	N	67	ASP	N-CA-C	-11.77	79.22	111.00
3	1	1060	TYR	CB-CG-CD1	11.74	128.05	121.00
9	T	747	PHE	CB-CG-CD1	-11.74	112.58	120.80
7	M	832	PHE	CB-CG-CD1	11.73	129.01	120.80
7	O	110	ARG	NE-CZ-NH1	11.73	126.17	120.30
9	R	607	ARG	NE-CZ-NH2	-11.71	114.44	120.30
9	T	209	ARG	NE-CZ-NH2	-11.71	114.45	120.30
9	R	747	PHE	CB-CG-CD1	-11.69	112.62	120.80
9	R	209	ARG	NE-CZ-NH2	-11.66	114.47	120.30
3	Z	1060	TYR	CB-CG-CD1	11.65	127.99	121.00
6	F	314	TYR	CB-CG-CD2	-11.65	114.01	121.00
2	0	1170	ARG	NE-CZ-NH2	-11.64	114.48	120.30
7	O	943	ARG	NE-CZ-NH2	-11.64	114.48	120.30
7	M	110	ARG	NE-CZ-NH1	11.61	126.10	120.30
8	N	1432	ARG	NE-CZ-NH2	11.60	126.10	120.30
9	T	217	ARG	NE-CZ-NH2	11.60	126.10	120.30
3	Z	1178	ARG	NE-CZ-NH1	11.59	126.09	120.30
3	Z	512	ARG	NE-CZ-NH2	-11.58	114.51	120.30
7	O	1195	PHE	CB-CG-CD1	11.56	128.89	120.80
2	Y	1170	ARG	NE-CZ-NH2	-11.55	114.52	120.30
3	1	1178	ARG	NE-CZ-NH1	11.55	126.08	120.30
7	O	1366	ARG	NE-CZ-NH2	-11.55	114.53	120.30
7	M	1195	PHE	CB-CG-CD1	11.54	128.88	120.80
7	M	943	ARG	NE-CZ-NH2	-11.53	114.53	120.30
8	P	1432	ARG	NE-CZ-NH2	11.53	126.06	120.30
3	1	512	ARG	NE-CZ-NH2	-11.51	114.54	120.30
6	L	314	TYR	CB-CG-CD2	-11.50	114.10	121.00
5	B	313	TYR	CB-CG-CD1	11.47	127.88	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	1521	PHE	CB-CG-CD2	-11.47	112.77	120.80
2	Y	1230	PHE	CB-CG-CD1	-11.44	112.79	120.80
8	N	1521	PHE	CB-CG-CD2	-11.44	112.79	120.80
3	Z	240	ARG	NE-CZ-NH2	-11.44	114.58	120.30
9	R	217	ARG	NE-CZ-NH2	11.43	126.02	120.30
5	H	313	TYR	CB-CG-CD1	11.41	127.85	121.00
2	0	1230	PHE	CB-CG-CD1	-11.40	112.82	120.80
8	P	89	PHE	CB-CG-CD2	-11.39	112.83	120.80
3	Z	1187	TYR	CB-CG-CD2	-11.39	114.17	121.00
7	M	1366	ARG	NE-CZ-NH2	-11.37	114.62	120.30
8	N	89	PHE	CB-CG-CD2	-11.35	112.86	120.80
3	Z	554	TYR	CB-CG-CD2	-11.33	114.20	121.00
3	1	274	PHE	CB-CG-CD2	-11.33	112.87	120.80
3	Z	274	PHE	CB-CG-CD2	-11.32	112.88	120.80
3	1	841	ARG	NE-CZ-NH1	11.31	125.95	120.30
3	1	1187	TYR	CB-CG-CD2	-11.31	114.22	121.00
9	T	811	ARG	NE-CZ-NH2	-11.30	114.65	120.30
3	Z	841	ARG	NE-CZ-NH1	11.29	125.95	120.30
7	O	1527	ARG	NE-CZ-NH1	-11.29	114.65	120.30
3	1	554	TYR	CB-CG-CD2	-11.26	114.24	121.00
7	O	171	TYR	CB-CG-CD2	-11.24	114.26	121.00
9	S	754	ARG	NE-CZ-NH2	11.23	125.92	120.30
3	1	240	ARG	NE-CZ-NH2	-11.21	114.70	120.30
7	O	1469	ARG	NE-CZ-NH1	11.18	125.89	120.30
2	Y	949	PHE	CB-CG-CD1	-11.18	112.97	120.80
9	R	811	ARG	NE-CZ-NH2	-11.17	114.72	120.30
2	0	949	PHE	CB-CG-CD1	-11.16	112.99	120.80
8	P	67	ASP	N-CA-C	-11.15	80.89	111.00
11	V	377	PHE	CB-CG-CD1	-11.14	113.00	120.80
11	X	377	PHE	CB-CG-CD1	-11.12	113.02	120.80
7	M	1469	ARG	NE-CZ-NH1	11.10	125.85	120.30
7	M	171	TYR	CB-CG-CD2	-11.08	114.35	121.00
8	N	648	ARG	NE-CZ-NH2	-11.08	114.76	120.30
9	Q	754	ARG	NE-CZ-NH2	11.06	125.83	120.30
8	N	1247	PHE	CB-CG-CD1	11.05	128.54	120.80
3	Z	1382	TYR	CB-CG-CD2	11.03	127.62	121.00
8	P	1247	PHE	CB-CG-CD1	11.02	128.52	120.80
7	M	184	ASP	CB-CG-OD2	11.01	128.21	118.30
9	S	417	ARG	NE-CZ-NH2	-10.99	114.80	120.30
7	O	228	PHE	CB-CG-CD2	10.97	128.48	120.80
7	M	1527	ARG	NE-CZ-NH1	-10.97	114.81	120.30
7	M	228	PHE	CB-CG-CD2	10.96	128.47	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	Q	650	TYR	CB-CG-CD1	10.95	127.57	121.00
3	1	853	PHE	CB-CG-CD2	-10.95	113.14	120.80
8	P	648	ARG	NE-CZ-NH2	-10.95	114.83	120.30
3	1	1382	TYR	CB-CG-CD2	10.95	127.57	121.00
7	O	184	ASP	CB-CG-OD2	10.94	128.15	118.30
7	M	188	ARG	NE-CZ-NH2	-10.93	114.84	120.30
6	F	310	ARG	NE-CZ-NH2	-10.92	114.84	120.30
7	O	188	ARG	NE-CZ-NH2	-10.87	114.86	120.30
3	Z	853	PHE	CB-CG-CD2	-10.86	113.19	120.80
8	P	1106	PHE	CB-CG-CD1	-10.86	113.20	120.80
4	A	658	TYR	CB-CG-CD2	-10.86	114.48	121.00
9	S	650	TYR	CB-CG-CD1	10.86	127.52	121.00
9	Q	417	ARG	NE-CZ-NH2	-10.84	114.88	120.30
7	M	489	TYR	CB-CG-CD1	-10.83	114.50	121.00
9	Q	691	ARG	NE-CZ-NH2	-10.83	114.89	120.30
4	G	639	ASP	CB-CG-OD1	-10.82	108.56	118.30
11	X	276	TYR	CB-CG-CD1	10.81	127.49	121.00
4	G	658	TYR	CB-CG-CD2	-10.81	114.52	121.00
2	0	1012	ARG	NE-CZ-NH1	-10.80	114.90	120.30
11	V	276	TYR	CB-CG-CD1	10.79	127.47	121.00
4	A	639	ASP	CB-CG-OD1	-10.79	108.59	118.30
8	N	1106	PHE	CB-CG-CD1	-10.77	113.26	120.80
7	O	1412	TYR	CG-CD2-CE2	-10.76	112.69	121.30
7	O	489	TYR	CB-CG-CD1	-10.75	114.55	121.00
8	N	252	TYR	CB-CG-CD1	10.73	127.44	121.00
7	M	1412	TYR	CG-CD2-CE2	-10.72	112.72	121.30
8	P	252	TYR	CB-CG-CD1	10.72	127.43	121.00
9	S	691	ARG	NE-CZ-NH2	-10.71	114.94	120.30
3	1	646	TYR	CB-CG-CD1	-10.71	114.58	121.00
5	H	469	ARG	NE-CZ-NH1	-10.71	114.95	120.30
2	0	1225	PHE	CB-CG-CD1	-10.70	113.31	120.80
6	L	310	ARG	NE-CZ-NH2	-10.69	114.95	120.30
5	B	469	ARG	NE-CZ-NH1	-10.66	114.97	120.30
2	Y	1012	ARG	NE-CZ-NH1	-10.65	114.97	120.30
3	Z	646	TYR	CB-CG-CD1	-10.65	114.61	121.00
2	0	1428	TYR	CB-CG-CD1	-10.65	114.61	121.00
3	1	106	ARG	NE-CZ-NH2	-10.65	114.98	120.30
7	M	739	ARG	NE-CZ-NH2	-10.63	114.98	120.30
7	O	1569	TYR	CB-CG-CD2	-10.60	114.64	121.00
7	O	739	ARG	NE-CZ-NH2	-10.60	115.00	120.30
2	Y	1225	PHE	CB-CG-CD1	-10.59	113.39	120.80
2	Y	1428	TYR	CB-CG-CD1	-10.58	114.65	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	L	325	TYR	CB-CG-CD1	10.57	127.34	121.00
7	O	713	PHE	CB-CG-CD1	-10.57	113.40	120.80
2	Y	201	TYR	CB-CG-CD2	10.53	127.32	121.00
6	F	325	TYR	CB-CG-CD1	10.51	127.31	121.00
7	M	713	PHE	CB-CG-CD1	-10.51	113.44	120.80
2	0	201	TYR	CB-CG-CD2	10.51	127.31	121.00
3	Z	106	ARG	NE-CZ-NH2	-10.49	115.06	120.30
7	M	1569	TYR	CB-CG-CD2	-10.46	114.72	121.00
7	O	1635	ARG	NE-CZ-NH2	-10.46	115.07	120.30
7	O	237	PHE	CB-CG-CD1	10.40	128.08	120.80
8	P	1082	PHE	CB-CG-CD1	10.40	128.08	120.80
7	M	1635	ARG	NE-CZ-NH2	-10.38	115.11	120.30
2	Y	1427	TYR	CB-CG-CD2	-10.37	114.78	121.00
8	N	1217	ARG	NE-CZ-NH1	10.35	125.47	120.30
4	J	680	TYR	CB-CG-CD1	10.35	127.21	121.00
8	P	421	PHE	CB-CG-CD2	10.34	128.04	120.80
4	D	680	TYR	CB-CG-CD1	10.32	127.19	121.00
7	M	237	PHE	CB-CG-CD1	10.32	128.02	120.80
2	0	1427	TYR	CB-CG-CD2	-10.31	114.81	121.00
3	Z	138	PHE	CB-CG-CD1	-10.29	113.59	120.80
8	N	421	PHE	CB-CG-CD2	10.27	127.99	120.80
5	B	397	ARG	NE-CZ-NH1	10.25	125.42	120.30
7	O	212	PHE	CB-CG-CD1	10.22	127.95	120.80
3	1	138	PHE	CB-CG-CD1	-10.19	113.67	120.80
7	M	212	PHE	CB-CG-CD1	10.18	127.93	120.80
8	N	1082	PHE	CB-CG-CD1	10.14	127.90	120.80
5	H	397	ARG	NE-CZ-NH1	10.13	125.36	120.30
11	V	276	TYR	CB-CG-CD2	-10.13	114.92	121.00
2	Y	696	ARG	NE-CZ-NH2	-10.12	115.24	120.30
6	C	281	ASP	CB-CG-OD2	10.12	127.41	118.30
3	Z	127	ASP	CB-CG-OD2	-10.12	109.19	118.30
8	P	1217	ARG	NE-CZ-NH1	10.11	125.36	120.30
7	M	112	TYR	CB-CG-CD2	10.11	127.07	121.00
4	A	801	PHE	CB-CG-CD2	10.11	127.88	120.80
11	X	276	TYR	CB-CG-CD2	-10.11	114.94	121.00
3	1	127	ASP	CB-CG-OD2	-10.09	109.22	118.30
8	P	922	PHE	CB-CG-CD2	10.09	127.86	120.80
11	X	377	PHE	CB-CG-CD2	10.08	127.86	120.80
7	O	418	TYR	CB-CG-CD2	-10.08	114.95	121.00
7	M	418	TYR	CB-CG-CD2	-10.07	114.96	121.00
4	G	801	PHE	CB-CG-CD2	10.06	127.84	120.80
7	O	112	TYR	CB-CG-CD2	10.05	127.03	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	922	PHE	CB-CG-CD2	10.05	127.83	120.80
7	M	671	PHE	CB-CG-CD1	-10.04	113.77	120.80
9	R	546	ARG	NE-CZ-NH1	10.04	125.32	120.30
7	O	671	PHE	CB-CG-CD1	-10.04	113.77	120.80
9	Q	551	ARG	NE-CZ-NH1	10.03	125.31	120.30
9	T	546	ARG	NE-CZ-NH1	10.02	125.31	120.30
6	I	281	ASP	CB-CG-OD2	10.01	127.31	118.30
9	S	551	ARG	NE-CZ-NH1	10.00	125.30	120.30
6	L	306	ASP	CB-CG-OD2	-9.99	109.31	118.30
3	Z	1287	PHE	CB-CG-CD1	-9.98	113.81	120.80
3	1	1351	TYR	CG-CD2-CE2	-9.98	113.31	121.30
4	G	801	PHE	CB-CG-CD1	-9.98	113.81	120.80
11	V	377	PHE	CB-CG-CD2	9.98	127.78	120.80
4	A	801	PHE	CB-CG-CD1	-9.97	113.82	120.80
3	Z	1351	TYR	CG-CD2-CE2	-9.96	113.33	121.30
6	F	306	ASP	CB-CG-OD2	-9.96	109.33	118.30
3	1	1287	PHE	CB-CG-CD1	-9.96	113.83	120.80
7	M	680	PHE	CB-CG-CD1	9.95	127.77	120.80
7	M	785	TYR	CB-CG-CD2	9.91	126.94	121.00
7	O	680	PHE	CB-CG-CD1	9.90	127.73	120.80
8	P	323	TYR	CB-CG-CD1	9.89	126.94	121.00
4	J	658	TYR	CB-CG-CD2	-9.88	115.07	121.00
7	O	785	TYR	CB-CG-CD2	9.88	126.92	121.00
2	0	696	ARG	NE-CZ-NH2	-9.87	115.36	120.30
2	Y	417	TYR	CB-CG-CD2	-9.83	115.10	121.00
7	M	1496	ASP	CB-CG-OD2	-9.82	109.46	118.30
2	Y	652	TYR	CB-CG-CD1	-9.82	115.11	121.00
8	N	1259	PHE	CB-CG-CD1	-9.81	113.93	120.80
8	P	1259	PHE	CB-CG-CD1	-9.81	113.93	120.80
8	N	323	TYR	CB-CG-CD1	9.80	126.88	121.00
9	T	547	TYR	CB-CG-CD2	9.79	126.87	121.00
2	0	652	TYR	CB-CG-CD1	-9.78	115.14	121.00
7	O	1496	ASP	CB-CG-OD2	-9.77	109.50	118.30
4	D	658	TYR	CB-CG-CD2	-9.76	115.14	121.00
7	O	251	ASP	CB-CG-OD2	-9.76	109.52	118.30
9	Q	696	TYR	CB-CG-CD2	-9.75	115.15	121.00
3	1	843	TYR	CB-CG-CD2	-9.74	115.15	121.00
3	1	1327	ARG	NE-CZ-NH2	-9.74	115.43	120.30
8	N	844	TYR	CB-CG-CD2	9.73	126.84	121.00
7	M	943	ARG	NE-CZ-NH1	9.73	125.16	120.30
3	1	883	TYR	CB-CG-CD2	-9.73	115.16	121.00
9	S	696	TYR	CB-CG-CD2	-9.72	115.17	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	251	ASP	CB-CG-OD2	-9.71	109.56	118.30
2	0	876	ARG	NE-CZ-NH1	9.71	125.16	120.30
8	P	844	TYR	CB-CG-CD2	9.71	126.83	121.00
9	Q	469	TYR	CB-CG-CD2	-9.70	115.18	121.00
8	P	102	PHE	CB-CG-CD2	9.70	127.59	120.80
3	Z	843	TYR	CB-CG-CD2	-9.70	115.18	121.00
3	Z	883	TYR	CB-CG-CD2	-9.70	115.18	121.00
2	0	417	TYR	CB-CG-CD2	-9.69	115.18	121.00
9	R	547	TYR	CB-CG-CD2	9.68	126.81	121.00
7	O	182	ARG	NE-CZ-NH2	-9.68	115.46	120.30
8	N	102	PHE	CB-CG-CD2	9.66	127.56	120.80
7	M	48	ARG	NE-CZ-NH1	9.66	125.13	120.30
4	D	745	TYR	CB-CG-CD2	-9.65	115.21	121.00
8	N	1446	PHE	CB-CG-CD1	-9.65	114.04	120.80
3	1	421	PHE	CB-CG-CD1	9.64	127.55	120.80
4	J	745	TYR	CB-CG-CD2	-9.62	115.23	121.00
3	Z	421	PHE	CB-CG-CD1	9.59	127.52	120.80
7	M	182	ARG	NE-CZ-NH2	-9.59	115.50	120.30
8	P	1534	TYR	CB-CG-CD2	-9.59	115.24	121.00
8	N	1534	TYR	CB-CG-CD2	-9.59	115.25	121.00
8	N	1104	ASP	CB-CG-OD2	-9.57	109.68	118.30
3	Z	1230	ASP	CB-CG-OD2	-9.57	109.69	118.30
7	M	1015	ARG	NE-CZ-NH1	-9.57	115.52	120.30
7	O	943	ARG	NE-CZ-NH1	9.57	125.08	120.30
5	B	469	ARG	NE-CZ-NH2	-9.56	115.52	120.30
3	1	1230	ASP	CB-CG-OD2	-9.56	109.70	118.30
8	P	411	PHE	CB-CG-CD2	9.55	127.48	120.80
5	K	518	ARG	NE-CZ-NH2	-9.53	115.53	120.30
8	P	1446	PHE	CB-CG-CD1	-9.53	114.13	120.80
7	O	48	ARG	NE-CZ-NH1	9.53	125.06	120.30
11	V	360	TYR	CB-CG-CD2	-9.52	115.29	121.00
8	P	1104	ASP	CB-CG-OD2	-9.51	109.74	118.30
2	0	1460	ARG	NE-CZ-NH2	-9.51	115.55	120.30
5	E	518	ARG	NE-CZ-NH2	-9.51	115.55	120.30
8	N	411	PHE	CB-CG-CD2	9.51	127.45	120.80
9	R	636	ARG	NE-CZ-NH1	-9.51	115.55	120.30
3	Z	1327	ARG	NE-CZ-NH2	-9.50	115.55	120.30
2	Y	876	ARG	NE-CZ-NH1	9.50	125.05	120.30
9	Q	650	TYR	CB-CG-CD2	-9.50	115.30	121.00
3	Z	949	ARG	NE-CZ-NH1	9.50	125.05	120.30
11	X	360	TYR	CB-CG-CD2	-9.49	115.31	121.00
7	O	237	PHE	CB-CG-CD2	-9.48	114.16	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	318	TYR	CB-CG-CD2	9.47	126.68	121.00
9	T	422	ARG	NE-CZ-NH2	-9.47	115.57	120.30
9	R	422	ARG	NE-CZ-NH2	-9.47	115.57	120.30
3	1	766	PHE	CB-CG-CD2	-9.46	114.17	120.80
3	Z	766	PHE	CB-CG-CD2	-9.46	114.18	120.80
9	S	469	TYR	CB-CG-CD2	-9.44	115.33	121.00
8	N	476	ASP	CB-CG-OD2	9.44	126.80	118.30
8	N	1251	TYR	CG-CD2-CE2	-9.43	113.76	121.30
8	N	648	ARG	NE-CZ-NH1	9.42	125.01	120.30
2	Y	643	THR	CA-CB-CG2	-9.42	99.22	112.40
7	M	237	PHE	CB-CG-CD2	-9.41	114.21	120.80
2	Y	1460	ARG	NE-CZ-NH2	-9.41	115.59	120.30
7	O	1015	ARG	NE-CZ-NH1	-9.41	115.59	120.30
10	W	318	TYR	CB-CG-CD2	9.41	126.64	121.00
2	0	643	THR	CA-CB-CG2	-9.40	99.24	112.40
3	1	949	ARG	NE-CZ-NH1	9.39	125.00	120.30
9	S	650	TYR	CB-CG-CD2	-9.39	115.36	121.00
5	K	411	ARG	NE-CZ-NH2	-9.39	115.61	120.30
8	P	476	ASP	CB-CG-OD2	9.38	126.75	118.30
8	N	216	TYR	CB-CG-CD1	9.38	126.63	121.00
3	Z	348	ASP	CB-CG-OD1	9.38	126.74	118.30
5	H	469	ARG	NE-CZ-NH2	-9.38	115.61	120.30
8	P	1156	PHE	CB-CG-CD1	9.37	127.36	120.80
8	P	648	ARG	NE-CZ-NH1	9.37	124.98	120.30
8	N	1156	PHE	CB-CG-CD1	9.36	127.35	120.80
8	P	1251	TYR	CG-CD2-CE2	-9.35	113.82	121.30
5	E	411	ARG	NE-CZ-NH2	-9.32	115.64	120.30
3	1	983	TYR	CB-CG-CD1	-9.31	115.41	121.00
8	P	216	TYR	CB-CG-CD1	9.31	126.59	121.00
5	E	463	LEU	CB-CG-CD1	9.30	126.80	111.00
9	R	629	ARG	NE-CZ-NH2	-9.29	115.66	120.30
7	O	1195	PHE	CB-CG-CD2	-9.28	114.31	120.80
3	1	348	ASP	CB-CG-OD1	9.26	126.64	118.30
3	1	1005	TYR	CG-CD1-CE1	9.24	128.69	121.30
10	W	318	TYR	CB-CG-CD1	-9.24	115.45	121.00
9	T	629	ARG	NE-CZ-NH2	-9.24	115.68	120.30
5	K	463	LEU	CB-CG-CD1	9.22	126.67	111.00
7	M	1164	PHE	CB-CG-CD2	-9.21	114.35	120.80
9	T	636	ARG	NE-CZ-NH1	-9.21	115.69	120.30
8	P	720	ARG	NE-CZ-NH1	9.19	124.90	120.30
8	N	398	ARG	NE-CZ-NH1	9.19	124.89	120.30
3	Z	983	TYR	CB-CG-CD1	-9.19	115.49	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
10	U	318	TYR	CB-CG-CD1	-9.18	115.49	121.00
9	R	386	TYR	CB-CG-CD2	-9.17	115.50	121.00
3	Z	849	PHE	CB-CG-CD1	-9.16	114.39	120.80
7	M	692	TYR	CB-CG-CD1	-9.15	115.51	121.00
3	Z	1005	TYR	CG-CD1-CE1	9.15	128.62	121.30
7	M	1195	PHE	CB-CG-CD2	-9.15	114.40	120.80
9	T	386	TYR	CB-CG-CD2	-9.15	115.51	121.00
8	N	1104	ASP	CB-CG-OD1	9.14	126.53	118.30
3	1	849	PHE	CB-CG-CD1	-9.14	114.40	120.80
8	P	207	ASP	CB-CG-OD1	-9.14	110.07	118.30
10	W	348	ALA	N-CA-CB	9.13	122.89	110.10
10	U	348	ALA	N-CA-CB	9.12	122.87	110.10
3	Z	1240	ARG	NE-CZ-NH1	9.12	124.86	120.30
8	N	1233	PHE	CB-CG-CD1	9.11	127.17	120.80
3	Z	1223	PHE	CB-CG-CD1	9.10	127.17	120.80
8	N	1251	TYR	CB-CG-CD1	-9.10	115.54	121.00
8	P	1251	TYR	CB-CG-CD1	-9.10	115.54	121.00
7	O	1164	PHE	CB-CG-CD2	-9.09	114.44	120.80
7	M	1154	ARG	NE-CZ-NH2	-9.09	115.76	120.30
7	O	692	TYR	CB-CG-CD1	-9.07	115.56	121.00
8	P	1104	ASP	CB-CG-OD1	9.07	126.46	118.30
8	P	1233	PHE	CB-CG-CD1	9.06	127.14	120.80
3	1	1223	PHE	CB-CG-CD1	9.06	127.14	120.80
8	P	398	ARG	NE-CZ-NH1	9.06	124.83	120.30
8	N	720	ARG	NE-CZ-NH1	9.04	124.82	120.30
2	0	380	TYR	CB-CG-CD1	-9.04	115.58	121.00
7	O	832	PHE	CB-CG-CD2	-9.03	114.48	120.80
9	Q	636	ARG	NE-CZ-NH2	-9.02	115.79	120.30
7	O	516	ARG	NE-CZ-NH1	9.02	124.81	120.30
3	1	905	ARG	NE-CZ-NH1	9.02	124.81	120.30
7	M	832	PHE	CB-CG-CD2	-9.01	114.50	120.80
3	1	1240	ARG	NE-CZ-NH1	9.00	124.80	120.30
7	O	1154	ARG	NE-CZ-NH2	-9.00	115.80	120.30
3	1	380	ASP	CB-CG-OD2	-9.00	110.20	118.30
9	R	342	ARG	NE-CZ-NH2	8.98	124.79	120.30
5	E	446	ARG	NE-CZ-NH1	8.97	124.79	120.30
3	Z	905	ARG	NE-CZ-NH1	8.97	124.79	120.30
3	1	948	ARG	NE-CZ-NH1	8.97	124.79	120.30
9	T	342	ARG	NE-CZ-NH2	8.97	124.78	120.30
5	B	469	ARG	NH1-CZ-NH2	8.96	129.26	119.40
2	Y	397	TYR	CB-CG-CD2	8.95	126.37	121.00
8	N	207	ASP	CB-CG-OD1	-8.95	110.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	632	ASP	CB-CG-OD1	-8.93	110.26	118.30
2	Y	867	TYR	CB-CG-CD2	-8.92	115.65	121.00
3	Z	380	ASP	CB-CG-OD2	-8.92	110.27	118.30
5	H	469	ARG	NH1-CZ-NH2	8.91	129.20	119.40
8	N	480	ASP	CB-CG-OD2	-8.90	110.29	118.30
9	S	636	ARG	NE-CZ-NH2	-8.90	115.85	120.30
2	0	867	TYR	CB-CG-CD2	-8.90	115.66	121.00
8	N	134	ARG	NE-CZ-NH1	-8.89	115.85	120.30
2	Y	380	TYR	CB-CG-CD1	-8.89	115.67	121.00
2	0	1146	TYR	CG-CD2-CE2	8.89	128.41	121.30
5	K	446	ARG	NE-CZ-NH1	8.89	124.74	120.30
2	Y	408	ARG	NE-CZ-NH2	8.88	124.74	120.30
3	1	1016	ASP	CB-CG-OD1	8.88	126.29	118.30
9	S	338	PHE	CB-CG-CD2	-8.87	114.59	120.80
9	Q	338	PHE	CB-CG-CD2	-8.87	114.59	120.80
2	0	1344	PHE	CB-CG-CD2	-8.86	114.59	120.80
8	P	480	ASP	CB-CG-OD2	-8.87	110.32	118.30
9	R	632	ASP	CB-CG-OD1	-8.86	110.32	118.30
2	0	624	PHE	CB-CG-CD2	-8.86	114.60	120.80
2	Y	624	PHE	CB-CG-CD2	-8.86	114.60	120.80
3	Z	1016	ASP	CB-CG-OD1	8.86	126.27	118.30
8	N	1487	PHE	CB-CG-CD2	8.85	126.99	120.80
3	1	1213	LEU	CB-CA-C	-8.85	93.39	110.20
8	P	134	ARG	NE-CZ-NH1	-8.84	115.88	120.30
2	Y	1146	TYR	CG-CD2-CE2	8.84	128.37	121.30
3	1	770	ARG	NE-CZ-NH1	8.83	124.72	120.30
8	P	1327	ARG	NE-CZ-NH2	8.83	124.72	120.30
7	M	516	ARG	NE-CZ-NH1	8.83	124.72	120.30
2	0	397	TYR	CB-CG-CD2	8.83	126.30	121.00
2	0	853	PHE	CB-CG-CD1	-8.83	114.62	120.80
5	K	311	PHE	CB-CG-CD2	-8.81	114.64	120.80
2	Y	853	PHE	CB-CG-CD1	-8.80	114.64	120.80
7	M	1231	TYR	CB-CG-CD1	-8.80	115.72	121.00
2	0	278	ARG	NE-CZ-NH2	-8.77	115.92	120.30
2	0	408	ARG	NE-CZ-NH2	8.76	124.68	120.30
9	S	226	ARG	NE-CZ-NH1	8.76	124.68	120.30
5	E	311	PHE	CB-CG-CD2	-8.75	114.67	120.80
8	N	1652	PHE	CB-CG-CD1	-8.75	114.67	120.80
2	0	409	ALA	N-CA-CB	8.75	122.35	110.10
2	Y	409	ALA	N-CA-CB	8.74	122.34	110.10
9	R	417	ARG	NE-CZ-NH1	8.74	124.67	120.30
8	P	1652	PHE	CB-CG-CD1	-8.74	114.68	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	770	ARG	NE-CZ-NH1	8.74	124.67	120.30
7	O	1231	TYR	CB-CG-CD1	-8.74	115.75	121.00
2	0	935	PHE	CB-CG-CD1	8.73	126.91	120.80
2	Y	1344	PHE	CB-CG-CD2	-8.73	114.69	120.80
9	T	412	TYR	CB-CG-CD1	8.71	126.23	121.00
8	N	167	ASP	CB-CG-OD1	8.71	126.14	118.30
3	1	440	ARG	NE-CZ-NH1	8.71	124.66	120.30
7	M	1247	ARG	NE-CZ-NH2	-8.71	115.95	120.30
7	M	1513	TYR	CB-CG-CD1	-8.71	115.78	121.00
8	N	1327	ARG	NE-CZ-NH2	8.71	124.65	120.30
3	Z	440	ARG	NE-CZ-NH1	8.70	124.65	120.30
2	Y	935	PHE	CB-CG-CD1	8.69	126.89	120.80
2	0	278	ARG	NE-CZ-NH1	8.69	124.64	120.30
7	O	1324	ARG	NE-CZ-NH2	-8.68	115.96	120.30
5	H	353	TYR	CB-CG-CD2	-8.67	115.80	121.00
8	P	1487	PHE	CB-CG-CD2	8.67	126.87	120.80
3	Z	948	ARG	NE-CZ-NH1	8.66	124.63	120.30
7	M	1324	ARG	NE-CZ-NH2	-8.65	115.98	120.30
3	Z	1068	ARG	NE-CZ-NH2	-8.64	115.98	120.30
5	B	353	TYR	CB-CG-CD2	-8.64	115.82	121.00
8	N	184	ASP	CB-CG-OD2	-8.64	110.53	118.30
3	1	171	TYR	CB-CG-CD2	-8.62	115.83	121.00
3	1	1327	ARG	NE-CZ-NH1	8.61	124.60	120.30
7	O	1237	TYR	CB-CG-CD1	8.60	126.16	121.00
8	P	167	ASP	CB-CG-OD1	8.60	126.04	118.30
2	Y	278	ARG	NE-CZ-NH1	8.60	124.60	120.30
9	Q	226	ARG	NE-CZ-NH1	8.60	124.60	120.30
10	U	308	TYR	CB-CG-CD1	8.60	126.16	121.00
2	Y	1011	ARG	NE-CZ-NH2	8.59	124.60	120.30
7	O	1247	ARG	NE-CZ-NH2	-8.59	116.00	120.30
7	M	774	ARG	NE-CZ-NH1	-8.59	116.00	120.30
8	N	878	PHE	CB-CG-CD2	8.59	126.81	120.80
9	T	226	ARG	NE-CZ-NH1	-8.58	116.01	120.30
7	M	482	PHE	CB-CG-CD2	-8.58	114.80	120.80
7	O	1572	ASN	N-CA-C	-8.58	87.84	111.00
9	R	226	ARG	NE-CZ-NH1	-8.57	116.01	120.30
8	P	707	PHE	CB-CG-CD2	-8.57	114.80	120.80
8	P	878	PHE	CB-CG-CD2	8.57	126.80	120.80
7	O	1453	ARG	NE-CZ-NH2	8.57	124.58	120.30
8	P	184	ASP	CB-CG-OD2	-8.57	110.59	118.30
2	Y	278	ARG	NE-CZ-NH2	-8.57	116.02	120.30
8	N	1642	ARG	NE-CZ-NH1	8.57	124.58	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	1237	TYR	CB-CG-CD1	8.56	126.14	121.00
2	Y	914	TYR	CB-CG-CD2	-8.56	115.86	121.00
7	M	1572	ASN	N-CA-C	-8.55	87.90	111.00
8	P	862	ARG	NE-CZ-NH1	8.55	124.58	120.30
7	O	482	PHE	CB-CG-CD2	-8.54	114.82	120.80
8	N	862	ARG	NE-CZ-NH1	8.54	124.57	120.30
4	G	694	ASP	CB-CG-OD2	-8.53	110.62	118.30
7	O	1513	TYR	CB-CG-CD1	-8.53	115.88	121.00
9	R	412	TYR	CB-CG-CD1	8.53	126.12	121.00
3	1	1071	TYR	CB-CG-CD1	8.52	126.11	121.00
4	J	802	ASP	CB-CG-OD1	8.52	125.97	118.30
10	W	308	TYR	CB-CG-CD1	8.52	126.11	121.00
3	Z	171	TYR	CB-CG-CD2	-8.51	115.89	121.00
4	D	802	ASP	CB-CG-OD1	8.51	125.96	118.30
8	N	707	PHE	CB-CG-CD2	-8.50	114.85	120.80
7	O	774	ARG	NE-CZ-NH1	-8.49	116.05	120.30
9	T	417	ARG	NE-CZ-NH1	8.49	124.55	120.30
2	Y	198	ASP	CB-CG-OD2	-8.49	110.66	118.30
8	N	256	THR	CA-CB-CG2	-8.49	100.51	112.40
2	0	914	TYR	CB-CG-CD2	-8.49	115.91	121.00
9	Q	408	ARG	NE-CZ-NH2	-8.48	116.06	120.30
8	P	256	THR	CA-CB-CG2	-8.48	100.53	112.40
3	1	892	PHE	CB-CG-CD1	-8.47	114.87	120.80
7	M	489	TYR	CB-CG-CD2	8.46	126.08	121.00
2	0	198	ASP	CB-CG-OD2	-8.47	110.68	118.30
4	A	694	ASP	CB-CG-OD2	-8.46	110.69	118.30
8	N	382	PHE	CB-CG-CD2	-8.45	114.88	120.80
8	P	421	PHE	CB-CG-CD1	-8.45	114.89	120.80
3	Z	551	TYR	CB-CG-CD1	-8.44	115.94	121.00
3	1	551	TYR	CB-CG-CD1	-8.43	115.94	121.00
9	S	760	PHE	CB-CG-CD2	8.43	126.70	120.80
3	1	1068	ARG	NE-CZ-NH2	-8.43	116.08	120.30
3	1	1079	PHE	CB-CG-CD1	-8.43	114.90	120.80
9	S	290	TYR	CG-CD1-CE1	8.43	128.04	121.30
8	N	421	PHE	CB-CG-CD1	-8.42	114.90	120.80
2	0	704	THR	CA-CB-CG2	-8.42	100.61	112.40
7	M	1453	ARG	NE-CZ-NH2	8.42	124.51	120.30
9	Q	290	TYR	CG-CD1-CE1	8.42	128.03	121.30
8	P	1642	ARG	NE-CZ-NH1	8.42	124.51	120.30
3	Z	710	TYR	CB-CG-CD1	-8.42	115.95	121.00
9	S	407	TYR	CB-CG-CD2	-8.41	115.95	121.00
9	Q	407	TYR	CB-CG-CD2	-8.41	115.96	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	0	1011	ARG	NE-CZ-NH2	8.41	124.50	120.30
9	S	408	ARG	NE-CZ-NH2	-8.41	116.10	120.30
8	N	21	PHE	CB-CG-CD1	-8.40	114.92	120.80
3	Z	1327	ARG	NE-CZ-NH1	8.40	124.50	120.30
7	M	771	ARG	NE-CZ-NH2	-8.40	116.10	120.30
3	Z	892	PHE	CB-CG-CD1	-8.40	114.92	120.80
3	Z	1079	PHE	CB-CG-CD1	-8.40	114.92	120.80
8	P	220	PHE	CB-CG-CD2	-8.39	114.93	120.80
2	Y	704	THR	CA-CB-CG2	-8.39	100.66	112.40
3	Z	1071	TYR	CB-CG-CD1	8.39	126.03	121.00
7	O	489	TYR	CB-CG-CD2	8.38	126.03	121.00
7	O	1510	ASP	CB-CG-OD2	-8.38	110.76	118.30
3	1	986	ARG	NE-CZ-NH1	8.37	124.49	120.30
9	Q	760	PHE	CB-CG-CD2	8.37	126.66	120.80
8	P	382	PHE	CB-CG-CD2	-8.37	114.94	120.80
7	O	745	ARG	NE-CZ-NH2	-8.36	116.12	120.30
8	P	21	PHE	CB-CG-CD1	-8.36	114.95	120.80
3	1	849	PHE	CB-CG-CD2	8.34	126.64	120.80
3	Z	849	PHE	CB-CG-CD2	8.34	126.64	120.80
7	O	771	ARG	NE-CZ-NH2	-8.34	116.13	120.30
9	Q	690	ARG	NE-CZ-NH1	8.34	124.47	120.30
7	M	1510	ASP	CB-CG-OD2	-8.33	110.81	118.30
7	O	282	PHE	CB-CG-CD2	-8.31	114.98	120.80
9	S	690	ARG	NE-CZ-NH1	8.31	124.45	120.30
7	O	913	TYR	CB-CG-CD2	-8.31	116.02	121.00
8	P	295	PHE	CB-CG-CD1	-8.30	114.99	120.80
7	M	282	PHE	CB-CG-CD2	-8.30	114.99	120.80
4	G	714	PHE	CB-CG-CD1	8.30	126.61	120.80
8	N	184	ASP	CB-CG-OD1	8.29	125.77	118.30
3	1	710	TYR	CB-CG-CD1	-8.29	116.02	121.00
8	P	184	ASP	CB-CG-OD1	8.29	125.77	118.30
6	F	306	ASP	CB-CG-OD1	8.29	125.76	118.30
8	N	1349	TYR	CG-CD2-CE2	-8.29	114.67	121.30
3	1	1057	TYR	CB-CG-CD1	-8.29	116.03	121.00
3	Z	1182	ARG	NE-CZ-NH2	-8.29	116.16	120.30
9	S	317	ASP	CB-CG-OD2	-8.29	110.84	118.30
3	Z	1223	PHE	CB-CG-CD2	-8.28	115.00	120.80
6	L	306	ASP	CB-CG-OD1	8.28	125.75	118.30
3	Z	1057	TYR	CB-CG-CD1	-8.27	116.04	121.00
5	K	518	ARG	NE-CZ-NH1	8.26	124.43	120.30
5	E	518	ARG	NE-CZ-NH1	8.26	124.43	120.30
7	M	913	TYR	CB-CG-CD2	-8.26	116.05	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	816	TYR	CB-CG-CD1	-8.26	116.05	121.00
8	N	295	PHE	CB-CG-CD1	-8.25	115.02	120.80
9	Q	317	ASP	CB-CG-OD2	-8.25	110.87	118.30
3	1	1223	PHE	CB-CG-CD2	-8.25	115.03	120.80
2	Y	1428	TYR	CB-CG-CD2	8.25	125.95	121.00
3	Z	1074	ARG	NE-CZ-NH1	8.25	124.42	120.30
7	M	745	ARG	NE-CZ-NH2	-8.25	116.18	120.30
2	0	909	PHE	CB-CG-CD2	8.23	126.56	120.80
9	R	816	TYR	CB-CG-CD1	-8.23	116.06	121.00
2	Y	909	PHE	CB-CG-CD2	8.23	126.56	120.80
8	P	1349	TYR	CG-CD2-CE2	-8.23	114.72	121.30
2	0	1428	TYR	CB-CG-CD2	8.22	125.93	121.00
9	R	371	PHE	CB-CG-CD1	8.21	126.55	120.80
4	J	745	TYR	CB-CG-CD1	8.21	125.92	121.00
8	N	1534	TYR	CB-CG-CD1	8.20	125.92	121.00
3	1	822	PHE	CB-CG-CD2	-8.20	115.06	120.80
3	Z	986	ARG	NE-CZ-NH1	8.19	124.39	120.30
3	Z	545	TYR	CB-CG-CD1	-8.18	116.09	121.00
4	D	745	TYR	CB-CG-CD1	8.18	125.91	121.00
3	1	419	ASP	CB-CG-OD2	-8.17	110.94	118.30
2	Y	1146	TYR	CZ-CE2-CD2	-8.17	112.45	119.80
3	1	1182	ARG	NE-CZ-NH2	-8.16	116.22	120.30
3	1	545	TYR	CB-CG-CD1	-8.15	116.11	121.00
3	1	1074	ARG	NE-CZ-NH1	8.13	124.37	120.30
4	A	714	PHE	CB-CG-CD1	8.13	126.49	120.80
7	O	508	TYR	CB-CG-CD1	-8.13	116.12	121.00
2	0	365	ARG	NE-CZ-NH2	-8.12	116.24	120.30
8	P	1490	ARG	NE-CZ-NH1	-8.12	116.24	120.30
9	R	386	TYR	CB-CG-CD1	8.12	125.87	121.00
2	0	1146	TYR	CZ-CE2-CD2	-8.12	112.50	119.80
9	T	371	PHE	CB-CG-CD1	8.10	126.47	120.80
7	M	508	TYR	CB-CG-CD1	-8.09	116.14	121.00
8	P	1534	TYR	CB-CG-CD1	8.09	125.86	121.00
3	Z	419	ASP	CB-CG-OD2	-8.09	111.02	118.30
3	Z	822	PHE	CB-CG-CD2	-8.09	115.14	120.80
3	1	1033	PHE	CB-CG-CD1	-8.07	115.15	120.80
8	N	1490	ARG	NE-CZ-NH1	-8.07	116.27	120.30
3	Z	421	PHE	CG-CD2-CE2	8.06	129.67	120.80
8	N	916	TYR	CB-CG-CD1	8.05	125.83	121.00
3	1	421	PHE	CG-CD2-CE2	8.04	129.65	120.80
2	Y	659	PHE	CB-CG-CD2	8.03	126.42	120.80
7	M	755	TYR	CB-CG-CD2	8.03	125.82	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	1033	PHE	CB-CG-CD1	-8.02	115.19	120.80
8	P	411	PHE	CB-CG-CD1	-8.02	115.19	120.80
7	O	755	TYR	CB-CG-CD2	8.01	125.81	121.00
8	N	21	PHE	CB-CG-CD2	8.00	126.40	120.80
3	Z	348	ASP	CB-CG-OD2	-7.99	111.11	118.30
2	0	1282	ASP	CB-CG-OD1	7.98	125.49	118.30
7	M	755	TYR	CB-CG-CD1	-7.98	116.21	121.00
2	0	659	PHE	CB-CG-CD2	7.98	126.39	120.80
9	T	477	TYR	CB-CG-CD2	-7.98	116.21	121.00
9	T	386	TYR	CB-CG-CD1	7.98	125.79	121.00
8	P	1072	TYR	CB-CG-CD1	7.98	125.79	121.00
2	Y	365	ARG	NE-CZ-NH2	-7.97	116.31	120.30
8	N	135	PHE	CB-CG-CD1	7.97	126.38	120.80
2	Y	1282	ASP	CB-CG-OD1	7.95	125.46	118.30
2	Y	200	GLU	N-CA-CB	7.95	124.90	110.60
7	O	755	TYR	CB-CG-CD1	-7.95	116.23	121.00
8	P	704	ASP	CB-CG-OD1	7.94	125.45	118.30
2	0	200	GLU	N-CA-CB	7.94	124.89	110.60
8	N	1072	TYR	CB-CG-CD1	7.92	125.75	121.00
8	P	916	TYR	CB-CG-CD1	7.91	125.75	121.00
8	N	411	PHE	CB-CG-CD1	-7.91	115.27	120.80
5	H	346	GLN	N-CA-CB	7.90	124.82	110.60
9	R	477	TYR	CB-CG-CD2	-7.90	116.26	121.00
5	H	440	PHE	CB-CG-CD1	7.88	126.31	120.80
8	P	1313	ARG	NE-CZ-NH2	-7.88	116.36	120.30
8	N	1313	ARG	NE-CZ-NH2	-7.87	116.36	120.30
8	P	21	PHE	CB-CG-CD2	7.87	126.31	120.80
5	B	440	PHE	CB-CG-CD1	7.87	126.31	120.80
8	P	135	PHE	CB-CG-CD1	7.87	126.31	120.80
3	Z	937	ARG	NE-CZ-NH2	-7.87	116.37	120.30
3	Z	431	ARG	NE-CZ-NH1	7.87	124.23	120.30
8	N	398	ARG	NE-CZ-NH2	-7.86	116.37	120.30
5	B	346	GLN	N-CA-CB	7.86	124.74	110.60
5	H	462	ARG	NE-CZ-NH1	7.85	124.22	120.30
8	N	704	ASP	CB-CG-OD1	7.85	125.36	118.30
3	Z	1071	TYR	CB-CG-CD2	-7.84	116.29	121.00
5	K	393	ASP	CB-CG-OD2	-7.84	111.24	118.30
3	1	348	ASP	CB-CG-OD2	-7.84	111.25	118.30
7	M	807	ASP	CB-CG-OD2	-7.83	111.26	118.30
7	O	1657	ASP	CB-CG-OD2	-7.82	111.26	118.30
7	M	1657	ASP	CB-CG-OD2	-7.82	111.27	118.30
8	N	758	TYR	CG-CD2-CE2	7.81	127.55	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	0	1232	ARG	NE-CZ-NH1	7.81	124.20	120.30
2	0	1331	ARG	NE-CZ-NH2	-7.80	116.40	120.30
5	E	393	ASP	CB-CG-OD2	-7.80	111.28	118.30
7	M	1598	PHE	CB-CG-CD2	7.79	126.25	120.80
3	1	433	TYR	CB-CG-CD1	-7.79	116.33	121.00
5	B	462	ARG	NE-CZ-NH1	7.79	124.19	120.30
3	1	431	ARG	NE-CZ-NH1	7.79	124.19	120.30
3	1	1053	ARG	NE-CZ-NH2	-7.78	116.41	120.30
4	A	702	ARG	NE-CZ-NH2	-7.78	116.41	120.30
8	N	733	ARG	NE-CZ-NH1	7.78	124.19	120.30
9	Q	725	GLU	N-CA-CB	7.77	124.58	110.60
4	J	658	TYR	CB-CG-CD1	7.77	125.66	121.00
7	O	1598	PHE	CB-CG-CD2	7.76	126.23	120.80
2	Y	1331	ARG	NE-CZ-NH2	-7.76	116.42	120.30
4	D	658	TYR	CB-CG-CD1	7.76	125.66	121.00
9	S	725	GLU	N-CA-CB	7.75	124.56	110.60
2	0	205	ASP	N-CA-CB	7.75	124.55	110.60
7	M	1657	ASP	CB-CG-OD1	7.75	125.27	118.30
3	Z	983	TYR	CG-CD1-CE1	-7.74	115.11	121.30
3	Z	1053	ARG	NE-CZ-NH2	-7.74	116.43	120.30
3	Z	1101	TYR	CB-CG-CD1	7.74	125.64	121.00
8	N	1435	ASP	CB-CG-OD1	7.74	125.27	118.30
7	O	1066	ASP	CB-CG-OD2	-7.74	111.33	118.30
2	Y	448	PHE	CB-CG-CD1	-7.74	115.38	120.80
7	O	807	ASP	CB-CG-OD2	-7.74	111.33	118.30
3	1	1071	TYR	CB-CG-CD2	-7.73	116.36	121.00
7	M	335	ASP	CB-CG-OD2	-7.73	111.34	118.30
9	Q	523	ARG	NE-CZ-NH2	-7.73	116.44	120.30
3	1	937	ARG	NE-CZ-NH2	-7.72	116.44	120.30
2	Y	899	MET	CG-SD-CE	-7.72	87.85	100.20
2	0	899	MET	CG-SD-CE	-7.72	87.85	100.20
7	O	1657	ASP	CB-CG-OD1	7.71	125.24	118.30
2	0	448	PHE	CB-CG-CD1	-7.71	115.40	120.80
7	O	1532	ARG	NE-CZ-NH1	7.71	124.16	120.30
3	Z	402	ARG	NE-CZ-NH1	7.71	124.15	120.30
4	G	702	ARG	NE-CZ-NH2	-7.71	116.44	120.30
3	Z	949	ARG	NE-CZ-NH2	-7.71	116.45	120.30
2	Y	1088	PHE	CB-CG-CD1	7.70	126.19	120.80
7	M	816	PHE	CB-CG-CD1	7.70	126.19	120.80
3	1	983	TYR	CG-CD1-CE1	-7.70	115.14	121.30
9	S	541	TYR	CG-CD2-CE2	-7.70	115.14	121.30
2	Y	205	ASP	N-CA-CB	7.70	124.45	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	1066	ASP	CB-CG-OD2	-7.70	111.37	118.30
9	Q	217	ARG	NE-CZ-NH2	7.69	124.15	120.30
8	P	758	TYR	CG-CD2-CE2	7.68	127.45	121.30
2	Y	1154	ASP	CB-CG-OD2	-7.68	111.39	118.30
2	Y	1232	ARG	NE-CZ-NH1	7.68	124.14	120.30
9	Q	422	ARG	NE-CZ-NH1	7.67	124.14	120.30
8	P	323	TYR	CB-CG-CD2	-7.67	116.40	121.00
8	P	398	ARG	NE-CZ-NH2	-7.67	116.47	120.30
9	S	422	ARG	NE-CZ-NH1	7.66	124.13	120.30
8	N	209	VAL	CA-CB-CG1	7.66	122.39	110.90
3	1	1044	TYR	CB-CG-CD1	7.66	125.60	121.00
3	Z	433	TYR	CB-CG-CD1	-7.66	116.41	121.00
2	Y	1288	ALA	N-CA-CB	7.65	120.81	110.10
7	M	1532	ARG	NE-CZ-NH1	7.64	124.12	120.30
2	0	1288	ALA	N-CA-CB	7.64	120.80	110.10
8	P	209	VAL	CA-CB-CG1	7.64	122.36	110.90
7	O	335	ASP	CB-CG-OD2	-7.64	111.42	118.30
7	O	816	PHE	CB-CG-CD1	7.64	126.15	120.80
4	A	805	ARG	NE-CZ-NH1	7.63	124.12	120.30
8	N	127	TYR	CB-CG-CD1	-7.63	116.42	121.00
8	N	1495	TRP	CB-CG-CD2	7.63	136.52	126.60
9	S	523	ARG	NE-CZ-NH2	-7.63	116.48	120.30
7	M	1679	TYR	CB-CG-CD1	7.63	125.58	121.00
6	F	447	PHE	CB-CG-CD2	-7.63	115.46	120.80
3	1	402	ARG	NE-CZ-NH1	7.63	124.11	120.30
8	P	1495	TRP	CB-CG-CD2	7.62	136.51	126.60
2	0	1154	ASP	CB-CG-OD2	-7.62	111.44	118.30
5	K	449	ASP	CB-CG-OD1	7.62	125.16	118.30
8	P	1435	ASP	CB-CG-OD1	7.62	125.16	118.30
9	Q	541	TYR	CG-CD2-CE2	-7.62	115.20	121.30
3	1	214	PHE	CB-CG-CD2	7.61	126.13	120.80
5	E	449	ASP	CB-CG-OD1	7.61	125.15	118.30
3	Z	1108	PHE	CB-CG-CD1	-7.59	115.48	120.80
4	D	725	VAL	CG1-CB-CG2	-7.59	98.75	110.90
3	Z	1044	TYR	CB-CG-CD1	7.59	125.55	121.00
7	M	300	MET	CG-SD-CE	-7.59	88.06	100.20
9	Q	640	SER	N-CA-CB	7.59	121.88	110.50
9	T	496	TYR	CB-CG-CD1	7.59	125.55	121.00
3	Z	295	PHE	CB-CG-CD1	7.58	126.11	120.80
3	1	925	ARG	NE-CZ-NH1	7.58	124.09	120.30
7	M	1097	TYR	CB-CG-CD2	7.58	125.55	121.00
8	N	323	TYR	CB-CG-CD2	-7.58	116.45	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1	949	ARG	NE-CZ-NH2	-7.58	116.51	120.30
6	L	447	PHE	CB-CG-CD2	-7.58	115.49	120.80
3	1	1101	TYR	CB-CG-CD1	7.58	125.55	121.00
4	J	725	VAL	CG1-CB-CG2	-7.58	98.78	110.90
7	O	300	MET	CG-SD-CE	-7.57	88.08	100.20
3	1	1108	PHE	CB-CG-CD1	-7.56	115.51	120.80
9	S	640	SER	N-CA-CB	7.56	121.84	110.50
2	Y	126	TYR	CB-CG-CD2	-7.56	116.46	121.00
3	1	295	PHE	CB-CG-CD1	7.56	126.09	120.80
6	L	311	ASP	CB-CG-OD2	-7.55	111.50	118.30
8	P	114	TYR	CB-CG-CD2	-7.54	116.47	121.00
4	G	682	ASP	CB-CG-OD2	-7.54	111.51	118.30
7	O	1679	TYR	CB-CG-CD1	7.54	125.53	121.00
3	1	999	ASP	CB-CG-OD1	7.54	125.08	118.30
9	S	217	ARG	NE-CZ-NH2	7.54	124.07	120.30
2	Y	1325	PHE	CB-CG-CD2	-7.53	115.53	120.80
9	T	551	ARG	NE-CZ-NH1	7.53	124.07	120.30
2	Y	198	ASP	CB-CG-OD1	7.53	125.08	118.30
2	0	126	TYR	CB-CG-CD2	-7.53	116.48	121.00
4	G	805	ARG	NE-CZ-NH1	7.53	124.06	120.30
8	N	114	TYR	CB-CG-CD2	-7.52	116.49	121.00
3	1	1001	ARG	NE-CZ-NH1	7.52	124.06	120.30
8	P	127	TYR	CB-CG-CD1	-7.52	116.49	121.00
2	0	1325	PHE	CB-CG-CD2	-7.51	115.54	120.80
8	P	733	ARG	NE-CZ-NH1	7.51	124.06	120.30
2	0	1088	PHE	CB-CG-CD1	7.50	126.05	120.80
3	Z	214	PHE	CB-CG-CD2	7.50	126.05	120.80
8	N	1158	TYR	CB-CG-CD2	7.50	125.50	121.00
3	Z	999	ASP	CB-CG-OD1	7.50	125.05	118.30
6	F	311	ASP	CB-CG-OD2	-7.50	111.56	118.30
9	R	496	TYR	CB-CG-CD1	7.50	125.50	121.00
2	Y	1059	TYR	CB-CG-CD1	-7.49	116.51	121.00
2	0	198	ASP	CB-CG-OD1	7.49	125.04	118.30
7	O	1097	TYR	CB-CG-CD2	7.48	125.49	121.00
8	P	707	PHE	CB-CG-CD1	7.48	126.03	120.80
7	M	241	PHE	CB-CG-CD1	7.47	126.03	120.80
7	O	110	ARG	NE-CZ-NH2	-7.46	116.57	120.30
8	P	1380	ASP	CB-CG-OD2	-7.46	111.58	118.30
2	0	391	MET	CG-SD-CE	-7.46	88.26	100.20
2	Y	391	MET	CG-SD-CE	-7.46	88.27	100.20
8	N	707	PHE	CB-CG-CD1	7.46	126.02	120.80
3	Z	1001	ARG	NE-CZ-NH1	7.44	124.02	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1	117	TYR	CB-CG-CD1	7.44	125.46	121.00
8	P	753	TYR	CB-CG-CD2	7.44	125.46	121.00
9	Q	511	ALA	N-CA-CB	7.43	120.51	110.10
9	R	551	ARG	NE-CZ-NH1	7.43	124.02	120.30
2	0	400	ARG	NE-CZ-NH2	-7.43	116.58	120.30
7	M	110	ARG	NE-CZ-NH2	-7.43	116.58	120.30
3	1	1060	TYR	CB-CG-CD2	-7.43	116.54	121.00
4	D	665	TRP	CB-CG-CD1	-7.43	117.34	127.00
3	1	1005	TYR	CD1-CE1-CZ	-7.42	113.12	119.80
7	O	241	PHE	CB-CG-CD1	7.42	125.99	120.80
9	S	294	MET	CG-SD-CE	-7.42	88.33	100.20
8	N	1380	ASP	CB-CG-OD2	-7.42	111.63	118.30
9	S	511	ALA	N-CA-CB	7.42	120.48	110.10
4	A	682	ASP	CB-CG-OD2	-7.41	111.63	118.30
8	N	89	PHE	CB-CG-CD1	7.41	125.99	120.80
9	Q	294	MET	CG-SD-CE	-7.41	88.34	100.20
9	S	317	ASP	CB-CG-OD1	7.41	124.97	118.30
2	Y	762	ASP	CB-CG-OD1	-7.41	111.63	118.30
4	G	802	ASP	CB-CG-OD1	-7.41	111.63	118.30
4	J	665	TRP	CB-CG-CD1	-7.41	117.37	127.00
8	P	72	ARG	NE-CZ-NH2	-7.40	116.60	120.30
8	P	89	PHE	CB-CG-CD1	7.40	125.98	120.80
3	Z	925	ARG	NE-CZ-NH1	7.39	123.99	120.30
9	Q	630	ARG	NE-CZ-NH1	7.39	123.99	120.30
9	S	454	TYR	CB-CG-CD1	-7.39	116.57	121.00
3	Z	103	PHE	CB-CG-CD1	-7.38	115.63	120.80
3	Z	1060	TYR	CB-CG-CD2	-7.38	116.57	121.00
9	Q	338	PHE	CB-CG-CD1	7.38	125.97	120.80
8	P	1158	TYR	CB-CG-CD2	7.38	125.43	121.00
3	Z	1275	THR	CA-CB-CG2	-7.38	102.07	112.40
8	P	1597	ARG	NE-CZ-NH2	-7.38	116.61	120.30
8	P	463	PHE	CB-CG-CD1	7.37	125.96	120.80
8	P	1446	PHE	CB-CG-CD2	7.37	125.96	120.80
3	Z	117	TYR	CB-CG-CD1	7.37	125.42	121.00
6	I	300	ASP	CB-CG-OD1	7.37	124.93	118.30
8	N	758	TYR	CB-CG-CD2	7.37	125.42	121.00
7	M	744	TYR	CB-CG-CD1	-7.36	116.58	121.00
2	0	1256	VAL	CA-CB-CG2	-7.36	99.86	110.90
2	0	1059	TYR	CB-CG-CD1	-7.36	116.58	121.00
8	P	613	GLU	CB-CG-CD	7.36	134.07	114.20
4	A	802	ASP	CB-CG-OD1	-7.36	111.68	118.30
6	C	300	ASP	CB-CG-OD1	7.35	124.92	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	613	GLU	CB-CG-CD	7.35	134.05	114.20
3	1	1271	ARG	NE-CZ-NH1	7.35	123.97	120.30
9	Q	317	ASP	CB-CG-OD1	7.34	124.91	118.30
8	N	463	PHE	CB-CG-CD1	7.34	125.94	120.80
8	N	706	THR	CA-CB-CG2	-7.34	102.12	112.40
8	N	1116	ASP	CB-CG-OD1	7.34	124.91	118.30
9	Q	454	TYR	CB-CG-CD1	-7.34	116.60	121.00
7	O	1271	PHE	CB-CG-CD1	-7.34	115.66	120.80
3	1	237	PHE	CB-CG-CD1	7.34	125.94	120.80
2	Y	1154	ASP	CB-CG-OD1	7.34	124.90	118.30
2	0	762	ASP	CB-CG-OD1	-7.33	111.70	118.30
3	1	1275	THR	CA-CB-CG2	-7.33	102.14	112.40
7	M	1490	ARG	NE-CZ-NH1	7.33	123.96	120.30
8	P	706	THR	CA-CB-CG2	-7.33	102.14	112.40
3	Z	1271	ARG	NE-CZ-NH1	7.32	123.96	120.30
3	Z	1005	TYR	CD1-CE1-CZ	-7.32	113.21	119.80
8	N	1446	PHE	CB-CG-CD2	7.32	125.92	120.80
7	O	744	TYR	CB-CG-CD1	-7.32	116.61	121.00
9	T	500	GLU	OE1-CD-OE2	7.32	132.08	123.30
9	S	630	ARG	NE-CZ-NH1	7.32	123.96	120.30
8	P	389	PHE	CB-CG-CD2	-7.31	115.68	120.80
9	R	500	GLU	OE1-CD-OE2	7.31	132.07	123.30
9	S	338	PHE	CB-CG-CD1	7.31	125.92	120.80
2	Y	1256	VAL	CA-CB-CG2	-7.31	99.94	110.90
7	O	559	ALA	N-CA-CB	7.31	120.33	110.10
7	M	559	ALA	N-CA-CB	7.30	120.33	110.10
9	Q	277	TYR	CB-CG-CD2	7.30	125.38	121.00
7	M	1431	ARG	NE-CZ-NH1	-7.30	116.65	120.30
8	N	1597	ARG	NE-CZ-NH2	-7.30	116.65	120.30
8	N	953	TYR	CB-CG-CD1	7.29	125.38	121.00
2	0	218	ARG	NE-CZ-NH1	7.29	123.95	120.30
2	Y	400	ARG	NE-CZ-NH2	-7.29	116.66	120.30
8	P	135	PHE	CB-CG-CD2	-7.28	115.71	120.80
8	N	753	TYR	CB-CG-CD2	7.27	125.36	121.00
2	0	1219	ARG	NE-CZ-NH1	-7.27	116.67	120.30
3	1	103	PHE	CB-CG-CD1	-7.27	115.71	120.80
9	S	209	ARG	NE-CZ-NH1	7.27	123.93	120.30
9	Q	209	ARG	NE-CZ-NH1	7.26	123.93	120.30
11	X	370	LEU	CB-CG-CD2	7.26	123.34	111.00
5	H	353	TYR	CB-CG-CD1	7.25	125.35	121.00
9	S	277	TYR	CB-CG-CD2	7.25	125.35	121.00
8	N	135	PHE	CB-CG-CD2	-7.24	115.73	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	G	639	ASP	CB-CG-OD2	7.23	124.81	118.30
9	Q	724	ARG	NE-CZ-NH2	-7.23	116.69	120.30
8	N	1054	PHE	CB-CG-CD1	-7.23	115.74	120.80
8	P	953	TYR	CB-CG-CD1	7.23	125.34	121.00
7	M	48	ARG	NH1-CZ-NH2	-7.22	111.46	119.40
11	V	370	LEU	CB-CG-CD2	7.22	123.27	111.00
7	O	48	ARG	NH1-CZ-NH2	-7.22	111.46	119.40
8	P	1054	PHE	CB-CG-CD1	-7.22	115.75	120.80
4	A	639	ASP	CB-CG-OD2	7.21	124.79	118.30
7	M	739	ARG	NE-CZ-NH1	7.21	123.91	120.30
3	Z	539	TYR	CB-CG-CD1	7.21	125.33	121.00
7	M	1271	PHE	CB-CG-CD1	-7.21	115.75	120.80
7	O	1490	ARG	NE-CZ-NH1	7.21	123.90	120.30
3	Z	268	ARG	NE-CZ-NH1	7.20	123.90	120.30
8	P	1116	ASP	CB-CG-OD1	7.20	124.78	118.30
3	Z	284	TRP	CE2-CD2-CG	-7.20	101.54	107.30
6	F	302	ASP	CB-CG-OD2	-7.20	111.82	118.30
2	0	1154	ASP	CB-CG-OD1	7.20	124.78	118.30
3	1	575	ARG	NE-CZ-NH1	7.18	123.89	120.30
3	Z	575	ARG	NE-CZ-NH1	7.18	123.89	120.30
5	H	518	ARG	NE-CZ-NH2	-7.18	116.71	120.30
3	Z	237	PHE	CB-CG-CD1	7.17	125.82	120.80
7	O	739	ARG	NE-CZ-NH1	7.17	123.89	120.30
9	S	724	ARG	NE-CZ-NH2	-7.17	116.71	120.30
6	L	302	ASP	CB-CG-OD2	-7.17	111.85	118.30
8	P	463	PHE	CB-CG-CD2	-7.17	115.78	120.80
2	0	1225	PHE	CB-CG-CD2	7.17	125.82	120.80
3	Z	1351	TYR	CB-CG-CD1	7.16	125.30	121.00
7	O	1203	TYR	CB-CG-CD1	-7.16	116.70	121.00
2	0	281	ARG	NE-CZ-NH1	7.16	123.88	120.30
2	Y	281	ARG	NE-CZ-NH1	7.15	123.88	120.30
8	N	389	PHE	CB-CG-CD2	-7.15	115.79	120.80
9	R	764	ASP	CB-CG-OD1	7.15	124.74	118.30
9	T	311	THR	CA-CB-CG2	-7.15	102.39	112.40
3	1	284	TRP	CE2-CD2-CG	-7.15	101.58	107.30
9	T	638	TYR	CG-CD1-CE1	-7.15	115.58	121.30
8	N	332	ARG	CD-NE-CZ	7.14	133.60	123.60
3	1	1079	PHE	CB-CG-CD2	7.14	125.80	120.80
8	N	463	PHE	CB-CG-CD2	-7.13	115.81	120.80
7	O	582	PHE	CB-CG-CD1	7.13	125.79	120.80
7	O	729	MET	CG-SD-CE	-7.13	88.80	100.20
8	P	441	PRO	N-CD-CG	7.12	113.89	103.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	1225	PHE	CB-CG-CD2	7.12	125.79	120.80
8	P	332	ARG	CD-NE-CZ	7.12	133.57	123.60
5	B	353	TYR	CB-CG-CD1	7.12	125.27	121.00
5	E	458	GLU	OE1-CD-OE2	7.12	131.84	123.30
2	Y	218	ARG	NE-CZ-NH1	7.12	123.86	120.30
7	O	516	ARG	NE-CZ-NH2	-7.12	116.74	120.30
5	B	518	ARG	NE-CZ-NH2	-7.11	116.74	120.30
9	R	311	THR	CA-CB-CG2	-7.11	102.44	112.40
7	M	729	MET	CG-SD-CE	-7.11	88.82	100.20
8	N	1113	PHE	CB-CG-CD1	7.11	125.77	120.80
2	0	577	PHE	CB-CG-CD1	7.11	125.77	120.80
11	V	355	TRP	CB-CG-CD1	-7.10	117.76	127.00
5	K	458	GLU	OE1-CD-OE2	7.10	131.82	123.30
9	R	638	TYR	CG-CD1-CE1	-7.10	115.62	121.30
2	Y	577	PHE	CB-CG-CD1	7.09	125.77	120.80
8	P	1113	PHE	CB-CG-CD1	7.09	125.77	120.80
5	E	309	ARG	NE-CZ-NH2	-7.09	116.75	120.30
5	E	469	ARG	NE-CZ-NH1	7.09	123.84	120.30
8	P	758	TYR	CB-CG-CD2	7.09	125.25	121.00
2	0	1124	SER	N-CA-CB	7.08	121.13	110.50
11	X	288	PHE	CB-CG-CD1	7.08	125.76	120.80
11	V	288	PHE	CB-CG-CD1	7.08	125.76	120.80
3	1	268	ARG	NE-CZ-NH1	7.08	123.84	120.30
3	1	843	TYR	CB-CG-CD1	7.08	125.25	121.00
9	T	764	ASP	CB-CG-OD1	7.07	124.67	118.30
2	0	124	ARG	NE-CZ-NH2	-7.07	116.76	120.30
2	Y	1124	SER	N-CA-CB	7.07	121.10	110.50
7	M	1203	TYR	CB-CG-CD1	-7.07	116.76	121.00
8	N	441	PRO	N-CD-CG	7.07	113.80	103.20
4	J	680	TYR	CB-CG-CD2	-7.07	116.76	121.00
2	0	650	TYR	CB-CG-CD2	7.07	125.24	121.00
8	P	1372	THR	CA-CB-CG2	-7.07	102.51	112.40
7	M	516	ARG	NE-CZ-NH2	-7.06	116.77	120.30
9	R	651	ASP	CB-CG-OD2	-7.06	111.95	118.30
2	0	1026	TYR	CB-CG-CD1	-7.06	116.77	121.00
5	K	309	ARG	NE-CZ-NH2	-7.05	116.77	120.30
2	Y	269	ASP	CB-CG-OD2	7.05	124.65	118.30
7	O	1431	ARG	NE-CZ-NH1	-7.05	116.78	120.30
2	Y	909	PHE	CB-CG-CD1	-7.04	115.87	120.80
11	X	355	TRP	CB-CG-CD1	-7.04	117.84	127.00
3	1	539	TYR	CB-CG-CD1	7.04	125.22	121.00
3	Z	1351	TYR	CZ-CE2-CD2	7.03	126.13	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	1474	PHE	CB-CG-CD1	-7.03	115.88	120.80
2	0	909	PHE	CB-CG-CD1	-7.03	115.88	120.80
2	0	467	PHE	CB-CG-CD1	7.03	125.72	120.80
2	0	201	TYR	CG-CD1-CE1	7.03	126.92	121.30
2	0	995	PHE	CB-CG-CD2	7.03	125.72	120.80
3	Z	843	TYR	CB-CG-CD1	7.02	125.21	121.00
5	K	469	ARG	NE-CZ-NH1	7.02	123.81	120.30
8	P	1349	TYR	CB-CG-CD1	-7.02	116.79	121.00
8	N	1372	THR	CA-CB-CG2	-7.01	102.58	112.40
2	Y	598	PHE	CB-CG-CD1	7.01	125.71	120.80
2	0	598	PHE	CB-CG-CD1	7.01	125.70	120.80
7	M	1474	PHE	CB-CG-CD1	-7.00	115.90	120.80
3	1	733	ARG	NE-CZ-NH1	-7.00	116.80	120.30
2	Y	1219	ARG	NE-CZ-NH1	-7.00	116.80	120.30
2	Y	201	TYR	CG-CD1-CE1	7.00	126.90	121.30
7	O	486	TYR	CB-CG-CD1	-7.00	116.80	121.00
3	Z	733	ARG	NE-CZ-NH1	-7.00	116.80	120.30
7	M	582	PHE	CB-CG-CD1	7.00	125.70	120.80
2	0	145	PHE	CB-CG-CD2	7.00	125.70	120.80
2	0	583	TYR	CB-CG-CD1	-7.00	116.80	121.00
5	B	401	ALA	N-CA-CB	7.00	119.89	110.10
2	Y	1026	TYR	CB-CG-CD1	-6.99	116.80	121.00
4	D	689	SER	N-CA-CB	6.99	120.98	110.50
9	R	692	MET	CG-SD-CE	-6.99	89.02	100.20
8	N	1349	TYR	CB-CG-CD1	-6.98	116.81	121.00
2	Y	467	PHE	CB-CG-CD1	6.98	125.69	120.80
7	M	23	ASP	CB-CG-OD2	-6.98	112.02	118.30
9	T	816	TYR	CB-CG-CD2	6.98	125.19	121.00
2	0	269	ASP	CB-CG-OD2	6.98	124.58	118.30
3	Z	577	PHE	CB-CG-CD2	-6.96	115.92	120.80
6	C	386	ASP	CB-CG-OD2	-6.96	112.03	118.30
4	D	680	TYR	CB-CG-CD2	-6.96	116.83	121.00
3	1	1351	TYR	CZ-CE2-CD2	6.96	126.06	119.80
8	N	737	ASP	CB-CG-OD1	6.95	124.56	118.30
4	J	689	SER	N-CA-CB	6.95	120.92	110.50
8	P	1124	ASP	CB-CG-OD2	-6.95	112.05	118.30
3	1	856	ASN	CB-CG-OD1	-6.95	107.70	121.60
3	Z	1079	PHE	CB-CG-CD2	6.95	125.66	120.80
8	P	1486	GLU	N-CA-CB	-6.94	98.10	110.60
9	T	692	MET	CG-SD-CE	-6.94	89.09	100.20
3	1	577	PHE	CB-CG-CD2	-6.94	115.94	120.80
9	S	394	TYR	CB-CG-CD2	-6.94	116.83	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	124	PHE	CB-CG-CD1	-6.94	115.94	120.80
5	H	411	ARG	CD-NE-CZ	-6.94	113.88	123.60
7	M	437	ASP	CB-CG-OD1	6.94	124.55	118.30
8	N	1308	TYR	CB-CG-CD2	-6.94	116.84	121.00
7	M	849	ASP	CB-CG-OD1	6.93	124.54	118.30
2	Y	995	PHE	CB-CG-CD2	6.93	125.65	120.80
10	U	345	TYR	CB-CG-CD2	-6.93	116.84	121.00
7	O	526	PHE	CB-CG-CD1	-6.93	115.95	120.80
2	Y	650	TYR	CB-CG-CD2	6.92	125.16	121.00
7	O	849	ASP	CB-CG-OD1	6.92	124.53	118.30
7	O	23	ASP	CB-CG-OD2	-6.92	112.07	118.30
9	T	651	ASP	CB-CG-OD2	-6.92	112.07	118.30
5	B	411	ARG	CD-NE-CZ	-6.92	113.92	123.60
3	1	106	ARG	NE-CZ-NH1	6.92	123.76	120.30
3	Z	856	ASN	CB-CG-OD1	-6.92	107.77	121.60
3	1	1351	TYR	CB-CG-CD1	6.92	125.15	121.00
2	Y	124	ARG	NE-CZ-NH2	-6.91	116.84	120.30
6	C	456	ARG	NE-CZ-NH2	6.91	123.76	120.30
8	N	567	ARG	NE-CZ-NH2	-6.91	116.84	120.30
2	0	1391	PHE	CB-CG-CD2	-6.91	115.96	120.80
2	Y	583	TYR	CB-CG-CD1	-6.91	116.85	121.00
6	C	456	ARG	NH1-CZ-NH2	-6.91	111.80	119.40
2	0	577	PHE	CB-CG-CD2	-6.91	115.96	120.80
7	O	437	ASP	CB-CG-OD1	6.91	124.52	118.30
7	M	1153	TYR	CB-CG-CD2	-6.91	116.86	121.00
2	Y	145	PHE	CB-CG-CD2	6.91	125.63	120.80
2	0	158	ASP	CB-CG-OD1	6.91	124.52	118.30
8	N	1486	GLU	N-CA-CB	-6.90	98.18	110.60
8	P	114	TYR	CD1-CE1-CZ	6.90	126.01	119.80
8	N	114	TYR	CD1-CE1-CZ	6.90	126.01	119.80
8	N	1124	ASP	CB-CG-OD2	-6.90	112.09	118.30
7	O	1153	TYR	CB-CG-CD2	-6.90	116.86	121.00
3	Z	380	ASP	CB-CG-OD1	6.89	124.50	118.30
5	H	401	ALA	N-CA-CB	6.89	119.75	110.10
2	Y	133	TYR	CB-CG-CD1	-6.89	116.86	121.00
7	O	1013	TYR	CB-CG-CD1	6.89	125.14	121.00
2	Y	1088	PHE	N-CA-CB	6.89	123.00	110.60
7	M	526	PHE	CB-CG-CD1	-6.89	115.98	120.80
8	P	1308	TYR	CB-CG-CD2	-6.89	116.87	121.00
9	Q	394	TYR	CB-CG-CD2	-6.89	116.87	121.00
7	O	124	PHE	CB-CG-CD1	-6.89	115.98	120.80
9	T	85	ALA	N-CA-CB	6.88	119.73	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	106	ARG	NE-CZ-NH1	6.88	123.74	120.30
2	Y	158	ASP	CB-CG-OD1	6.87	124.48	118.30
2	0	1088	PHE	N-CA-CB	6.87	122.97	110.60
5	B	441	GLN	N-CA-CB	6.87	122.96	110.60
2	0	133	TYR	CB-CG-CD1	-6.87	116.88	121.00
6	I	386	ASP	CB-CG-OD2	-6.87	112.12	118.30
9	S	546	ARG	NE-CZ-NH2	6.87	123.73	120.30
9	T	811	ARG	NE-CZ-NH1	6.86	123.73	120.30
6	I	456	ARG	NH1-CZ-NH2	-6.86	111.85	119.40
3	Z	268	ARG	NE-CZ-NH2	-6.86	116.87	120.30
3	1	380	ASP	CB-CG-OD1	6.86	124.47	118.30
9	R	85	ALA	N-CA-CB	6.85	119.70	110.10
5	H	441	GLN	N-CA-CB	6.85	122.94	110.60
9	Q	469	TYR	CB-CG-CD1	6.85	125.11	121.00
9	R	209	ARG	NE-CZ-NH1	6.85	123.73	120.30
8	P	1342	LEU	CB-CG-CD1	6.85	122.65	111.00
10	W	345	TYR	CB-CG-CD2	-6.85	116.89	121.00
8	P	567	ARG	NE-CZ-NH2	-6.85	116.87	120.30
8	N	252	TYR	CB-CG-CD2	-6.85	116.89	121.00
2	Y	126	TYR	CB-CG-CD1	6.85	125.11	121.00
8	N	1342	LEU	CB-CG-CD1	6.85	122.64	111.00
3	Z	1230	ASP	CB-CG-OD1	6.85	124.46	118.30
7	M	486	TYR	CB-CG-CD1	-6.84	116.89	121.00
2	Y	1391	PHE	CB-CG-CD2	-6.83	116.02	120.80
3	Z	79	HIS	N-CA-CB	6.83	122.90	110.60
3	1	1213	LEU	CA-C-O	6.83	134.45	120.10
8	P	252	TYR	CB-CG-CD2	-6.83	116.90	121.00
7	O	471	ASP	CB-CG-OD1	6.83	124.45	118.30
2	Y	577	PHE	CB-CG-CD2	-6.83	116.02	120.80
8	N	912	TRP	CG-CD1-NE1	-6.83	103.27	110.10
9	R	816	TYR	CB-CG-CD2	6.82	125.09	121.00
9	Q	386	TYR	CB-CG-CD1	6.82	125.09	121.00
8	P	1308	TYR	CB-CG-CD1	6.82	125.09	121.00
3	Z	969	ARG	NE-CZ-NH1	-6.82	116.89	120.30
7	M	224	ASP	CB-CG-OD2	-6.82	112.16	118.30
3	1	1230	ASP	CB-CG-OD1	6.82	124.43	118.30
9	S	469	TYR	CB-CG-CD1	6.82	125.09	121.00
7	M	1029	SER	N-CA-CB	6.81	120.72	110.50
6	I	336	PHE	CB-CG-CD2	6.81	125.57	120.80
3	Z	1074	ARG	NE-CZ-NH2	-6.81	116.89	120.30
7	O	1227	THR	CA-CB-CG2	-6.81	102.86	112.40
7	M	1013	TYR	CB-CG-CD1	6.81	125.08	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1	969	ARG	NE-CZ-NH1	-6.81	116.90	120.30
7	M	471	ASP	CB-CG-OD1	6.80	124.42	118.30
7	M	1412	TYR	CB-CG-CD2	-6.80	116.92	121.00
3	Z	1280	ASP	CB-CG-OD1	6.79	124.42	118.30
7	M	1013	TYR	CG-CD1-CE1	-6.79	115.87	121.30
3	1	79	HIS	N-CA-CB	6.79	122.82	110.60
6	C	336	PHE	CB-CG-CD2	6.79	125.55	120.80
9	S	530	ARG	NE-CZ-NH1	-6.79	116.91	120.30
8	N	1308	TYR	CB-CG-CD1	6.79	125.07	121.00
2	0	690	ASN	N-CA-CB	6.79	122.81	110.60
3	1	743	PHE	CB-CG-CD1	-6.79	116.05	120.80
9	Q	290	TYR	CG-CD2-CE2	-6.78	115.88	121.30
9	R	811	ARG	NE-CZ-NH1	6.78	123.69	120.30
11	X	378	ARG	N-CA-CB	6.78	122.81	110.60
3	1	268	ARG	NE-CZ-NH2	-6.78	116.91	120.30
3	1	1280	ASP	CB-CG-OD1	6.78	124.40	118.30
8	P	1263	TYR	CB-CG-CD1	-6.78	116.93	121.00
9	S	386	TYR	CB-CG-CD1	6.78	125.07	121.00
3	Z	297	SER	N-CA-CB	6.78	120.66	110.50
7	O	282	PHE	CB-CG-CD1	6.78	125.54	120.80
7	O	1029	SER	N-CA-CB	6.78	120.67	110.50
8	N	1420	VAL	CA-CB-CG2	-6.77	100.74	110.90
3	1	1074	ARG	NE-CZ-NH2	-6.77	116.91	120.30
8	N	671	LEU	CB-CG-CD2	6.77	122.51	111.00
11	V	378	ARG	N-CA-CB	6.77	122.78	110.60
8	P	68	HIS	N-CA-C	-6.77	92.72	111.00
2	Y	522	ALA	N-CA-CB	6.77	119.58	110.10
2	Y	690	ASN	N-CA-CB	6.77	122.78	110.60
3	1	97	PHE	CB-CG-CD2	-6.77	116.06	120.80
8	N	906	TYR	CB-CG-CD1	-6.77	116.94	121.00
9	Q	682	GLU	N-CA-CB	6.77	122.78	110.60
8	P	912	TRP	CG-CD1-NE1	-6.76	103.33	110.10
8	P	737	ASP	CB-CG-OD1	6.76	124.39	118.30
7	M	1227	THR	CA-CB-CG2	-6.76	102.94	112.40
2	0	126	TYR	CB-CG-CD1	6.76	125.06	121.00
3	1	1350	TRP	CB-CG-CD2	-6.76	117.81	126.60
6	I	456	ARG	NE-CZ-NH2	6.76	123.68	120.30
7	O	1412	TYR	CB-CG-CD2	-6.76	116.94	121.00
7	O	224	ASP	CB-CG-OD2	-6.76	112.22	118.30
2	0	1097	TYR	CB-CG-CD2	-6.75	116.95	121.00
8	P	671	LEU	CB-CG-CD2	6.75	122.48	111.00
8	N	332	ARG	NE-CZ-NH1	6.75	123.67	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	332	ARG	NE-CZ-NH1	6.75	123.67	120.30
9	S	682	GLU	N-CA-CB	6.75	122.75	110.60
8	P	906	TYR	CB-CG-CD1	-6.75	116.95	121.00
7	O	1052	LEU	CB-CG-CD2	-6.75	99.53	111.00
7	M	488	PHE	CB-CG-CD2	6.74	125.52	120.80
8	N	912	TRP	CB-CG-CD2	-6.74	117.84	126.60
7	M	982	PHE	CB-CG-CD2	-6.73	116.09	120.80
7	M	282	PHE	CB-CG-CD1	6.73	125.51	120.80
2	0	522	ALA	N-CA-CB	6.73	119.53	110.10
2	Y	881	THR	CA-CB-CG2	-6.73	102.98	112.40
2	Y	1313	VAL	CG1-CB-CG2	-6.73	100.13	110.90
3	1	297	SER	N-CA-CB	6.73	120.59	110.50
7	M	1099	TYR	CG-CD2-CE2	-6.73	115.92	121.30
7	O	671	PHE	CB-CG-CD2	6.73	125.51	120.80
3	Z	743	PHE	CB-CG-CD1	-6.72	116.09	120.80
7	M	1052	LEU	CB-CG-CD2	-6.72	99.57	111.00
9	T	209	ARG	NE-CZ-NH1	6.72	123.66	120.30
8	P	1420	VAL	CA-CB-CG2	-6.72	100.82	110.90
8	N	1183	PHE	CB-CG-CD2	-6.72	116.10	120.80
9	R	619	PHE	CB-CG-CD1	6.72	125.50	120.80
4	D	750	THR	CA-CB-CG2	-6.71	103.00	112.40
11	X	270	ALA	N-CA-CB	6.71	119.50	110.10
7	M	184	ASP	CB-CG-OD1	-6.71	112.26	118.30
2	Y	1201	TRP	CA-CB-CG	6.71	126.44	113.70
9	R	342	ARG	NH1-CZ-NH2	-6.71	112.02	119.40
9	Q	546	ARG	NE-CZ-NH2	6.70	123.65	120.30
2	0	881	THR	CA-CB-CG2	-6.70	103.01	112.40
2	0	1313	VAL	CG1-CB-CG2	-6.70	100.17	110.90
9	S	290	TYR	CG-CD2-CE2	-6.70	115.94	121.30
5	K	392	LEU	CB-CG-CD1	6.70	122.39	111.00
8	P	912	TRP	CB-CG-CD2	-6.70	117.89	126.60
5	E	421	THR	CA-CB-CG2	-6.70	103.02	112.40
7	M	671	PHE	CB-CG-CD2	6.70	125.49	120.80
7	M	774	ARG	NH1-CZ-NH2	6.70	126.77	119.40
4	J	750	THR	CA-CB-CG2	-6.70	103.03	112.40
5	E	392	LEU	CB-CG-CD1	6.69	122.38	111.00
3	Z	646	TYR	CB-CG-CD2	6.69	125.02	121.00
7	O	1013	TYR	CG-CD1-CE1	-6.69	115.95	121.30
8	N	1239	ASP	CB-CG-OD1	-6.69	112.28	118.30
6	C	343	ASP	CB-CG-OD2	-6.68	112.28	118.30
8	N	106	ARG	NE-CZ-NH2	6.68	123.64	120.30
5	K	421	THR	CA-CB-CG2	-6.68	103.04	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	1181	THR	CA-CB-CG2	-6.68	103.05	112.40
2	Y	250	ALA	CB-CA-C	-6.68	100.08	110.10
7	O	1005	PHE	CB-CG-CD1	-6.68	116.13	120.80
8	N	1263	TYR	CB-CG-CD1	-6.67	117.00	121.00
7	O	1099	TYR	CG-CD2-CE2	-6.67	115.96	121.30
5	B	397	ARG	NE-CZ-NH2	-6.67	116.96	120.30
8	N	441	PRO	CA-N-CD	-6.67	102.16	111.50
8	N	1271	LEU	CB-CG-CD2	6.67	122.34	111.00
11	V	270	ALA	N-CA-CB	6.67	119.44	110.10
8	P	1181	THR	CA-CB-CG2	-6.67	103.06	112.40
7	O	184	ASP	CB-CG-OD1	-6.67	112.30	118.30
9	Q	710	ASN	N-CA-CB	6.67	122.60	110.60
3	1	983	TYR	CB-CG-CD2	6.67	125.00	121.00
8	P	441	PRO	CA-N-CD	-6.67	102.17	111.50
3	Z	1350	TRP	CB-CG-CD2	-6.66	117.94	126.60
8	N	481	THR	CA-CB-CG2	-6.66	103.07	112.40
7	M	1005	PHE	CB-CG-CD1	-6.66	116.14	120.80
9	Q	530	ARG	NE-CZ-NH1	-6.66	116.97	120.30
2	0	1201	TRP	CA-CB-CG	6.66	126.35	113.70
9	T	342	ARG	NH1-CZ-NH2	-6.66	112.08	119.40
8	N	16	THR	CA-CB-CG2	-6.65	103.08	112.40
2	Y	632	TYR	CB-CG-CD1	-6.65	117.01	121.00
9	T	477	TYR	CB-CG-CD1	6.65	124.99	121.00
2	Y	294	TRP	CD1-CG-CD2	-6.64	100.98	106.30
8	P	1183	PHE	CB-CG-CD2	-6.64	116.15	120.80
7	O	982	PHE	CB-CG-CD2	-6.64	116.15	120.80
8	P	16	THR	CA-CB-CG2	-6.64	103.11	112.40
2	Y	1097	TYR	CB-CG-CD2	-6.64	117.02	121.00
8	P	481	THR	CA-CB-CG2	-6.64	103.11	112.40
8	P	1271	LEU	CB-CG-CD2	6.64	122.28	111.00
8	N	1199	TYR	CB-CG-CD2	-6.63	117.02	121.00
7	O	488	PHE	CB-CG-CD2	6.63	125.44	120.80
8	N	1087	TYR	CD1-CE1-CZ	-6.63	113.83	119.80
8	P	1087	TYR	CD1-CE1-CZ	-6.63	113.83	119.80
8	P	327	PHE	CB-CG-CD1	6.63	125.44	120.80
2	0	632	TYR	CB-CG-CD1	-6.63	117.02	121.00
9	R	620	LEU	CB-CG-CD2	6.62	122.26	111.00
9	R	438	MET	CG-SD-CE	-6.62	89.60	100.20
10	W	354	ALA	N-CA-CB	6.62	119.37	110.10
6	I	343	ASP	CB-CG-OD2	-6.62	112.34	118.30
8	N	68	HIS	N-CA-C	-6.62	93.13	111.00
9	R	804	ASP	CB-CG-OD2	-6.62	112.34	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	797	LEU	CB-CG-CD2	6.61	122.24	111.00
7	O	1203	TYR	CB-CG-CD2	6.61	124.97	121.00
7	M	1122	TRP	N-CA-C	-6.61	93.15	111.00
9	T	438	MET	CG-SD-CE	-6.61	89.63	100.20
3	Z	445	SER	N-CA-CB	6.61	120.41	110.50
3	Z	1333	GLU	N-CA-CB	6.61	122.49	110.60
9	T	619	PHE	CB-CG-CD1	6.61	125.43	120.80
9	T	620	LEU	CB-CG-CD2	6.61	122.23	111.00
7	M	1153	TYR	CB-CG-CD1	6.61	124.96	121.00
2	0	250	ALA	CB-CA-C	-6.61	100.19	110.10
3	1	822	PHE	CG-CD2-CE2	-6.61	113.53	120.80
3	1	646	TYR	CB-CG-CD2	6.60	124.96	121.00
7	O	771	ARG	CA-CB-CG	6.60	127.93	113.40
9	S	710	ASN	N-CA-CB	6.60	122.49	110.60
4	D	665	TRP	CD2-CE2-CZ2	-6.60	114.38	122.30
7	O	1150	PHE	CB-CG-CD1	6.60	125.42	120.80
7	O	1122	TRP	N-CA-C	-6.60	93.19	111.00
10	U	354	ALA	N-CA-CB	6.59	119.33	110.10
4	G	797	LEU	CB-CG-CD2	6.59	122.21	111.00
7	O	774	ARG	NH1-CZ-NH2	6.59	126.65	119.40
7	M	771	ARG	CA-CB-CG	6.59	127.90	113.40
4	J	665	TRP	CD2-CE2-CZ2	-6.59	114.39	122.30
6	C	387	TYR	CZ-CE2-CD2	-6.59	113.87	119.80
8	N	1498	GLY	O-C-N	6.59	133.24	122.70
5	H	397	ARG	NE-CZ-NH2	-6.59	117.01	120.30
2	Y	1427	TYR	CB-CG-CD1	6.58	124.95	121.00
3	Z	97	PHE	CB-CG-CD2	-6.58	116.19	120.80
3	1	1333	GLU	N-CA-CB	6.58	122.44	110.60
2	0	294	TRP	CD1-CG-CD2	-6.58	101.04	106.30
5	B	323	LEU	CB-CA-C	6.58	122.69	110.20
7	M	774	ARG	NE-CZ-NH2	-6.57	117.01	120.30
7	M	977	ARG	NE-CZ-NH1	6.57	123.58	120.30
8	N	327	PHE	CB-CG-CD1	6.57	125.40	120.80
2	0	914	TYR	CB-CG-CD1	6.57	124.94	121.00
7	O	1402	ARG	NE-CZ-NH1	6.57	123.58	120.30
9	R	477	TYR	CB-CG-CD1	6.56	124.94	121.00
6	I	387	TYR	CZ-CE2-CD2	-6.56	113.89	119.80
2	Y	914	TYR	CB-CG-CD1	6.56	124.94	121.00
8	P	388	ASN	CA-CB-CG	-6.56	98.97	113.40
9	Q	477	TYR	CD1-CE1-CZ	6.56	125.70	119.80
7	M	1366	ARG	NE-CZ-NH1	6.56	123.58	120.30
8	P	1498	GLY	O-C-N	6.56	133.19	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	388	ASN	CA-CB-CG	-6.56	98.98	113.40
2	0	145	PHE	CB-CG-CD1	-6.55	116.21	120.80
7	O	977	ARG	NE-CZ-NH1	6.55	123.58	120.30
8	P	1239	ASP	CB-CG-OD1	-6.55	112.41	118.30
7	M	1099	TYR	CB-CG-CD2	-6.55	117.07	121.00
3	1	862	LEU	CB-CG-CD1	6.54	122.13	111.00
3	Z	822	PHE	CG-CD2-CE2	-6.54	113.61	120.80
3	Z	1289	MET	CG-SD-CE	6.54	110.67	100.20
7	O	1366	ARG	NE-CZ-NH1	6.54	123.57	120.30
2	0	1427	TYR	CB-CG-CD1	6.54	124.92	121.00
3	1	445	SER	N-CA-CB	6.54	120.31	110.50
9	S	290	TYR	CB-CG-CD1	-6.54	117.08	121.00
2	Y	145	PHE	CB-CG-CD1	-6.54	116.22	120.80
3	1	1289	MET	CG-SD-CE	6.54	110.66	100.20
9	Q	290	TYR	CB-CG-CD1	-6.53	117.08	121.00
8	P	1199	TYR	CB-CG-CD2	-6.53	117.08	121.00
3	Z	862	LEU	CB-CG-CD1	6.53	122.09	111.00
9	Q	794	TYR	CB-CG-CD2	-6.53	117.08	121.00
2	Y	1207	ARG	NE-CZ-NH2	-6.52	117.04	120.30
7	M	563	SER	CB-CA-C	6.52	122.48	110.10
2	0	98	SER	N-CA-CB	6.52	120.28	110.50
5	K	329	HIS	N-CA-CB	6.51	122.33	110.60
2	Y	1442	SER	N-CA-CB	6.51	120.27	110.50
2	0	1442	SER	N-CA-CB	6.51	120.27	110.50
7	O	1153	TYR	CB-CG-CD1	6.51	124.91	121.00
8	P	106	ARG	NE-CZ-NH2	6.51	123.55	120.30
8	P	680	ASP	CB-CG-OD2	-6.51	112.44	118.30
7	M	741	GLY	N-CA-C	-6.51	96.83	113.10
7	O	563	SER	CB-CA-C	6.51	122.46	110.10
7	O	741	GLY	N-CA-C	-6.50	96.84	113.10
2	Y	98	SER	N-CA-CB	6.50	120.25	110.50
7	M	736	PHE	CB-CG-CD2	6.50	125.35	120.80
9	S	562	LEU	CB-CG-CD2	6.50	122.04	111.00
7	M	492	ARG	NE-CZ-NH2	-6.49	117.05	120.30
7	O	1099	TYR	CB-CG-CD2	-6.49	117.10	121.00
5	E	329	HIS	N-CA-CB	6.49	122.28	110.60
9	S	794	TYR	CB-CG-CD2	-6.49	117.11	121.00
9	Q	562	LEU	CB-CG-CD2	6.49	122.03	111.00
7	M	1364	TYR	CG-CD1-CE1	-6.49	116.11	121.30
5	B	353	TYR	CG-CD1-CE1	-6.48	116.11	121.30
7	M	1150	PHE	CB-CG-CD1	6.48	125.34	120.80
3	Z	983	TYR	CB-CG-CD2	6.48	124.89	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	1237	TYR	CB-CG-CD2	-6.48	117.11	121.00
7	O	736	PHE	CB-CG-CD2	6.48	125.34	120.80
4	D	702	ARG	N-CA-CB	6.48	122.26	110.60
3	Z	755	TYR	CG-CD2-CE2	-6.47	116.12	121.30
3	Z	1187	TYR	CG-CD1-CE1	6.47	126.48	121.30
8	P	922	PHE	CB-CG-CD1	-6.47	116.27	120.80
9	S	477	TYR	CD1-CE1-CZ	6.47	125.62	119.80
2	0	447	TYR	CB-CG-CD2	6.47	124.88	121.00
8	P	1156	PHE	CB-CG-CD2	-6.46	116.28	120.80
8	N	1083	ALA	N-CA-CB	6.46	119.15	110.10
7	M	1203	TYR	CB-CG-CD2	6.46	124.88	121.00
4	G	714	PHE	CB-CG-CD2	-6.46	116.28	120.80
8	N	680	ASP	CB-CG-OD2	-6.46	112.49	118.30
3	1	1187	TYR	CG-CD1-CE1	6.46	126.47	121.30
8	P	683	ASP	CB-CG-OD1	6.46	124.11	118.30
9	T	273	VAL	CA-CB-CG1	-6.45	101.22	110.90
9	R	691	ARG	NE-CZ-NH2	-6.45	117.07	120.30
9	T	691	ARG	NE-CZ-NH2	-6.45	117.08	120.30
2	Y	109	ASP	CB-CG-OD2	-6.45	112.50	118.30
3	1	366	TYR	CB-CG-CD2	-6.45	117.13	121.00
7	O	1598	PHE	CG-CD1-CE1	6.45	127.89	120.80
9	T	804	ASP	CB-CG-OD2	-6.45	112.50	118.30
8	N	1156	PHE	CB-CG-CD2	-6.45	116.29	120.80
4	J	702	ARG	N-CA-CB	6.45	122.20	110.60
7	O	492	ARG	NE-CZ-NH2	-6.44	117.08	120.30
2	0	1329	ASP	CB-CG-OD2	-6.44	112.50	118.30
9	S	669	ASP	CB-CG-OD1	-6.44	112.50	118.30
9	R	273	VAL	CA-CB-CG1	-6.44	101.24	110.90
3	1	1136	ARG	NE-CZ-NH2	6.44	123.52	120.30
7	O	774	ARG	NE-CZ-NH2	-6.43	117.08	120.30
7	M	345	ARG	NE-CZ-NH1	-6.43	117.08	120.30
2	0	1207	ARG	NE-CZ-NH2	-6.43	117.08	120.30
3	1	1360	SER	N-CA-CB	6.43	120.14	110.50
7	O	269	TYR	CB-CG-CD1	-6.43	117.14	121.00
2	0	496	PHE	N-CA-CB	6.43	122.17	110.60
3	1	214	PHE	CB-CG-CD1	-6.43	116.30	120.80
5	H	353	TYR	CG-CD1-CE1	-6.42	116.16	121.30
7	O	1364	TYR	CG-CD1-CE1	-6.42	116.16	121.30
8	P	1083	ALA	N-CA-CB	6.42	119.09	110.10
7	M	1598	PHE	CG-CD1-CE1	6.42	127.86	120.80
3	1	843	TYR	CG-CD2-CE2	-6.41	116.17	121.30
8	N	683	ASP	CB-CG-OD1	6.41	124.07	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	0	867	TYR	CB-CG-CD1	6.41	124.84	121.00
2	0	109	ASP	CB-CG-OD2	-6.40	112.54	118.30
8	N	1425	TYR	CZ-CE2-CD2	6.40	125.56	119.80
9	Q	669	ASP	CB-CG-OD1	-6.40	112.54	118.30
3	Z	1360	SER	N-CA-CB	6.40	120.10	110.50
7	O	934	ASP	CB-CG-OD1	6.39	124.05	118.30
3	Z	843	TYR	CG-CD2-CE2	-6.39	116.19	121.30
8	N	922	PHE	CB-CG-CD1	-6.39	116.33	120.80
3	Z	366	TYR	CB-CG-CD2	-6.38	117.17	121.00
7	O	1237	TYR	CB-CG-CD2	-6.38	117.17	121.00
9	T	749	ASP	CB-CG-OD1	6.38	124.05	118.30
7	M	269	TYR	CB-CG-CD1	-6.38	117.17	121.00
7	M	354	ARG	NE-CZ-NH1	-6.38	117.11	120.30
8	N	1380	ASP	CB-CG-OD1	6.38	124.04	118.30
2	Y	447	TYR	CB-CG-CD2	6.38	124.83	121.00
2	Y	867	TYR	CB-CG-CD1	6.38	124.83	121.00
9	Q	657	VAL	CG1-CB-CG2	-6.38	100.69	110.90
4	J	809	ASP	CB-CG-OD2	-6.38	112.56	118.30
9	T	572	CYS	O-C-N	-6.38	112.49	122.70
8	P	1392	PHE	CB-CG-CD1	-6.37	116.34	120.80
7	O	345	ARG	NE-CZ-NH1	-6.37	117.12	120.30
8	P	1425	TYR	CZ-CE2-CD2	6.37	125.53	119.80
3	Z	1054	PHE	CB-CG-CD1	-6.36	116.34	120.80
3	1	755	TYR	CG-CD2-CE2	-6.36	116.21	121.30
2	Y	127	TYR	CB-CG-CD2	-6.36	117.19	121.00
9	S	657	VAL	CG1-CB-CG2	-6.36	100.73	110.90
8	N	1171	ARG	NE-CZ-NH1	6.36	123.48	120.30
8	P	330	TYR	CG-CD1-CE1	6.36	126.38	121.30
8	P	1380	ASP	CB-CG-OD1	6.36	124.02	118.30
2	Y	496	PHE	N-CA-CB	6.35	122.03	110.60
3	Z	214	PHE	CB-CG-CD1	-6.35	116.35	120.80
9	R	572	CYS	O-C-N	-6.35	112.54	122.70
9	S	619	PHE	CZ-CE2-CD2	-6.34	112.49	120.10
4	A	714	PHE	CB-CG-CD2	-6.34	116.36	120.80
3	Z	948	ARG	NE-CZ-NH2	-6.34	117.13	120.30
7	O	1544	PHE	CB-CG-CD2	6.34	125.24	120.80
3	Z	718	ARG	NE-CZ-NH1	6.34	123.47	120.30
5	K	346	GLN	N-CA-CB	6.34	122.01	110.60
2	Y	619	THR	N-CA-C	-6.34	93.89	111.00
7	O	731	PHE	CB-CG-CD2	-6.34	116.36	120.80
4	D	726	VAL	CA-CB-CG1	-6.33	101.40	110.90
7	O	816	PHE	CB-CG-CD2	-6.33	116.36	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	354	ARG	NE-CZ-NH1	-6.33	117.13	120.30
9	Q	251	ALA	CB-CA-C	-6.33	100.60	110.10
8	N	1392	PHE	CB-CG-CD1	-6.33	116.37	120.80
7	M	934	ASP	CB-CG-OD1	6.33	123.99	118.30
7	O	245	ARG	NE-CZ-NH2	-6.33	117.14	120.30
5	E	346	GLN	N-CA-CB	6.32	121.98	110.60
6	F	389	ARG	NH1-CZ-NH2	6.32	126.36	119.40
3	1	1054	PHE	CB-CG-CD1	-6.32	116.38	120.80
9	R	749	ASP	CB-CG-OD1	6.32	123.99	118.30
7	O	1635	ARG	NE-CZ-NH1	6.32	123.46	120.30
2	0	619	THR	N-CA-C	-6.32	93.94	111.00
3	Z	1136	ARG	NE-CZ-NH2	6.32	123.46	120.30
9	T	539	ALA	CB-CA-C	-6.32	100.62	110.10
6	F	396	THR	CA-CB-CG2	-6.32	103.56	112.40
9	S	823	ARG	NE-CZ-NH1	6.32	123.46	120.30
9	Q	619	PHE	CZ-CE2-CD2	-6.31	112.52	120.10
2	Y	1329	ASP	CB-CG-OD2	-6.31	112.62	118.30
7	M	1013	TYR	CZ-CE2-CD2	6.31	125.48	119.80
7	M	731	PHE	CB-CG-CD2	-6.31	116.39	120.80
8	N	330	TYR	CG-CD1-CE1	6.31	126.35	121.30
3	1	1164	PHE	CD1-CE1-CZ	6.31	127.67	120.10
6	L	396	THR	CA-CB-CG2	-6.31	103.57	112.40
8	N	685	TYR	N-CA-CB	6.30	121.95	110.60
9	R	516	PHE	CB-CG-CD2	6.30	125.21	120.80
4	J	726	VAL	CA-CB-CG1	-6.30	101.44	110.90
5	K	313	TYR	CB-CG-CD1	-6.30	117.22	121.00
9	S	251	ALA	CB-CA-C	-6.30	100.64	110.10
9	Q	412	TYR	CB-CG-CD2	-6.30	117.22	121.00
7	M	816	PHE	CB-CG-CD2	-6.30	116.39	120.80
9	S	473	ARG	NE-CZ-NH2	-6.30	117.15	120.30
5	E	422	LEU	N-CA-CB	6.29	122.99	110.40
7	M	1635	ARG	NE-CZ-NH1	6.29	123.45	120.30
11	X	360	TYR	CB-CG-CD1	6.29	124.78	121.00
9	S	238	PHE	CB-CG-CD2	-6.29	116.40	120.80
9	Q	238	PHE	CB-CG-CD2	-6.29	116.40	120.80
9	Q	473	ARG	NE-CZ-NH2	-6.29	117.16	120.30
8	P	685	TYR	N-CA-CB	6.29	121.92	110.60
9	S	412	TYR	CB-CG-CD2	-6.29	117.23	121.00
11	V	360	TYR	CB-CG-CD1	6.29	124.77	121.00
7	M	1544	PHE	CB-CG-CD2	6.28	125.20	120.80
3	1	1057	TYR	CG-CD2-CE2	-6.28	116.27	121.30
3	Z	83	SER	N-CA-CB	6.28	119.92	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	0	127	TYR	CB-CG-CD2	-6.28	117.23	121.00
6	L	389	ARG	NH1-CZ-NH2	6.28	126.31	119.40
9	Q	412	TYR	CB-CG-CD1	6.28	124.77	121.00
9	T	629	ARG	NE-CZ-NH1	6.28	123.44	120.30
8	P	1247	PHE	CB-CG-CD2	-6.27	116.41	120.80
3	Z	816	TYR	CG-CD2-CE2	6.27	126.32	121.30
4	G	712	ASP	CB-CG-OD2	-6.27	112.66	118.30
7	O	1013	TYR	CZ-CE2-CD2	6.27	125.45	119.80
3	Z	1188	ARG	NE-CZ-NH1	6.27	123.44	120.30
4	A	710	PHE	CB-CG-CD2	-6.27	116.41	120.80
3	1	1188	ARG	NE-CZ-NH1	6.27	123.44	120.30
8	N	955	PHE	CB-CG-CD2	-6.27	116.41	120.80
4	D	680	TYR	CG-CD2-CE2	6.27	126.31	121.30
8	N	1247	PHE	CB-CG-CD2	-6.27	116.41	120.80
2	Y	133	TYR	CB-CG-CD2	6.27	124.76	121.00
9	R	539	ALA	CB-CA-C	-6.27	100.70	110.10
8	P	955	PHE	CB-CG-CD2	-6.26	116.42	120.80
3	1	948	ARG	NE-CZ-NH2	-6.26	117.17	120.30
3	1	83	SER	N-CA-CB	6.26	119.89	110.50
3	1	718	ARG	NE-CZ-NH1	6.26	123.43	120.30
4	D	809	ASP	CB-CG-OD2	-6.26	112.67	118.30
4	G	710	PHE	CB-CG-CD2	-6.26	116.42	120.80
6	F	274	ARG	NE-CZ-NH1	-6.25	117.17	120.30
9	R	215	TYR	CD1-CE1-CZ	6.25	125.43	119.80
2	0	1385	PHE	CB-CG-CD2	-6.25	116.42	120.80
5	K	422	LEU	N-CA-CB	6.25	122.91	110.40
2	0	369	TYR	CB-CG-CD1	-6.25	117.25	121.00
2	Y	1232	ARG	NE-CZ-NH2	-6.25	117.17	120.30
8	P	685	TYR	CB-CG-CD1	6.25	124.75	121.00
7	M	1402	ARG	NE-CZ-NH1	6.25	123.42	120.30
3	1	1184	ASP	CB-CG-OD2	-6.24	112.68	118.30
8	P	1171	ARG	NE-CZ-NH1	6.24	123.42	120.30
5	B	537	TYR	C-N-CA	6.24	137.29	121.70
5	E	313	TYR	CB-CG-CD1	-6.24	117.26	121.00
7	M	642	PHE	CB-CG-CD2	-6.24	116.43	120.80
10	U	345	TYR	CB-CG-CD1	6.24	124.74	121.00
8	P	1482	ASP	CB-CG-OD1	6.23	123.91	118.30
2	0	1210	PHE	CB-CG-CD1	-6.23	116.44	120.80
8	P	343	ASP	CB-CG-OD1	-6.23	112.69	118.30
7	M	535	PHE	CB-CG-CD2	6.23	125.16	120.80
6	F	456	ARG	NE-CZ-NH1	6.23	123.41	120.30
7	M	5	ALA	N-CA-CB	6.23	118.82	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	852	PHE	CB-CG-CD1	6.23	125.16	120.80
6	L	343	ASP	CB-CG-OD2	-6.23	112.69	118.30
3	1	816	TYR	CG-CD2-CE2	6.22	126.28	121.30
7	M	431	PHE	CB-CG-CD2	-6.22	116.45	120.80
2	Y	1385	PHE	CB-CG-CD2	-6.22	116.45	120.80
7	O	1484	ARG	NH1-CZ-NH2	-6.22	112.56	119.40
9	T	587	THR	CA-CB-CG2	-6.22	103.69	112.40
7	M	565	TYR	CB-CG-CD1	-6.22	117.27	121.00
2	Y	285	ALA	CB-CA-C	-6.21	100.78	110.10
2	Y	369	TYR	CB-CG-CD1	-6.21	117.27	121.00
7	O	295	ARG	NE-CZ-NH2	-6.21	117.19	120.30
2	0	133	TYR	CB-CG-CD2	6.21	124.73	121.00
7	O	642	PHE	CB-CG-CD2	-6.21	116.45	120.80
3	Z	1164	PHE	CD1-CE1-CZ	6.21	127.55	120.10
9	T	215	TYR	CD1-CE1-CZ	6.21	125.39	119.80
2	0	285	ALA	CB-CA-C	-6.20	100.80	110.10
3	Z	1016	ASP	CB-CG-OD2	-6.20	112.72	118.30
8	N	343	ASP	CB-CG-OD1	-6.20	112.72	118.30
7	O	5	ALA	N-CA-CB	6.20	118.78	110.10
3	1	1016	ASP	CB-CG-OD2	-6.20	112.72	118.30
2	Y	1210	PHE	CB-CG-CD1	-6.20	116.46	120.80
4	J	809	ASP	CB-CG-OD1	6.20	123.88	118.30
9	S	412	TYR	CB-CG-CD1	6.20	124.72	121.00
2	Y	1468	TYR	CG-CD2-CE2	-6.20	116.34	121.30
7	M	1484	ARG	NE-CZ-NH2	-6.20	117.20	120.30
2	0	1430	LEU	CB-CG-CD1	6.20	121.53	111.00
5	H	537	TYR	C-N-CA	6.20	137.19	121.70
7	O	1484	ARG	NE-CZ-NH2	-6.19	117.20	120.30
2	Y	1430	LEU	CB-CG-CD1	6.19	121.52	111.00
8	N	1487	PHE	CB-CG-CD1	-6.19	116.47	120.80
2	0	445	ARG	CD-NE-CZ	6.19	132.27	123.60
9	T	516	PHE	CB-CG-CD2	6.19	125.13	120.80
7	M	692	TYR	CB-CG-CD2	6.19	124.71	121.00
6	F	343	ASP	CB-CG-OD2	-6.18	112.73	118.30
5	K	313	TYR	CA-CB-CG	-6.18	101.66	113.40
7	O	431	PHE	CB-CG-CD2	-6.18	116.47	120.80
6	L	274	ARG	NE-CZ-NH1	-6.18	117.21	120.30
4	D	809	ASP	CB-CG-OD1	6.18	123.86	118.30
8	N	1365	ARG	NE-CZ-NH2	-6.18	117.21	120.30
9	R	629	ARG	NE-CZ-NH1	6.18	123.39	120.30
6	L	322	THR	CA-CB-OG1	6.17	121.97	109.00
7	O	14	SER	N-CA-CB	6.17	119.76	110.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	1057	TYR	CG-CD2-CE2	-6.17	116.36	121.30
7	M	1104	ASN	N-CA-CB	6.17	121.71	110.60
2	0	269	ASP	CB-CG-OD1	-6.17	112.75	118.30
7	O	1104	ASN	N-CA-CB	6.17	121.71	110.60
9	T	690	ARG	NE-CZ-NH2	-6.17	117.22	120.30
5	E	313	TYR	CA-CB-CG	-6.17	101.68	113.40
9	R	586	PHE	CB-CG-CD2	6.16	125.11	120.80
2	0	829	ILE	C-N-CA	6.16	137.10	121.70
2	0	1232	ARG	NE-CZ-NH2	-6.16	117.22	120.30
3	1	998	TYR	CB-CG-CD1	6.16	124.69	121.00
9	T	586	PHE	CB-CG-CD2	6.16	125.11	120.80
3	1	1080	VAL	CA-CB-CG1	6.15	120.13	110.90
7	M	14	SER	N-CA-CB	6.15	119.73	110.50
2	0	381	VAL	CA-CB-CG2	-6.15	101.67	110.90
7	M	1484	ARG	NH1-CZ-NH2	-6.15	112.63	119.40
4	J	680	TYR	CG-CD2-CE2	6.15	126.22	121.30
3	Z	1053	ARG	NE-CZ-NH1	6.15	123.38	120.30
8	N	685	TYR	CB-CG-CD1	6.15	124.69	121.00
9	T	630	ARG	NE-CZ-NH1	6.15	123.37	120.30
7	O	692	TYR	CB-CG-CD2	6.14	124.69	121.00
6	F	322	THR	CA-CB-OG1	6.14	121.89	109.00
9	Q	760	PHE	CB-CG-CD1	-6.14	116.50	120.80
7	M	245	ARG	NE-CZ-NH2	-6.14	117.23	120.30
9	R	587	THR	CA-CB-CG2	-6.14	103.81	112.40
9	Q	249	ARG	NE-CZ-NH1	6.13	123.37	120.30
9	R	799	LYS	CA-CB-CG	6.13	126.89	113.40
2	Y	445	ARG	CD-NE-CZ	6.13	132.19	123.60
9	R	630	ARG	NE-CZ-NH1	6.13	123.37	120.30
9	R	690	ARG	NE-CZ-NH2	-6.13	117.23	120.30
7	M	1666	MET	CG-SD-CE	-6.13	90.39	100.20
7	O	535	PHE	CB-CG-CD2	6.13	125.09	120.80
7	O	245	ARG	NE-CZ-NH1	6.13	123.36	120.30
3	Z	1080	VAL	CA-CB-CG1	6.13	120.09	110.90
4	A	712	ASP	CB-CG-OD2	-6.13	112.78	118.30
9	T	799	LYS	CA-CB-CG	6.13	126.88	113.40
2	Y	829	ILE	C-N-CA	6.13	137.01	121.70
8	N	1482	ASP	CB-CG-OD1	6.12	123.81	118.30
7	M	938	ALA	CB-CA-C	-6.12	100.92	110.10
2	Y	124	ARG	NH1-CZ-NH2	-6.12	112.67	119.40
2	Y	381	VAL	CA-CB-CG2	-6.12	101.72	110.90
9	S	79	SER	N-CA-CB	6.12	119.68	110.50
3	Z	1018	TYR	CB-CG-CD1	6.12	124.67	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	80	GLU	OE1-CD-OE2	6.12	130.64	123.30
7	M	1412	TYR	CZ-CE2-CD2	6.11	125.30	119.80
3	1	998	TYR	CB-CG-CD2	-6.11	117.33	121.00
7	O	1050	ASP	CB-CG-OD1	-6.11	112.80	118.30
7	O	1412	TYR	CZ-CE2-CD2	6.11	125.30	119.80
7	O	1666	MET	CG-SD-CE	-6.11	90.43	100.20
9	S	760	PHE	CB-CG-CD1	-6.11	116.52	120.80
3	1	1269	LEU	CB-CG-CD2	6.10	121.38	111.00
9	Q	79	SER	N-CA-CB	6.10	119.65	110.50
10	W	345	TYR	CB-CG-CD1	6.10	124.66	121.00
2	0	1468	TYR	CG-CD2-CE2	-6.10	116.42	121.30
3	1	502	ILE	N-CA-C	-6.10	94.54	111.00
7	O	80	GLU	OE1-CD-OE2	6.10	130.62	123.30
3	Z	502	ILE	N-CA-C	-6.10	94.54	111.00
2	Y	1157	PHE	CB-CG-CD1	-6.09	116.53	120.80
2	0	1157	PHE	CB-CG-CD1	-6.09	116.53	120.80
7	M	233	TYR	CG-CD1-CE1	6.09	126.17	121.30
3	1	1018	TYR	CB-CG-CD1	6.09	124.66	121.00
8	P	1365	ARG	NE-CZ-NH2	-6.09	117.25	120.30
2	Y	931	ASP	CB-CG-OD1	6.09	123.78	118.30
3	Z	402	ARG	NE-CZ-NH2	-6.09	117.26	120.30
6	I	396	THR	CA-CB-CG2	-6.09	103.88	112.40
6	L	456	ARG	NE-CZ-NH1	6.09	123.34	120.30
7	M	1569	TYR	CZ-CE2-CD2	6.08	125.28	119.80
9	Q	823	ARG	NE-CZ-NH1	6.08	123.34	120.30
2	0	124	ARG	NH1-CZ-NH2	-6.08	112.71	119.40
3	1	905	ARG	NE-CZ-NH2	-6.08	117.26	120.30
8	N	247	PHE	CB-CG-CD1	-6.07	116.55	120.80
3	1	228	PHE	CB-CG-CD2	6.07	125.05	120.80
7	O	455	ASP	CB-CG-OD2	-6.07	112.83	118.30
9	R	263	MET	CB-CA-C	-6.07	98.26	110.40
7	M	455	ASP	CB-CG-OD2	-6.07	112.84	118.30
9	R	723	ILE	CA-CB-CG1	-6.07	99.47	111.00
8	P	449	ASP	CB-CG-OD2	-6.07	112.84	118.30
8	P	1309	ARG	NE-CZ-NH1	6.07	123.33	120.30
7	M	245	ARG	NE-CZ-NH1	6.07	123.33	120.30
3	1	935	TYR	CB-CG-CD1	-6.07	117.36	121.00
9	S	829	TYR	CB-CG-CD1	6.07	124.64	121.00
7	O	565	TYR	CB-CG-CD1	-6.06	117.36	121.00
8	P	180	LYS	CA-CB-CG	6.06	126.73	113.40
8	P	1170	ASP	CB-CG-OD2	-6.06	112.85	118.30
8	P	1487	PHE	CB-CG-CD1	-6.06	116.56	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	723	ILE	CA-CB-CG1	-6.06	99.49	111.00
2	Y	269	ASP	CB-CG-OD1	-6.06	112.85	118.30
2	Y	1230	PHE	CB-CG-CD2	6.06	125.04	120.80
8	N	555	PHE	CB-CG-CD2	-6.06	116.56	120.80
9	S	191	ASN	C-N-CA	6.06	136.84	121.70
3	Z	228	PHE	CB-CG-CD2	6.05	125.04	120.80
6	I	341	ASP	CB-CG-OD2	6.05	123.75	118.30
4	J	644	TRP	CB-CG-CD1	6.05	134.87	127.00
8	P	247	PHE	CB-CG-CD1	-6.05	116.56	120.80
3	Z	1269	LEU	CB-CG-CD2	6.05	121.29	111.00
8	N	227	ILE	C-N-CA	6.05	136.83	121.70
3	1	402	ARG	NE-CZ-NH2	-6.05	117.27	120.30
9	R	18	ALA	N-CA-CB	6.05	118.57	110.10
8	N	180	LYS	CA-CB-CG	6.05	126.70	113.40
7	O	233	TYR	CG-CD1-CE1	6.05	126.14	121.30
9	S	249	ARG	NE-CZ-NH1	6.04	123.32	120.30
8	N	758	TYR	CZ-CE2-CD2	-6.04	114.36	119.80
3	1	1212	PRO	N-CA-C	6.04	127.81	112.10
4	J	788	ASP	CB-CG-OD2	-6.04	112.86	118.30
7	O	938	ALA	CB-CA-C	-6.04	101.04	110.10
9	T	451	ASP	CB-CG-OD1	6.04	123.74	118.30
3	Z	935	TYR	CB-CG-CD1	-6.04	117.38	121.00
7	O	1569	TYR	CZ-CE2-CD2	6.04	125.24	119.80
9	T	263	MET	CB-CA-C	-6.04	98.32	110.40
2	Y	856	TYR	CB-CG-CD1	-6.04	117.38	121.00
3	Z	905	ARG	NE-CZ-NH2	-6.04	117.28	120.30
9	S	457	TYR	CB-CG-CD1	-6.04	117.38	121.00
4	D	644	TRP	CB-CG-CD1	6.04	134.85	127.00
8	N	1099	PHE	CB-CG-CD2	-6.04	116.58	120.80
9	Q	191	ASN	C-N-CA	6.04	136.79	121.70
2	Y	1218	TYR	CB-CG-CD1	-6.03	117.38	121.00
3	Z	998	TYR	CB-CG-CD2	-6.03	117.38	121.00
8	P	852	PHE	CB-CG-CD1	6.03	125.02	120.80
6	C	396	THR	CA-CB-CG2	-6.03	103.96	112.40
9	Q	541	TYR	CD1-CE1-CZ	-6.03	114.37	119.80
2	0	1230	PHE	CB-CG-CD2	6.03	125.02	120.80
4	J	710	PHE	CB-CG-CD1	6.03	125.02	120.80
6	C	341	ASP	CB-CG-OD2	6.03	123.72	118.30
9	Q	829	TYR	CB-CG-CD1	6.03	124.62	121.00
3	1	1277	ARG	NE-CZ-NH1	-6.03	117.29	120.30
6	C	306	ASP	CB-CG-OD2	-6.03	112.88	118.30
9	S	501	MET	CG-SD-CE	-6.03	90.56	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1	1053	ARG	NE-CZ-NH1	6.02	123.31	120.30
6	I	306	ASP	CB-CG-OD2	-6.02	112.88	118.30
3	Z	127	ASP	CB-CG-OD1	6.02	123.72	118.30
4	D	788	ASP	CB-CG-OD2	-6.02	112.88	118.30
8	P	24	ASP	CB-CG-OD2	-6.02	112.88	118.30
3	Z	998	TYR	CB-CG-CD1	6.02	124.61	121.00
8	N	24	ASP	CB-CG-OD2	-6.02	112.89	118.30
9	T	18	ALA	N-CA-CB	6.01	118.52	110.10
9	R	451	ASP	CB-CG-OD1	6.01	123.71	118.30
3	1	127	ASP	CB-CG-OD1	6.01	123.71	118.30
4	A	752	ASP	N-CA-CB	6.00	121.41	110.60
8	N	1309	ARG	NE-CZ-NH1	6.00	123.30	120.30
9	Q	501	MET	CG-SD-CE	-6.00	90.60	100.20
7	M	918	PHE	CB-CG-CD1	6.00	125.00	120.80
3	1	821	ALA	N-CA-CB	6.00	118.50	110.10
7	O	1157	TRP	CE2-CD2-CG	-6.00	102.50	107.30
8	P	758	TYR	CZ-CE2-CD2	-6.00	114.40	119.80
3	Z	816	TYR	CZ-CE2-CD2	-6.00	114.40	119.80
3	1	816	TYR	CZ-CE2-CD2	-6.00	114.41	119.80
8	P	555	PHE	CB-CG-CD2	-5.99	116.61	120.80
9	Q	282	PHE	CB-CG-CD1	-5.99	116.61	120.80
7	O	112	TYR	CG-CD2-CE2	-5.99	116.51	121.30
8	N	1170	ASP	CB-CG-OD2	-5.99	112.91	118.30
9	S	18	ALA	N-CA-CB	5.99	118.48	110.10
4	A	720	ALA	N-CA-CB	5.99	118.48	110.10
3	1	150	VAL	CA-CB-CG2	-5.99	101.92	110.90
7	M	1368	ARG	NE-CZ-NH2	-5.98	117.31	120.30
7	M	295	ARG	NE-CZ-NH2	-5.98	117.31	120.30
3	1	351	ARG	NH1-CZ-NH2	-5.98	112.82	119.40
9	T	607	ARG	NE-CZ-NH1	5.98	123.29	120.30
8	P	1087	TYR	CG-CD1-CE1	5.98	126.08	121.30
6	I	350	PHE	CB-CG-CD1	5.98	124.98	120.80
7	O	918	PHE	CB-CG-CD1	5.98	124.99	120.80
7	M	1050	ASP	CB-CG-OD1	-5.98	112.92	118.30
9	Q	457	TYR	CB-CG-CD1	-5.98	117.41	121.00
2	Y	1380	ASP	CB-CG-OD2	-5.97	112.92	118.30
8	P	1099	PHE	CB-CG-CD2	-5.97	116.62	120.80
3	Z	821	ALA	N-CA-CB	5.97	118.45	110.10
9	S	541	TYR	CD1-CE1-CZ	-5.97	114.43	119.80
9	S	757	ALA	N-CA-CB	5.97	118.45	110.10
3	1	1243	ASP	CB-CG-OD2	-5.97	112.93	118.30
3	1	404	PHE	CB-CG-CD2	5.96	124.97	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	138	PHE	CB-CG-CD2	5.96	124.97	120.80
5	K	299	TRP	CD1-NE1-CE2	-5.96	103.64	109.00
3	Z	1148	ASP	CB-CG-OD1	-5.96	112.94	118.30
2	Y	653	ARG	NE-CZ-NH1	5.96	123.28	120.30
5	E	299	TRP	CD1-NE1-CE2	-5.96	103.64	109.00
4	G	720	ALA	N-CA-CB	5.96	118.44	110.10
8	P	1536	TRP	NE1-CE2-CZ2	5.96	136.95	130.40
4	D	710	PHE	CB-CG-CD1	5.95	124.97	120.80
7	M	929	TYR	CB-CG-CD2	-5.95	117.43	121.00
8	N	1536	TRP	NE1-CE2-CZ2	5.95	136.95	130.40
7	O	929	TYR	CB-CG-CD2	-5.95	117.43	121.00
9	Q	829	TYR	CB-CG-CD2	-5.95	117.43	121.00
3	1	1213	LEU	CA-C-N	-5.95	104.11	117.20
2	0	1380	ASP	CB-CG-OD2	-5.95	112.95	118.30
3	Z	1377	ASP	CB-CG-OD1	-5.94	112.95	118.30
8	N	449	ASP	CB-CG-OD2	-5.94	112.95	118.30
4	G	686	ALA	N-CA-CB	5.94	118.42	110.10
4	G	752	ASP	N-CA-CB	5.94	121.29	110.60
3	Z	349	GLN	CB-CA-C	-5.94	98.52	110.40
2	Y	281	ARG	NE-CZ-NH2	-5.94	117.33	120.30
2	Y	387	LEU	N-CA-C	-5.94	94.97	111.00
7	M	1157	TRP	CE2-CD2-CG	-5.94	102.55	107.30
2	0	1162	TYR	CB-CG-CD1	5.94	124.56	121.00
9	R	101	PRO	N-CA-CB	5.94	110.42	103.30
9	Q	757	ALA	N-CA-CB	5.93	118.41	110.10
2	0	931	ASP	CB-CG-OD1	5.93	123.64	118.30
3	1	349	GLN	CB-CA-C	-5.93	98.53	110.40
3	1	1377	ASP	CB-CG-OD1	-5.93	112.96	118.30
2	Y	369	TYR	CB-CG-CD2	5.93	124.56	121.00
3	Z	351	ARG	NH1-CZ-NH2	-5.93	112.88	119.40
3	Z	1230	ASP	N-CA-CB	5.93	121.28	110.60
9	S	101	PRO	N-CA-CB	5.93	110.42	103.30
7	O	1060	LEU	CB-CG-CD1	5.93	121.08	111.00
9	S	98	PRO	N-CA-CB	5.93	110.41	103.30
2	Y	1398	PHE	CB-CG-CD2	5.92	124.95	120.80
7	M	1060	LEU	CB-CG-CD1	5.92	121.07	111.00
8	N	202	THR	CA-CB-CG2	-5.92	104.11	112.40
8	N	1087	TYR	CG-CD1-CE1	5.92	126.04	121.30
2	Y	243	PHE	CB-CG-CD1	5.92	124.94	120.80
8	N	811	ASP	CB-CG-OD1	5.92	123.63	118.30
9	Q	101	PRO	N-CA-CB	5.92	110.40	103.30
3	Z	738	GLU	OE1-CD-OE2	-5.92	116.20	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	0	387	LEU	N-CA-C	-5.92	95.02	111.00
4	A	686	ALA	N-CA-CB	5.92	118.38	110.10
3	1	1230	ASP	N-CA-CB	5.91	121.24	110.60
7	O	1510	ASP	CB-CG-OD1	5.91	123.62	118.30
9	S	100	PRO	N-CA-CB	5.91	110.39	103.30
3	Z	150	VAL	CA-CB-CG2	-5.91	102.04	110.90
6	C	336	PHE	CB-CG-CD1	-5.91	116.66	120.80
9	T	101	PRO	N-CA-CB	5.91	110.39	103.30
7	M	112	TYR	CG-CD2-CE2	-5.91	116.58	121.30
9	R	607	ARG	NE-CZ-NH1	5.91	123.25	120.30
6	L	440	VAL	CG1-CB-CG2	-5.91	101.45	110.90
2	Y	939	ASP	CB-CG-OD2	-5.91	112.98	118.30
4	A	685	MET	CG-SD-CE	-5.91	90.75	100.20
2	0	856	TYR	CB-CG-CD1	-5.91	117.46	121.00
3	1	433	TYR	CG-CD1-CE1	-5.91	116.58	121.30
3	1	1148	ASP	CB-CG-OD1	-5.91	112.98	118.30
4	G	685	MET	CG-SD-CE	-5.91	90.75	100.20
9	S	33	PRO	N-CA-CB	5.90	110.38	103.30
6	F	440	VAL	CG1-CB-CG2	-5.90	101.46	110.90
2	0	1203	TYR	CB-CG-CD2	-5.90	117.46	121.00
2	0	1218	TYR	CB-CG-CD1	-5.90	117.46	121.00
7	M	839	SER	N-CA-CB	5.90	119.35	110.50
2	0	939	ASP	CB-CG-OD2	-5.90	112.99	118.30
2	0	1459	ASP	CB-CG-OD2	-5.90	112.99	118.30
9	S	829	TYR	CB-CG-CD2	-5.90	117.46	121.00
2	Y	1203	TYR	CB-CG-CD2	-5.90	117.46	121.00
9	T	100	PRO	N-CA-CB	5.90	110.38	103.30
7	M	494	GLU	CB-CA-C	-5.89	98.61	110.40
9	Q	100	PRO	N-CA-CB	5.89	110.37	103.30
7	O	1672	MET	CA-CB-CG	5.89	123.32	113.30
9	T	836	ASP	CB-CG-OD2	-5.89	113.00	118.30
6	C	350	PHE	CB-CG-CD1	5.89	124.92	120.80
3	1	738	GLU	OE1-CD-OE2	-5.89	116.23	123.30
9	T	33	PRO	N-CA-CB	5.89	110.37	103.30
7	O	494	GLU	CB-CA-C	-5.89	98.62	110.40
9	Q	33	PRO	N-CA-CB	5.89	110.37	103.30
8	N	455	PHE	CB-CG-CD1	5.89	124.92	120.80
8	P	569	LEU	CB-CG-CD1	5.88	121.00	111.00
2	0	1148	ALA	CB-CA-C	5.88	118.92	110.10
2	0	842	TYR	CB-CG-CD2	5.88	124.53	121.00
2	0	241	PHE	CB-CG-CD1	-5.88	116.69	120.80
7	O	1150	PHE	CG-CD1-CE1	5.88	127.27	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	124	PHE	CG-CD2-CE2	-5.88	114.34	120.80
2	0	641	VAL	CA-CB-CG2	-5.88	102.08	110.90
3	1	138	PHE	CB-CG-CD2	5.88	124.91	120.80
7	O	124	PHE	CG-CD2-CE2	-5.88	114.33	120.80
2	Y	1148	ALA	CB-CA-C	5.87	118.91	110.10
9	Q	98	PRO	N-CA-CB	5.87	110.35	103.30
8	P	202	THR	CA-CB-CG2	-5.87	104.18	112.40
2	Y	1459	ASP	CB-CG-OD2	-5.87	113.02	118.30
7	M	1672	MET	CA-CB-CG	5.87	123.28	113.30
9	R	100	PRO	N-CA-CB	5.87	110.35	103.30
8	N	777	ASP	CB-CG-OD1	-5.87	113.02	118.30
8	P	811	ASP	CB-CG-OD1	5.87	123.58	118.30
7	M	1150	PHE	CG-CD1-CE1	5.87	127.25	120.80
7	M	1510	ASP	CB-CG-OD1	5.87	123.58	118.30
9	S	282	PHE	CB-CG-CD1	-5.86	116.70	120.80
9	S	619	PHE	CG-CD2-CE2	5.86	127.25	120.80
3	1	1349	ASP	CB-CG-OD2	-5.86	113.02	118.30
2	Y	641	VAL	CA-CB-CG2	-5.86	102.11	110.90
7	O	839	SER	N-CA-CB	5.86	119.29	110.50
8	N	569	LEU	CB-CG-CD1	5.86	120.96	111.00
2	0	281	ARG	NE-CZ-NH2	-5.86	117.37	120.30
2	Y	979	ALA	N-CA-CB	5.86	118.30	110.10
6	F	336	PHE	CB-CG-CD2	-5.86	116.70	120.80
2	0	1398	PHE	CB-CG-CD2	5.86	124.90	120.80
8	P	455	PHE	CB-CG-CD1	5.85	124.90	120.80
2	Y	1162	TYR	CB-CG-CD1	5.85	124.51	121.00
2	0	693	GLU	O-C-N	-5.85	113.33	122.70
3	1	231	TYR	CG-CD2-CE2	5.85	125.98	121.30
2	Y	693	GLU	O-C-N	-5.85	113.34	122.70
3	Z	1277	ARG	NE-CZ-NH1	-5.85	117.38	120.30
3	Z	730	VAL	CG1-CB-CG2	-5.84	101.55	110.90
7	M	335	ASP	CB-CG-OD1	5.84	123.56	118.30
9	Q	290	TYR	CD1-CE1-CZ	-5.84	114.54	119.80
2	0	493	PHE	CB-CG-CD1	-5.84	116.71	120.80
2	Y	1428	TYR	CD1-CE1-CZ	5.84	125.06	119.80
3	1	1145	THR	CA-CB-CG2	-5.84	104.22	112.40
2	0	369	TYR	CB-CG-CD2	5.84	124.50	121.00
2	Y	209	HIS	CA-CB-CG	5.84	123.53	113.60
3	Z	404	PHE	CB-CG-CD2	5.84	124.89	120.80
3	Z	1145	THR	CA-CB-CG2	-5.84	104.23	112.40
7	M	1542	ASN	N-CA-CB	5.84	121.11	110.60
9	R	836	ASP	CB-CG-OD2	-5.83	113.05	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	209	VAL	CA-CB-CG2	-5.83	102.15	110.90
9	Q	531	ASP	CB-CG-OD1	-5.83	113.05	118.30
9	R	33	PRO	N-CA-CB	5.83	110.30	103.30
2	0	1329	ASP	CB-CG-OD1	5.83	123.55	118.30
7	O	43	LYS	CA-CB-CG	5.83	126.23	113.40
9	S	531	ASP	CB-CG-OD1	-5.83	113.05	118.30
4	A	802	ASP	CB-CG-OD2	5.83	123.55	118.30
7	O	878	TYR	CG-CD1-CE1	5.83	125.96	121.30
2	Y	1468	TYR	CB-CG-CD2	-5.83	117.50	121.00
9	Q	619	PHE	CG-CD2-CE2	5.83	127.21	120.80
2	0	1428	TYR	CD1-CE1-CZ	5.83	125.04	119.80
9	S	267	ASP	CB-CG-OD2	-5.83	113.06	118.30
9	T	519	ASP	CB-CG-OD2	-5.83	113.06	118.30
3	1	730	VAL	CG1-CB-CG2	-5.82	101.58	110.90
8	P	209	VAL	CA-CB-CG2	-5.82	102.17	110.90
7	O	227	ASP	CB-CG-OD1	5.82	123.54	118.30
6	I	336	PHE	CB-CG-CD1	-5.82	116.72	120.80
2	0	209	HIS	CA-CB-CG	5.82	123.49	113.60
7	M	878	TYR	CG-CD1-CE1	5.82	125.95	121.30
9	S	290	TYR	CD1-CE1-CZ	-5.82	114.56	119.80
3	Z	433	TYR	CG-CD1-CE1	-5.82	116.65	121.30
5	H	462	ARG	NE-CZ-NH2	-5.82	117.39	120.30
9	T	454	TYR	CB-CG-CD1	5.82	124.49	121.00
7	O	1542	ASN	N-CA-CB	5.81	121.06	110.60
2	Y	842	TYR	CB-CG-CD2	5.81	124.49	121.00
7	M	43	LYS	CA-CB-CG	5.81	126.19	113.40
8	N	672	VAL	CA-CB-CG1	-5.81	102.18	110.90
4	G	802	ASP	CB-CG-OD2	5.81	123.53	118.30
7	O	2	LYS	N-CA-C	-5.81	95.32	111.00
8	P	603	ASP	CB-CG-OD1	5.81	123.53	118.30
3	Z	1349	ASP	CB-CG-OD2	-5.81	113.07	118.30
3	1	1289	MET	N-CA-CB	5.81	121.06	110.60
2	Y	493	PHE	CB-CG-CD1	-5.81	116.74	120.80
8	P	1360	ASN	CB-CG-OD1	-5.81	109.99	121.60
7	O	1368	ARG	NE-CZ-NH2	-5.80	117.40	120.30
7	M	2	LYS	N-CA-C	-5.80	95.34	111.00
4	A	707	LEU	CB-CG-CD2	5.80	120.86	111.00
7	M	227	ASP	CB-CG-OD1	5.80	123.52	118.30
8	N	1360	ASN	CB-CG-OD1	-5.80	110.01	121.60
3	1	755	TYR	CB-CG-CD1	-5.80	117.52	121.00
2	0	653	ARG	NE-CZ-NH1	5.79	123.20	120.30
2	Y	241	PHE	CB-CG-CD1	-5.79	116.75	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	129	SER	N-CA-CB	5.79	119.19	110.50
2	Y	137	ARG	NE-CZ-NH1	-5.79	117.41	120.30
9	Q	696	TYR	CB-CG-CD1	5.79	124.47	121.00
7	O	762	ALA	N-CA-CB	5.79	118.20	110.10
3	Z	231	TYR	CG-CD2-CE2	5.79	125.93	121.30
7	O	1528	VAL	CA-CB-CG2	-5.79	102.22	110.90
7	M	1528	VAL	CA-CB-CG2	-5.79	102.22	110.90
7	O	956	VAL	CG1-CB-CG2	-5.79	101.64	110.90
7	M	762	ALA	N-CA-CB	5.78	118.20	110.10
8	P	777	ASP	CB-CG-OD1	-5.78	113.10	118.30
2	0	404	THR	CA-CB-CG2	-5.78	104.31	112.40
8	N	987	SER	O-C-N	5.78	131.95	122.70
4	G	656	GLU	CB-CG-CD	-5.78	98.59	114.20
7	O	1633	TYR	CB-CG-CD2	-5.78	117.53	121.00
2	Y	193	TRP	CH2-CZ2-CE2	5.78	123.18	117.40
4	A	656	GLU	CB-CG-CD	-5.78	98.60	114.20
2	0	1343	LEU	CB-CG-CD1	5.78	120.82	111.00
9	T	583	THR	CA-CB-OG1	5.77	121.12	109.00
3	Z	437	SER	N-CA-CB	5.77	119.16	110.50
3	Z	1289	MET	N-CA-CB	5.77	120.99	110.60
7	M	956	VAL	CG1-CB-CG2	-5.77	101.66	110.90
2	0	129	SER	N-CA-CB	5.77	119.16	110.50
2	0	1468	TYR	CB-CG-CD2	-5.77	117.54	121.00
6	C	385	GLU	O-C-N	-5.77	113.47	122.70
9	R	583	THR	CA-CB-OG1	5.77	121.12	109.00
2	Y	404	THR	CA-CB-CG2	-5.77	104.32	112.40
8	N	603	ASP	CB-CG-OD1	5.77	123.49	118.30
9	R	829	TYR	CB-CG-CD1	-5.77	117.54	121.00
6	L	336	PHE	CB-CG-CD2	-5.77	116.76	120.80
3	Z	449	ASP	CB-CG-OD1	5.77	123.49	118.30
7	M	106	TYR	CB-CG-CD1	5.77	124.46	121.00
4	D	665	TRP	CE2-CD2-CG	-5.76	102.69	107.30
8	P	987	SER	O-C-N	5.76	131.92	122.70
3	1	437	SER	N-CA-CB	5.76	119.14	110.50
3	Z	755	TYR	CB-CG-CD1	-5.76	117.54	121.00
6	C	387	TYR	CB-CG-CD1	5.76	124.45	121.00
7	M	432	LEU	CB-CG-CD1	5.76	120.79	111.00
2	Y	538	SER	N-CA-CB	5.76	119.14	110.50
3	Z	1243	ASP	CB-CG-OD2	-5.76	113.12	118.30
9	Q	458	SER	N-CA-CB	5.76	119.14	110.50
3	1	601	VAL	N-CA-C	-5.76	95.45	111.00
3	Z	575	ARG	NE-CZ-NH2	-5.75	117.42	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	R	519	ASP	CB-CG-OD2	-5.75	113.12	118.30
8	N	441	PRO	N-CA-CB	5.75	110.20	103.30
2	0	979	ALA	N-CA-CB	5.75	118.15	110.10
3	Z	601	VAL	N-CA-C	-5.75	95.47	111.00
9	Q	220	PHE	CB-CA-C	5.75	121.90	110.40
6	I	385	GLU	O-C-N	-5.75	113.50	122.70
9	S	458	SER	N-CA-CB	5.75	119.13	110.50
9	S	462	PHE	CB-CG-CD1	5.75	124.83	120.80
2	Y	1343	LEU	CB-CG-CD1	5.75	120.77	111.00
3	Z	1044	TYR	CB-CG-CD2	-5.75	117.55	121.00
6	I	387	TYR	CB-CG-CD1	5.75	124.45	121.00
7	O	792	ASP	CB-CG-OD1	-5.75	113.13	118.30
8	P	441	PRO	N-CA-CB	5.75	110.20	103.30
7	O	48	ARG	NE-CZ-NH2	5.75	123.17	120.30
2	Y	1392	PRO	N-CA-CB	5.74	110.19	103.30
6	I	398	VAL	CA-CB-CG2	-5.74	102.29	110.90
2	0	538	SER	N-CA-CB	5.74	119.11	110.50
8	N	893	TYR	CD1-CE1-CZ	5.74	124.97	119.80
3	1	994	ARG	NH1-CZ-NH2	-5.74	113.09	119.40
4	G	707	LEU	CB-CG-CD2	5.74	120.75	111.00
4	J	809	ASP	CB-CA-C	5.74	121.87	110.40
2	0	380	TYR	CD1-CE1-CZ	-5.74	114.64	119.80
2	0	193	TRP	CH2-CZ2-CE2	5.73	123.13	117.40
3	1	579	TYR	N-CA-C	-5.73	95.52	111.00
3	Z	994	ARG	NH1-CZ-NH2	-5.73	113.10	119.40
9	R	454	TYR	CB-CG-CD1	5.73	124.44	121.00
2	0	243	PHE	CB-CG-CD1	5.73	124.81	120.80
2	0	458	GLU	CB-CA-C	-5.73	98.94	110.40
8	P	18	VAL	CA-CB-CG2	-5.73	102.31	110.90
8	P	67	ASP	CB-CA-C	-5.73	98.94	110.40
9	S	220	PHE	CB-CA-C	5.73	121.86	110.40
5	B	462	ARG	NE-CZ-NH2	-5.73	117.44	120.30
3	Z	1042	ARG	NE-CZ-NH2	5.73	123.16	120.30
9	Q	267	ASP	CB-CG-OD2	-5.73	113.15	118.30
3	1	561	LEU	CB-CG-CD2	5.73	120.74	111.00
2	Y	102	ASP	CB-CG-OD2	-5.72	113.15	118.30
5	B	393	ASP	N-CA-CB	5.72	120.91	110.60
8	P	871	SER	CB-CA-C	-5.72	99.22	110.10
8	N	148	VAL	CA-CB-CG2	-5.72	102.32	110.90
8	N	244	PHE	CB-CG-CD1	5.72	124.81	120.80
3	1	449	ASP	CB-CG-OD1	5.72	123.45	118.30
8	P	672	VAL	CA-CB-CG1	-5.72	102.32	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	18	VAL	CA-CB-CG2	-5.72	102.32	110.90
2	Y	458	GLU	CB-CA-C	-5.72	98.96	110.40
2	Y	509	PHE	CB-CG-CD1	-5.72	116.80	120.80
3	Z	579	TYR	N-CA-C	-5.72	95.56	111.00
4	D	809	ASP	CB-CA-C	5.72	121.84	110.40
7	M	792	ASP	CB-CG-OD1	-5.72	113.15	118.30
7	O	432	LEU	CB-CG-CD1	5.72	120.72	111.00
7	M	1342	TYR	CG-CD2-CE2	-5.72	116.73	121.30
2	0	102	ASP	CB-CG-OD2	-5.72	113.15	118.30
8	P	148	VAL	CA-CB-CG2	-5.72	102.32	110.90
9	S	552	VAL	CG1-CB-CG2	-5.72	101.75	110.90
6	C	387	TYR	CG-CD2-CE2	5.72	125.87	121.30
8	N	557	TYR	CD1-CE1-CZ	-5.72	114.66	119.80
7	O	106	TYR	CB-CG-CD1	5.72	124.43	121.00
2	Y	380	TYR	CD1-CE1-CZ	-5.71	114.66	119.80
5	H	393	ASP	N-CA-CB	5.71	120.89	110.60
6	C	398	VAL	CA-CB-CG2	-5.71	102.33	110.90
4	D	681	SER	N-CA-CB	5.71	119.06	110.50
2	0	1392	PRO	N-CA-CB	5.71	110.15	103.30
8	N	871	SER	CB-CA-C	-5.71	99.26	110.10
9	R	571	LEU	CB-CG-CD2	5.71	120.70	111.00
6	I	456	ARG	NE-CZ-NH1	5.71	123.15	120.30
7	M	1482	THR	CA-CB-CG2	-5.70	104.42	112.40
7	O	181	PHE	CB-CG-CD2	-5.70	116.81	120.80
2	Y	776	LEU	CB-CG-CD1	5.70	120.69	111.00
2	Y	1203	TYR	CZ-CE2-CD2	5.70	124.93	119.80
2	Y	1329	ASP	CB-CG-OD1	5.70	123.43	118.30
9	R	71	TYR	N-CA-CB	5.70	120.86	110.60
3	1	1090	LYS	O-C-N	-5.70	113.58	122.70
7	O	1482	THR	CA-CB-CG2	-5.70	104.42	112.40
8	P	449	ASP	CB-CG-OD1	5.70	123.43	118.30
8	P	1384	ASP	CB-CG-OD1	5.70	123.43	118.30
9	R	286	THR	CA-CB-CG2	-5.70	104.42	112.40
4	J	665	TRP	CE2-CD2-CG	-5.70	102.74	107.30
8	P	43	PHE	CG-CD2-CE2	-5.70	114.53	120.80
9	R	494	TYR	CB-CG-CD2	-5.70	117.58	121.00
7	O	1342	TYR	CG-CD2-CE2	-5.70	116.74	121.30
8	P	417	THR	CA-CB-CG2	-5.70	104.42	112.40
2	0	218	ARG	NE-CZ-NH2	-5.69	117.45	120.30
8	P	1226	PHE	CB-CG-CD1	-5.69	116.81	120.80
9	Q	462	PHE	CB-CG-CD1	5.69	124.78	120.80
3	1	575	ARG	NE-CZ-NH2	-5.69	117.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	829	TYR	CB-CG-CD1	-5.69	117.58	121.00
7	M	1070	TYR	CG-CD2-CE2	-5.69	116.75	121.30
5	B	419	LEU	CB-CG-CD1	-5.69	101.33	111.00
8	P	1521	PHE	CG-CD1-CE1	-5.69	114.54	120.80
2	0	137	ARG	NE-CZ-NH1	-5.69	117.46	120.30
8	P	123	ASP	O-C-N	-5.69	113.60	122.70
7	M	207	MET	CA-CB-CG	5.68	122.96	113.30
8	N	123	ASP	O-C-N	-5.68	113.61	122.70
9	Q	552	VAL	CG1-CB-CG2	-5.68	101.80	110.90
4	J	681	SER	N-CA-CB	5.68	119.03	110.50
8	N	505	VAL	CA-CB-CG2	-5.68	102.38	110.90
8	N	758	TYR	CD1-CG-CD2	-5.68	111.65	117.90
8	N	1226	PHE	CB-CG-CD1	-5.68	116.82	120.80
5	H	419	LEU	CB-CG-CD1	-5.68	101.34	111.00
7	O	1070	TYR	CG-CD2-CE2	-5.68	116.75	121.30
9	T	571	LEU	CB-CG-CD2	5.68	120.66	111.00
9	Q	315	LYS	N-CA-C	-5.68	95.66	111.00
9	S	315	LYS	N-CA-C	-5.68	95.66	111.00
8	N	417	THR	CA-CB-CG2	-5.68	104.45	112.40
9	T	286	THR	CA-CB-CG2	-5.68	104.45	112.40
8	N	43	PHE	CG-CD2-CE2	-5.67	114.56	120.80
8	P	369	LEU	CB-CA-C	-5.67	99.42	110.20
8	P	557	TYR	CD1-CE1-CZ	-5.67	114.69	119.80
2	0	776	LEU	CB-CG-CD1	5.67	120.64	111.00
3	Z	1090	LYS	O-C-N	-5.67	113.63	122.70
7	O	207	MET	CA-CB-CG	5.67	122.94	113.30
8	N	369	LEU	CB-CA-C	-5.67	99.43	110.20
2	0	1105	TYR	CB-CG-CD2	-5.67	117.60	121.00
3	1	104	ARG	NE-CZ-NH1	5.67	123.13	120.30
4	J	657	GLN	CG-CD-OE1	-5.67	110.26	121.60
8	P	452	PHE	CB-CG-CD2	-5.67	116.83	120.80
9	S	696	TYR	CB-CG-CD1	5.67	124.40	121.00
7	M	1633	TYR	CB-CG-CD2	-5.67	117.60	121.00
7	O	335	ASP	CB-CG-OD1	5.67	123.40	118.30
9	S	671	ASP	CB-CG-OD1	5.67	123.40	118.30
2	Y	455	PHE	CB-CG-CD2	5.67	124.77	120.80
3	Z	561	LEU	CB-CG-CD2	5.66	120.63	111.00
8	N	1521	PHE	CG-CD1-CE1	-5.66	114.57	120.80
9	Q	676	GLY	N-CA-C	-5.66	98.94	113.10
5	H	471	LYS	O-C-N	-5.66	113.64	122.70
2	0	455	PHE	CB-CG-CD2	5.66	124.76	120.80
7	O	1469	ARG	NE-CZ-NH2	-5.66	117.47	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	720	ARG	NE-CZ-NH2	-5.66	117.47	120.30
9	S	676	GLY	N-CA-C	-5.66	98.95	113.10
2	Y	1105	TYR	CB-CG-CD2	-5.66	117.61	121.00
3	1	579	TYR	CG-CD1-CE1	-5.66	116.77	121.30
4	D	657	GLN	CG-CD-OE1	-5.66	110.29	121.60
8	P	31	ALA	N-CA-CB	5.66	118.02	110.10
3	Z	900	ASP	N-CA-CB	5.66	120.78	110.60
2	Y	1398	PHE	CB-CG-CD1	-5.65	116.84	120.80
5	E	437	TRP	N-CA-CB	5.65	120.78	110.60
2	0	1203	TYR	CZ-CE2-CD2	5.65	124.89	119.80
9	T	71	TYR	N-CA-CB	5.65	120.78	110.60
5	B	332	GLN	O-C-N	-5.65	113.66	122.70
6	C	456	ARG	NE-CZ-NH1	5.65	123.12	120.30
9	T	320	TRP	CG-CD2-CE3	-5.65	128.81	133.90
8	N	720	ARG	NE-CZ-NH2	-5.65	117.48	120.30
6	I	387	TYR	CG-CD2-CE2	5.65	125.82	121.30
8	P	893	TYR	CD1-CE1-CZ	5.65	124.88	119.80
8	P	244	PHE	CB-CG-CD1	5.65	124.75	120.80
5	K	353	TYR	CB-CG-CD1	-5.64	117.61	121.00
7	O	435	PHE	O-C-N	5.64	131.73	122.70
9	T	577	ARG	NE-CZ-NH2	5.64	123.12	120.30
7	M	181	PHE	CB-CG-CD2	-5.64	116.85	120.80
3	Z	579	TYR	CG-CD1-CE1	-5.64	116.79	121.30
3	Z	1060	TYR	CD1-CE1-CZ	5.64	124.88	119.80
8	N	449	ASP	CB-CG-OD1	5.64	123.38	118.30
9	Q	814	MET	CG-SD-CE	-5.64	91.18	100.20
8	N	31	ALA	N-CA-CB	5.64	117.99	110.10
3	1	1044	TYR	CB-CG-CD2	-5.64	117.62	121.00
8	N	1199	TYR	CZ-CE2-CD2	-5.63	114.73	119.80
3	1	900	ASP	N-CA-CB	5.63	120.74	110.60
8	P	182	PHE	CB-CG-CD2	-5.63	116.86	120.80
8	P	505	VAL	CA-CB-CG2	-5.63	102.45	110.90
9	Q	394	TYR	CG-CD1-CE1	-5.63	116.80	121.30
5	H	332	GLN	O-C-N	-5.63	113.69	122.70
9	R	320	TRP	CG-CD2-CE3	-5.63	128.83	133.90
7	M	1521	THR	CA-CB-CG2	-5.63	104.52	112.40
5	K	437	TRP	N-CA-CB	5.63	120.73	110.60
8	P	639	PHE	CB-CG-CD1	5.63	124.74	120.80
8	P	1022	TYR	CB-CG-CD1	5.63	124.38	121.00
8	P	1199	TYR	CZ-CE2-CD2	-5.63	114.73	119.80
9	S	814	MET	CG-SD-CE	-5.63	91.20	100.20
3	Z	1017	ASP	CB-CG-OD2	-5.63	113.24	118.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	1469	ARG	NE-CZ-NH2	-5.63	117.49	120.30
7	O	1406	TYR	N-CA-CB	5.63	120.73	110.60
7	M	851	LEU	CB-CG-CD2	5.62	120.56	111.00
8	N	452	PHE	CB-CG-CD2	-5.62	116.86	120.80
9	T	325	LEU	N-CA-CB	5.62	121.65	110.40
7	M	1455	THR	CA-CB-OG1	5.62	120.80	109.00
7	O	1521	THR	CA-CB-CG2	-5.62	104.53	112.40
8	N	135	PHE	CZ-CE2-CD2	5.62	126.84	120.10
9	R	394	TYR	CZ-CE2-CD2	-5.62	114.74	119.80
9	T	494	TYR	CB-CG-CD2	-5.62	117.63	121.00
3	Z	295	PHE	CB-CG-CD2	-5.62	116.87	120.80
5	E	330	VAL	CA-CB-CG2	-5.62	102.47	110.90
9	R	325	LEU	N-CA-CB	5.62	121.64	110.40
2	0	205	ASP	CB-CG-OD2	-5.62	113.24	118.30
3	1	295	PHE	CB-CG-CD2	-5.62	116.87	120.80
7	M	877	ASP	CB-CG-OD1	-5.62	113.25	118.30
7	O	877	ASP	CB-CG-OD1	-5.62	113.25	118.30
5	B	471	LYS	O-C-N	-5.61	113.72	122.70
2	0	91	ARG	NE-CZ-NH2	-5.61	117.49	120.30
3	1	1123	PHE	CB-CG-CD1	-5.61	116.87	120.80
7	O	1455	THR	CA-CB-OG1	5.61	120.79	109.00
2	0	1416	PHE	CG-CD1-CE1	-5.61	114.63	120.80
7	M	435	PHE	O-C-N	5.61	131.68	122.70
2	Y	1468	TYR	CD1-CG-CD2	5.61	124.07	117.90
7	M	1117	THR	CA-CB-OG1	5.61	120.78	109.00
3	1	1212	PRO	N-CD-CG	5.61	111.61	103.20
8	P	758	TYR	CD1-CG-CD2	-5.61	111.73	117.90
5	H	513	LEU	N-CA-CB	5.61	121.61	110.40
7	O	851	LEU	CB-CG-CD2	5.61	120.53	111.00
9	T	651	ASP	CB-CG-OD1	5.61	123.34	118.30
8	N	182	PHE	CB-CG-CD2	-5.60	116.88	120.80
9	Q	671	ASP	CB-CG-OD1	5.60	123.34	118.30
3	1	1017	ASP	CB-CG-OD2	-5.60	113.26	118.30
7	O	661	VAL	CG1-CB-CG2	-5.60	101.94	110.90
9	R	826	ARG	NE-CZ-NH2	5.60	123.10	120.30
2	0	509	PHE	CB-CG-CD1	-5.60	116.88	120.80
3	Z	853	PHE	CZ-CE2-CD2	-5.60	113.38	120.10
7	M	1406	TYR	N-CA-CB	5.60	120.68	110.60
2	0	1434	ILE	CA-CB-CG2	5.60	122.09	110.90
5	H	411	ARG	NE-CZ-NH2	-5.60	117.50	120.30
7	O	1117	THR	CA-CB-OG1	5.60	120.75	109.00
2	Y	91	ARG	NE-CZ-NH2	-5.59	117.50	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	C	438	ALA	CB-CA-C	-5.59	101.71	110.10
8	N	639	PHE	CB-CG-CD1	5.59	124.72	120.80
8	N	754	TYR	CB-CG-CD2	5.59	124.36	121.00
7	O	915	ALA	CB-CA-C	-5.59	101.71	110.10
9	S	665	LEU	CB-CA-C	-5.59	99.57	110.20
8	N	1022	TYR	CB-CG-CD1	5.59	124.36	121.00
9	Q	665	LEU	CB-CA-C	-5.59	99.58	110.20
7	M	1569	TYR	CG-CD1-CE1	5.59	125.77	121.30
9	T	469	TYR	CD1-CE1-CZ	5.59	124.83	119.80
5	B	513	LEU	N-CA-CB	5.59	121.58	110.40
3	Z	1212	PRO	N-CD-CG	5.59	111.58	103.20
3	Z	104	ARG	NE-CZ-NH1	5.58	123.09	120.30
6	C	281	ASP	CB-CG-OD1	-5.58	113.28	118.30
7	M	1503	THR	CA-CB-CG2	-5.58	104.58	112.40
7	M	48	ARG	NE-CZ-NH2	5.58	123.09	120.30
4	J	805	ARG	NE-CZ-NH2	-5.58	117.51	120.30
9	T	394	TYR	CZ-CE2-CD2	-5.58	114.78	119.80
5	B	411	ARG	NE-CZ-NH2	-5.58	117.51	120.30
2	Y	1463	ARG	NE-CZ-NH1	5.58	123.09	120.30
5	E	369	VAL	CG1-CB-CG2	5.58	119.83	110.90
3	1	554	TYR	CD1-CE1-CZ	-5.58	114.78	119.80
3	1	1116	TYR	CB-CG-CD2	-5.58	117.65	121.00
6	F	270	PRO	CA-N-CD	-5.58	103.69	111.50
2	Y	218	ARG	NE-CZ-NH2	-5.57	117.51	120.30
2	Y	1434	ILE	CA-CB-CG2	5.57	122.05	110.90
7	M	915	ALA	CB-CA-C	-5.57	101.74	110.10
2	0	1468	TYR	CD1-CG-CD2	5.57	124.03	117.90
8	P	135	PHE	CZ-CE2-CD2	5.57	126.79	120.10
7	O	692	TYR	CG-CD2-CE2	-5.57	116.84	121.30
2	0	1398	PHE	CB-CG-CD1	-5.57	116.90	120.80
6	I	438	ALA	CB-CA-C	-5.57	101.75	110.10
9	R	651	ASP	CB-CG-OD1	5.57	123.31	118.30
3	Z	507	TYR	CB-CG-CD2	-5.57	117.66	121.00
8	N	1384	ASP	CB-CG-OD1	5.57	123.31	118.30
7	O	1513	TYR	CB-CG-CD2	5.57	124.34	121.00
9	T	586	PHE	CB-CG-CD1	-5.56	116.91	120.80
2	Y	1176	ASP	CB-CG-OD2	-5.56	113.30	118.30
7	M	1100	LEU	CB-CG-CD2	5.56	120.46	111.00
10	U	343	VAL	N-CA-C	-5.56	95.98	111.00
3	1	621	PHE	CD1-CG-CD2	5.56	125.53	118.30
9	T	339	TYR	CZ-CE2-CD2	-5.56	114.80	119.80
9	S	290	TYR	CB-CG-CD2	5.56	124.34	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	K	330	VAL	CA-CB-CG2	-5.56	102.56	110.90
7	O	1100	LEU	CB-CG-CD2	5.56	120.45	111.00
7	O	1569	TYR	CG-CD1-CE1	5.56	125.75	121.30
8	P	1204	ALA	CB-CA-C	-5.56	101.77	110.10
10	W	343	VAL	N-CA-C	-5.55	96.00	111.00
9	S	547	TYR	CD1-CE1-CZ	5.55	124.80	119.80
3	Z	1173	LEU	CB-CG-CD1	5.55	120.44	111.00
6	C	270	PRO	N-CA-CB	5.55	109.96	103.30
9	Q	290	TYR	CB-CG-CD2	5.55	124.33	121.00
6	I	281	ASP	CB-CG-OD1	-5.55	113.30	118.30
7	M	692	TYR	CG-CD2-CE2	-5.55	116.86	121.30
7	M	1513	TYR	CB-CG-CD2	5.55	124.33	121.00
5	H	340	GLU	OE1-CD-OE2	5.55	129.96	123.30
9	Q	588	VAL	CA-CB-CG1	5.55	119.22	110.90
7	O	1503	THR	CA-CB-CG2	-5.55	104.63	112.40
8	N	1243	ASP	CB-CG-OD1	5.55	123.29	118.30
9	R	469	TYR	CD1-CE1-CZ	5.55	124.79	119.80
9	S	588	VAL	CA-CB-CG1	5.55	119.22	110.90
9	Q	816	TYR	CG-CD2-CE2	-5.54	116.87	121.30
7	O	481	PHE	CB-CG-CD1	-5.54	116.92	120.80
5	E	353	TYR	CB-CG-CD1	-5.54	117.67	121.00
7	M	661	VAL	CG1-CB-CG2	-5.54	102.03	110.90
7	M	1306	TRP	CB-CG-CD2	5.54	133.81	126.60
3	Z	554	TYR	CD1-CE1-CZ	-5.54	114.81	119.80
9	Q	222	PHE	CB-CG-CD2	-5.54	116.92	120.80
2	Y	1416	PHE	CG-CD1-CE1	-5.54	114.71	120.80
8	N	1309	ARG	CG-CD-NE	-5.54	100.17	111.80
4	D	805	ARG	NE-CZ-NH2	-5.54	117.53	120.30
3	1	975	ASP	CB-CG-OD2	5.54	123.28	118.30
7	M	51	LEU	CB-CG-CD2	5.53	120.41	111.00
3	1	1060	TYR	CD1-CE1-CZ	5.53	124.78	119.80
3	Z	1116	TYR	CB-CG-CD2	-5.53	117.68	121.00
3	Z	239	ASP	CB-CG-OD2	5.53	123.28	118.30
3	Z	621	PHE	CD1-CG-CD2	5.53	125.49	118.30
8	N	1204	ALA	CB-CA-C	-5.53	101.80	110.10
2	0	1463	ARG	NE-CZ-NH1	5.53	123.07	120.30
6	L	270	PRO	CA-N-CD	-5.53	103.76	111.50
7	O	1306	TRP	CB-CG-CD2	5.53	133.79	126.60
8	P	1270	LYS	CA-CB-CG	5.53	125.57	113.40
8	P	754	TYR	CB-CG-CD2	5.53	124.32	121.00
8	P	1243	ASP	CB-CG-OD1	5.53	123.27	118.30
9	S	394	TYR	CG-CD1-CE1	-5.53	116.88	121.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	B	340	GLU	OE1-CD-OE2	5.53	129.93	123.30
9	Q	816	TYR	CB-CG-CD2	-5.53	117.69	121.00
3	1	844	PHE	N-CA-CB	5.52	120.54	110.60
5	K	397	ARG	NE-CZ-NH2	-5.52	117.54	120.30
9	R	339	TYR	CZ-CE2-CD2	-5.52	114.83	119.80
11	V	355	TRP	CB-CG-CD2	5.52	133.78	126.60
9	R	523	ARG	NE-CZ-NH2	-5.52	117.54	120.30
3	1	239	ASP	CB-CG-OD2	5.52	123.27	118.30
2	Y	923	ASP	CB-CG-OD1	-5.52	113.33	118.30
7	O	51	LEU	CB-CG-CD2	5.52	120.38	111.00
2	Y	99	LYS	CB-CA-C	-5.51	99.37	110.40
7	M	1244	ASN	CB-CG-OD1	5.51	132.63	121.60
9	S	222	PHE	CB-CG-CD2	-5.51	116.94	120.80
3	Z	421	PHE	CZ-CE2-CD2	-5.51	113.48	120.10
7	O	1244	ASN	CB-CG-OD1	5.51	132.63	121.60
9	Q	765	ASP	CB-CG-OD1	5.51	123.26	118.30
3	1	1173	LEU	CB-CG-CD1	5.51	120.37	111.00
3	Z	264	ILE	CA-CB-CG1	5.50	121.46	111.00
9	S	789	LEU	N-CA-CB	5.50	121.41	110.40
3	Z	761	VAL	CA-CB-CG1	-5.50	102.65	110.90
3	Z	844	PHE	N-CA-CB	5.50	120.50	110.60
9	R	577	ARG	NE-CZ-NH2	5.50	123.05	120.30
6	I	270	PRO	N-CA-CB	5.50	109.90	103.30
2	0	1176	ASP	CB-CG-OD2	-5.50	113.35	118.30
8	P	1309	ARG	CG-CD-NE	-5.50	100.25	111.80
3	Z	135	PHE	CG-CD1-CE1	5.50	126.85	120.80
3	1	761	VAL	CA-CB-CG1	-5.50	102.65	110.90
5	H	313	TYR	CB-CG-CD2	-5.50	117.70	121.00
4	J	803	ALA	N-CA-CB	5.50	117.80	110.10
3	1	853	PHE	CZ-CE2-CD2	-5.50	113.50	120.10
8	N	67	ASP	CB-CA-C	-5.50	99.41	110.40
2	0	923	ASP	CB-CG-OD1	-5.50	113.35	118.30
3	1	175	THR	N-CA-CB	5.50	120.74	110.30
3	1	421	PHE	CZ-CE2-CD2	-5.50	113.51	120.10
3	1	1164	PHE	CG-CD1-CE1	-5.50	114.76	120.80
3	1	1238	TRP	CE2-CD2-CG	5.49	111.69	107.30
9	S	765	ASP	CB-CG-OD1	5.49	123.24	118.30
8	N	906	TYR	CG-CD1-CE1	-5.49	116.91	121.30
11	V	347	TYR	CZ-CE2-CD2	5.49	124.74	119.80
8	N	1222	LEU	C-N-CA	5.49	135.42	121.70
8	N	1270	LYS	CA-CB-CG	5.49	125.47	113.40
2	0	99	LYS	CB-CA-C	-5.49	99.42	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	205	ASP	CB-CG-OD2	-5.49	113.36	118.30
4	D	803	ALA	N-CA-CB	5.49	117.78	110.10
9	Q	789	LEU	N-CA-CB	5.49	121.37	110.40
3	1	171	TYR	CZ-CE2-CD2	-5.49	114.86	119.80
3	1	507	TYR	CB-CG-CD2	-5.49	117.71	121.00
8	N	1143	GLN	CA-CB-CG	5.48	125.46	113.40
8	P	1222	LEU	C-N-CA	5.48	135.41	121.70
8	P	1143	GLN	CA-CB-CG	5.48	125.46	113.40
9	T	704	ARG	NE-CZ-NH2	5.48	123.04	120.30
8	P	1521	PHE	CD1-CG-CD2	5.48	125.42	118.30
9	S	816	TYR	CG-CD2-CE2	-5.48	116.92	121.30
3	Z	1238	TRP	CE2-CD2-CG	5.48	111.68	107.30
8	N	24	ASP	CB-CG-OD1	5.48	123.23	118.30
9	S	739	MET	CG-SD-CE	-5.48	91.44	100.20
3	Z	1123	PHE	CB-CG-CD1	-5.48	116.97	120.80
3	1	1214	ASP	N-CA-CB	-5.48	100.74	110.60
4	J	652	ALA	N-CA-CB	5.48	117.77	110.10
8	P	92	SER	N-CA-CB	5.48	118.71	110.50
3	Z	175	THR	N-CA-CB	5.47	120.70	110.30
9	R	547	TYR	CG-CD2-CE2	-5.47	116.92	121.30
9	S	612	HIS	CA-CB-CG	-5.47	104.29	113.60
9	T	547	TYR	CG-CD2-CE2	-5.47	116.92	121.30
2	Y	1462	PHE	CG-CD2-CE2	-5.47	114.78	120.80
3	1	264	ILE	CA-CB-CG1	5.47	121.40	111.00
9	Q	547	TYR	CD1-CE1-CZ	5.47	124.72	119.80
9	Q	739	MET	CG-SD-CE	-5.47	91.45	100.20
4	J	702	ARG	NE-CZ-NH2	5.47	123.03	120.30
8	P	24	ASP	CB-CG-OD1	5.47	123.22	118.30
5	B	313	TYR	CB-CG-CD2	-5.47	117.72	121.00
9	S	447	ASP	N-CA-CB	5.47	120.44	110.60
9	Q	612	HIS	CA-CB-CG	-5.46	104.31	113.60
3	1	115	ASP	CB-CG-OD1	-5.46	113.38	118.30
5	H	401	ALA	CB-CA-C	-5.46	101.91	110.10
3	Z	640	ALA	N-CA-CB	5.46	117.75	110.10
4	A	685	MET	CA-CB-CG	5.46	122.58	113.30
7	M	565	TYR	CB-CG-CD2	5.46	124.28	121.00
5	B	537	TYR	CG-CD2-CE2	-5.46	116.93	121.30
4	G	744	ALA	N-CA-CB	5.46	117.74	110.10
3	Z	171	TYR	CZ-CE2-CD2	-5.46	114.89	119.80
4	D	639	ASP	N-CA-CB	5.46	120.42	110.60
9	R	586	PHE	CB-CG-CD1	-5.46	116.98	120.80
7	O	1070	TYR	CZ-CE2-CD2	5.46	124.71	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1	135	PHE	CG-CD1-CE1	5.46	126.80	120.80
11	X	347	TYR	CZ-CE2-CD2	5.45	124.71	119.80
8	P	1490	ARG	NH1-CZ-NH2	5.45	125.40	119.40
4	A	744	ALA	N-CA-CB	5.45	117.73	110.10
3	Z	975	ASP	CB-CG-OD2	5.45	123.20	118.30
5	E	397	ARG	NE-CZ-NH2	-5.45	117.58	120.30
7	M	481	PHE	CB-CG-CD1	-5.45	116.99	120.80
7	M	1250	LYS	N-CA-CB	5.45	120.41	110.60
8	N	92	SER	N-CA-CB	5.45	118.67	110.50
9	T	474	PHE	C-N-CA	5.45	135.32	121.70
7	O	759	ASP	CB-CG-OD1	5.45	123.20	118.30
8	P	906	TYR	CG-CD1-CE1	-5.45	116.94	121.30
3	1	1248	ALA	N-CA-CB	5.44	117.72	110.10
8	P	730	ILE	N-CA-C	-5.44	96.30	111.00
3	Z	539	TYR	CB-CG-CD2	-5.44	117.73	121.00
4	D	652	ALA	N-CA-CB	5.44	117.72	110.10
9	R	474	PHE	C-N-CA	5.44	135.31	121.70
7	O	1037	ASN	CA-CB-CG	-5.44	101.43	113.40
9	T	826	ARG	NE-CZ-NH2	5.44	123.02	120.30
9	Q	561	THR	N-CA-CB	5.44	120.64	110.30
5	K	440	PHE	N-CA-CB	5.44	120.39	110.60
2	0	379	ALA	N-CA-CB	5.44	117.71	110.10
8	P	1344	PHE	CB-CG-CD2	-5.44	116.99	120.80
5	H	361	ARG	NE-CZ-NH1	5.44	123.02	120.30
3	Z	612	TYR	CG-CD2-CE2	5.44	125.65	121.30
9	Q	447	ASP	N-CA-CB	5.44	120.39	110.60
7	O	72	PHE	CB-CG-CD1	-5.44	117.00	120.80
8	N	730	ILE	N-CA-C	-5.43	96.33	111.00
11	X	355	TRP	CB-CG-CD2	5.43	133.66	126.60
4	A	658	TYR	CB-CG-CD1	5.43	124.26	121.00
5	H	458	GLU	N-CA-CB	5.43	120.37	110.60
9	S	386	TYR	CG-CD2-CE2	5.43	125.64	121.30
3	Z	830	MET	CG-SD-CE	-5.42	91.52	100.20
9	R	704	ARG	NE-CZ-NH2	5.42	123.01	120.30
3	1	727	ARG	NE-CZ-NH2	5.42	123.01	120.30
7	O	1250	LYS	N-CA-CB	5.42	120.36	110.60
7	O	1431	ARG	NE-CZ-NH2	-5.42	117.59	120.30
9	S	816	TYR	CB-CG-CD2	-5.42	117.75	121.00
3	1	1042	ARG	NE-CZ-NH2	5.42	123.01	120.30
2	Y	379	ALA	N-CA-CB	5.42	117.69	110.10
8	N	1344	PHE	CB-CG-CD2	-5.42	117.00	120.80
8	N	1490	ARG	NH1-CZ-NH2	5.42	125.36	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	521	LYS	CB-CA-C	-5.42	99.56	110.40
7	O	31	ASP	CB-CG-OD1	5.42	123.18	118.30
5	B	458	GLU	N-CA-CB	5.42	120.35	110.60
7	M	31	ASP	CB-CG-OD1	5.42	123.17	118.30
3	Z	1248	ALA	N-CA-CB	5.41	117.68	110.10
7	M	1221	LEU	CB-CG-CD1	-5.41	101.80	111.00
3	1	851	ASP	CB-CA-C	-5.41	99.57	110.40
2	Y	407	ALA	CB-CA-C	-5.41	101.98	110.10
3	1	640	ALA	N-CA-CB	5.41	117.68	110.10
8	P	770	HIS	O-C-N	-5.41	114.04	122.70
9	S	268	ILE	C-N-CA	5.41	135.23	121.70
7	M	1037	ASN	CA-CB-CG	-5.41	101.50	113.40
4	G	685	MET	CA-CB-CG	5.41	122.50	113.30
8	P	920	LEU	CB-CG-CD2	-5.41	101.80	111.00
2	0	521	LYS	CB-CA-C	-5.41	99.58	110.40
2	0	1247	SER	N-CA-C	-5.41	96.40	111.00
5	H	537	TYR	CG-CD2-CE2	-5.41	116.97	121.30
8	N	945	ASP	N-CA-C	-5.41	96.40	111.00
8	P	945	ASP	N-CA-C	-5.41	96.40	111.00
8	N	758	TYR	CG-CD1-CE1	5.41	125.62	121.30
2	0	201	TYR	CD1-CG-CD2	-5.41	111.95	117.90
8	P	216	TYR	CG-CD1-CE1	-5.41	116.97	121.30
9	S	561	THR	N-CA-CB	5.40	120.57	110.30
5	E	440	PHE	N-CA-CB	5.40	120.33	110.60
7	M	72	PHE	CB-CG-CD1	-5.40	117.02	120.80
7	M	696	PHE	CZ-CE2-CD2	5.40	126.58	120.10
2	0	407	ALA	CB-CA-C	-5.40	102.00	110.10
3	1	830	MET	CG-SD-CE	-5.40	91.56	100.20
9	T	725	GLU	N-CA-CB	5.40	120.32	110.60
5	B	401	ALA	CB-CA-C	-5.40	102.00	110.10
8	N	216	TYR	CG-CD1-CE1	-5.40	116.98	121.30
3	1	990	THR	CA-CB-CG2	-5.40	104.84	112.40
2	Y	493	PHE	CD1-CE1-CZ	-5.39	113.63	120.10
7	O	736	PHE	CB-CG-CD1	-5.39	117.02	120.80
11	X	360	TYR	CD1-CE1-CZ	-5.39	114.95	119.80
8	N	1521	PHE	CD1-CG-CD2	5.39	125.31	118.30
3	1	1271	ARG	NE-CZ-NH2	-5.39	117.60	120.30
9	Q	268	ILE	C-N-CA	5.39	135.16	121.70
2	0	1462	PHE	CG-CD2-CE2	-5.39	114.88	120.80
7	O	1221	LEU	CB-CG-CD1	-5.39	101.84	111.00
3	Z	727	ARG	NE-CZ-NH2	5.38	122.99	120.30
9	T	523	ARG	NE-CZ-NH2	-5.38	117.61	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	696	PHE	CZ-CE2-CD2	5.38	126.56	120.10
11	X	358	LEU	CB-CG-CD1	5.38	120.15	111.00
8	N	770	HIS	O-C-N	-5.38	114.09	122.70
10	U	340	ILE	CA-CB-CG1	5.38	121.22	111.00
2	Y	201	TYR	CD1-CG-CD2	-5.38	111.98	117.90
2	Y	1247	SER	N-CA-C	-5.38	96.48	111.00
3	1	853	PHE	CB-CG-CD1	5.38	124.57	120.80
7	O	500	TRP	CG-CD2-CE3	5.38	138.74	133.90
8	N	680	ASP	CB-CG-OD1	5.38	123.14	118.30
9	Q	706	ILE	N-CA-C	-5.38	96.48	111.00
3	1	431	ARG	NE-CZ-NH2	-5.38	117.61	120.30
4	D	702	ARG	NE-CZ-NH2	5.38	122.99	120.30
6	I	448	THR	CA-CB-CG2	-5.38	104.88	112.40
7	M	1070	TYR	CZ-CE2-CD2	5.37	124.64	119.80
2	0	1185	TYR	CG-CD1-CE1	-5.37	117.00	121.30
4	G	658	TYR	CB-CG-CD1	5.37	124.22	121.00
3	1	801	LEU	CB-CG-CD1	5.37	120.13	111.00
3	1	97	PHE	N-CA-CB	5.37	120.27	110.60
7	O	251	ASP	CB-CG-OD1	5.37	123.13	118.30
9	T	300	THR	CA-CB-CG2	-5.37	104.88	112.40
9	T	661	LEU	CB-CG-CD1	5.37	120.12	111.00
9	T	699	ASN	CA-CB-CG	-5.37	101.59	113.40
9	R	153	ASN	C-N-CA	5.37	135.12	121.70
2	0	493	PHE	CD1-CE1-CZ	-5.37	113.66	120.10
3	Z	115	ASP	CB-CG-OD1	-5.37	113.47	118.30
9	Q	223	ASN	N-CA-CB	5.37	120.26	110.60
11	V	358	LEU	CB-CG-CD1	5.37	120.12	111.00
10	W	340	ILE	CA-CB-CG1	5.37	121.19	111.00
7	M	656	VAL	CA-CB-CG2	-5.36	102.86	110.90
9	S	768	VAL	CA-CB-CG2	5.36	118.95	110.90
8	P	816	ALA	CB-CA-C	-5.36	102.06	110.10
9	S	706	ILE	N-CA-C	-5.36	96.53	111.00
9	Q	576	LEU	N-CA-CB	5.36	121.12	110.40
4	J	767	VAL	O-C-N	-5.36	114.12	122.70
3	Z	851	ASP	CB-CA-C	-5.36	99.68	110.40
7	M	418	TYR	CB-CG-CD1	5.36	124.21	121.00
9	S	223	ASN	N-CA-CB	5.36	120.24	110.60
3	Z	904	TYR	CB-CG-CD2	-5.36	117.79	121.00
9	R	555	GLU	OE1-CD-OE2	5.36	129.73	123.30
3	1	404	PHE	CG-CD2-CE2	5.36	126.69	120.80
7	O	1563	LEU	N-CA-C	-5.36	96.54	111.00
7	M	500	TRP	CG-CD2-CE3	5.35	138.72	133.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	920	LEU	CB-CG-CD2	-5.35	101.90	111.00
8	P	1495	TRP	CB-CG-CD1	-5.35	120.04	127.00
2	Y	1467	SER	N-CA-CB	5.35	118.53	110.50
4	A	649	THR	CA-CB-OG1	5.35	120.24	109.00
5	E	371	GLN	CA-CB-CG	5.35	125.17	113.40
9	R	300	THR	CA-CB-CG2	-5.35	104.91	112.40
3	1	539	TYR	CB-CG-CD2	-5.35	117.79	121.00
3	Z	97	PHE	N-CA-CB	5.35	120.23	110.60
9	S	576	LEU	N-CA-CB	5.35	121.10	110.40
3	Z	801	LEU	CB-CG-CD1	5.35	120.09	111.00
3	Z	990	THR	CA-CB-CG2	-5.35	104.91	112.40
7	M	1040	THR	N-CA-CB	5.35	120.46	110.30
3	Z	1164	PHE	CG-CD1-CE1	-5.35	114.92	120.80
9	R	699	ASN	CA-CB-CG	-5.35	101.64	113.40
9	R	725	GLU	N-CA-CB	5.35	120.23	110.60
3	1	904	TYR	CB-CG-CD2	-5.35	117.79	121.00
3	1	1391	LYS	N-CA-CB	5.35	120.23	110.60
7	O	565	TYR	CB-CG-CD2	5.35	124.21	121.00
8	P	758	TYR	CG-CD1-CE1	5.35	125.58	121.30
8	P	1339	PHE	CB-CG-CD2	5.35	124.54	120.80
2	Y	1109	PHE	CB-CG-CD1	5.35	124.54	120.80
8	P	844	TYR	CD1-CE1-CZ	-5.35	114.99	119.80
3	Z	1391	LYS	N-CA-CB	5.34	120.22	110.60
7	M	736	PHE	CB-CG-CD1	-5.34	117.06	120.80
7	O	656	VAL	CA-CB-CG2	-5.34	102.88	110.90
2	0	143	GLY	CA-C-O	5.34	130.22	120.60
7	O	144	ILE	C-N-CA	5.34	135.06	121.70
11	V	360	TYR	CD1-CE1-CZ	-5.34	114.99	119.80
2	0	259	THR	CA-CB-CG2	-5.34	104.92	112.40
4	G	649	THR	CA-CB-OG1	5.34	120.22	109.00
8	P	247	PHE	N-CA-CB	5.34	120.21	110.60
9	S	287	ASP	CB-CG-OD1	5.34	123.11	118.30
9	S	456	ARG	CD-NE-CZ	-5.34	116.12	123.60
2	Y	1159	TYR	CG-CD2-CE2	-5.34	117.03	121.30
6	C	448	THR	CA-CB-CG2	-5.34	104.92	112.40
2	0	1467	SER	N-CA-CB	5.34	118.51	110.50
4	D	712	ASP	CB-CG-OD1	5.34	123.10	118.30
7	M	251	ASP	CB-CG-OD1	5.34	123.10	118.30
8	N	783	PHE	CB-CG-CD2	-5.34	117.06	120.80
8	N	1495	TRP	CB-CG-CD1	-5.34	120.06	127.00
9	R	238	PHE	CG-CD2-CE2	5.34	126.67	120.80
2	0	1444	PHE	CB-CG-CD1	5.34	124.53	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	1	241	THR	CA-CB-CG2	-5.34	104.93	112.40
9	T	153	ASN	C-N-CA	5.34	135.04	121.70
3	Z	431	ARG	NE-CZ-NH2	-5.33	117.63	120.30
7	M	1431	ARG	NE-CZ-NH2	-5.33	117.63	120.30
9	R	546	ARG	NH1-CZ-NH2	-5.33	113.53	119.40
8	P	942	PRO	N-CD-CG	5.33	111.20	103.20
9	T	526	LYS	N-CA-CB	5.33	120.20	110.60
3	1	1123	PHE	CG-CD2-CE2	-5.33	114.93	120.80
3	Z	818	ASP	C-N-CA	5.33	135.03	121.70
7	M	144	ILE	C-N-CA	5.33	135.03	121.70
9	Q	386	TYR	CG-CD2-CE2	5.33	125.56	121.30
7	O	418	TYR	CB-CG-CD1	5.33	124.20	121.00
3	Z	427	THR	CA-CB-CG2	-5.33	104.94	112.40
7	M	484	SER	N-CA-CB	5.33	118.49	110.50
7	M	1563	LEU	N-CA-C	-5.33	96.61	111.00
2	0	270	VAL	CA-CB-CG2	-5.33	102.91	110.90
4	G	658	TYR	O-C-N	-5.33	114.17	122.70
6	I	310	ARG	NE-CZ-NH2	-5.33	117.64	120.30
9	S	366	SER	N-CA-CB	5.33	118.49	110.50
3	Z	844	PHE	CB-CG-CD1	-5.32	117.07	120.80
7	M	205	ALA	N-CA-CB	5.32	117.55	110.10
9	R	526	LYS	N-CA-CB	5.32	120.18	110.60
9	R	661	LEU	CB-CG-CD1	5.32	120.05	111.00
3	1	612	TYR	CG-CD2-CE2	5.32	125.56	121.30
8	P	922	PHE	CD1-CE1-CZ	-5.32	113.71	120.10
8	N	247	PHE	N-CA-CB	5.32	120.18	110.60
9	Q	768	VAL	CA-CB-CG2	5.32	118.88	110.90
8	P	680	ASP	CB-CG-OD1	5.32	123.09	118.30
2	Y	652	TYR	CG-CD2-CE2	-5.32	117.05	121.30
4	D	767	VAL	O-C-N	-5.32	114.19	122.70
9	R	749	ASP	CB-CG-OD2	-5.32	113.51	118.30
3	Z	1340	LYS	N-CA-CB	5.32	120.17	110.60
4	A	658	TYR	O-C-N	-5.32	114.19	122.70
7	M	1398	SER	N-CA-CB	5.32	118.47	110.50
8	N	1524	TYR	CB-CG-CD1	-5.32	117.81	121.00
2	Y	421	VAL	CA-CB-CG1	-5.31	102.93	110.90
8	N	816	ALA	CB-CA-C	-5.31	102.13	110.10
2	Y	143	GLY	CA-C-O	5.31	130.16	120.60
8	N	942	PRO	N-CD-CG	5.31	111.17	103.20
5	H	535	LYS	N-CA-CB	5.31	120.16	110.60
7	O	484	SER	N-CA-CB	5.31	118.47	110.50
2	Y	272	ASP	CB-CA-C	-5.31	99.78	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	973	ARG	NE-CZ-NH1	5.31	122.95	120.30
4	A	686	ALA	CB-CA-C	-5.31	102.14	110.10
9	Q	456	ARG	CD-NE-CZ	-5.31	116.17	123.60
7	O	56	ILE	CA-CB-CG1	5.31	121.09	111.00
8	P	783	PHE	CB-CG-CD2	-5.31	117.08	120.80
9	T	555	GLU	OE1-CD-OE2	5.31	129.67	123.30
9	Q	523	ARG	NE-CZ-NH1	5.31	122.95	120.30
4	G	686	ALA	CB-CA-C	-5.31	102.14	110.10
9	T	238	PHE	CG-CD2-CE2	5.31	126.64	120.80
3	Z	241	THR	CA-CB-CG2	-5.30	104.97	112.40
3	Z	404	PHE	CG-CD2-CE2	5.30	126.64	120.80
9	S	523	ARG	NE-CZ-NH1	5.30	122.95	120.30
2	Y	138	GLU	N-CA-CB	5.30	120.14	110.60
2	Y	270	VAL	CA-CB-CG2	-5.30	102.95	110.90
3	1	1340	LYS	N-CA-CB	5.30	120.14	110.60
9	S	72	LEU	O-C-N	5.30	131.18	122.70
8	N	844	TYR	CD1-CE1-CZ	-5.30	115.03	119.80
2	0	1228	THR	CA-CB-CG2	-5.30	104.98	112.40
5	H	335	TRP	CE2-CD2-CG	-5.30	103.06	107.30
7	O	1040	THR	N-CA-CB	5.30	120.37	110.30
9	S	810	ALA	CB-CA-C	-5.30	102.15	110.10
5	B	344	SER	N-CA-CB	5.30	118.45	110.50
8	P	568	ILE	O-C-N	-5.30	114.22	122.70
8	P	955	PHE	CB-CG-CD1	5.30	124.51	120.80
9	Q	287	ASP	CB-CG-OD1	5.30	123.07	118.30
9	Q	366	SER	N-CA-CB	5.30	118.45	110.50
9	Q	810	ALA	CB-CA-C	-5.30	102.15	110.10
2	0	138	GLU	N-CA-CB	5.30	120.13	110.60
7	O	205	ALA	N-CA-CB	5.29	117.51	110.10
2	Y	1185	TYR	CG-CD1-CE1	-5.29	117.06	121.30
7	M	56	ILE	CA-CB-CG1	5.29	121.06	111.00
7	M	184	ASP	N-CA-CB	5.29	120.13	110.60
2	Y	980	SER	N-CA-C	-5.29	96.71	111.00
5	E	467	LYS	O-C-N	-5.29	114.23	122.70
3	1	818	ASP	C-N-CA	5.29	134.93	121.70
8	P	1199	TYR	CG-CD1-CE1	-5.29	117.07	121.30
2	Y	979	ALA	CB-CA-C	-5.29	102.17	110.10
5	B	361	ARG	NE-CZ-NH1	5.29	122.94	120.30
8	N	568	ILE	O-C-N	-5.29	114.24	122.70
2	0	421	VAL	CA-CB-CG1	-5.29	102.97	110.90
2	0	1176	ASP	CB-CG-OD1	5.29	123.06	118.30
3	1	427	THR	CA-CB-CG2	-5.29	104.99	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	P	216	TYR	CD1-CE1-CZ	5.29	124.56	119.80
9	T	546	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
2	Y	1228	THR	CA-CB-CG2	-5.29	105.00	112.40
9	R	816	TYR	CG-CD1-CE1	-5.29	117.07	121.30
2	0	1109	PHE	CB-CG-CD1	5.29	124.50	120.80
4	A	709	ASN	CB-CG-OD1	5.29	132.17	121.60
2	0	272	ASP	CB-CA-C	-5.29	99.83	110.40
2	0	980	SER	N-CA-C	-5.29	96.73	111.00
5	H	344	SER	N-CA-CB	5.29	118.43	110.50
5	B	394	THR	CA-CB-CG2	-5.28	105.00	112.40
5	B	535	LYS	N-CA-CB	5.28	120.11	110.60
8	N	1620	THR	N-CA-C	-5.28	96.74	111.00
9	Q	811	ARG	NE-CZ-NH1	5.28	122.94	120.30
3	Z	1123	PHE	CG-CD2-CE2	-5.28	114.99	120.80
4	D	685	MET	CG-SD-CE	-5.28	91.75	100.20
8	N	922	PHE	CD1-CE1-CZ	-5.28	113.76	120.10
9	Q	72	LEU	O-C-N	5.28	131.15	122.70
2	0	979	ALA	CB-CA-C	-5.28	102.18	110.10
8	N	617	TYR	N-CA-CB	5.28	120.10	110.60
4	J	685	MET	CG-SD-CE	-5.28	91.76	100.20
9	T	382	LEU	CB-CA-C	-5.28	100.17	110.20
7	M	759	ASP	CB-CG-OD1	5.28	123.05	118.30
9	Q	424	ASN	CB-CG-OD1	-5.28	111.05	121.60
7	O	1398	SER	N-CA-CB	5.28	118.41	110.50
9	S	811	ARG	NE-CZ-NH1	5.28	122.94	120.30
9	T	749	ASP	CB-CG-OD2	-5.27	113.55	118.30
7	M	1156	TYR	CB-CG-CD2	-5.27	117.84	121.00
8	N	970	LEU	CB-CG-CD1	5.27	119.96	111.00
9	Q	294	MET	O-C-N	-5.27	114.26	122.70
2	0	1159	TYR	CG-CD2-CE2	-5.27	117.08	121.30
3	Z	1271	ARG	NE-CZ-NH2	-5.27	117.67	120.30
8	N	1642	ARG	NH1-CZ-NH2	-5.27	113.60	119.40
5	K	467	LYS	O-C-N	-5.27	114.27	122.70
8	P	970	LEU	CB-CG-CD1	5.27	119.96	111.00
4	A	797	LEU	CB-CG-CD1	-5.27	102.04	111.00
4	J	712	ASP	CB-CG-OD1	5.27	123.04	118.30
6	F	313	ALA	CB-CA-C	-5.27	102.20	110.10
9	Q	262	SER	O-C-N	5.26	131.12	122.70
6	L	313	ALA	CB-CA-C	-5.26	102.20	110.10
2	Y	1176	ASP	CB-CG-OD1	5.26	123.04	118.30
3	Z	268	ARG	CD-NE-CZ	-5.26	116.23	123.60
2	Y	787	ARG	NE-CZ-NH2	5.26	122.93	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	Y	790	PHE	N-CA-CB	5.26	120.07	110.60
6	F	336	PHE	O-C-N	-5.26	114.28	122.70
7	M	1667	VAL	CA-CB-CG2	-5.26	103.01	110.90
6	C	310	ARG	NE-CZ-NH2	-5.26	117.67	120.30
9	R	516	PHE	CD1-CG-CD2	-5.26	111.46	118.30
2	0	424	SER	N-CA-CB	5.26	118.39	110.50
3	1	1244	SER	N-CA-CB	5.26	118.39	110.50
5	H	394	THR	CA-CB-CG2	-5.26	105.04	112.40
2	0	1349	MET	C-N-CA	5.26	134.84	121.70
2	Y	259	THR	CA-CB-CG2	-5.26	105.04	112.40
7	M	1643	ARG	NH1-CZ-NH2	5.26	125.18	119.40
2	0	790	PHE	N-CA-CB	5.26	120.06	110.60
5	B	335	TRP	CE2-CD2-CG	-5.25	103.10	107.30
7	M	981	ALA	CB-CA-C	-5.25	102.22	110.10
7	M	1530	GLU	N-CA-CB	5.25	120.06	110.60
6	L	336	PHE	O-C-N	-5.25	114.29	122.70
7	O	1530	GLU	N-CA-CB	5.25	120.06	110.60
8	P	1620	THR	N-CA-C	-5.25	96.82	111.00
2	Y	1349	MET	C-N-CA	5.25	134.83	121.70
2	0	1352	ASN	N-CA-CB	5.25	120.05	110.60
3	1	217	SER	N-CA-CB	5.25	118.38	110.50
3	1	1320	LYS	N-CA-CB	5.25	120.05	110.60
2	0	1413	VAL	CB-CA-C	5.25	121.37	111.40
3	1	353	VAL	CA-CB-CG1	-5.25	103.03	110.90
3	1	1307	VAL	CA-CB-CG2	-5.25	103.03	110.90
7	O	112	TYR	CZ-CE2-CD2	5.25	124.52	119.80
2	Y	424	SER	N-CA-CB	5.25	118.37	110.50
3	Z	217	SER	N-CA-CB	5.25	118.37	110.50
8	N	216	TYR	CD1-CE1-CZ	5.25	124.52	119.80
3	Z	353	VAL	CA-CB-CG1	-5.24	103.03	110.90
8	N	1209	ALA	N-CA-CB	5.24	117.44	110.10
9	R	792	SER	N-CA-CB	5.24	118.36	110.50
9	S	424	ASN	CB-CG-OD1	-5.24	111.11	121.60
9	S	531	ASP	CB-CG-OD2	5.24	123.02	118.30
4	D	744	ALA	CB-CA-C	-5.24	102.24	110.10
2	Y	578	VAL	CA-CB-CG1	5.24	118.76	110.90
8	N	114	TYR	CG-CD1-CE1	-5.24	117.11	121.30
3	1	1350	TRP	CB-CG-CD1	5.24	133.81	127.00
4	G	709	ASN	CB-CG-OD1	5.24	132.08	121.60
8	P	242	TYR	CG-CD1-CE1	-5.24	117.11	121.30
3	Z	853	PHE	CB-CG-CD1	5.24	124.47	120.80
8	N	685	TYR	CD1-CE1-CZ	5.24	124.52	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	928	SER	N-CA-CB	5.24	118.36	110.50
7	M	260	MET	N-CA-CB	5.24	120.03	110.60
8	N	259	SER	N-CA-CB	5.24	118.36	110.50
8	P	617	TYR	N-CA-CB	5.24	120.03	110.60
8	P	928	SER	N-CA-CB	5.24	118.36	110.50
9	T	792	SER	N-CA-CB	5.24	118.36	110.50
2	Y	1444	PHE	CB-CG-CD1	5.24	124.47	120.80
5	E	335	TRP	CZ3-CH2-CZ2	-5.24	115.32	121.60
8	N	1349	TYR	CD1-CG-CD2	5.24	123.66	117.90
2	0	787	ARG	NE-CZ-NH2	5.24	122.92	120.30
5	K	335	TRP	CZ3-CH2-CZ2	-5.24	115.32	121.60
3	Z	1164	PHE	CB-CG-CD2	-5.23	117.14	120.80
2	0	1170	ARG	NE-CZ-NH1	5.23	122.92	120.30
7	O	184	ASP	N-CA-CB	5.23	120.02	110.60
8	P	1524	TYR	CB-CG-CD1	-5.23	117.86	121.00
2	Y	765	ILE	C-N-CA	5.23	134.78	121.70
3	Z	1244	SER	N-CA-CB	5.23	118.35	110.50
8	N	1339	PHE	CB-CG-CD2	5.23	124.46	120.80
3	1	1164	PHE	CB-CG-CD2	-5.23	117.14	120.80
8	P	837	ASP	CB-CG-OD1	-5.23	113.59	118.30
9	R	382	LEU	CB-CA-C	-5.23	100.26	110.20
4	J	744	ALA	CB-CA-C	-5.23	102.25	110.10
8	P	114	TYR	CG-CD1-CE1	-5.23	117.12	121.30
8	P	1642	ARG	NH1-CZ-NH2	-5.23	113.65	119.40
9	Q	531	ASP	CB-CG-OD2	5.23	123.01	118.30
2	0	765	ILE	C-N-CA	5.23	134.77	121.70
7	O	1667	VAL	CA-CB-CG2	-5.23	103.06	110.90
3	Z	1307	VAL	CA-CB-CG2	-5.23	103.06	110.90
7	M	1334	THR	CA-CB-CG2	-5.23	105.08	112.40
3	1	1249	PRO	CA-N-CD	-5.23	104.18	111.50
7	O	1087	CYS	CA-CB-SG	-5.23	104.59	114.00
8	P	1039	PHE	CG-CD1-CE1	-5.23	115.05	120.80
3	1	181	ILE	N-CA-C	-5.22	96.89	111.00
3	1	1279	THR	CA-CB-CG2	-5.22	105.09	112.40
8	P	877	LEU	CB-CG-CD1	-5.22	102.12	111.00
8	P	1209	ALA	N-CA-CB	5.22	117.41	110.10
8	N	242	TYR	CG-CD1-CE1	-5.22	117.12	121.30
8	P	259	SER	N-CA-CB	5.22	118.33	110.50
4	G	797	LEU	CB-CG-CD1	-5.22	102.12	111.00
9	S	262	SER	O-C-N	5.22	131.05	122.70
11	X	366	ALA	N-CA-CB	5.22	117.41	110.10
4	A	793	LEU	O-C-N	5.22	131.05	122.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	1611	TYR	CB-CG-CD2	-5.22	117.87	121.00
3	1	1386	ARG	NE-CZ-NH2	5.22	122.91	120.30
9	T	516	PHE	CD1-CG-CD2	-5.22	111.51	118.30
2	Y	1413	VAL	CB-CA-C	5.22	121.31	111.40
8	N	781	ASP	CB-CG-OD2	-5.22	113.60	118.30
3	1	268	ARG	CD-NE-CZ	-5.22	116.29	123.60
4	G	793	LEU	O-C-N	5.22	131.05	122.70
7	M	1087	CYS	CA-CB-SG	-5.22	104.61	114.00
8	N	558	LYS	N-CA-CB	5.22	119.99	110.60
8	N	916	TYR	CB-CG-CD2	-5.22	117.87	121.00
8	P	1349	TYR	CD1-CG-CD2	5.22	123.64	117.90
3	1	856	ASN	CB-CA-C	5.21	120.83	110.40
8	N	877	LEU	CB-CG-CD1	-5.21	102.14	111.00
7	O	1073	MET	CG-SD-CE	5.21	108.54	100.20
2	Y	1352	ASN	N-CA-CB	5.21	119.98	110.60
3	Z	1249	PRO	CA-N-CD	-5.21	104.20	111.50
3	Z	1320	LYS	N-CA-CB	5.21	119.98	110.60
4	D	693	ILE	CA-CB-CG1	5.21	120.90	111.00
7	M	1323	THR	N-CA-CB	5.21	120.20	110.30
8	N	1039	PHE	CG-CD1-CE1	-5.21	115.07	120.80
3	1	822	PHE	CD1-CG-CD2	5.21	125.08	118.30
7	M	1523	PHE	CB-CG-CD2	-5.21	117.15	120.80
3	Z	181	ILE	N-CA-C	-5.21	96.94	111.00
7	M	1073	MET	CG-SD-CE	5.21	108.53	100.20
2	0	578	VAL	CA-CB-CG1	5.21	118.71	110.90
8	P	584	ASP	CB-CG-OD2	-5.21	113.61	118.30
2	Y	768	PRO	N-CD-CG	5.21	111.01	103.20
4	A	677	SER	N-CA-CB	5.21	118.31	110.50
7	O	1323	THR	N-CA-CB	5.21	120.19	110.30
7	O	981	ALA	CB-CA-C	-5.20	102.30	110.10
2	Y	397	TYR	CG-CD1-CE1	5.20	125.46	121.30
3	Z	1386	ARG	NE-CZ-NH2	5.20	122.90	120.30
2	0	192	LEU	CB-CG-CD2	5.20	119.84	111.00
2	0	1285	ILE	N-CA-C	-5.20	96.95	111.00
8	N	430	ALA	N-CA-CB	5.20	117.38	110.10
2	0	1108	VAL	CA-CB-CG1	5.20	118.70	110.90
3	Z	856	ASN	CB-CA-C	5.20	120.80	110.40
8	N	888	TYR	CD1-CE1-CZ	5.20	124.48	119.80
8	N	1313	ARG	N-CA-CB	5.20	119.96	110.60
2	Y	1170	ARG	NE-CZ-NH1	5.20	122.90	120.30
2	Y	1268	VAL	CA-CB-CG1	5.20	118.69	110.90
7	O	155	LEU	N-CA-CB	5.20	120.79	110.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	584	ASP	CB-CG-OD2	-5.20	113.62	118.30
8	P	617	TYR	CB-CG-CD1	-5.20	117.88	121.00
2	Y	1219	ARG	NE-CZ-NH2	5.19	122.90	120.30
9	R	245	ALA	N-CA-CB	5.19	117.37	110.10
2	0	1268	VAL	CA-CB-CG1	5.19	118.69	110.90
7	O	1156	TYR	CB-CG-CD2	-5.19	117.89	121.00
8	P	781	ASP	CB-CG-OD2	-5.19	113.63	118.30
2	Y	1108	VAL	CA-CB-CG1	5.19	118.68	110.90
7	M	155	LEU	N-CA-CB	5.19	120.78	110.40
9	Q	600	ILE	C-N-CD	5.19	139.30	128.40
11	V	366	ALA	N-CA-CB	5.19	117.37	110.10
2	0	135	PHE	CB-CG-CD2	-5.19	117.17	120.80
7	O	188	ARG	CG-CD-NE	-5.19	100.90	111.80
6	C	313	ALA	CB-CA-C	-5.19	102.32	110.10
2	0	397	TYR	CG-CD1-CE1	5.19	125.45	121.30
3	Z	1279	THR	CA-CB-CG2	-5.19	105.14	112.40
7	M	188	ARG	CG-CD-NE	-5.19	100.91	111.80
2	0	768	PRO	N-CD-CG	5.19	110.98	103.20
2	0	973	ARG	NE-CZ-NH1	5.19	122.89	120.30
7	O	260	MET	N-CA-CB	5.19	119.94	110.60
9	T	245	ALA	N-CA-CB	5.19	117.36	110.10
2	0	1219	ARG	NE-CZ-NH2	5.19	122.89	120.30
4	G	677	SER	N-CA-CB	5.19	118.28	110.50
4	J	693	ILE	CA-CB-CG1	5.19	120.85	111.00
2	Y	119	PRO	N-CD-CG	5.18	110.97	103.20
7	M	112	TYR	CZ-CE2-CD2	5.18	124.47	119.80
8	N	1199	TYR	CG-CD1-CE1	-5.18	117.15	121.30
2	0	652	TYR	CG-CD2-CE2	-5.18	117.15	121.30
3	1	978	ASN	N-CA-CB	5.18	119.93	110.60
2	Y	135	PHE	CB-CG-CD2	-5.18	117.17	120.80
9	Q	680	ASN	C-N-CA	5.18	134.66	121.70
7	O	70	PHE	N-CA-CB	-5.18	101.27	110.60
8	P	497	ILE	CA-CB-CG2	-5.18	100.53	110.90
8	P	1313	ARG	N-CA-CB	5.18	119.93	110.60
9	T	474	PHE	CB-CG-CD1	-5.18	117.17	120.80
5	E	309	ARG	N-CA-C	-5.18	97.02	111.00
3	Z	444	GLY	O-C-N	5.18	130.98	122.70
3	Z	642	SER	N-CA-CB	5.18	118.27	110.50
7	M	1251	ARG	NE-CZ-NH2	5.18	122.89	120.30
8	P	558	LYS	N-CA-CB	5.18	119.92	110.60
8	N	837	ASP	CB-CG-OD1	-5.17	113.64	118.30
8	N	955	PHE	CB-CG-CD1	5.17	124.42	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	O	249	ASP	CB-CG-OD1	5.17	122.96	118.30
7	O	1643	ARG	NH1-CZ-NH2	5.17	125.09	119.40
2	Y	192	LEU	CB-CG-CD2	5.17	119.79	111.00
7	M	1431	ARG	NH1-CZ-NH2	5.17	125.09	119.40
9	Q	644	TYR	CG-CD2-CE2	5.17	125.44	121.30
8	P	430	ALA	N-CA-CB	5.17	117.34	110.10
9	S	294	MET	O-C-N	-5.17	114.42	122.70
8	P	1063	ASP	O-C-N	5.17	130.97	122.70
4	J	788	ASP	CB-CG-OD1	5.17	122.95	118.30
7	M	70	PHE	N-CA-CB	-5.17	101.30	110.60
3	1	140	ARG	NE-CZ-NH1	-5.17	117.72	120.30
3	1	444	GLY	O-C-N	5.17	130.97	122.70
8	P	1538	ASP	CB-CG-OD1	5.17	122.95	118.30
9	T	776	ILE	O-C-N	-5.17	114.43	122.70
9	S	680	ASN	C-N-CA	5.17	134.61	121.70
9	T	816	TYR	CG-CD1-CE1	-5.17	117.17	121.30
3	Z	890	GLU	O-C-N	-5.16	114.44	122.70
3	1	582	THR	CA-CB-OG1	5.16	119.84	109.00
7	O	106	TYR	CG-CD1-CE1	-5.16	117.17	121.30
9	R	449	GLU	CB-CA-C	-5.16	100.08	110.40
2	Y	1285	ILE	N-CA-C	-5.16	97.07	111.00
2	0	438	ALA	CB-CA-C	5.16	117.84	110.10
7	O	1523	PHE	CB-CG-CD2	-5.16	117.19	120.80
8	P	888	TYR	CD1-CE1-CZ	5.16	124.44	119.80
9	T	449	GLU	CB-CA-C	-5.16	100.08	110.40
8	N	1538	ASP	CB-CG-OD1	5.16	122.94	118.30
3	1	642	SER	N-CA-CB	5.16	118.24	110.50
6	I	313	ALA	CB-CA-C	-5.16	102.36	110.10
9	S	644	TYR	CG-CD2-CE2	5.16	125.43	121.30
2	Y	673	TYR	CG-CD1-CE1	5.16	125.43	121.30
3	Z	908	GLU	CG-CD-OE1	-5.16	107.99	118.30
7	M	249	ASP	CB-CG-OD1	5.16	122.94	118.30
2	0	606	GLN	N-CA-C	-5.16	97.08	111.00
9	T	520	SER	N-CA-C	-5.15	97.08	111.00
2	0	1280	TYR	CD1-CE1-CZ	-5.15	115.16	119.80
2	Y	438	ALA	CB-CA-C	5.15	117.83	110.10
7	M	467	LEU	N-CA-CB	5.15	120.70	110.40
2	0	1181	PHE	CG-CD1-CE1	-5.15	115.14	120.80
8	N	1063	ASP	O-C-N	5.15	130.94	122.70
5	E	317	ASN	N-CA-C	5.15	124.89	111.00
5	K	309	ARG	N-CA-C	-5.15	97.10	111.00
2	Y	283	PHE	N-CA-C	-5.14	97.11	111.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	1350	TRP	CB-CG-CD1	5.14	133.69	127.00
9	R	474	PHE	N-CA-CB	5.14	119.86	110.60
2	0	1022	ASP	CB-CA-C	-5.14	100.11	110.40
7	O	1431	ARG	NH1-CZ-NH2	5.14	125.06	119.40
8	P	914	ASP	CB-CG-OD1	5.14	122.93	118.30
9	T	474	PHE	N-CA-CB	5.14	119.86	110.60
7	M	106	TYR	CG-CD1-CE1	-5.14	117.19	121.30
8	N	497	ILE	CA-CB-CG2	-5.14	100.62	110.90
3	1	770	ARG	NE-CZ-NH2	-5.14	117.73	120.30
8	P	685	TYR	CD1-CE1-CZ	5.14	124.43	119.80
2	Y	431	ASN	N-CA-CB	5.14	119.85	110.60
9	S	417	ARG	NE-CZ-NH1	5.14	122.87	120.30
2	0	431	ASN	N-CA-CB	5.14	119.85	110.60
7	O	1334	THR	CA-CB-CG2	-5.14	105.21	112.40
2	Y	606	GLN	N-CA-C	-5.14	97.13	111.00
3	Z	582	THR	CA-CB-OG1	5.14	119.79	109.00
7	M	543	VAL	CA-CB-CG2	-5.14	103.19	110.90
7	M	1368	ARG	NE-CZ-NH1	5.14	122.87	120.30
8	N	886	ASP	CB-CG-OD2	-5.14	113.68	118.30
8	P	72	ARG	NE-CZ-NH1	5.14	122.87	120.30
8	P	1611	TYR	CB-CG-CD2	-5.14	117.92	121.00
2	0	283	PHE	N-CA-C	-5.13	97.14	111.00
7	O	459	ASP	CB-CG-OD1	5.13	122.92	118.30
9	T	493	ASP	CB-CG-OD1	5.13	122.92	118.30
3	Z	822	PHE	CD1-CG-CD2	5.13	124.97	118.30
8	N	479	ALA	N-CA-CB	5.13	117.28	110.10
7	O	467	LEU	N-CA-CB	5.13	120.66	110.40
9	T	710	ASN	N-CA-CB	5.13	119.83	110.60
8	P	555	PHE	CB-CG-CD1	5.13	124.39	120.80
3	Z	740	MET	CA-CB-CG	5.13	122.02	113.30
3	Z	978	ASN	N-CA-CB	5.13	119.83	110.60
7	M	1437	LEU	O-C-N	5.13	130.91	122.70
8	N	661	MET	CG-SD-CE	-5.13	91.99	100.20
9	R	776	ILE	O-C-N	-5.13	114.50	122.70
2	0	119	PRO	N-CD-CG	5.13	110.89	103.20
8	P	479	ALA	N-CA-CB	5.13	117.28	110.10
2	Y	1022	ASP	CB-CA-C	-5.13	100.15	110.40
2	Y	1181	PHE	CG-CD1-CE1	-5.13	115.16	120.80
3	Z	871	VAL	CA-CB-CG2	-5.13	103.21	110.90
3	1	908	GLU	CG-CD-OE1	-5.13	108.05	118.30
8	P	916	TYR	CB-CG-CD2	-5.12	117.92	121.00
3	1	844	PHE	CB-CG-CD1	-5.12	117.22	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	1121	THR	CA-CB-CG2	-5.12	105.23	112.40
8	N	300	SER	CB-CA-C	5.12	119.82	110.10
9	R	520	SER	N-CA-C	-5.12	97.18	111.00
9	R	710	ASN	N-CA-CB	5.12	119.81	110.60
8	P	753	TYR	CG-CD2-CE2	5.12	125.39	121.30
9	Q	605	GLU	N-CA-CB	5.12	119.81	110.60
5	K	325	THR	N-CA-C	5.12	124.81	111.00
8	P	603	ASP	CB-CG-OD2	-5.12	113.70	118.30
9	S	605	GLU	N-CA-CB	5.12	119.81	110.60
3	Z	883	TYR	CG-CD1-CE1	-5.11	117.21	121.30
3	Z	964	VAL	CA-CB-CG1	5.11	118.57	110.90
8	P	623	ASP	CB-CA-C	5.11	120.63	110.40
2	Y	1340	TRP	CH2-CZ2-CE2	5.11	122.51	117.40
5	E	541	THR	CA-CB-CG2	-5.11	105.24	112.40
8	N	623	ASP	CB-CA-C	5.11	120.62	110.40
3	Z	140	ARG	NE-CZ-NH1	-5.11	117.75	120.30
3	1	871	VAL	CA-CB-CG2	-5.11	103.23	110.90
7	O	1013	TYR	CG-CD2-CE2	-5.11	117.21	121.30
7	O	1437	LEU	O-C-N	5.11	130.88	122.70
8	P	295	PHE	CG-CD2-CE2	-5.11	115.18	120.80
2	0	1340	TRP	CH2-CZ2-CE2	5.11	122.51	117.40
8	P	262	SER	N-CA-CB	5.11	118.16	110.50
8	N	295	PHE	CG-CD2-CE2	-5.11	115.18	120.80
8	N	914	ASP	CB-CG-OD1	5.11	122.89	118.30
7	O	543	VAL	CA-CB-CG2	-5.11	103.24	110.90
6	L	456	ARG	NE-CZ-NH2	-5.10	117.75	120.30
8	P	246	ASN	N-CA-CB	5.10	119.79	110.60
7	M	1013	TYR	CG-CD2-CE2	-5.10	117.22	121.30
6	C	447	PHE	CB-CG-CD1	5.10	124.37	120.80
3	1	740	MET	CA-CB-CG	5.10	121.97	113.30
3	1	890	GLU	O-C-N	-5.10	114.54	122.70
3	1	964	VAL	CA-CB-CG1	5.10	118.55	110.90
7	O	623	VAL	CG1-CB-CG2	5.10	119.06	110.90
8	P	683	ASP	CB-CG-OD2	-5.10	113.71	118.30
7	O	1650	GLU	OE1-CD-OE2	5.10	129.42	123.30
4	D	788	ASP	CB-CG-OD1	5.10	122.89	118.30
5	K	541	THR	CA-CB-CG2	-5.10	105.27	112.40
9	S	385	GLU	OE1-CD-OE2	5.10	129.41	123.30
7	M	31	ASP	CB-CG-OD2	-5.09	113.72	118.30
6	L	404	ASP	CB-CG-OD2	5.09	122.89	118.30
7	O	96	ASP	CB-CG-OD2	5.09	122.89	118.30
8	P	661	MET	CG-SD-CE	-5.09	92.05	100.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	Z	144	THR	CA-CB-CG2	-5.09	105.27	112.40
8	N	1443	THR	CA-CB-CG2	-5.09	105.27	112.40
8	P	823	ILE	O-C-N	-5.09	114.55	122.70
2	Y	502	SER	N-CA-CB	5.09	118.14	110.50
2	Y	617	ALA	N-CA-C	-5.09	97.25	111.00
8	N	246	ASN	N-CA-CB	5.09	119.76	110.60
9	R	493	ASP	CB-CG-OD1	5.09	122.88	118.30
2	0	673	TYR	CG-CD1-CE1	5.09	125.37	121.30
8	P	886	ASP	CB-CG-OD2	-5.09	113.72	118.30
3	Z	510	CYS	N-CA-C	-5.09	97.27	111.00
9	Q	404	GLY	O-C-N	5.09	130.84	122.70
8	P	300	SER	CB-CA-C	5.08	119.76	110.10
7	M	1650	GLU	OE1-CD-OE2	5.08	129.40	123.30
8	N	1605	PHE	CA-CB-CG	-5.08	101.70	113.90
7	O	430	PHE	CA-CB-CG	5.08	126.10	113.90
8	P	914	ASP	C-N-CA	5.08	134.41	121.70
11	X	360	TYR	CZ-CE2-CD2	5.08	124.38	119.80
2	Y	1280	TYR	CD1-CE1-CZ	-5.08	115.23	119.80
2	0	617	ALA	N-CA-C	-5.08	97.28	111.00
6	I	447	PHE	CB-CG-CD1	5.08	124.36	120.80
8	N	888	TYR	CG-CD1-CE1	-5.08	117.24	121.30
9	Q	516	PHE	CB-CG-CD1	-5.08	117.24	120.80
3	1	510	CYS	N-CA-C	-5.08	97.28	111.00
7	M	579	ARG	NE-CZ-NH2	-5.08	117.76	120.30
3	1	144	THR	CA-CB-CG2	-5.08	105.29	112.40
3	1	1081	LEU	O-C-N	-5.08	111.45	121.10
7	O	216	LEU	CB-CG-CD2	-5.08	102.36	111.00
9	R	474	PHE	CB-CG-CD1	-5.08	117.25	120.80
7	M	572	PHE	CB-CG-CD2	-5.08	117.25	120.80
8	N	555	PHE	CB-CG-CD1	5.08	124.35	120.80
3	1	644	ALA	N-CA-CB	5.08	117.20	110.10
5	K	449	ASP	CB-CG-OD2	-5.08	113.73	118.30
7	O	1405	PHE	CB-CG-CD2	-5.08	117.25	120.80
9	S	586	PHE	CB-CG-CD2	5.08	124.35	120.80
3	Z	937	ARG	CG-CD-NE	-5.07	101.14	111.80
7	M	1394	SER	C-N-CD	5.07	139.05	128.40
8	N	823	ILE	O-C-N	-5.07	114.58	122.70
2	0	967	LEU	CA-C-N	5.07	128.36	117.20
6	I	311	ASP	CB-CG-OD2	-5.07	113.73	118.30
5	B	437	TRP	CG-CD1-NE1	5.07	115.17	110.10
7	M	623	VAL	CG1-CB-CG2	5.07	119.02	110.90
7	O	1121	THR	CA-CB-CG2	-5.07	105.30	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	0	405	THR	N-CA-CB	5.07	119.94	110.30
2	0	455	PHE	N-CA-CB	5.07	119.73	110.60
4	G	641	VAL	CB-CA-C	5.07	121.03	111.40
8	P	650	ASP	CB-CG-OD2	-5.07	113.74	118.30
2	Y	659	PHE	CG-CD1-CE1	5.07	126.38	120.80
5	E	449	ASP	CB-CG-OD2	-5.07	113.74	118.30
11	V	368	ARG	NE-CZ-NH1	5.07	122.83	120.30
3	Z	770	ARG	NE-CZ-NH2	-5.07	117.77	120.30
7	M	430	PHE	CA-CB-CG	5.07	126.06	113.90
8	N	262	SER	N-CA-CB	5.07	118.10	110.50
2	Y	455	PHE	N-CA-CB	5.06	119.71	110.60
7	O	101	ASN	CB-CG-OD1	-5.06	111.47	121.60
2	Y	121	LEU	CB-CG-CD1	5.06	119.60	111.00
4	A	641	VAL	CB-CA-C	5.06	121.02	111.40
7	M	216	LEU	CB-CG-CD2	-5.06	102.40	111.00
7	M	764	VAL	CA-CB-CG2	5.06	118.49	110.90
7	O	793	TYR	CB-CG-CD1	5.06	124.04	121.00
2	Y	1090	GLU	OE1-CD-OE2	-5.06	117.23	123.30
8	N	683	ASP	CB-CG-OD2	-5.06	113.75	118.30
3	1	1284	PRO	CA-N-CD	-5.06	104.42	111.50
6	I	393	ASP	CB-CG-OD2	5.06	122.85	118.30
7	O	1394	SER	C-N-CD	5.06	139.03	128.40
3	Z	274	PHE	CD1-CG-CD2	5.06	124.87	118.30
4	A	717	LYS	N-CA-CB	5.06	119.70	110.60
5	E	313	TYR	CD1-CE1-CZ	-5.06	115.25	119.80
7	M	899	PHE	CB-CG-CD1	-5.06	117.26	120.80
9	Q	586	PHE	CB-CG-CD2	5.06	124.34	120.80
2	0	502	SER	N-CA-CB	5.06	118.08	110.50
7	M	1406	TYR	CB-CG-CD1	5.06	124.03	121.00
3	1	937	ARG	CG-CD-NE	-5.06	101.18	111.80
2	0	121	LEU	CB-CG-CD1	5.05	119.59	111.00
2	0	276	HIS	CA-CB-CG	-5.05	105.01	113.60
3	1	274	PHE	CD1-CG-CD2	5.05	124.87	118.30
8	P	1605	PHE	CA-CB-CG	-5.05	101.77	113.90
9	S	404	GLY	O-C-N	5.05	130.79	122.70
11	X	368	ARG	NE-CZ-NH1	5.05	122.83	120.30
3	Z	1081	LEU	O-C-N	-5.05	111.50	121.10
7	M	459	ASP	CB-CG-OD1	5.05	122.85	118.30
2	Y	276	HIS	CA-CB-CG	-5.05	105.01	113.60
7	M	96	ASP	CB-CG-OD2	5.05	122.85	118.30
8	N	914	ASP	C-N-CA	5.05	134.33	121.70
2	0	1395	CYS	N-CA-CB	5.05	119.69	110.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	M	101	ASN	CB-CG-OD1	-5.05	111.50	121.60
8	N	1643	ASP	CB-CG-OD1	5.05	122.84	118.30
3	1	1323	TYR	CB-CG-CD2	-5.05	117.97	121.00
5	K	330	VAL	CA-CB-CG1	5.05	118.47	110.90
7	O	1406	TYR	CB-CG-CD1	5.05	124.03	121.00
8	N	1022	TYR	CB-CG-CD2	-5.05	117.97	121.00
9	Q	385	GLU	OE1-CD-OE2	5.05	129.36	123.30
9	R	697	PHE	CD1-CG-CD2	-5.05	111.74	118.30
2	0	659	PHE	CG-CD1-CE1	5.05	126.35	120.80
9	S	679	ASP	CB-CG-OD1	5.05	122.84	118.30
2	Y	967	LEU	CA-C-N	5.04	128.30	117.20
8	N	1097	LEU	CB-CG-CD2	5.04	119.58	111.00
2	Y	298	TYR	N-CA-CB	5.04	119.68	110.60
7	O	572	PHE	CB-CG-CD2	-5.04	117.27	120.80
2	Y	243	PHE	N-CA-CB	5.04	119.68	110.60
8	N	476	ASP	N-CA-C	-5.04	97.39	111.00
2	0	1090	GLU	OE1-CD-OE2	-5.04	117.25	123.30
2	Y	1395	CYS	N-CA-CB	5.04	119.67	110.60
2	0	298	TYR	N-CA-CB	5.04	119.67	110.60
9	T	823	ARG	CD-NE-CZ	5.04	130.66	123.60
9	Q	747	PHE	CG-CD2-CE2	-5.04	115.26	120.80
9	R	823	ARG	CD-NE-CZ	5.04	130.65	123.60
3	1	1299	LYS	CB-CA-C	5.04	120.48	110.40
8	P	1097	LEU	CB-CG-CD2	5.04	119.57	111.00
5	E	330	VAL	CA-CB-CG1	5.04	118.46	110.90
9	R	456	ARG	CB-CA-C	-5.04	100.33	110.40
2	Y	294	TRP	CE2-CD2-CG	5.04	111.33	107.30
4	G	717	LYS	N-CA-CB	5.04	119.67	110.60
2	Y	243	PHE	CB-CA-C	-5.03	100.33	110.40
3	Z	1284	PRO	CA-N-CD	-5.03	104.45	111.50
6	C	311	ASP	CB-CG-OD2	-5.03	113.77	118.30
6	F	272	GLN	CG-CD-OE1	-5.03	111.53	121.60
6	F	404	ASP	CB-CG-OD2	5.03	122.83	118.30
9	R	146	LEU	CB-CA-C	-5.03	100.64	110.20
7	O	31	ASP	CB-CG-OD2	-5.03	113.77	118.30
9	S	499	SER	N-CA-CB	5.03	118.05	110.50
9	T	697	PHE	CD1-CG-CD2	-5.03	111.76	118.30
2	Y	1416	PHE	CD1-CG-CD2	5.03	124.84	118.30
3	Z	1302	ALA	CB-CA-C	5.03	117.65	110.10
2	0	243	PHE	N-CA-CB	5.03	119.65	110.60
3	1	148	ASP	CB-CG-OD1	5.03	122.83	118.30
6	I	442	THR	CA-CB-CG2	-5.03	105.36	112.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	T	611	LEU	CB-CG-CD1	-5.03	102.45	111.00
2	Y	405	THR	N-CA-CB	5.03	119.85	110.30
9	S	372	LYS	N-CA-CB	5.03	119.65	110.60
3	Z	1299	LYS	CB-CA-C	5.03	120.45	110.40
11	V	360	TYR	CZ-CE2-CD2	5.03	124.32	119.80
2	0	1416	PHE	CD1-CG-CD2	5.03	124.83	118.30
3	1	883	TYR	CG-CD1-CE1	-5.03	117.28	121.30
9	T	456	ARG	CB-CA-C	-5.03	100.35	110.40
8	N	617	TYR	CB-CG-CD1	-5.02	117.98	121.00
2	Y	1261	ARG	NH1-CZ-NH2	-5.02	113.88	119.40
3	Z	644	ALA	N-CA-CB	5.02	117.13	110.10
8	N	603	ASP	CB-CG-OD2	-5.02	113.78	118.30
6	L	272	GLN	CG-CD-OE1	-5.02	111.55	121.60
3	Z	536	HIS	CB-CA-C	-5.02	100.36	110.40
5	E	446	ARG	NE-CZ-NH2	-5.02	117.79	120.30
7	M	659	ASN	CB-CA-C	-5.02	100.36	110.40
7	M	1553	LEU	N-CA-CB	5.02	120.44	110.40
5	H	437	TRP	CG-CD1-NE1	5.02	115.12	110.10
8	P	1443	THR	CA-CB-CG2	-5.02	105.37	112.40
9	S	232	PHE	CB-CG-CD2	-5.02	117.29	120.80
9	R	359	ASN	CA-CB-CG	-5.02	102.36	113.40
9	S	638	TYR	CG-CD1-CE1	-5.02	117.29	121.30
9	T	359	ASN	CA-CB-CG	-5.02	102.36	113.40
9	Q	499	SER	N-CA-CB	5.02	118.02	110.50
5	B	523	LEU	CB-CG-CD2	5.01	119.53	111.00
7	M	705	ASP	CB-CG-OD1	5.01	122.81	118.30
5	K	457	ASN	O-C-N	-5.01	114.68	122.70
7	M	793	TYR	CB-CG-CD1	5.01	124.01	121.00
3	1	536	HIS	CB-CA-C	-5.01	100.38	110.40
8	P	888	TYR	CG-CD1-CE1	-5.01	117.29	121.30
9	S	747	PHE	CG-CD2-CE2	-5.01	115.29	120.80
2	0	365	ARG	NH1-CZ-NH2	5.01	124.91	119.40
2	0	489	ALA	N-CA-CB	-5.01	103.09	110.10
8	P	1154	GLU	N-CA-CB	5.01	119.61	110.60
8	P	1281	MET	CG-SD-CE	-5.01	92.19	100.20
9	R	226	ARG	NH1-CZ-NH2	5.00	124.91	119.40
7	O	669	THR	C-N-CA	5.00	134.21	121.70
8	P	476	ASP	N-CA-C	-5.00	97.49	111.00
6	F	468	ALA	N-CA-CB	5.00	117.11	110.10
9	R	611	LEU	CB-CG-CD1	-5.00	102.49	111.00
2	0	1282	ASP	CB-CG-OD2	-5.00	113.80	118.30
7	M	1097	TYR	CB-CG-CD1	-5.00	118.00	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	N	862	ARG	NE-CZ-NH2	-5.00	117.80	120.30
7	O	1553	LEU	N-CA-CB	5.00	120.40	110.40
9	S	277	TYR	CA-CB-CG	-5.00	103.90	113.40

There are no chirality outliers.

All (380) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	0	1011	ARG	Sidechain
2	0	1012	ARG	Sidechain
2	0	1019	ARG	Sidechain
2	0	1059	TYR	Sidechain
2	0	107	TYR	Sidechain
2	0	1146	TYR	Sidechain
2	0	1219	ARG	Sidechain
2	0	1235	PHE	Sidechain
2	0	127	TYR	Sidechain
2	0	1284	ARG	Sidechain
2	0	1428	TYR	Sidechain
2	0	1460	ARG	Sidechain
2	0	154	PHE	Sidechain
2	0	181	ARG	Sidechain
2	0	313	CYS	Peptide
2	0	380	TYR	Sidechain
2	0	397	TYR	Sidechain
2	0	408	ARG	Sidechain
2	0	417	TYR	Sidechain
2	0	447	TYR	Sidechain
2	0	454	ARG	Sidechain
2	0	461	ARG	Sidechain
2	0	491	ARG	Sidechain
2	0	509	PHE	Sidechain
2	0	538	SER	Peptide
2	0	583	TYR	Sidechain
2	0	592	TYR	Sidechain
2	0	705	MET	Peptide
2	0	771	TYR	Sidechain
2	0	787	ARG	Sidechain
2	0	792	THR	Peptide
2	0	842	TYR	Sidechain
2	0	856	TYR	Sidechain
2	0	973	ARG	Sidechain

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Mol	Chain	Res	Type	Group
3	1	1042	ARG	Sidechain
3	1	1044	TYR	Sidechain
3	1	1060	TYR	Sidechain
3	1	1068	ARG	Sidechain
3	1	1079	PHE	Sidechain
3	1	1083	TYR	Sidechain
3	1	1100	PHE	Sidechain
3	1	1101	TYR	Sidechain
3	1	1136	ARG	Sidechain
3	1	117	TYR	Sidechain
3	1	1178	ARG	Sidechain
3	1	1188	ARG	Sidechain
3	1	1277	ARG	Sidechain
3	1	1287	PHE	Sidechain
3	1	1323	TYR	Sidechain
3	1	1351	TYR	Sidechain
3	1	166	PHE	Sidechain
3	1	240	ARG	Sidechain
3	1	242	HIS	Sidechain
3	1	266	TYR	Sidechain
3	1	288	TYR	Sidechain
3	1	351	ARG	Sidechain
3	1	355	HIS	Sidechain
3	1	404	PHE	Sidechain
3	1	431	ARG	Sidechain
3	1	512	ARG	Sidechain
3	1	554	TYR	Sidechain
3	1	635	TYR	Sidechain
3	1	666	SER	Peptide
3	1	710	TYR	Sidechain
3	1	773	PHE	Sidechain
3	1	816	TYR	Sidechain
3	1	836	TYR	Sidechain
3	1	850	HIS	Sidechain
3	1	883	TYR	Sidechain
3	1	904	TYR	Sidechain
3	1	986	ARG	Sidechain
1	7	83	UNK	Mainchain
1	8	83	UNK	Mainchain
4	A	658	TYR	Sidechain
5	B	373	ARG	Sidechain
5	B	397	ARG	Sidechain

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Mol	Chain	Res	Type	Group
5	B	411	ARG	Sidechain
6	C	314	TYR	Sidechain
6	C	389	ARG	Sidechain
4	D	800	HIS	Sidechain
5	E	313	TYR	Sidechain
5	E	373	ARG	Sidechain
5	E	522	TYR	Sidechain
6	F	325	TYR	Sidechain
4	G	658	TYR	Sidechain
5	H	373	ARG	Sidechain
5	H	397	ARG	Sidechain
5	H	411	ARG	Sidechain
6	I	314	TYR	Sidechain
6	I	389	ARG	Sidechain
4	J	800	HIS	Sidechain
5	K	313	TYR	Sidechain
5	K	522	TYR	Sidechain
6	L	325	TYR	Sidechain
7	M	1005	PHE	Sidechain
7	M	1013	TYR	Sidechain
7	M	1041	PHE	Sidechain
7	M	1074	ARG	Sidechain
7	M	1154	ARG	Sidechain
7	M	1156	TYR	Sidechain
7	M	1183	TYR	Sidechain
7	M	12	TYR	Sidechain
7	M	1231	TYR	Sidechain
7	M	1286	PHE	Sidechain
7	M	1292	ARG	Sidechain
7	M	1342	TYR	Sidechain
7	M	1349	PHE	Sidechain
7	M	1368	ARG	Sidechain
7	M	1412	TYR	Sidechain
7	M	150	PHE	Sidechain
7	M	1635	ARG	Sidechain
7	M	171	TYR	Sidechain
7	M	185	PHE	Sidechain
7	M	238	PHE	Sidechain
7	M	284	TYR	Sidechain
7	M	296	ARG	Sidechain
7	M	359	GLN	Peptide
7	M	412	ASN	Peptide

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Mol	Chain	Res	Type	Group
7	M	480	ARG	Sidechain
7	M	482	PHE	Sidechain
7	M	486	TYR	Sidechain
7	M	495	TYR	Sidechain
7	M	544	TYR	Sidechain
7	M	545	HIS	Sidechain
7	M	546	TYR	Sidechain
7	M	654	PHE	Sidechain
7	M	674	PHE	Sidechain
7	M	677	SER	Peptide
7	M	680	PHE	Sidechain
7	M	692	TYR	Sidechain
7	M	693	ARG	Sidechain
7	M	703	TYR	Sidechain
7	M	752	TYR	Sidechain
7	M	793	TYR	Sidechain
7	M	918	PHE	Sidechain
7	M	929	TYR	Sidechain
7	M	951	ARG	Sidechain
7	M	982	PHE	Sidechain
8	N	1072	TYR	Sidechain
8	N	1111	HIS	Sidechain
8	N	1263	TYR	Sidechain
8	N	1313	ARG	Sidechain
8	N	1349	TYR	Sidechain
8	N	1534	TYR	Sidechain
8	N	1597	ARG	Sidechain
8	N	1633	ARG	Sidechain
8	N	1642	ARG	Sidechain
8	N	242	TYR	Sidechain
8	N	244	PHE	Sidechain
8	N	330	TYR	Sidechain
8	N	375	TYR	Sidechain
8	N	421	PHE	Sidechain
8	N	460	ILE	Peptide
8	N	475	TYR	Sidechain
8	N	617	TYR	Sidechain
8	N	648	ARG	Sidechain
8	N	660	PHE	Sidechain
8	N	685	TYR	Sidechain
8	N	844	TYR	Sidechain
8	N	862	ARG	Sidechain

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Mol	Chain	Res	Type	Group
8	N	88	PHE	Sidechain
8	N	888	TYR	Sidechain
8	N	906	TYR	Sidechain
8	N	916	TYR	Sidechain
7	O	1005	PHE	Sidechain
7	O	1013	TYR	Sidechain
7	O	1041	PHE	Sidechain
7	O	1154	ARG	Sidechain
7	O	1156	TYR	Sidechain
7	O	1183	TYR	Sidechain
7	O	12	TYR	Sidechain
7	O	1231	TYR	Sidechain
7	O	1286	PHE	Sidechain
7	O	1292	ARG	Sidechain
7	O	1342	TYR	Sidechain
7	O	1349	PHE	Sidechain
7	O	1368	ARG	Sidechain
7	O	1412	TYR	Sidechain
7	O	150	PHE	Sidechain
7	O	1513	TYR	Sidechain
7	O	1635	ARG	Sidechain
7	O	171	TYR	Sidechain
7	O	185	PHE	Sidechain
7	O	238	PHE	Sidechain
7	O	284	TYR	Sidechain
7	O	296	ARG	Sidechain
7	O	359	GLN	Peptide
7	O	412	ASN	Peptide
7	O	480	ARG	Sidechain
7	O	482	PHE	Sidechain
7	O	486	TYR	Sidechain
7	O	495	TYR	Sidechain
7	O	510	PHE	Sidechain
7	O	544	TYR	Sidechain
7	O	545	HIS	Sidechain
7	O	546	TYR	Sidechain
7	O	654	PHE	Sidechain
7	O	674	PHE	Sidechain
7	O	677	SER	Peptide
7	O	680	PHE	Sidechain
7	O	692	TYR	Sidechain
7	O	693	ARG	Sidechain

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Mol	Chain	Res	Type	Group
7	O	703	TYR	Sidechain
7	O	752	TYR	Sidechain
7	O	793	TYR	Sidechain
7	O	918	PHE	Sidechain
7	O	929	TYR	Sidechain
7	O	951	ARG	Sidechain
7	O	982	PHE	Sidechain
8	P	1072	TYR	Sidechain
8	P	1111	HIS	Sidechain
8	P	1263	TYR	Sidechain
8	P	1313	ARG	Sidechain
8	P	1349	TYR	Sidechain
8	P	1534	TYR	Sidechain
8	P	1597	ARG	Sidechain
8	P	1633	ARG	Sidechain
8	P	1642	ARG	Sidechain
8	P	242	TYR	Sidechain
8	P	244	PHE	Sidechain
8	P	330	TYR	Sidechain
8	P	375	TYR	Sidechain
8	P	421	PHE	Sidechain
8	P	460	ILE	Peptide
8	P	475	TYR	Sidechain
8	P	617	TYR	Sidechain
8	P	648	ARG	Sidechain
8	P	660	PHE	Sidechain
8	P	685	TYR	Sidechain
8	P	72	ARG	Sidechain
8	P	844	TYR	Sidechain
8	P	862	ARG	Sidechain
8	P	88	PHE	Sidechain
8	P	888	TYR	Sidechain
8	P	906	TYR	Sidechain
8	P	916	TYR	Sidechain
9	Q	199	ARG	Sidechain
9	Q	215	TYR	Sidechain
9	Q	339	TYR	Sidechain
9	Q	371	PHE	Sidechain
9	Q	374	TYR	Sidechain
9	Q	454	TYR	Sidechain
9	Q	469	TYR	Sidechain
9	Q	478	TYR	Sidechain

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Mol	Chain	Res	Type	Group
9	Q	556	TYR	Sidechain
9	Q	650	TYR	Sidechain
9	Q	707	HIS	Sidechain
9	Q	727	TYR	Sidechain
9	Q	728	PHE	Sidechain
9	Q	754	ARG	Sidechain
9	Q	794	TYR	Sidechain
9	Q	816	TYR	Sidechain
9	R	217	ARG	Sidechain
9	R	238	PHE	Sidechain
9	R	249	ARG	Sidechain
9	R	290	TYR	Sidechain
9	R	394	TYR	Sidechain
9	R	412	TYR	Sidechain
9	R	456	ARG	Sidechain
9	R	473	ARG	Sidechain
9	R	494	TYR	Sidechain
9	R	496	TYR	Sidechain
9	R	523	ARG	Sidechain
9	R	546	ARG	Sidechain
9	R	547	TYR	Sidechain
9	R	577	ARG	Sidechain
9	R	614	ARG	Sidechain
9	R	727	TYR	Sidechain
9	R	811	ARG	Sidechain
9	S	199	ARG	Sidechain
9	S	215	TYR	Sidechain
9	S	339	TYR	Sidechain
9	S	370	TYR	Sidechain
9	S	371	PHE	Sidechain
9	S	374	TYR	Sidechain
9	S	454	TYR	Sidechain
9	S	469	TYR	Sidechain
9	S	478	TYR	Sidechain
9	S	556	TYR	Sidechain
9	S	650	TYR	Sidechain
9	S	707	HIS	Sidechain
9	S	727	TYR	Sidechain
9	S	728	PHE	Sidechain
9	S	754	ARG	Sidechain
9	S	794	TYR	Sidechain
9	S	816	TYR	Sidechain

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Mol	Chain	Res	Type	Group
9	T	217	ARG	Sidechain
9	T	238	PHE	Sidechain
9	T	249	ARG	Sidechain
9	T	290	TYR	Sidechain
9	T	394	TYR	Sidechain
9	T	412	TYR	Sidechain
9	T	456	ARG	Sidechain
9	T	473	ARG	Sidechain
9	T	494	TYR	Sidechain
9	T	496	TYR	Sidechain
9	T	523	ARG	Sidechain
9	T	546	ARG	Sidechain
9	T	547	TYR	Sidechain
9	T	577	ARG	Sidechain
9	T	614	ARG	Sidechain
9	T	727	TYR	Sidechain
9	T	811	ARG	Sidechain
10	U	280	PHE	Sidechain
10	U	318	TYR	Sidechain
11	V	377	PHE	Sidechain
10	W	318	TYR	Sidechain
11	X	377	PHE	Sidechain
2	Y	1011	ARG	Sidechain
2	Y	1012	ARG	Sidechain
2	Y	1019	ARG	Sidechain
2	Y	1059	TYR	Sidechain
2	Y	107	TYR	Sidechain
2	Y	1146	TYR	Sidechain
2	Y	1219	ARG	Sidechain
2	Y	1235	PHE	Sidechain
2	Y	1242	PHE	Sidechain
2	Y	127	TYR	Sidechain
2	Y	1284	ARG	Sidechain
2	Y	1428	TYR	Sidechain
2	Y	1460	ARG	Sidechain
2	Y	154	PHE	Sidechain
2	Y	181	ARG	Sidechain
2	Y	313	CYS	Peptide
2	Y	380	TYR	Sidechain
2	Y	397	TYR	Sidechain
2	Y	408	ARG	Sidechain
2	Y	417	TYR	Sidechain

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Mol	Chain	Res	Type	Group
2	Y	447	TYR	Sidechain
2	Y	454	ARG	Sidechain
2	Y	461	ARG	Sidechain
2	Y	491	ARG	Sidechain
2	Y	509	PHE	Sidechain
2	Y	538	SER	Peptide
2	Y	583	TYR	Sidechain
2	Y	592	TYR	Sidechain
2	Y	705	MET	Peptide
2	Y	771	TYR	Sidechain
2	Y	787	ARG	Sidechain
2	Y	792	THR	Peptide
2	Y	842	TYR	Sidechain
2	Y	856	TYR	Sidechain
2	Y	973	ARG	Sidechain
3	Z	1042	ARG	Sidechain
3	Z	1044	TYR	Sidechain
3	Z	1060	TYR	Sidechain
3	Z	1068	ARG	Sidechain
3	Z	1079	PHE	Sidechain
3	Z	1083	TYR	Sidechain
3	Z	1100	PHE	Sidechain
3	Z	1101	TYR	Sidechain
3	Z	1136	ARG	Sidechain
3	Z	117	TYR	Sidechain
3	Z	1178	ARG	Sidechain
3	Z	1188	ARG	Sidechain
3	Z	1277	ARG	Sidechain
3	Z	1287	PHE	Sidechain
3	Z	1323	TYR	Sidechain
3	Z	1351	TYR	Sidechain
3	Z	166	PHE	Sidechain
3	Z	240	ARG	Sidechain
3	Z	242	HIS	Sidechain
3	Z	266	TYR	Sidechain
3	Z	288	TYR	Sidechain
3	Z	351	ARG	Sidechain
3	Z	355	HIS	Sidechain
3	Z	404	PHE	Sidechain
3	Z	431	ARG	Sidechain
3	Z	512	ARG	Sidechain
3	Z	554	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	Z	635	TYR	Sidechain
3	Z	666	SER	Peptide
3	Z	710	TYR	Sidechain
3	Z	773	PHE	Sidechain
3	Z	816	TYR	Sidechain
3	Z	836	TYR	Sidechain
3	Z	850	HIS	Sidechain
3	Z	883	TYR	Sidechain
3	Z	904	TYR	Sidechain
3	Z	986	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	3	80	0	18	18	0
1	4	80	0	18	17	0
1	7	85	0	20	34	0
1	8	85	0	20	33	0
1	a	40	0	12	0	0
1	b	175	0	37	0	0
1	c	85	0	18	0	0
1	d	110	0	25	0	0
1	e	185	0	39	0	0
1	f	40	0	12	0	0
1	g	175	0	37	0	0
1	h	85	0	21	0	0
1	i	110	0	24	0	0
1	j	185	0	39	0	0
1	k	65	0	19	0	0
1	l	65	0	19	0	0
1	m	125	0	28	0	0
1	n	125	0	28	0	0
2	0	10015	0	10047	88	0
2	Y	10015	0	10047	69	0
3	1	9319	0	9286	182	0
3	Z	9319	0	9286	161	0
4	A	1315	0	1275	17	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
4	D	1345	0	1287	44	0
4	G	1315	0	1275	18	0
4	J	1347	0	1292	31	0
5	B	1771	0	1832	72	0
5	E	1771	0	1832	112	0
5	H	1771	0	1832	30	0
5	K	1771	0	1832	129	0
6	C	1347	0	1376	14	0
6	F	1381	0	1391	37	0
6	I	1347	0	1376	30	0
6	L	1381	0	1391	59	0
7	M	13334	0	13379	337	0
7	O	13334	0	13379	359	0
8	N	13181	0	13422	324	0
8	P	13190	0	13436	262	0
9	Q	5961	0	5621	82	0
9	R	5983	0	5599	194	0
9	S	5961	0	5621	87	0
9	T	5988	0	5600	195	0
10	U	745	0	752	74	0
10	W	745	0	752	89	0
11	V	710	0	692	132	0
11	X	710	0	692	165	0
All	All	138272	0	136036	2816	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 11.

All (2816) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:617:TYR:CD1	8:N:617:TYR:CE1	1.75	1.71
8:P:617:TYR:CD1	8:P:617:TYR:CE1	1.76	1.70
8:P:617:TYR:CE1	8:P:617:TYR:CZ	1.79	1.66
8:N:617:TYR:CE1	8:N:617:TYR:CZ	1.79	1.66
8:P:617:TYR:CD1	8:P:617:TYR:CG	1.83	1.65
8:N:617:TYR:CD1	8:N:617:TYR:CG	1.83	1.64
7:O:1189:MET:CB	8:P:248:GLN:HG2	1.28	1.63
8:P:617:TYR:CG	8:P:617:TYR:CD2	1.83	1.63
7:M:1189:MET:CB	8:N:248:GLN:HG2	1.28	1.63
8:N:617:TYR:CG	8:N:617:TYR:CD2	1.83	1.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:617:TYR:CZ	8:P:617:TYR:CE2	1.80	1.62
8:N:617:TYR:CZ	8:N:617:TYR:CE2	1.80	1.61
7:O:1382:TYR:CD2	8:P:748:HIS:CE1	1.82	1.61
4:A:796:ILE:HG22	9:Q:24:GLU:CB	1.11	1.57
7:O:1386:LYS:CG	8:P:688:THR:CG2	1.78	1.57
7:M:1386:LYS:CG	8:N:688:THR:CG2	1.78	1.56
10:W:276:ILE:HG13	10:W:283:ILE:CD1	1.35	1.56
7:M:1389:ILE:CG2	8:N:687:LYS:HG2	1.18	1.55
8:N:216:TYR:HA	8:N:220:PHE:CD1	1.32	1.55
7:M:1389:ILE:HG21	8:N:687:LYS:CG	1.32	1.55
5:B:323:LEU:CD2	5:B:338:ALA:CB	1.83	1.54
5:K:517:GLN:HE22	9:T:23:ASN:CB	0.92	1.52
5:K:316:VAL:CG1	5:K:348:ILE:CD1	1.84	1.51
3:1:494:ASN:HB2	3:1:512:ARG:CB	1.37	1.51
7:M:1386:LYS:HG2	8:N:688:THR:CG2	1.06	1.51
7:O:1386:LYS:HG2	8:P:688:THR:CG2	1.06	1.51
10:U:321:GLU:HB2	11:V:293:HIS:CD2	1.45	1.50
7:M:384:MET:HG2	7:M:766:GLN:NE2	1.22	1.50
7:O:384:MET:HG2	7:O:766:GLN:NE2	1.21	1.50
7:O:1671:VAL:HG11	9:T:166:LYS:CB	1.03	1.50
10:W:321:GLU:HB2	11:X:293:HIS:CD2	1.45	1.50
7:O:1382:TYR:CD2	8:P:748:HIS:HE1	1.20	1.49
11:X:289:SER:CB	11:X:294:ILE:CD1	1.81	1.49
7:M:1189:MET:HG2	8:N:248:GLN:CB	1.39	1.49
3:Z:1213:LEU:CD1	3:Z:1215:TYR:CG	1.96	1.48
5:K:517:GLN:NE2	9:T:23:ASN:CB	1.73	1.48
7:O:1189:MET:HG2	8:P:248:GLN:CB	1.39	1.48
11:V:355:TRP:CD1	11:V:400:ILE:HB	1.47	1.47
11:X:355:TRP:CD1	11:X:400:ILE:HB	1.47	1.47
4:A:796:ILE:CG2	9:Q:24:GLU:CB	1.91	1.46
7:M:1191:SER:CB	8:N:757:LYS:HA	1.46	1.46
7:O:1191:SER:CB	8:P:757:LYS:HA	1.46	1.46
11:X:289:SER:HB3	11:X:294:ILE:CD1	1.32	1.46
9:T:436:LEU:HD12	9:T:462:PHE:CZ	1.51	1.45
9:R:436:LEU:HD12	9:R:462:PHE:CZ	1.51	1.45
5:E:314:ASN:HD21	5:E:348:ILE:CB	1.26	1.44
5:B:323:LEU:HD11	5:B:339:MET:N	1.16	1.44
11:V:355:TRP:NE1	11:V:400:ILE:HB	1.32	1.44
11:X:355:TRP:NE1	11:X:400:ILE:HB	1.33	1.43
7:O:1381:LEU:HD11	7:O:1385:PHE:CZ	1.53	1.43
3:Z:1213:LEU:HD13	3:Z:1215:TYR:CD1	1.53	1.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:795:LYS:NZ	9:R:21:LYS:CB	1.83	1.41
1:3:2:UNK:H	5:E:316:VAL:CB	1.34	1.41
11:V:273:VAL:HB	11:V:356:VAL:CG2	1.51	1.41
11:X:273:VAL:HB	11:X:356:VAL:CG2	1.51	1.41
3:Z:1213:LEU:HD11	3:Z:1215:TYR:CG	1.55	1.40
1:4:5:UNK:CB	5:K:315:LYS:HD3	1.50	1.40
5:B:320:GLU:OE1	5:B:348:ILE:CD1	1.70	1.39
7:O:1671:VAL:CG1	9:T:166:LYS:CB	1.99	1.39
11:X:289:SER:CA	11:X:294:ILE:HD13	1.52	1.39
7:M:1559:LEU:CD2	7:O:1642:LYS:HE3	1.52	1.39
3:Z:1213:LEU:HD22	3:Z:1215:TYR:CE2	1.57	1.38
5:B:323:LEU:CD2	5:B:338:ALA:HB1	1.41	1.38
9:S:594:GLY:CA	10:W:324:LYS:HE2	1.51	1.38
11:X:289:SER:CB	11:X:294:ILE:HD11	1.42	1.38
5:B:323:LEU:HD21	5:B:338:ALA:C	1.43	1.38
9:Q:594:GLY:CA	10:U:324:LYS:HE2	1.51	1.38
7:M:1386:LYS:CG	8:N:688:THR:HG23	1.42	1.37
7:O:1386:LYS:CG	8:P:688:THR:HG23	1.42	1.37
3:Z:1213:LEU:CD2	3:Z:1215:TYR:CE2	2.08	1.36
5:B:323:LEU:CD1	5:B:339:MET:HA	1.51	1.36
1:3:2:UNK:N	5:E:316:VAL:HG12	1.34	1.36
7:M:1642:LYS:HE3	7:O:1559:LEU:CD2	1.55	1.36
5:H:413:LEU:HB2	6:I:373:PHE:CE2	1.58	1.36
5:E:314:ASN:ND2	5:E:348:ILE:HB	1.08	1.35
11:V:273:VAL:CB	11:V:356:VAL:HG23	1.57	1.35
11:X:273:VAL:CB	11:X:356:VAL:HG23	1.57	1.34
7:M:1382:TYR:CG	8:N:748:HIS:HE1	1.46	1.34
1:3:2:UNK:H	5:E:316:VAL:CG1	1.40	1.34
3:1:494:ASN:CB	3:1:512:ARG:CB	2.04	1.34
8:P:761:PHE:CE1	8:P:764:LYS:HD3	1.62	1.34
8:N:761:PHE:CE1	8:N:764:LYS:HD3	1.62	1.33
5:H:413:LEU:CB	6:I:373:PHE:HE2	1.43	1.32
5:H:413:LEU:CB	6:I:373:PHE:CE2	2.10	1.31
1:3:2:UNK:N	5:E:316:VAL:CG1	1.91	1.31
1:7:72:UNK:CB	9:R:426:PRO:HB3	1.59	1.30
7:M:1382:TYR:CD2	8:N:748:HIS:CE1	2.19	1.30
10:U:262:ILE:HG23	10:U:265:SER:OG	1.21	1.29
10:U:266:ILE:CG1	10:U:336:ASN:HD22	1.44	1.29
9:T:436:LEU:CD1	9:T:462:PHE:HZ	1.42	1.29
9:R:436:LEU:CD1	9:R:462:PHE:HZ	1.43	1.29
7:M:1382:TYR:CE2	8:N:748:HIS:NE2	1.97	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:436:LEU:CD1	9:R:462:PHE:CZ	2.13	1.28
5:H:413:LEU:HB2	6:I:373:PHE:CZ	1.68	1.28
9:T:436:LEU:CD1	9:T:462:PHE:CZ	2.12	1.28
7:M:1386:LYS:NZ	8:N:683:ASP:OD2	1.63	1.28
5:K:456:THR:O	5:K:460:TRP:CD1	1.87	1.28
5:B:323:LEU:HD21	5:B:338:ALA:CA	1.62	1.28
5:E:456:THR:O	5:E:460:TRP:CD1	1.87	1.28
1:8:72:UNK:CB	9:T:426:PRO:HB3	1.63	1.27
7:O:1386:LYS:NZ	8:P:683:ASP:OD2	1.63	1.27
3:1:494:ASN:CB	3:1:512:ARG:HB2	1.64	1.27
10:W:304:LYS:HB3	11:X:270:ALA:O	1.32	1.27
5:B:323:LEU:CD1	5:B:339:MET:CA	2.11	1.27
10:U:268:LEU:CA	10:U:283:ILE:HD11	0.80	1.27
7:M:1561:LEU:C	7:M:1580:VAL:HG11	1.52	1.27
4:J:806:SER:HB3	9:T:35:ALA:CB	1.65	1.27
7:O:1189:MET:CG	8:P:248:GLN:HG2	1.61	1.27
7:M:1189:MET:CG	8:N:248:GLN:HG2	1.61	1.27
10:U:268:LEU:HA	10:U:283:ILE:CD1	0.79	1.27
7:O:1561:LEU:C	7:O:1580:VAL:HG11	1.52	1.26
1:7:76:UNK:CB	9:R:429:THR:CB	2.13	1.26
1:8:76:UNK:CB	9:T:429:THR:CB	2.13	1.26
7:M:1561:LEU:N	7:M:1580:VAL:HG21	1.47	1.25
8:N:64:SER:HB3	8:N:73:SER:OG	1.31	1.25
10:U:262:ILE:CG2	10:U:265:SER:OG	1.83	1.25
1:7:80:UNK:CB	9:R:431:SER:O	1.83	1.25
1:8:80:UNK:CB	9:T:431:SER:O	1.84	1.25
7:O:1561:LEU:N	7:O:1580:VAL:HG21	1.47	1.25
8:P:1357:CYS:SG	9:T:453:VAL:HG11	1.77	1.24
5:B:323:LEU:HD11	5:B:339:MET:CA	1.66	1.24
7:M:1559:LEU:HD21	7:O:1642:LYS:CE	1.66	1.24
8:N:1357:CYS:SG	9:R:453:VAL:HG11	1.77	1.24
8:P:288:LEU:HD11	8:P:328:ILE:CG2	1.66	1.24
8:N:288:LEU:HD11	8:N:328:ILE:CG2	1.66	1.24
9:T:675:VAL:CG2	9:T:728:PHE:CE2	2.19	1.23
9:R:675:VAL:CG2	9:R:728:PHE:CE2	2.19	1.23
8:P:461:CYS:O	8:P:556:LEU:HD12	1.24	1.23
7:O:1408:LEU:O	7:O:1412:TYR:HD2	1.17	1.23
7:M:1408:LEU:O	7:M:1412:TYR:HD2	1.17	1.23
3:1:1177:VAL:CG2	3:1:1215:TYR:CZ	2.20	1.23
7:M:1189:MET:HG2	8:N:248:GLN:CG	1.67	1.22
7:O:1189:MET:HG2	8:P:248:GLN:CG	1.67	1.22

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1642:LYS:CE	7:O:1559:LEU:HD21	1.68	1.22
1:4:2:UNK:H2	5:K:314:ASN:CG	1.43	1.22
8:N:276:ASN:O	8:N:381:VAL:HG11	1.37	1.22
7:O:1381:LEU:CD1	7:O:1385:PHE:CZ	2.23	1.21
8:P:276:ASN:O	8:P:381:VAL:HG11	1.37	1.21
7:O:1189:MET:HB3	8:P:249:ASP:N	1.56	1.21
7:M:1189:MET:HB3	8:N:249:ASP:N	1.56	1.21
4:D:796:ILE:CD1	5:E:513:LEU:HD21	1.71	1.20
8:P:273:LEU:O	8:P:284:ILE:O	1.59	1.20
8:N:273:LEU:O	8:N:284:ILE:O	1.59	1.20
7:M:1191:SER:HB3	8:N:757:LYS:CA	1.71	1.20
5:K:316:VAL:CG1	5:K:348:ILE:HD11	1.55	1.20
7:O:341:PHE:CZ	7:O:652:ALA:HA	1.76	1.20
10:W:276:ILE:CG1	10:W:283:ILE:CD1	2.17	1.20
11:X:273:VAL:CB	11:X:356:VAL:CG2	2.14	1.20
7:M:341:PHE:CZ	7:M:652:ALA:HA	1.77	1.20
7:O:1191:SER:HB3	8:P:757:LYS:CA	1.72	1.20
7:M:1189:MET:CB	8:N:249:ASP:N	2.06	1.19
11:V:273:VAL:CB	11:V:356:VAL:CG2	2.14	1.19
7:O:1189:MET:CB	8:P:249:ASP:N	2.06	1.19
4:J:806:SER:CB	9:T:35:ALA:HB2	1.73	1.19
1:7:80:UNK:HA	9:R:430:LEU:O	1.38	1.19
3:Z:1191:LEU:HD13	3:Z:1215:TYR:OH	1.38	1.19
7:M:1189:MET:H	8:N:248:GLN:CG	1.53	1.19
7:O:1189:MET:H	8:P:248:GLN:CG	1.53	1.19
7:O:1382:TYR:OH	8:P:744:LEU:HD23	1.42	1.19
1:8:80:UNK:HA	9:T:430:LEU:O	1.38	1.19
6:L:350:PHE:CE1	6:L:373:PHE:CE1	2.30	1.19
10:W:266:ILE:HG12	10:W:336:ASN:OD1	1.39	1.19
7:M:1189:MET:CG	8:N:248:GLN:CG	2.20	1.18
5:K:316:VAL:CG1	5:K:348:ILE:HD12	1.52	1.18
7:O:1189:MET:CG	8:P:248:GLN:CG	2.20	1.18
3:1:492:TYR:O	3:1:511:VAL:HG13	1.00	1.18
11:X:289:SER:CA	11:X:294:ILE:CD1	2.13	1.18
5:B:323:LEU:HB2	5:B:342:LYS:NZ	1.57	1.17
4:G:810:ASN:HB2	9:S:35:ALA:CB	1.73	1.17
7:M:1389:ILE:HG13	8:N:686:GLY:O	1.42	1.17
5:B:320:GLU:OE1	5:B:348:ILE:HD13	1.22	1.17
4:D:795:LYS:HZ1	9:R:21:LYS:CB	1.44	1.17
4:D:796:ILE:HD13	5:E:513:LEU:CD2	1.75	1.17
7:O:1389:ILE:HG13	8:P:686:GLY:O	1.42	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1382:TYR:CG	8:N:748:HIS:CE1	2.33	1.17
7:O:990:ILE:HG13	7:O:995:VAL:CG1	1.73	1.17
7:O:1382:TYR:CZ	8:P:744:LEU:HD23	1.78	1.17
9:T:675:VAL:CG2	9:T:728:PHE:HE2	1.57	1.17
9:R:675:VAL:CG2	9:R:728:PHE:HE2	1.57	1.16
10:U:268:LEU:CD1	10:U:283:ILE:HG13	1.74	1.16
3:1:1191:LEU:CD1	3:1:1213:LEU:CD2	2.23	1.16
1:7:76:UNK:CB	9:R:429:THR:HB	1.74	1.16
8:N:275:LEU:HD11	8:N:382:PHE:CB	1.76	1.16
8:P:275:LEU:HD11	8:P:382:PHE:CB	1.76	1.16
1:8:76:UNK:CB	9:T:429:THR:HB	1.74	1.16
5:B:323:LEU:HD11	5:B:338:ALA:C	1.64	1.15
7:M:332:VAL:O	7:M:338:MET:O	1.64	1.15
3:1:494:ASN:HB2	3:1:512:ARG:CA	1.76	1.15
7:O:332:VAL:O	7:O:338:MET:O	1.64	1.15
6:L:354:LEU:HD21	6:L:369:LEU:HD11	1.25	1.15
5:E:517:GLN:HG3	9:R:24:GLU:CB	1.77	1.15
8:N:216:TYR:CA	8:N:220:PHE:CD1	2.29	1.15
5:K:316:VAL:HG12	5:K:348:ILE:CD1	1.75	1.15
7:O:384:MET:CG	7:O:766:GLN:NE2	2.08	1.15
7:M:384:MET:CG	7:M:766:GLN:NE2	2.08	1.15
7:M:1386:LYS:HG3	8:N:688:THR:HG23	1.19	1.15
3:Z:1173:LEU:HB2	3:Z:1218:ILE:HG21	1.22	1.14
8:N:613:GLU:CG	8:N:617:TYR:CD1	2.30	1.14
7:O:1386:LYS:HG3	8:P:688:THR:HG23	1.19	1.14
8:P:613:GLU:CG	8:P:617:TYR:CD1	2.30	1.14
10:W:321:GLU:CB	11:X:293:HIS:CD2	2.28	1.14
3:Z:1213:LEU:HD13	3:Z:1215:TYR:CG	1.70	1.14
3:Z:1213:LEU:HD11	3:Z:1215:TYR:CD2	1.83	1.14
7:M:1191:SER:CB	8:N:757:LYS:CA	2.24	1.14
3:1:1173:LEU:CD2	3:1:1218:ILE:CD1	2.24	1.14
7:O:1191:SER:CB	8:P:757:LYS:CA	2.24	1.14
9:T:278:LEU:HD22	9:T:433:GLU:HB3	1.19	1.14
1:7:76:UNK:CB	9:R:429:THR:CG2	2.26	1.14
5:B:323:LEU:CD1	5:B:339:MET:N	2.10	1.14
7:M:1189:MET:CB	8:N:248:GLN:CG	2.23	1.14
10:U:321:GLU:CB	11:V:293:HIS:CD2	2.28	1.14
11:V:355:TRP:CD1	11:V:400:ILE:CB	2.30	1.14
7:O:1189:MET:CB	8:P:248:GLN:CG	2.23	1.14
8:P:275:LEU:CD1	8:P:382:PHE:HB2	1.76	1.14
11:X:355:TRP:CD1	11:X:400:ILE:CB	2.30	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:275:LEU:CD1	8:N:382:PHE:HB2	1.77	1.14
9:R:278:LEU:HD22	9:R:433:GLU:HB3	1.19	1.14
1:7:76:UNK:CB	9:R:429:THR:HG21	1.76	1.13
2:0:516:LEU:HD21	2:0:598:PHE:CZ	1.81	1.13
8:N:613:GLU:CG	8:N:617:TYR:CD2	2.30	1.13
5:K:316:VAL:HG13	5:K:348:ILE:CD1	1.61	1.13
8:P:613:GLU:CG	8:P:617:TYR:CD2	2.30	1.13
1:8:76:UNK:CB	9:T:429:THR:CG2	2.26	1.13
7:M:1393:ASN:HD21	8:N:687:LYS:HE2	1.09	1.13
1:8:76:UNK:CB	9:T:429:THR:HG21	1.77	1.13
7:M:381:THR:HA	7:M:703:TYR:CB	1.79	1.12
3:1:492:TYR:O	3:1:511:VAL:CG1	1.96	1.12
6:L:434:THR:HA	6:L:438:ALA:HB2	1.21	1.13
7:O:381:THR:HA	7:O:703:TYR:CB	1.79	1.12
4:A:800:HIS:CE1	9:Q:27:GLU:CB	2.31	1.12
3:1:493:ILE:HG22	3:1:512:ARG:O	1.46	1.12
10:W:276:ILE:HG13	10:W:283:ILE:HD11	1.29	1.12
7:M:1336:ILE:HD13	7:M:1383:GLN:HG3	1.18	1.12
7:O:984:THR:O	7:O:988:SER:N	1.83	1.12
10:U:268:LEU:HD12	10:U:283:ILE:HG13	1.14	1.12
8:P:529:LEU:HD21	8:P:531:ILE:HD11	1.23	1.11
8:N:65:SER:OG	8:N:83:VAL:HG11	1.50	1.11
8:N:613:GLU:CG	8:N:617:TYR:CZ	2.33	1.11
2:0:516:LEU:CD2	2:0:535:VAL:HG11	1.80	1.11
3:1:1177:VAL:HG22	3:1:1215:TYR:CZ	1.82	1.11
7:O:1336:ILE:HD13	7:O:1383:GLN:HG3	1.18	1.11
8:P:613:GLU:CG	8:P:617:TYR:CZ	2.33	1.11
8:N:613:GLU:CG	8:N:617:TYR:CE1	2.32	1.11
7:O:381:THR:HA	7:O:703:TYR:HB3	1.22	1.11
4:J:669:LEU:HD21	5:K:369:VAL:HG12	1.33	1.11
8:P:613:GLU:CG	8:P:617:TYR:CE1	2.32	1.11
7:M:381:THR:HA	7:M:703:TYR:HB3	1.22	1.10
5:K:380:LEU:CD2	6:L:314:TYR:HE2	1.64	1.10
5:E:380:LEU:CD2	6:F:314:TYR:HE2	1.63	1.10
7:O:1189:MET:HB3	8:P:248:GLN:HG2	1.16	1.10
9:T:668:SER:HB3	9:T:673:PRO:HB2	1.20	1.10
5:E:517:GLN:HE21	9:R:24:GLU:CA	1.63	1.10
7:M:383:ASN:O	7:M:766:GLN:HB3	1.52	1.10
7:M:1189:MET:HB3	8:N:248:GLN:HG2	1.16	1.10
8:N:613:GLU:CG	8:N:617:TYR:CE2	2.35	1.10
8:N:741:LYS:O	8:N:744:LEU:HG	1.52	1.10

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:383:ASN:O	7:O:766:GLN:HB3	1.52	1.10
8:P:613:GLU:CG	8:P:617:TYR:CE2	2.35	1.10
10:U:266:ILE:HG13	10:U:336:ASN:HD22	0.94	1.10
11:X:273:VAL:HB	11:X:356:VAL:HG22	1.34	1.10
5:B:323:LEU:CD2	5:B:338:ALA:HB3	1.80	1.10
5:B:323:LEU:HD22	5:B:338:ALA:HB3	1.34	1.10
9:R:668:SER:HB3	9:R:673:PRO:HB2	1.20	1.10
10:U:268:LEU:HD12	10:U:283:ILE:CG1	1.82	1.10
11:V:273:VAL:HB	11:V:356:VAL:HG22	1.34	1.10
7:O:1386:LYS:CG	8:P:688:THR:HG22	1.59	1.10
7:M:1386:LYS:CG	8:N:688:THR:HG22	1.59	1.09
9:R:432:ILE:HD11	9:R:477:TYR:CG	1.88	1.09
3:1:493:ILE:HG22	3:1:494:ASN:N	1.60	1.09
9:T:432:ILE:HD11	9:T:477:TYR:CG	1.88	1.09
2:0:516:LEU:HD23	2:0:535:VAL:HG11	1.11	1.09
5:K:360:GLN:O	5:K:363:GLN:HG2	1.52	1.09
7:O:1392:ILE:HG12	7:O:1437:LEU:CD1	1.81	1.09
5:E:360:GLN:O	5:E:363:GLN:HG2	1.52	1.09
7:M:1393:ASN:HD21	8:N:687:LYS:CE	1.65	1.09
3:1:1183:ILE:HG13	3:1:1213:LEU:HD11	1.17	1.09
7:O:1189:MET:CA	8:P:249:ASP:OD1	2.00	1.09
7:O:1382:TYR:CE2	8:P:748:HIS:CE1	2.41	1.09
1:3:2:UNK:H	5:E:316:VAL:HB	1.11	1.09
7:M:1392:ILE:HG12	7:M:1437:LEU:CD1	1.81	1.09
7:M:1408:LEU:O	7:M:1412:TYR:CD2	2.03	1.09
9:Q:601:PRO:HB2	9:Q:605:GLU:HB2	1.24	1.09
4:A:803:ALA:HB1	9:Q:31:ASN:CB	1.82	1.09
6:F:455:GLU:OE1	6:F:456:ARG:HD2	1.52	1.09
11:V:273:VAL:CG2	11:V:356:VAL:HG23	1.81	1.09
2:0:1310:ASP:OD2	2:0:1311:PHE:CE2	2.05	1.09
11:X:273:VAL:CG2	11:X:356:VAL:HG23	1.81	1.09
7:O:1408:LEU:O	7:O:1412:TYR:CD2	2.03	1.08
3:Z:1210:ALA:HB2	3:Z:1218:ILE:CD1	1.83	1.08
9:Q:594:GLY:HA3	10:U:324:LYS:HE2	1.30	1.08
9:R:407:TYR:CE1	9:R:428:VAL:HG12	1.88	1.08
3:1:494:ASN:CB	3:1:512:ARG:HB3	1.83	1.08
9:T:407:TYR:CE1	9:T:428:VAL:HG12	1.88	1.08
5:K:318:GLU:HA	5:K:346:GLN:HA	1.09	1.08
9:Q:594:GLY:HA2	10:U:324:LYS:HE2	1.31	1.08
7:O:384:MET:HA	7:O:766:GLN:OE1	1.51	1.08
8:P:613:GLU:CG	8:P:617:TYR:CG	2.35	1.08

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:273:VAL:HG23	11:X:356:VAL:O	1.54	1.08
1:4:2:UNK:H	5:K:316:VAL:HB	1.17	1.08
7:M:1189:MET:CG	8:N:248:GLN:CB	2.32	1.08
8:N:613:GLU:CG	8:N:617:TYR:CG	2.35	1.08
11:V:273:VAL:HG23	11:V:356:VAL:O	1.53	1.08
7:O:1189:MET:CG	8:P:248:GLN:CB	2.32	1.08
7:O:1386:LYS:HG2	8:P:688:THR:HG21	1.27	1.08
7:M:384:MET:HA	7:M:766:GLN:OE1	1.51	1.07
7:M:1386:LYS:HG2	8:N:688:THR:HG21	1.28	1.07
3:1:1173:LEU:CD2	3:1:1218:ILE:HD11	1.84	1.07
5:K:317:ASN:HD22	5:K:348:ILE:HD13	1.19	1.07
3:1:917:GLU:HG3	3:1:918:MET:H	1.18	1.07
9:S:594:GLY:HA3	10:W:324:LYS:HE2	1.30	1.07
3:Z:917:GLU:HG3	3:Z:918:MET:H	1.17	1.07
3:Z:1210:ALA:HB2	3:Z:1218:ILE:HD12	1.26	1.07
3:Z:1213:LEU:CD1	3:Z:1215:TYR:CD2	2.35	1.07
9:S:594:GLY:HA2	10:W:324:LYS:HE2	1.31	1.07
5:B:320:GLU:OE1	5:B:348:ILE:HD11	1.55	1.07
7:M:1560:GLY:C	7:M:1580:VAL:HG21	1.74	1.07
7:O:1560:GLY:C	7:O:1580:VAL:HG21	1.74	1.07
10:W:271:ALA:HA	10:W:283:ILE:HG21	1.28	1.07
5:B:323:LEU:CB	5:B:342:LYS:HZ1	1.66	1.06
8:N:216:TYR:HA	8:N:220:PHE:CE1	1.89	1.06
3:1:1173:LEU:HD23	3:1:1218:ILE:CD1	1.84	1.06
3:1:1191:LEU:CD1	3:1:1213:LEU:HD22	1.80	1.06
7:O:1191:SER:HB2	8:P:757:LYS:HB3	1.38	1.06
10:W:321:GLU:CB	11:X:293:HIS:HD2	1.63	1.06
7:M:1191:SER:HB2	8:N:757:LYS:HB3	1.38	1.06
10:U:321:GLU:CB	11:V:293:HIS:HD2	1.63	1.06
8:N:761:PHE:HE2	8:N:765:PHE:CE2	1.73	1.06
7:O:1374:LYS:HE3	7:O:1418:SER:O	1.54	1.06
8:N:216:TYR:CA	8:N:220:PHE:HD1	1.68	1.05
11:V:274:PHE:HA	11:V:355:TRP:HA	1.32	1.05
8:P:761:PHE:HE2	8:P:765:PHE:CE2	1.73	1.05
11:X:298:PHE:HD1	11:X:299:GLN:HG3	1.20	1.05
3:Z:1215:TYR:HB2	3:Z:1218:ILE:HD11	1.38	1.05
8:N:761:PHE:CZ	8:N:765:PHE:CZ	2.43	1.05
2:0:516:LEU:HA	2:0:537:LYS:NZ	1.70	1.05
3:1:1177:VAL:HG21	3:1:1215:TYR:CZ	1.88	1.05
8:P:761:PHE:CZ	8:P:765:PHE:CZ	2.43	1.05
11:X:274:PHE:HA	11:X:355:TRP:HA	1.32	1.05

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:7:72:UNK:CB	9:R:426:PRO:CB	2.35	1.05
2:Y:1019:ARG:CB	9:R:246:ASN:HB2	1.86	1.05
8:P:227:ILE:HD13	8:P:255:GLU:HG2	1.06	1.05
10:U:268:LEU:HA	10:U:283:ILE:HD12	1.38	1.05
11:V:273:VAL:CB	11:V:356:VAL:O	2.05	1.05
2:0:1019:ARG:CB	9:T:246:ASN:HB2	1.86	1.05
3:1:1184:ASP:HB2	3:1:1187:TYR:HD2	1.14	1.05
11:X:273:VAL:CB	11:X:356:VAL:O	2.05	1.04
7:M:1382:TYR:CE2	8:N:748:HIS:CE1	2.41	1.04
3:1:1173:LEU:HB3	3:1:1218:ILE:HD13	1.35	1.04
7:O:1382:TYR:CG	8:P:748:HIS:HE1	1.75	1.04
1:3:4:UNK:CB	5:E:316:VAL:HG23	1.88	1.04
5:E:317:ASN:O	5:E:348:ILE:HD11	1.56	1.04
10:U:321:GLU:HB2	11:V:293:HIS:NE2	1.72	1.04
10:W:321:GLU:HB2	11:X:293:HIS:NE2	1.72	1.04
8:P:613:GLU:CD	8:P:617:TYR:CG	2.31	1.04
7:M:1562:ASP:OD2	9:T:173:LYS:CB	2.05	1.04
8:N:613:GLU:CD	8:N:617:TYR:CG	2.31	1.04
11:X:274:PHE:HB3	11:X:355:TRP:CD2	1.93	1.04
8:N:64:SER:CB	8:N:73:SER:OG	2.06	1.03
11:V:274:PHE:HB3	11:V:355:TRP:CD2	1.93	1.03
5:H:413:LEU:CA	6:I:373:PHE:HE2	1.68	1.03
3:Z:1215:TYR:HB2	3:Z:1218:ILE:CD1	1.87	1.03
4:A:709:ASN:ND2	4:D:631:SER:O	1.90	1.03
2:0:516:LEU:HD23	2:0:535:VAL:CG1	1.88	1.03
5:K:316:VAL:HG11	5:K:348:ILE:HD12	1.38	1.03
7:M:1191:SER:CB	8:N:757:LYS:CB	2.35	1.03
7:M:1386:LYS:HG2	8:N:688:THR:HG22	1.09	1.03
8:N:223:PHE:CE2	8:N:258:ILE:HG22	1.94	1.03
10:U:266:ILE:CG1	10:U:336:ASN:ND2	2.21	1.03
4:G:709:ASN:ND2	4:J:631:SER:O	1.90	1.03
7:O:1191:SER:CB	8:P:757:LYS:CB	2.35	1.03
10:W:276:ILE:HG13	10:W:283:ILE:HD12	1.34	1.03
5:B:323:LEU:HB3	5:B:335:TRP:HH2	1.18	1.03
7:M:341:PHE:CZ	7:M:652:ALA:CA	2.40	1.03
3:1:493:ILE:HD12	3:1:513:LYS:HD3	1.40	1.03
7:O:341:PHE:CZ	7:O:652:ALA:CA	2.40	1.03
5:E:314:ASN:OD1	5:E:348:ILE:HD12	1.59	1.02
5:K:317:ASN:ND2	5:K:348:ILE:CD1	2.22	1.02
10:U:268:LEU:HA	10:U:283:ILE:CG1	1.89	1.02
11:V:394:GLN:O	11:V:398:CYS:HA	1.59	1.02

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:493:ILE:CG2	3:1:512:ARG:O	2.07	1.02
3:1:1191:LEU:HD12	3:1:1213:LEU:HD22	1.39	1.02
7:O:1386:LYS:HG2	8:P:688:THR:HG22	1.09	1.02
11:X:394:GLN:O	11:X:398:CYS:HA	1.58	1.02
10:U:266:ILE:HG13	10:U:336:ASN:ND2	1.75	1.02
5:K:317:ASN:HB2	5:K:348:ILE:HG12	1.41	1.02
7:O:341:PHE:HZ	7:O:652:ALA:HA	1.10	1.02
1:3:2:UNK:N	5:E:316:VAL:CB	2.17	1.01
7:M:1189:MET:HG2	8:N:248:GLN:HB2	1.03	1.01
7:M:1192:VAL:HG12	7:M:1193:ARG:H	1.24	1.01
7:O:1189:MET:HG2	8:P:248:GLN:HB2	1.03	1.01
10:W:266:ILE:CG1	10:W:336:ASN:OD1	2.08	1.01
7:O:990:ILE:HG13	7:O:995:VAL:HG13	1.04	1.01
11:X:273:VAL:CG1	11:X:356:VAL:CG2	2.38	1.01
1:7:72:UNK:CA	9:R:426:PRO:HB3	1.88	1.01
5:B:323:LEU:HD12	5:B:339:MET:HA	1.04	1.01
8:N:227:ILE:HD11	8:N:258:ILE:HG21	1.42	1.01
11:V:273:VAL:CG1	11:V:356:VAL:CG2	2.38	1.01
11:V:275:GLY:N	11:V:354:SER:O	1.93	1.01
3:1:493:ILE:CG2	3:1:494:ASN:H	1.70	1.01
3:1:494:ASN:HB3	3:1:512:ARG:HB2	1.41	1.01
7:O:1192:VAL:HG12	7:O:1193:ARG:H	1.24	1.01
7:O:1385:PHE:CE1	7:O:1426:VAL:HG22	1.94	1.01
8:P:613:GLU:CD	8:P:617:TYR:CZ	2.34	1.01
4:D:807:LEU:HD21	5:E:524:ASN:OD1	1.60	1.01
5:E:456:THR:O	5:E:460:TRP:HD1	1.37	1.01
7:M:341:PHE:HZ	7:M:652:ALA:HA	1.10	1.01
8:N:613:GLU:CD	8:N:617:TYR:CZ	2.33	1.01
4:G:810:ASN:HB2	9:S:35:ALA:HB3	1.37	1.01
11:X:275:GLY:N	11:X:354:SER:O	1.93	1.01
3:Z:1213:LEU:HD13	3:Z:1215:TYR:CE1	1.95	1.01
7:M:1189:MET:CA	8:N:248:GLN:HG2	1.91	1.01
8:N:274:GLY:HA2	8:N:284:ILE:CB	1.89	1.01
8:N:613:GLU:CD	8:N:617:TYR:CE2	2.34	1.01
5:K:456:THR:O	5:K:460:TRP:HD1	1.37	1.01
7:O:1189:MET:CA	8:P:248:GLN:HG2	1.91	1.01
5:B:323:LEU:HD22	5:B:338:ALA:CB	1.84	1.00
5:K:316:VAL:HG12	5:K:348:ILE:HD12	1.33	1.00
8:P:274:GLY:HA2	8:P:284:ILE:CB	1.89	1.00
8:P:613:GLU:CD	8:P:617:TYR:CE2	2.35	1.00
5:B:323:LEU:HB2	5:B:342:LYS:HZ2	1.26	1.00

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:384:MET:CG	7:M:766:GLN:HE22	1.70	1.00
7:M:1189:MET:HB3	8:N:248:GLN:CG	1.86	1.00
5:H:322:ILE:HG22	5:H:335:TRP:HH2	1.26	1.00
8:P:613:GLU:HG3	8:P:617:TYR:CE1	1.92	1.00
5:K:317:ASN:HD22	5:K:348:ILE:CD1	1.74	1.00
7:O:384:MET:CG	7:O:766:GLN:HE22	1.70	1.00
2:Y:1020:ASN:HB2	9:R:247:GLY:HA3	1.42	1.00
2:0:1020:ASN:HB2	9:T:247:GLY:HA3	1.42	1.00
5:B:323:LEU:HD21	5:B:338:ALA:CB	1.66	1.00
8:N:613:GLU:HG3	8:N:617:TYR:CE1	1.92	1.00
7:M:1382:TYR:CD1	8:N:748:HIS:HE1	1.78	1.00
11:V:275:GLY:H	11:V:354:SER:HB2	1.27	1.00
7:O:1189:MET:HB3	8:P:248:GLN:CG	1.86	1.00
7:M:1389:ILE:CG1	8:N:686:GLY:O	2.09	0.99
3:1:1173:LEU:HD22	3:1:1218:ILE:CD1	1.89	0.99
8:P:613:GLU:CD	8:P:617:TYR:CD1	2.35	0.99
11:X:275:GLY:H	11:X:354:SER:HB2	1.27	0.99
8:N:613:GLU:CD	8:N:617:TYR:CD1	2.35	0.99
3:1:1177:VAL:HG22	3:1:1215:TYR:CE1	1.96	0.99
7:O:1191:SER:HB2	8:P:757:LYS:CB	1.92	0.99
7:O:1389:ILE:CG1	8:P:686:GLY:O	2.09	0.99
10:W:271:ALA:HA	10:W:283:ILE:CG2	1.90	0.99
7:M:1191:SER:HB2	8:N:757:LYS:CB	1.93	0.99
3:1:493:ILE:HG22	3:1:494:ASN:H	0.85	0.99
7:M:1189:MET:SD	8:N:248:GLN:O	2.20	0.99
6:L:434:THR:HA	6:L:438:ALA:CB	1.92	0.99
11:X:274:PHE:HB3	11:X:355:TRP:CE3	1.96	0.99
5:E:517:GLN:NE2	9:R:24:GLU:CB	2.25	0.99
7:O:1189:MET:SD	8:P:248:GLN:O	2.20	0.99
7:O:1392:ILE:CD1	7:O:1437:LEU:HD13	1.93	0.99
7:M:1392:ILE:CD1	7:M:1437:LEU:HD13	1.93	0.99
11:V:274:PHE:HB3	11:V:355:TRP:CE3	1.97	0.99
3:Z:1173:LEU:CB	3:Z:1218:ILE:HG21	1.93	0.99
8:P:761:PHE:HE1	8:P:764:LYS:HD3	0.98	0.99
7:O:1561:LEU:N	7:O:1580:VAL:CG2	2.26	0.99
9:T:429:THR:HG23	9:T:434:ASP:HB3	1.45	0.99
5:B:323:LEU:CB	5:B:335:TRP:HH2	1.75	0.98
7:M:1561:LEU:N	7:M:1580:VAL:CG2	2.26	0.98
7:M:1336:ILE:CD1	7:M:1383:GLN:HG3	1.91	0.98
8:N:761:PHE:CE2	8:N:765:PHE:CE2	2.50	0.98
9:R:429:THR:HG23	9:R:434:ASP:HB3	1.45	0.98

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1382:TYR:CD2	8:P:748:HIS:ND1	2.32	0.98
11:X:273:VAL:CG2	11:X:356:VAL:O	2.09	0.98
4:A:800:HIS:HE1	9:Q:27:GLU:CB	1.72	0.98
9:Q:589:LEU:HA	9:Q:603:VAL:HG21	1.44	0.98
11:V:273:VAL:CG2	11:V:356:VAL:O	2.09	0.98
7:O:1336:ILE:CD1	7:O:1383:GLN:HG3	1.91	0.98
9:T:675:VAL:HG22	9:T:728:PHE:HE2	1.26	0.98
3:Z:1213:LEU:HD21	3:Z:1215:TYR:CE2	1.92	0.98
8:N:761:PHE:HE1	8:N:764:LYS:HD3	0.98	0.98
7:O:1193:ARG:O	7:O:1195:PHE:N	1.97	0.98
7:M:1193:ARG:O	7:M:1195:PHE:N	1.97	0.98
9:R:675:VAL:HG22	9:R:728:PHE:HE2	1.26	0.98
8:P:761:PHE:CE2	8:P:765:PHE:CE2	2.50	0.98
1:4:5:UNK:CB	5:K:315:LYS:CD	2.41	0.98
3:Z:1173:LEU:HB3	3:Z:1218:ILE:HG22	1.45	0.98
8:N:613:GLU:CD	8:N:617:TYR:CE1	2.36	0.98
8:P:613:GLU:CD	8:P:617:TYR:CE1	2.36	0.98
1:4:2:UNK:H2	5:K:314:ASN:ND2	1.59	0.98
7:M:1561:LEU:C	7:M:1580:VAL:CG1	2.33	0.97
11:V:289:SER:HA	11:V:294:ILE:HD12	1.45	0.97
7:O:1561:LEU:C	7:O:1580:VAL:CG1	2.33	0.97
3:Z:1173:LEU:CD2	3:Z:1205:LEU:HD21	1.94	0.97
3:1:1183:ILE:CG1	3:1:1213:LEU:HD11	1.94	0.97
9:T:325:LEU:H	11:X:376:ILE:HG13	1.28	0.97
11:X:289:SER:HA	11:X:294:ILE:CD1	1.83	0.97
5:H:322:ILE:HG22	5:H:335:TRP:CH2	2.00	0.97
8:N:225:ARG:O	8:N:228:ASN:HB2	1.63	0.97
3:1:1191:LEU:CD1	3:1:1213:LEU:HD23	1.93	0.97
9:R:325:LEU:H	11:V:376:ILE:HG13	1.28	0.97
9:Q:601:PRO:HB2	9:Q:605:GLU:CB	1.95	0.97
9:S:593:ILE:CG2	9:S:600:ILE:HG13	1.93	0.97
3:Z:917:GLU:HB2	3:Z:957:LEU:HD13	1.42	0.96
7:M:1189:MET:N	8:N:248:GLN:CG	2.28	0.96
5:K:317:ASN:HB2	5:K:348:ILE:CG1	1.94	0.96
7:O:1189:MET:HA	8:P:249:ASP:OD1	1.64	0.96
11:X:294:ILE:HA	11:X:361:ASN:ND2	1.80	0.96
1:7:80:UNK:CB	9:R:431:SER:C	2.33	0.96
11:V:355:TRP:NE1	11:V:400:ILE:CB	2.26	0.96
1:4:5:UNK:CA	5:K:315:LYS:HD3	1.95	0.96
7:M:1189:MET:CG	8:N:248:GLN:HB2	1.95	0.96
7:M:1189:MET:HE3	8:N:252:TYR:HB3	1.46	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:0:518:GLU:HB2	2:0:536:ILE:O	1.65	0.96
7:O:1189:MET:N	8:P:248:GLN:CG	2.28	0.96
8:P:227:ILE:CD1	8:P:255:GLU:HG2	1.95	0.96
1:8:80:UNK:CB	9:T:431:SER:C	2.33	0.96
7:O:1189:MET:CG	8:P:248:GLN:HB2	1.95	0.96
7:M:1189:MET:H	8:N:248:GLN:HG3	1.28	0.96
9:T:339:TYR:CE1	9:T:342:ARG:NH1	2.33	0.96
11:X:355:TRP:NE1	11:X:400:ILE:CB	2.27	0.96
9:R:339:TYR:CE1	9:R:342:ARG:NH1	2.33	0.96
3:1:917:GLU:HB2	3:1:957:LEU:HD13	1.42	0.96
5:K:318:GLU:HA	5:K:346:GLN:CA	1.95	0.96
3:1:1184:ASP:HB2	3:1:1187:TYR:CD2	2.00	0.96
7:O:1382:TYR:CZ	8:P:744:LEU:CD2	2.48	0.96
1:4:2:UNK:N	5:K:316:VAL:HB	1.80	0.96
2:Y:1358:GLU:HB3	3:1:787:ALA:N	1.81	0.96
7:O:1189:MET:H	8:P:248:GLN:HG3	1.29	0.96
7:O:1382:TYR:HD2	8:P:748:HIS:ND1	1.62	0.96
9:T:672:GLN:HB3	9:T:673:PRO:HD3	1.47	0.96
7:O:1191:SER:CB	8:P:757:LYS:HB3	1.95	0.95
8:P:1357:CYS:SG	9:T:453:VAL:CG1	2.53	0.95
7:M:1191:SER:CB	8:N:757:LYS:HB3	1.95	0.95
7:M:1392:ILE:HG21	7:M:1437:LEU:N	1.81	0.95
8:N:1357:CYS:SG	9:R:453:VAL:CG1	2.54	0.95
9:R:672:GLN:HB3	9:R:673:PRO:HD3	1.47	0.95
2:0:516:LEU:HA	2:0:537:LYS:HZ2	1.31	0.95
3:1:492:TYR:C	3:1:511:VAL:HG13	1.86	0.95
7:O:1380:ARG:HH11	7:O:1415:ARG:HE	1.13	0.95
7:M:1392:ILE:HG21	7:M:1437:LEU:CA	1.96	0.95
5:K:317:ASN:ND2	5:K:348:ILE:HD11	1.79	0.95
7:O:1392:ILE:HG21	7:O:1437:LEU:N	1.81	0.95
3:Z:1173:LEU:CB	3:Z:1218:ILE:CG2	2.44	0.95
7:M:341:PHE:CZ	7:M:652:ALA:CB	2.48	0.95
3:1:493:ILE:CD1	3:1:513:LYS:HD3	1.95	0.95
7:O:341:PHE:CZ	7:O:652:ALA:CB	2.48	0.95
3:1:1199:VAL:O	3:1:1200:LEU:HD23	1.66	0.95
8:P:613:GLU:CD	8:P:617:TYR:CD2	2.40	0.95
7:M:384:MET:HG2	7:M:766:GLN:HE22	1.20	0.95
8:N:613:GLU:CD	8:N:617:TYR:CD2	2.40	0.95
7:O:1392:ILE:HG21	7:O:1437:LEU:CA	1.96	0.95
1:8:72:UNK:CA	9:T:426:PRO:HB3	1.97	0.95
3:1:918:MET:HA	3:1:918:MET:CE	1.96	0.95

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:304:LYS:CB	11:X:270:ALA:O	2.14	0.94
3:Z:918:MET:HA	3:Z:918:MET:CE	1.96	0.94
3:Z:1213:LEU:HD22	3:Z:1215:TYR:CZ	2.01	0.94
7:M:384:MET:CE	7:M:760:ILE:HG23	1.96	0.94
7:M:1389:ILE:CG2	8:N:687:LYS:CG	2.11	0.94
5:B:323:LEU:CD2	5:B:338:ALA:C	2.35	0.94
11:X:296:GLU:O	11:X:346:LYS:HG3	1.65	0.94
8:N:741:LYS:HA	8:N:744:LEU:CD2	1.96	0.94
10:W:276:ILE:CD1	10:W:283:ILE:HD13	1.96	0.94
7:O:384:MET:HG2	7:O:766:GLN:HE22	1.20	0.94
7:O:384:MET:CE	7:O:760:ILE:HG23	1.97	0.94
4:D:636:THR:O	4:D:637:LEU:HB2	1.65	0.94
7:M:1642:LYS:HE3	7:O:1559:LEU:HD21	0.95	0.94
7:O:990:ILE:CG1	7:O:995:VAL:HG13	1.98	0.94
8:N:74:THR:HG21	8:N:162:HIS:CE1	2.02	0.94
8:N:613:GLU:HG2	8:N:617:TYR:CG	2.01	0.94
9:T:312:LYS:HE2	9:T:430:LEU:HD22	1.48	0.94
4:A:803:ALA:CB	9:Q:31:ASN:CB	2.45	0.94
9:R:312:LYS:HE2	9:R:430:LEU:HD22	1.47	0.94
10:W:276:ILE:HG13	10:W:283:ILE:HD13	1.49	0.93
1:4:2:UNK:N	5:K:314:ASN:OD1	2.01	0.93
3:Z:1191:LEU:CD1	3:Z:1215:TYR:OH	2.16	0.93
8:N:223:PHE:HE2	8:N:258:ILE:HG22	1.31	0.93
5:K:380:LEU:CD2	6:L:314:TYR:CE2	2.51	0.93
8:P:613:GLU:HG2	8:P:617:TYR:CG	2.01	0.93
1:4:2:UNK:N	5:K:314:ASN:ND2	2.16	0.93
5:E:380:LEU:CD2	6:F:314:TYR:CE2	2.51	0.93
7:O:383:ASN:O	7:O:766:GLN:CB	2.16	0.93
7:O:1381:LEU:HD11	7:O:1385:PHE:HZ	1.17	0.93
7:M:383:ASN:O	7:M:766:GLN:CB	2.16	0.93
7:M:1683:ASP:O	9:R:171:HIS:CB	2.16	0.93
7:O:1385:PHE:HE1	7:O:1426:VAL:HG22	1.34	0.93
3:Z:1174:LEU:O	3:Z:1177:VAL:HG12	1.69	0.93
10:U:268:LEU:N	10:U:283:ILE:HD11	1.83	0.93
4:J:793:LEU:HB3	6:L:439:ILE:CG2	1.99	0.93
6:L:455:GLU:OE1	9:T:71:TYR:CB	2.17	0.93
11:X:298:PHE:CD1	11:X:299:GLN:HG3	2.04	0.93
1:8:70:UNK:CB	9:T:469:TYR:CE1	2.51	0.92
4:D:793:LEU:HB3	6:F:439:ILE:CG2	1.99	0.92
7:O:1189:MET:HE3	8:P:249:ASP:HA	1.50	0.92
9:T:672:GLN:HB3	9:T:673:PRO:CD	1.98	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1559:LEU:HD21	7:O:1642:LYS:HE3	0.93	0.92
3:1:1173:LEU:HD23	3:1:1218:ILE:HD11	1.38	0.92
7:O:1189:MET:HB3	8:P:249:ASP:H	1.25	0.92
7:O:1191:SER:HB2	8:P:757:LYS:HA	1.49	0.92
7:M:1189:MET:HB3	8:N:249:ASP:H	1.25	0.92
8:N:74:THR:HG21	8:N:162:HIS:HE1	1.32	0.92
3:Z:1213:LEU:CD1	3:Z:1215:TYR:CD1	2.31	0.92
7:O:1381:LEU:HD11	7:O:1385:PHE:CE2	2.04	0.92
9:S:21:LYS:O	9:S:25:LEU:CB	2.18	0.92
10:W:276:ILE:CG1	10:W:283:ILE:HD13	1.99	0.92
1:7:80:UNK:CA	9:R:430:LEU:O	2.16	0.92
1:8:80:UNK:CA	9:T:430:LEU:O	2.16	0.92
1:8:72:UNK:CB	9:T:426:PRO:CB	2.46	0.92
3:Z:1210:ALA:CB	3:Z:1218:ILE:CD1	2.47	0.92
7:M:1191:SER:HB2	8:N:757:LYS:HA	1.49	0.92
9:R:21:LYS:O	9:R:25:LEU:CB	2.18	0.92
9:R:672:GLN:HB3	9:R:673:PRO:CD	1.98	0.91
3:1:494:ASN:CG	3:1:512:ARG:O	2.08	0.91
5:B:323:LEU:CB	5:B:342:LYS:NZ	2.28	0.91
7:O:1189:MET:HB2	8:P:249:ASP:CA	1.99	0.91
7:O:1189:MET:HG3	7:O:1190:TYR:HD1	1.32	0.91
9:S:593:ILE:HG22	9:S:600:ILE:HG13	1.50	0.91
5:E:517:GLN:CG	9:R:24:GLU:CB	2.47	0.91
7:M:1189:MET:HB2	8:N:249:ASP:N	1.85	0.91
7:M:1189:MET:HB2	8:N:249:ASP:CA	1.99	0.91
7:M:1189:MET:HG3	7:M:1190:TYR:HD1	1.32	0.91
8:P:529:LEU:CD2	8:P:531:ILE:HD11	1.99	0.91
11:X:294:ILE:HA	11:X:361:ASN:HD21	1.34	0.91
5:E:517:GLN:NE2	9:R:24:GLU:CA	2.32	0.91
5:E:517:GLN:NE2	9:R:24:GLU:O	2.03	0.91
7:O:1189:MET:HB2	8:P:249:ASP:N	1.85	0.91
5:B:323:LEU:CB	5:B:335:TRP:CH2	2.54	0.91
10:U:268:LEU:C	10:U:283:ILE:HD11	1.91	0.91
5:E:380:LEU:HD21	6:F:314:TYR:CE2	2.06	0.91
5:K:380:LEU:HD21	6:L:314:TYR:CE2	2.06	0.91
6:L:350:PHE:CZ	6:L:373:PHE:CZ	2.58	0.91
9:Q:116:ILE:HA	9:Q:120:GLU:CB	2.01	0.91
9:R:20:LYS:O	9:R:24:GLU:CB	2.19	0.91
5:K:316:VAL:O	5:K:348:ILE:HG13	1.69	0.91
7:O:1386:LYS:CD	8:P:688:THR:HG22	2.00	0.91
7:M:1386:LYS:CD	8:N:688:THR:HG22	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:917:GLU:HB2	3:Z:957:LEU:CD1	2.01	0.90
5:B:323:LEU:HD23	5:B:338:ALA:HB1	0.92	0.90
7:M:1193:ARG:O	7:M:1196:SER:N	2.04	0.90
3:1:917:GLU:HB2	3:1:957:LEU:CD1	2.01	0.90
7:O:1392:ILE:HG12	7:O:1437:LEU:HD13	1.53	0.90
9:T:21:LYS:O	9:T:25:LEU:CB	2.18	0.90
7:M:1392:ILE:HG12	7:M:1437:LEU:HD13	1.53	0.90
3:1:1191:LEU:HD13	3:1:1213:LEU:HD23	1.50	0.90
7:O:1193:ARG:O	7:O:1196:SER:N	2.04	0.90
7:O:985:GLN:HA	7:O:988:SER:HB3	1.54	0.90
11:X:289:SER:HA	11:X:294:ILE:HD13	0.91	0.90
5:H:413:LEU:HB3	6:I:373:PHE:CE2	2.03	0.90
8:N:64:SER:HB3	8:N:73:SER:HG	1.09	0.90
8:N:761:PHE:HE1	8:N:764:LYS:CD	1.84	0.90
9:R:338:PHE:CE2	9:R:342:ARG:HD2	2.07	0.90
9:S:20:LYS:O	9:S:24:GLU:CB	2.19	0.90
9:T:338:PHE:CE2	9:T:342:ARG:HD2	2.07	0.90
4:D:796:ILE:HD13	5:E:513:LEU:HD21	0.91	0.90
2:0:516:LEU:CD2	2:0:598:PHE:HZ	1.85	0.90
3:1:1170:GLN:OE1	3:1:1205:LEU:HD21	1.70	0.90
3:Z:1213:LEU:HD21	3:Z:1215:TYR:CD2	2.07	0.90
7:M:1558:ASP:HA	7:M:1582:LEU:HD21	1.54	0.90
8:N:761:PHE:HZ	8:N:765:PHE:CZ	1.86	0.90
8:P:761:PHE:HE1	8:P:764:LYS:CD	1.84	0.90
3:Z:1191:LEU:HD13	3:Z:1215:TYR:CZ	2.06	0.89
5:E:517:GLN:NE2	9:R:24:GLU:C	2.25	0.89
9:T:20:LYS:O	9:T:24:GLU:CB	2.19	0.89
8:P:761:PHE:HZ	8:P:765:PHE:CZ	1.86	0.89
7:O:1558:ASP:HA	7:O:1582:LEU:HD21	1.54	0.89
1:3:4:UNK:N	5:E:316:VAL:HG23	1.88	0.89
3:Z:1199:VAL:O	3:Z:1200:LEU:HD23	1.72	0.89
7:M:1585:PRO:HA	7:M:1659:ASN:HD21	1.36	0.89
7:M:1392:ILE:CG1	7:M:1437:LEU:HD13	2.02	0.89
3:1:1213:LEU:HG	3:1:1213:LEU:O	1.69	0.89
11:X:289:SER:CB	11:X:294:ILE:HD12	1.99	0.89
7:O:1392:ILE:CG1	7:O:1437:LEU:HD13	2.02	0.89
7:O:1585:PRO:HA	7:O:1659:ASN:HD21	1.36	0.89
1:4:2:UNK:N	5:K:314:ASN:CG	2.26	0.89
11:V:293:HIS:O	11:V:361:ASN:ND2	2.06	0.89
7:O:1191:SER:HB2	8:P:757:LYS:CA	1.97	0.89
10:W:276:ILE:CG1	10:W:283:ILE:HD11	1.92	0.89

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:795:LYS:HZ3	9:R:21:LYS:CB	1.66	0.89
7:M:1393:ASN:ND2	8:N:687:LYS:HE2	1.86	0.89
2:0:516:LEU:HG	2:0:537:LYS:HD3	1.54	0.89
9:T:158:ASN:O	9:T:162:LEU:CB	2.21	0.89
7:M:1191:SER:HB2	8:N:757:LYS:CA	1.97	0.88
9:R:675:VAL:HG21	9:R:728:PHE:CE2	2.06	0.88
9:T:675:VAL:HG21	9:T:728:PHE:CE2	2.05	0.88
7:O:1189:MET:HG3	7:O:1190:TYR:CD1	2.08	0.88
3:Z:1173:LEU:HB2	3:Z:1218:ILE:CG2	2.01	0.88
7:M:1189:MET:HG3	7:M:1190:TYR:CD1	2.08	0.88
5:H:413:LEU:HA	6:I:373:PHE:HE2	1.36	0.88
4:J:806:SER:HB3	9:T:35:ALA:HB2	0.89	0.88
6:L:350:PHE:CE1	6:L:373:PHE:HE1	1.85	0.88
7:O:1392:ILE:CG1	7:O:1437:LEU:CD1	2.52	0.88
9:T:669:ASP:H	9:T:673:PRO:CG	1.87	0.88
7:M:1392:ILE:CG1	7:M:1437:LEU:CD1	2.52	0.88
9:R:669:ASP:H	9:R:673:PRO:CG	1.87	0.88
2:0:516:LEU:CD2	2:0:598:PHE:CZ	2.56	0.88
3:1:1191:LEU:HD13	3:1:1215:TYR:OH	1.74	0.88
11:X:273:VAL:N	11:X:356:VAL:O	2.07	0.88
11:V:273:VAL:N	11:V:356:VAL:O	2.07	0.88
3:1:1173:LEU:HD22	3:1:1218:ILE:CG1	2.04	0.88
7:O:1382:TYR:HD2	8:P:748:HIS:CE1	1.59	0.88
3:1:1170:GLN:OE1	3:1:1205:LEU:CD2	2.22	0.88
4:J:669:LEU:CD2	5:K:369:VAL:HG12	2.04	0.88
10:W:321:GLU:HB2	11:X:293:HIS:HD2	1.11	0.88
3:Z:344:GLN:OE1	3:Z:497:CYS:HB2	1.73	0.87
5:B:323:LEU:HB3	5:B:335:TRP:CH2	2.09	0.87
7:M:1380:ARG:H	7:M:1380:ARG:HD2	1.37	0.87
9:R:472:SER:O	9:R:473:ARG:NH1	2.06	0.87
11:V:271:ILE:HA	11:V:386:PRO:HB3	1.54	0.87
10:U:321:GLU:HB2	11:V:293:HIS:HD2	1.11	0.87
7:O:1671:VAL:HG11	9:T:166:LYS:CA	2.04	0.87
11:X:271:ILE:HA	11:X:386:PRO:HB3	1.54	0.87
9:Q:594:GLY:CA	10:U:324:LYS:CE	2.47	0.87
7:O:984:THR:O	7:O:988:SER:HB2	1.74	0.87
9:T:472:SER:O	9:T:473:ARG:NH1	2.06	0.87
3:Z:1173:LEU:HB3	3:Z:1218:ILE:CG2	2.03	0.87
6:L:350:PHE:HE1	6:L:373:PHE:CE1	1.90	0.87
8:P:461:CYS:O	8:P:556:LEU:CD1	2.18	0.87
9:T:429:THR:HG23	9:T:434:ASP:CB	2.04	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:273:VAL:HG21	11:X:356:VAL:HG23	1.55	0.87
10:U:266:ILE:HG12	10:U:336:ASN:ND2	1.88	0.87
11:V:273:VAL:HG21	11:V:356:VAL:HG23	1.55	0.87
7:O:341:PHE:CE2	7:O:652:ALA:CB	2.57	0.87
9:S:594:GLY:CA	10:W:324:LYS:CE	2.47	0.87
7:M:341:PHE:CE2	7:M:652:ALA:CB	2.57	0.87
9:R:429:THR:HG23	9:R:434:ASP:CB	2.04	0.87
7:O:1191:SER:HB3	8:P:757:LYS:HA	0.87	0.87
7:O:1336:ILE:HD13	7:O:1383:GLN:CG	2.02	0.87
7:O:1561:LEU:H	7:O:1580:VAL:CB	1.88	0.87
7:M:1191:SER:HB3	8:N:757:LYS:HA	0.87	0.87
3:1:1173:LEU:CD2	3:1:1218:ILE:HD13	2.02	0.87
7:M:1336:ILE:HD13	7:M:1383:GLN:CG	2.03	0.86
7:M:1561:LEU:H	7:M:1580:VAL:CB	1.88	0.86
1:7:77:UNK:CB	9:R:435:TRP:CD1	2.58	0.86
9:T:675:VAL:HG23	9:T:728:PHE:CE2	2.07	0.86
1:8:77:UNK:CB	9:T:435:TRP:CD1	2.58	0.86
7:O:1392:ILE:HG12	7:O:1437:LEU:HD12	1.56	0.86
2:Y:1358:GLU:CB	3:1:787:ALA:N	2.37	0.86
5:E:314:ASN:ND2	5:E:348:ILE:CB	2.04	0.86
4:G:810:ASN:HB2	9:S:35:ALA:HB1	1.55	0.86
4:G:810:ASN:CB	9:S:35:ALA:CB	2.52	0.86
8:P:227:ILE:HD13	8:P:255:GLU:CG	1.99	0.86
9:R:675:VAL:HG23	9:R:728:PHE:CE2	2.08	0.86
11:V:273:VAL:HG11	11:V:356:VAL:CG2	2.05	0.86
11:X:273:VAL:HG11	11:X:356:VAL:CG2	2.05	0.86
8:P:613:GLU:HG2	8:P:617:TYR:CD1	2.08	0.86
7:M:984:THR:O	7:M:988:SER:N	2.09	0.86
7:M:1392:ILE:HG12	7:M:1437:LEU:HD12	1.56	0.86
8:N:613:GLU:HG2	8:N:617:TYR:CD1	2.08	0.86
7:O:1189:MET:HB2	8:P:249:ASP:HA	1.55	0.86
2:0:1019:ARG:HH11	9:T:245:ALA:HA	1.41	0.86
11:X:296:GLU:O	11:X:346:LYS:HE3	1.75	0.86
2:Y:1019:ARG:HH11	9:R:245:ALA:HA	1.41	0.85
10:U:266:ILE:HG12	10:U:336:ASN:HD22	1.38	0.85
7:O:984:THR:O	7:O:988:SER:CB	2.24	0.85
7:M:1189:MET:HB2	8:N:249:ASP:HA	1.56	0.85
7:M:1385:PHE:CE1	7:M:1426:VAL:HA	2.11	0.85
3:1:494:ASN:HB2	3:1:512:ARG:HB2	1.22	0.85
11:X:297:ASP:OD2	11:X:301:LEU:HG	1.75	0.85
11:X:355:TRP:HE1	11:X:400:ILE:HB	1.39	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:323:LEU:HD13	5:B:339:MET:HG3	1.57	0.85
5:B:323:LEU:HG	5:B:349:PRO:HG2	1.58	0.85
7:M:341:PHE:CE2	7:M:652:ALA:HB1	2.11	0.85
11:V:355:TRP:HE1	11:V:400:ILE:HB	1.38	0.85
7:O:341:PHE:CE2	7:O:652:ALA:HB1	2.11	0.85
3:Z:787:ALA:N	2:0:1358:GLU:HB3	1.92	0.85
7:M:1392:ILE:CG2	7:M:1437:LEU:HA	2.07	0.85
7:O:1189:MET:O	8:P:249:ASP:OD1	1.94	0.85
8:P:288:LEU:HD11	8:P:328:ILE:HG22	1.57	0.85
3:Z:1213:LEU:CD2	3:Z:1215:TYR:CD2	2.59	0.85
8:N:288:LEU:HD11	8:N:328:ILE:HG22	1.57	0.85
7:O:1392:ILE:CG2	7:O:1437:LEU:HA	2.07	0.85
5:K:316:VAL:HG13	5:K:348:ILE:HD11	0.85	0.85
8:N:71:LEU:O	8:N:75:ILE:HG13	1.77	0.85
9:Q:589:LEU:HA	9:Q:603:VAL:CG2	2.07	0.85
10:U:262:ILE:O	10:U:262:ILE:HG22	1.74	0.85
11:V:273:VAL:CA	11:V:356:VAL:O	2.25	0.84
3:1:1191:LEU:HD13	3:1:1215:TYR:CZ	2.11	0.84
3:1:1199:VAL:O	3:1:1200:LEU:CD2	2.25	0.84
10:W:304:LYS:N	11:X:271:ILE:HG12	1.91	0.84
7:M:1382:TYR:CD1	8:N:748:HIS:CE1	2.63	0.84
7:M:1392:ILE:CG2	7:M:1437:LEU:CA	2.56	0.84
8:N:314:ASP:OD2	8:N:361:LYS:NZ	2.08	0.84
10:U:262:ILE:HG23	10:U:265:SER:HG	1.03	0.84
3:1:1191:LEU:HD11	3:1:1213:LEU:CD2	2.05	0.84
11:X:273:VAL:CA	11:X:356:VAL:O	2.25	0.84
7:O:1392:ILE:CG2	7:O:1437:LEU:CA	2.56	0.84
1:3:2:UNK:N	5:E:316:VAL:HB	1.85	0.84
9:R:436:LEU:HD11	9:R:462:PHE:CZ	2.08	0.84
9:R:669:ASP:N	9:R:673:PRO:HG2	1.92	0.84
8:P:314:ASP:OD2	8:P:361:LYS:NZ	2.08	0.84
9:T:669:ASP:N	9:T:673:PRO:HG2	1.92	0.84
1:3:2:UNK:H2	5:E:316:VAL:HG12	1.05	0.84
9:T:436:LEU:HD11	9:T:462:PHE:CZ	2.08	0.84
8:N:761:PHE:CE2	8:N:765:PHE:CZ	2.66	0.84
10:W:276:ILE:N	10:W:283:ILE:HD11	1.92	0.84
3:1:1173:LEU:HD22	3:1:1218:ILE:HG12	1.57	0.84
9:S:584:LYS:HE2	9:S:636:ARG:HD2	1.57	0.84
7:M:1559:LEU:HD22	7:O:1642:LYS:HE3	1.56	0.84
6:L:354:LEU:HD21	6:L:369:LEU:CD1	2.07	0.84
8:P:761:PHE:CE2	8:P:765:PHE:CZ	2.66	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:1019:ARG:HB3	9:R:246:ASN:C	1.98	0.84
5:E:517:GLN:HE21	9:R:24:GLU:HA	1.41	0.84
8:N:744:LEU:CD1	8:N:745:HIS:ND1	2.41	0.84
5:B:323:LEU:HD13	5:B:339:MET:CG	2.08	0.84
2:0:1019:ARG:HB3	9:T:246:ASN:C	1.98	0.84
10:W:276:ILE:H	10:W:283:ILE:HD11	1.40	0.84
5:E:360:GLN:O	5:E:363:GLN:CG	2.26	0.83
7:M:1382:TYR:CD2	8:N:748:HIS:NE2	2.37	0.83
5:K:317:ASN:ND2	5:K:320:GLU:OE2	2.11	0.83
5:K:360:GLN:O	5:K:363:GLN:CG	2.26	0.83
7:M:1392:ILE:CG2	7:M:1437:LEU:N	2.41	0.83
8:P:288:LEU:CD1	8:P:328:ILE:CG2	2.55	0.83
8:P:613:GLU:OE2	8:P:617:TYR:CD2	2.31	0.83
8:N:288:LEU:CD1	8:N:328:ILE:CG2	2.55	0.83
8:N:613:GLU:OE2	8:N:617:TYR:CD2	2.31	0.83
11:V:273:VAL:CG1	11:V:356:VAL:HG22	2.07	0.83
3:Z:1215:TYR:CB	3:Z:1218:ILE:HG12	2.09	0.83
7:O:1392:ILE:CG2	7:O:1437:LEU:N	2.41	0.83
2:Y:1019:ARG:HD2	9:R:245:ALA:HA	1.61	0.83
7:O:381:THR:CA	7:O:703:TYR:HB3	2.06	0.83
2:0:1019:ARG:HD2	9:T:245:ALA:HA	1.61	0.83
11:X:274:PHE:HD2	11:X:355:TRP:CZ3	1.96	0.83
8:N:761:PHE:CZ	8:N:765:PHE:CE1	2.67	0.83
9:Q:603:VAL:HG23	9:Q:604:ILE:HG13	1.60	0.83
7:M:381:THR:CA	7:M:703:TYR:HB3	2.06	0.83
11:V:274:PHE:HD2	11:V:355:TRP:CZ3	1.97	0.83
8:P:761:PHE:CZ	8:P:765:PHE:CE1	2.67	0.83
11:V:355:TRP:CZ2	11:V:401:ASP:O	2.32	0.82
9:Q:594:GLY:HA3	10:U:324:LYS:CE	2.07	0.82
2:0:516:LEU:HD21	2:0:598:PHE:HZ	1.37	0.82
10:W:271:ALA:CA	10:W:283:ILE:CG2	2.56	0.82
11:X:355:TRP:CZ2	11:X:401:ASP:O	2.33	0.82
7:M:1561:LEU:O	7:M:1580:VAL:HG11	1.79	0.82
8:N:267:ILE:HG22	8:N:271:LEU:CD1	2.09	0.82
8:P:288:LEU:HD11	8:P:328:ILE:HG23	1.60	0.82
11:X:273:VAL:CB	11:X:356:VAL:HG22	1.98	0.82
7:M:1642:LYS:HE3	7:O:1559:LEU:HD22	1.58	0.82
8:N:288:LEU:HD11	8:N:328:ILE:HG23	1.60	0.82
7:O:1561:LEU:O	7:O:1580:VAL:HG11	1.79	0.82
11:V:273:VAL:CB	11:V:356:VAL:HG22	1.97	0.82
5:H:524:ASN:OD1	9:S:31:ASN:CB	2.28	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:1213:LEU:HD12	3:Z:1215:TYR:N	1.95	0.82
8:N:305:ASP:OD2	8:N:322:HIS:NE2	2.13	0.82
8:P:267:ILE:HG22	8:P:271:LEU:CD1	2.10	0.82
8:P:305:ASP:OD2	8:P:322:HIS:NE2	2.13	0.82
1:7:82:UNK:C	1:7:84:UNK:N	2.42	0.82
9:S:594:GLY:HA3	10:W:324:LYS:CE	2.07	0.82
1:8:82:UNK:C	1:8:84:UNK:N	2.42	0.82
7:O:990:ILE:HB	7:O:999:LYS:HZ1	1.44	0.82
8:N:71:LEU:HD12	8:N:72:ARG:N	1.93	0.82
3:Z:1191:LEU:HD22	3:Z:1213:LEU:CD2	2.10	0.82
5:B:517:GLN:OE1	9:Q:23:ASN:CB	2.28	0.82
8:N:744:LEU:HD11	8:N:745:HIS:ND1	1.95	0.82
3:1:1215:TYR:O	3:1:1218:ILE:HG22	1.80	0.82
7:O:1560:GLY:HA3	7:O:1580:VAL:HG23	1.61	0.82
7:M:1560:GLY:HA3	7:M:1580:VAL:HG23	1.61	0.81
9:R:339:TYR:HE1	9:R:342:ARG:NH1	1.75	0.81
7:O:1562:ASP:HA	7:O:1580:VAL:HG13	1.62	0.81
7:M:1562:ASP:HA	7:M:1580:VAL:HG13	1.62	0.81
7:M:1381:LEU:O	7:M:1385:PHE:CD2	2.33	0.81
9:R:668:SER:CB	9:R:673:PRO:HB2	2.07	0.81
3:1:1170:GLN:O	3:1:1173:LEU:HG	1.79	0.81
9:T:339:TYR:HE1	9:T:342:ARG:NH1	1.75	0.81
3:Z:1170:GLN:O	3:Z:1173:LEU:HG	1.80	0.81
3:Z:1174:LEU:O	3:Z:1177:VAL:CG1	2.29	0.81
8:N:613:GLU:OE1	8:N:617:TYR:CE1	2.33	0.81
5:K:517:GLN:HE22	9:T:23:ASN:CA	1.91	0.81
8:P:149:ILE:HG23	8:P:223:PHE:CD1	2.16	0.81
8:P:613:GLU:OE1	8:P:617:TYR:CE1	2.33	0.81
9:T:668:SER:CB	9:T:673:PRO:HB2	2.07	0.81
7:O:1381:LEU:CD1	7:O:1385:PHE:CE2	2.62	0.81
11:X:273:VAL:CG1	11:X:356:VAL:HG22	2.07	0.81
2:Y:1019:ARG:HB2	9:R:246:ASN:HB2	1.62	0.81
10:U:268:LEU:CB	10:U:283:ILE:HD11	2.08	0.81
11:V:397:GLY:HA3	11:V:399:LYS:HE3	1.63	0.81
7:O:1189:MET:CB	8:P:249:ASP:OD1	2.29	0.81
9:T:435:TRP:CH2	9:T:474:PHE:CE1	2.68	0.81
11:X:397:GLY:HA3	11:X:399:LYS:HE3	1.63	0.81
9:R:435:TRP:CH2	9:R:474:PHE:CE1	2.68	0.81
2:0:1019:ARG:HB2	9:T:246:ASN:HB2	1.62	0.81
3:Z:1173:LEU:HD21	3:Z:1205:LEU:HD21	1.62	0.81
5:E:517:GLN:HE21	9:R:24:GLU:CB	1.91	0.81

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1189:MET:CE	8:N:252:TYR:HB3	2.11	0.81
8:N:71:LEU:HB3	8:N:164:TYR:HE1	1.43	0.81
3:1:1146:SER:HA	9:T:447:ASP:OD1	1.79	0.81
11:X:274:PHE:HD2	11:X:355:TRP:CH2	1.99	0.81
3:Z:1146:SER:HA	9:R:447:ASP:OD1	1.79	0.80
7:O:1560:GLY:C	7:O:1580:VAL:CG2	2.49	0.80
7:M:1382:TYR:CZ	8:N:748:HIS:NE2	2.49	0.80
5:K:317:ASN:ND2	5:K:348:ILE:HD13	1.89	0.80
6:L:354:LEU:CD2	6:L:369:LEU:HD11	2.09	0.80
7:O:1189:MET:CE	8:P:252:TYR:HB3	2.11	0.80
3:Z:1191:LEU:HD22	3:Z:1213:LEU:HD23	1.61	0.80
7:M:1329:LEU:CD2	7:M:1380:ARG:NH2	2.43	0.80
7:M:1560:GLY:C	7:M:1580:VAL:CG2	2.49	0.80
8:N:327:PHE:CD1	8:N:389:PHE:HD2	1.99	0.80
1:3:4:UNK:CB	5:E:316:VAL:HA	2.11	0.80
11:V:274:PHE:HD2	11:V:355:TRP:CH2	2.00	0.80
7:M:1386:LYS:HG3	8:N:688:THR:CG2	1.85	0.80
2:0:1019:ARG:HB3	9:T:246:ASN:O	1.80	0.80
2:Y:1019:ARG:HB3	9:R:246:ASN:O	1.80	0.80
5:E:456:THR:C	5:E:460:TRP:HD1	1.84	0.80
8:N:64:SER:OG	8:N:73:SER:O	1.97	0.80
9:R:278:LEU:HD22	9:R:433:GLU:CB	2.09	0.80
5:K:456:THR:C	5:K:460:TRP:HD1	1.84	0.80
3:1:1173:LEU:CD1	3:1:1195:LEU:HD22	2.11	0.80
7:O:1386:LYS:HG3	8:P:688:THR:CG2	1.85	0.80
5:B:323:LEU:CB	5:B:323:LEU:CG	2.59	0.80
3:1:1177:VAL:HG21	3:1:1215:TYR:CE2	2.16	0.80
5:K:316:VAL:HG11	5:K:348:ILE:CD1	1.97	0.80
9:T:278:LEU:HD22	9:T:433:GLU:CB	2.09	0.80
11:V:270:ALA:HB2	11:V:357:LYS:HG3	1.62	0.79
2:Y:443:GLY:HA2	2:Y:519:THR:OG1	1.82	0.79
5:B:323:LEU:HG	5:B:342:LYS:NZ	1.97	0.79
7:M:384:MET:HE1	7:M:760:ILE:HG23	1.63	0.79
8:N:741:LYS:HA	8:N:744:LEU:HD21	1.64	0.79
5:K:318:GLU:CA	5:K:346:GLN:HA	2.02	0.79
11:X:289:SER:HB3	11:X:294:ILE:HD12	1.57	0.79
6:F:394:ILE:HD11	9:R:40:GLY:O	1.82	0.79
11:V:294:ILE:HG12	11:V:361:ASN:OD1	1.82	0.79
5:K:517:GLN:NE2	9:T:23:ASN:CA	2.45	0.79
4:J:765:LEU:HD23	5:K:460:TRP:CZ2	2.16	0.79
7:O:1189:MET:N	8:P:248:GLN:HG2	1.94	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:547:TYR:HB3	11:X:298:PHE:CD1	2.16	0.79
3:Z:1215:TYR:HB2	3:Z:1218:ILE:CG1	2.11	0.79
4:D:765:LEU:HD23	5:E:460:TRP:CZ2	2.16	0.79
5:E:380:LEU:HD21	6:F:314:TYR:HE2	1.44	0.79
7:M:1189:MET:N	8:N:248:GLN:HG2	1.94	0.79
3:1:1194:LYS:NZ	3:1:1208:ASP:O	2.13	0.79
6:L:350:PHE:CZ	6:L:373:PHE:CE1	2.71	0.79
1:7:83:UNK:O	9:R:285:TYR:OH	2.00	0.79
1:8:83:UNK:O	9:T:285:TYR:OH	2.00	0.79
8:N:223:PHE:HE2	8:N:258:ILE:CG2	1.95	0.79
7:O:384:MET:HE1	7:O:760:ILE:HG23	1.64	0.79
11:X:270:ALA:HB2	11:X:357:LYS:HG3	1.62	0.79
11:X:355:TRP:HD1	11:X:400:ILE:HD13	1.47	0.79
2:Y:1019:ARG:HB3	9:R:246:ASN:CA	2.13	0.79
3:Z:917:GLU:HG3	3:Z:918:MET:N	1.95	0.79
2:0:1019:ARG:HB3	9:T:246:ASN:CA	2.13	0.79
5:K:380:LEU:HD21	6:L:314:TYR:HE2	1.44	0.79
7:O:1392:ILE:HD11	7:O:1437:LEU:HD13	1.63	0.79
4:D:636:THR:C	4:D:637:LEU:CD2	2.50	0.79
7:M:1392:ILE:HD11	7:M:1437:LEU:HD13	1.63	0.79
7:M:1381:LEU:O	7:M:1385:PHE:HD2	1.66	0.79
11:V:355:TRP:HD1	11:V:400:ILE:HD13	1.47	0.79
8:N:223:PHE:CE2	8:N:258:ILE:CG2	2.66	0.78
3:1:917:GLU:HG3	3:1:918:MET:N	1.95	0.78
6:L:374:GLN:HE21	6:L:374:GLN:N	1.81	0.78
7:O:1189:MET:HB2	8:P:249:ASP:OD1	1.82	0.78
3:Z:1191:LEU:CD2	3:Z:1213:LEU:HD23	2.13	0.78
5:B:317:ASN:HB3	5:B:346:GLN:HG2	1.64	0.78
5:E:380:LEU:HD22	6:F:314:TYR:HE2	1.49	0.78
9:S:582:GLU:HG2	11:X:302:ARG:HH12	1.48	0.78
11:X:289:SER:OG	11:X:294:ILE:CD1	2.31	0.78
5:K:380:LEU:HD22	6:L:314:TYR:HE2	1.49	0.78
9:T:668:SER:HB3	9:T:673:PRO:CB	2.07	0.78
8:P:305:ASP:O	8:P:309:ASN:ND2	2.16	0.78
4:A:796:ILE:HG21	9:Q:24:GLU:CB	2.09	0.78
8:N:274:GLY:CA	8:N:284:ILE:CB	2.62	0.78
8:N:305:ASP:O	8:N:309:ASN:ND2	2.16	0.78
8:P:274:GLY:CA	8:P:284:ILE:CB	2.62	0.78
7:M:1382:TYR:CZ	8:N:748:HIS:CE1	2.72	0.78
3:1:1184:ASP:OD2	3:1:1187:TYR:CE2	2.36	0.78
5:E:436:MET:SD	6:F:370:ASP:CG	2.62	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:Q:592:LYS:HZ1	10:U:324:LYS:HD2	1.48	0.78
9:R:668:SER:HB3	9:R:673:PRO:CB	2.07	0.78
10:W:275:GLU:OE1	10:W:284:LYS:HD2	1.84	0.78
1:7:72:UNK:CB	9:R:426:PRO:CG	2.62	0.78
7:O:1382:TYR:HH	8:P:744:LEU:HD23	1.48	0.78
9:S:592:LYS:HZ1	10:W:324:LYS:HD2	1.48	0.78
4:D:636:THR:O	4:D:637:LEU:CB	2.30	0.78
7:M:1559:LEU:CD2	7:O:1642:LYS:CE	2.41	0.78
7:O:1561:LEU:H	7:O:1580:VAL:CG1	1.95	0.78
4:D:673:GLY:HA3	5:E:315:LYS:NZ	1.99	0.78
7:M:1561:LEU:H	7:M:1580:VAL:CG1	1.96	0.78
10:U:268:LEU:N	10:U:283:ILE:CD1	2.41	0.78
3:1:1173:LEU:HD11	3:1:1195:LEU:HD22	1.64	0.78
5:K:436:MET:SD	6:L:370:ASP:HB3	2.24	0.78
9:T:669:ASP:H	9:T:673:PRO:HG3	1.49	0.78
9:R:669:ASP:H	9:R:673:PRO:HG3	1.50	0.77
5:E:317:ASN:O	5:E:348:ILE:CD1	2.32	0.77
7:O:1189:MET:HA	8:P:249:ASP:CG	2.03	0.77
7:M:985:GLN:HA	7:M:988:SER:HB3	1.67	0.77
8:N:613:GLU:HG3	8:N:617:TYR:CZ	2.19	0.77
8:P:277:THR:CG2	8:P:381:VAL:HG21	2.15	0.77
8:P:613:GLU:HG3	8:P:617:TYR:CZ	2.19	0.77
9:S:593:ILE:HG21	9:S:599:ARG:HA	1.66	0.77
4:A:752:ASP:H	5:B:444:LEU:HD13	1.49	0.77
7:M:1186:SER:O	7:M:1192:VAL:HG13	1.83	0.77
8:N:277:THR:CG2	8:N:381:VAL:HG21	2.15	0.77
8:N:306:VAL:HG22	8:N:352:PHE:CG	2.20	0.77
9:R:407:TYR:CD1	9:R:428:VAL:HG12	2.20	0.77
3:1:1191:LEU:HD11	3:1:1213:LEU:CB	2.15	0.77
4:G:752:ASP:H	5:H:444:LEU:HD13	1.49	0.77
9:T:407:TYR:CD1	9:T:428:VAL:HG12	2.20	0.77
7:M:1189:MET:CB	8:N:248:GLN:C	2.52	0.77
8:N:306:VAL:HG22	8:N:352:PHE:CD1	2.20	0.77
8:P:306:VAL:HG22	8:P:352:PHE:CG	2.20	0.77
1:4:2:UNK:CA	5:K:314:ASN:OD1	2.33	0.77
7:O:1189:MET:CB	8:P:248:GLN:C	2.52	0.77
8:P:306:VAL:HG22	8:P:352:PHE:CD1	2.20	0.77
3:Z:1183:ILE:O	3:Z:1188:ARG:NH2	2.17	0.77
5:B:323:LEU:HA	5:B:349:PRO:HD2	1.66	0.77
7:M:335:ASP:OD2	7:M:857:GLY:HA3	1.84	0.77
7:O:1186:SER:O	7:O:1192:VAL:HG13	1.83	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1189:MET:C	8:P:249:ASP:OD1	2.22	0.77
11:X:275:GLY:N	11:X:354:SER:HB2	1.99	0.77
5:E:456:THR:C	5:E:460:TRP:CD1	2.57	0.77
5:H:413:LEU:HA	6:I:373:PHE:CE2	2.18	0.77
5:K:456:THR:C	5:K:460:TRP:CD1	2.57	0.77
11:V:275:GLY:N	11:V:354:SER:HB2	1.99	0.77
3:1:921:SER:HB3	3:1:924:SER:HB3	1.67	0.77
3:Z:921:SER:HB3	3:Z:924:SER:HB3	1.67	0.76
7:O:335:ASP:OD2	7:O:857:GLY:HA3	1.84	0.76
9:S:547:TYR:HB3	11:X:298:PHE:CG	2.19	0.76
11:X:355:TRP:CD1	11:X:400:ILE:CD1	2.69	0.76
7:M:1561:LEU:H	7:M:1580:VAL:HG11	1.46	0.76
8:N:273:LEU:HD13	8:N:328:ILE:HD13	1.67	0.76
11:V:355:TRP:CD1	11:V:400:ILE:CD1	2.69	0.76
7:O:1561:LEU:H	7:O:1580:VAL:HG11	1.46	0.76
8:P:273:LEU:HD13	8:P:328:ILE:HD13	1.67	0.76
3:Z:1209:CYS:O	3:Z:1213:LEU:HG	1.85	0.76
6:C:374:GLN:HA	6:C:374:GLN:HE21	1.50	0.76
6:F:314:TYR:OH	7:M:1030:ASN:ND2	2.19	0.76
5:K:317:ASN:CG	5:K:348:ILE:HD11	2.05	0.76
6:L:314:TYR:OH	7:O:1030:ASN:ND2	2.19	0.76
9:S:547:TYR:HB3	11:X:298:PHE:HB2	1.67	0.76
5:K:317:ASN:ND2	5:K:320:GLU:CD	2.39	0.76
7:M:1392:ILE:HG23	7:M:1437:LEU:HA	1.67	0.76
7:M:335:ASP:CG	7:M:857:GLY:HA3	2.06	0.76
7:M:341:PHE:CZ	7:M:652:ALA:HB2	2.20	0.76
11:V:273:VAL:HB	11:V:356:VAL:O	1.85	0.76
7:O:335:ASP:CG	7:O:857:GLY:HA3	2.06	0.76
7:O:341:PHE:CZ	7:O:652:ALA:HB2	2.21	0.76
7:O:1381:LEU:HD12	7:O:1385:PHE:CZ	2.21	0.76
7:O:1392:ILE:HG23	7:O:1437:LEU:HA	1.67	0.76
3:Z:787:ALA:N	2:0:1358:GLU:CB	2.48	0.75
10:W:276:ILE:HG21	10:W:282:VAL:HG21	1.68	0.75
11:X:273:VAL:HB	11:X:356:VAL:O	1.85	0.75
3:Z:1213:LEU:CD2	3:Z:1215:TYR:HE2	1.93	0.75
9:R:675:VAL:HG21	9:R:728:PHE:CZ	2.21	0.75
9:T:675:VAL:HG21	9:T:728:PHE:CZ	2.21	0.75
11:X:355:TRP:HD1	11:X:400:ILE:CD1	1.98	0.75
3:Z:1213:LEU:HD11	3:Z:1215:TYR:CB	2.17	0.75
8:N:216:TYR:CA	8:N:220:PHE:CE1	2.64	0.75
11:V:355:TRP:HD1	11:V:400:ILE:CD1	1.98	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:267:ILE:HG22	8:N:271:LEU:HD12	1.67	0.75
11:V:285:ILE:C	11:V:300:VAL:HG21	2.06	0.75
3:1:1183:ILE:HG13	3:1:1213:LEU:CD1	2.08	0.75
3:1:1170:GLN:HA	3:1:1173:LEU:HD21	1.69	0.75
8:P:267:ILE:HG22	8:P:271:LEU:HD12	1.67	0.75
1:4:5:UNK:HA	5:K:315:LYS:HD3	1.69	0.75
9:Q:602:GLY:O	9:Q:603:VAL:HG22	1.86	0.75
5:E:517:GLN:CD	9:R:24:GLU:CB	2.55	0.75
7:M:1189:MET:SD	8:N:248:GLN:C	2.65	0.75
10:U:304:LYS:N	11:V:271:ILE:HG12	2.02	0.75
7:O:1189:MET:SD	8:P:248:GLN:C	2.65	0.75
7:M:1642:LYS:CE	7:O:1559:LEU:CD2	2.44	0.74
10:U:321:GLU:CG	11:V:293:HIS:HD2	2.00	0.74
3:1:494:ASN:CB	3:1:512:ARG:O	2.35	0.74
3:1:1173:LEU:HD23	3:1:1218:ILE:HD13	1.63	0.74
3:1:1173:LEU:CB	3:1:1218:ILE:HD13	2.14	0.74
5:K:316:VAL:HG12	5:K:348:ILE:CG1	2.15	0.74
7:O:384:MET:HE2	7:O:760:ILE:HG23	1.69	0.74
10:W:321:GLU:CG	11:X:293:HIS:HD2	2.00	0.74
2:Y:1019:ARG:CG	9:R:246:ASN:HB2	2.18	0.74
3:Z:1170:GLN:HA	3:Z:1173:LEU:HD21	1.70	0.74
7:M:384:MET:HE2	7:M:760:ILE:HG23	1.69	0.74
7:M:1385:PHE:O	7:M:1389:ILE:HG12	1.87	0.74
2:0:1019:ARG:CG	9:T:246:ASN:HB2	2.18	0.74
7:M:335:ASP:OD1	7:M:856:GLU:C	2.26	0.74
9:R:436:LEU:HD12	9:R:462:PHE:HZ	0.61	0.74
7:O:335:ASP:OD1	7:O:856:GLU:C	2.26	0.74
9:S:599:ARG:NH2	9:S:605:GLU:OE2	2.19	0.74
9:T:436:LEU:HD12	9:T:462:PHE:HZ	0.61	0.74
7:M:1382:TYR:OH	8:N:744:LEU:HB2	1.88	0.74
2:0:1310:ASP:CG	2:0:1311:PHE:CD2	2.61	0.74
7:O:1385:PHE:O	7:O:1389:ILE:HG12	1.87	0.74
7:M:1560:GLY:HA3	7:M:1580:VAL:CG2	2.16	0.74
6:L:353:LEU:HD11	6:L:369:LEU:CD1	2.18	0.74
11:X:274:PHE:CA	11:X:355:TRP:HA	2.15	0.74
7:M:1189:MET:CG	8:N:248:GLN:C	2.56	0.74
8:N:285:GLN:HG2	8:N:331:TYR:HE2	1.51	0.74
11:V:274:PHE:CA	11:V:355:TRP:HA	2.14	0.74
7:O:1560:GLY:HA3	7:O:1580:VAL:CG2	2.16	0.74
9:T:339:TYR:CD1	9:T:342:ARG:NH1	2.54	0.74
9:R:339:TYR:CD1	9:R:342:ARG:NH1	2.54	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1189:MET:CG	8:P:248:GLN:C	2.56	0.74
9:S:593:ILE:HG23	9:S:600:ILE:HG13	1.67	0.74
5:E:380:LEU:CD1	6:F:314:TYR:CE2	2.71	0.74
8:N:305:ASP:OD2	8:N:322:HIS:CE1	2.41	0.74
8:P:305:ASP:OD2	8:P:322:HIS:CE1	2.41	0.74
7:M:1385:PHE:HE1	7:M:1426:VAL:HA	1.51	0.73
8:N:741:LYS:O	8:N:744:LEU:CG	2.32	0.73
4:J:806:SER:HB3	9:T:35:ALA:CA	2.17	0.73
7:O:984:THR:O	7:O:988:SER:CA	2.36	0.73
5:K:380:LEU:CD1	6:L:314:TYR:CE2	2.71	0.73
8:P:285:GLN:HG2	8:P:331:TYR:HE2	1.51	0.73
8:N:277:THR:HG22	8:N:381:VAL:HG21	1.69	0.73
8:N:744:LEU:HD12	8:N:745:HIS:N	2.02	0.73
7:O:1389:ILE:HG21	8:P:687:LYS:HB2	1.71	0.73
8:P:277:THR:HG22	8:P:381:VAL:HG21	1.69	0.73
8:P:288:LEU:HD11	8:P:328:ILE:HG21	1.68	0.73
3:Z:1215:TYR:CB	3:Z:1218:ILE:CD1	2.65	0.73
7:M:1562:ASP:N	7:M:1580:VAL:CG1	2.51	0.73
3:Z:1191:LEU:HD13	3:Z:1215:TYR:HH	1.51	0.73
7:O:1380:ARG:HH11	7:O:1415:ARG:NE	1.86	0.73
9:S:547:TYR:O	11:X:298:PHE:HB3	1.88	0.73
8:N:288:LEU:HD11	8:N:328:ILE:HG21	1.68	0.73
3:1:1191:LEU:HD11	3:1:1213:LEU:HD22	1.69	0.73
7:O:1562:ASP:N	7:O:1580:VAL:CG1	2.51	0.73
3:Z:1174:LEU:HA	3:Z:1177:VAL:HG12	1.71	0.73
4:D:806:SER:HB3	9:R:36:SER:HA	1.70	0.73
11:V:275:GLY:O	11:V:354:SER:HA	1.89	0.73
8:P:55:LEU:HD11	8:P:109:ARG:HE	1.52	0.73
1:8:76:UNK:CA	9:T:429:THR:HB	2.19	0.73
8:N:55:LEU:HD11	8:N:109:ARG:HE	1.52	0.73
9:Q:20:LYS:O	9:Q:24:GLU:N	2.22	0.73
3:1:494:ASN:CG	3:1:512:ARG:HB3	2.09	0.73
3:1:918:MET:HA	3:1:918:MET:HE3	1.71	0.73
11:X:275:GLY:O	11:X:354:SER:HA	1.89	0.73
1:7:76:UNK:CA	9:R:429:THR:HB	2.19	0.73
3:Z:918:MET:HA	3:Z:918:MET:HE3	1.71	0.73
10:W:262:ILE:HG13	10:W:336:ASN:HB3	1.70	0.73
6:F:455:GLU:HG3	9:R:63:SER:CB	2.17	0.72
5:H:322:ILE:HB	5:H:325:THR:HG22	1.71	0.72
8:P:529:LEU:HG	8:P:531:ILE:HG12	1.69	0.72
3:1:928:LEU:HD11	3:1:957:LEU:CD2	2.19	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:276:ILE:CB	10:W:283:ILE:HD11	2.18	0.72
2:Y:1310:ASP:O	2:Y:1310:ASP:OD1	2.06	0.72
11:X:274:PHE:CD2	11:X:355:TRP:CH2	2.78	0.72
3:Z:928:LEU:HD11	3:Z:957:LEU:CD2	2.19	0.72
7:M:990:ILE:HA	7:M:995:VAL:HG11	1.72	0.72
2:Y:1482:ASP:HB3	2:Y:1485:GLU:HB2	1.71	0.72
8:P:68:HIS:O	8:P:69:ASN:OD1	2.07	0.72
11:X:274:PHE:HA	11:X:355:TRP:CA	2.14	0.72
11:V:274:PHE:CD2	11:V:355:TRP:CH2	2.78	0.72
11:X:297:ASP:CG	11:X:301:LEU:HG	2.09	0.72
5:B:323:LEU:CG	5:B:342:LYS:HZ1	2.02	0.72
2:0:1482:ASP:HB3	2:0:1485:GLU:HB2	1.71	0.72
4:A:809:ASP:OD2	9:Q:36:SER:CB	2.38	0.72
5:E:316:VAL:HG13	5:E:348:ILE:HD13	1.69	0.72
7:M:384:MET:HA	7:M:766:GLN:CD	2.09	0.72
9:Q:588:VAL:HG12	9:Q:603:VAL:HG11	1.70	0.72
9:Q:593:ILE:CG2	9:Q:600:ILE:HG12	2.20	0.72
11:V:274:PHE:HA	11:V:355:TRP:CA	2.14	0.72
3:1:1183:ILE:HG22	3:1:1184:ASP:H	1.55	0.72
3:Z:1215:TYR:HB3	3:Z:1218:ILE:HG12	1.71	0.71
5:E:314:ASN:CG	5:E:348:ILE:HB	2.07	0.71
11:V:394:GLN:O	11:V:398:CYS:CA	2.36	0.71
3:1:494:ASN:OD1	3:1:512:ARG:HB3	1.90	0.71
7:O:384:MET:HA	7:O:766:GLN:CD	2.08	0.71
3:1:1215:TYR:HB2	3:1:1218:ILE:CG2	2.20	0.71
11:X:394:GLN:O	11:X:398:CYS:CA	2.36	0.71
7:M:1384:LEU:HD13	7:M:1412:TYR:HB2	1.72	0.71
2:0:1020:ASN:HB2	9:T:247:GLY:CA	2.20	0.71
4:J:669:LEU:HD21	5:K:369:VAL:CG1	2.18	0.71
7:O:1189:MET:HE1	8:P:252:TYR:CB	2.20	0.71
10:W:322:LEU:HG	10:W:322:LEU:O	1.91	0.71
2:Y:1020:ASN:HB2	9:R:247:GLY:CA	2.20	0.71
4:D:793:LEU:CB	6:F:439:ILE:HG21	2.21	0.71
8:N:55:LEU:CD2	8:N:109:ARG:HH21	2.03	0.71
2:0:1019:ARG:CB	9:T:246:ASN:CB	2.66	0.71
7:O:1384:LEU:HD13	7:O:1412:TYR:HB2	1.72	0.71
8:P:55:LEU:CD2	8:P:109:ARG:HH21	2.03	0.71
4:J:793:LEU:CB	6:L:439:ILE:HG21	2.21	0.71
2:Y:1019:ARG:CB	9:R:246:ASN:CB	2.67	0.71
3:Z:1210:ALA:CB	3:Z:1218:ILE:HD11	2.20	0.71
7:M:1386:LYS:NZ	8:N:683:ASP:CG	2.43	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1389:ILE:HG23	8:N:687:LYS:HG2	1.58	0.71
8:N:55:LEU:HD21	8:N:109:ARG:HH21	1.54	0.71
8:N:613:GLU:CB	8:N:617:TYR:CE2	2.73	0.71
3:1:1177:VAL:CG2	3:1:1215:TYR:CE1	2.67	0.71
7:O:1385:PHE:CE1	7:O:1426:VAL:HA	2.26	0.71
7:O:1561:LEU:N	7:O:1580:VAL:HG11	2.06	0.71
8:P:613:GLU:CB	8:P:617:TYR:CE2	2.73	0.71
8:P:55:LEU:HD21	8:P:109:ARG:HH21	1.54	0.71
10:W:271:ALA:CA	10:W:283:ILE:HG22	2.21	0.71
7:O:1189:MET:HE3	8:P:252:TYR:HB3	1.73	0.70
7:O:1189:MET:CE	8:P:252:TYR:CB	2.68	0.70
7:M:1189:MET:CE	8:N:252:TYR:CB	2.68	0.70
7:M:1561:LEU:N	7:M:1580:VAL:HG11	2.06	0.70
9:Q:588:VAL:O	9:Q:603:VAL:HG13	1.91	0.70
7:O:1386:LYS:NZ	8:P:683:ASP:CG	2.43	0.70
8:P:267:ILE:O	8:P:271:LEU:HD12	1.91	0.70
9:T:669:ASP:H	9:T:673:PRO:HG2	1.53	0.70
8:N:267:ILE:O	8:N:271:LEU:HD12	1.91	0.70
3:1:493:ILE:HD12	3:1:513:LYS:CD	2.19	0.70
3:1:1183:ILE:HG22	3:1:1184:ASP:N	2.05	0.70
7:M:1189:MET:CG	7:M:1190:TYR:HD1	2.05	0.70
2:0:516:LEU:CG	2:0:537:LYS:HD3	2.22	0.70
7:O:1189:MET:CG	7:O:1190:TYR:HD1	2.05	0.70
7:M:1188:THR:HG22	8:N:244:PHE:O	1.91	0.70
7:O:1188:THR:HG22	8:P:244:PHE:O	1.91	0.70
1:7:70:UNK:CB	9:R:469:TYR:CE1	2.75	0.70
1:8:74:UNK:HA	9:T:473:ARG:HG3	1.74	0.70
9:T:158:ASN:O	9:T:162:LEU:N	2.24	0.70
5:B:323:LEU:CG	5:B:342:LYS:NZ	2.55	0.70
4:D:807:LEU:CD2	5:E:524:ASN:OD1	2.40	0.70
9:R:669:ASP:H	9:R:673:PRO:HG2	1.53	0.70
2:0:1310:ASP:OD1	2:0:1311:PHE:CD2	2.44	0.70
5:K:372:ALA:HA	5:K:375:ILE:HD12	1.72	0.70
11:V:298:PHE:CD2	11:V:299:GLN:N	2.60	0.70
7:O:381:THR:HA	7:O:703:TYR:HB2	1.69	0.70
7:O:1192:VAL:HG12	7:O:1193:ARG:N	2.04	0.70
7:M:381:THR:HA	7:M:703:TYR:HB2	1.69	0.70
7:M:1192:VAL:HG12	7:M:1193:ARG:N	2.04	0.70
11:V:273:VAL:O	11:V:355:TRP:HA	1.91	0.70
11:X:273:VAL:O	11:X:355:TRP:HA	1.91	0.70
8:N:223:PHE:CZ	8:N:258:ILE:HG22	2.27	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:669:ASP:N	9:R:673:PRO:CG	2.54	0.69
8:P:1357:CYS:HG	9:T:453:VAL:HG11	1.56	0.69
9:S:599:ARG:NH2	9:S:605:GLU:CD	2.45	0.69
6:L:371:LYS:N	6:L:371:LYS:HD3	2.07	0.69
5:H:517:GLN:HE22	9:S:23:ASN:CB	2.04	0.69
9:T:669:ASP:N	9:T:673:PRO:CG	2.54	0.69
8:N:226:ASN:HA	8:N:229:SER:HB2	1.73	0.69
8:N:744:LEU:HD12	8:N:745:HIS:ND1	2.08	0.69
2:0:516:LEU:HD12	2:0:516:LEU:N	2.08	0.69
7:O:1336:ILE:CD1	7:O:1383:GLN:CG	2.67	0.69
10:W:276:ILE:HD12	10:W:283:ILE:HD13	1.74	0.69
6:F:353:LEU:HG	6:F:369:LEU:HD11	1.75	0.69
5:E:373:ARG:HH21	6:F:307:SER:CB	2.05	0.69
7:M:1336:ILE:CD1	7:M:1383:GLN:CG	2.67	0.69
10:U:322:LEU:HG	10:U:322:LEU:O	1.91	0.69
1:7:72:UNK:C	9:R:426:PRO:HB3	2.22	0.69
7:M:1384:LEU:HD13	7:M:1412:TYR:CB	2.23	0.69
6:I:374:GLN:HA	6:I:374:GLN:HE21	1.57	0.69
8:N:216:TYR:HA	8:N:220:PHE:HD1	0.87	0.69
8:N:1357:CYS:HG	9:R:453:VAL:HG11	1.57	0.69
7:M:1408:LEU:HB3	7:M:1412:TYR:HE2	1.57	0.68
3:1:494:ASN:HB2	3:1:512:ARG:C	2.13	0.68
11:X:272:ILE:HG22	11:X:355:TRP:CE3	2.28	0.68
7:M:1189:MET:CE	8:N:249:ASP:HA	2.23	0.68
8:N:74:THR:CG2	8:N:162:HIS:HE1	2.05	0.68
6:I:373:PHE:HA	6:I:376:LYS:HE3	1.73	0.68
2:Y:1086:ASN:HD22	2:Y:1094:ARG:HH22	1.42	0.68
9:Q:589:LEU:HD23	9:Q:603:VAL:HG21	1.75	0.68
2:0:1086:ASN:HD22	2:0:1094:ARG:HH22	1.42	0.68
7:O:1384:LEU:HD13	7:O:1412:TYR:CB	2.24	0.68
11:X:289:SER:OG	11:X:294:ILE:HD12	1.93	0.68
1:3:3:UNK:N	5:E:316:VAL:HB	2.08	0.68
5:B:413:LEU:HA	6:C:373:PHE:CE1	2.28	0.68
7:M:1393:ASN:ND2	8:N:687:LYS:CE	2.50	0.68
11:V:272:ILE:HG22	11:V:355:TRP:CE3	2.28	0.68
5:H:413:LEU:CA	6:I:373:PHE:CE2	2.61	0.68
6:L:350:PHE:CE1	6:L:373:PHE:CZ	2.79	0.68
1:3:4:UNK:N	5:E:316:VAL:CG2	2.56	0.68
2:0:517:LEU:HD13	2:0:517:LEU:O	1.94	0.68
3:1:1210:ALA:HB1	3:1:1218:ILE:HG23	1.76	0.68
7:O:1392:ILE:CG1	7:O:1437:LEU:HD12	2.22	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1561:LEU:N	7:O:1580:VAL:CB	2.54	0.68
1:3:4:UNK:CA	5:E:316:VAL:HG23	2.24	0.68
10:U:268:LEU:HD13	10:U:283:ILE:HG13	1.73	0.68
3:1:344:GLN:OE1	3:1:497:CYS:HB2	1.92	0.68
7:O:1385:PHE:CE1	7:O:1426:VAL:CG2	2.76	0.68
7:O:1408:LEU:HB3	7:O:1412:TYR:HE2	1.57	0.68
7:M:1561:LEU:N	7:M:1580:VAL:CB	2.54	0.68
6:L:455:GLU:HG2	9:T:63:SER:CB	2.23	0.68
7:O:1182:ASN:O	7:O:1186:SER:HB2	1.93	0.68
7:M:1182:ASN:O	7:M:1186:SER:HB2	1.93	0.68
10:U:262:ILE:HG22	10:U:265:SER:OG	1.92	0.68
9:S:547:TYR:HB3	11:X:298:PHE:CB	2.23	0.68
9:S:592:LYS:O	9:S:600:ILE:HD12	1.93	0.68
4:D:636:THR:O	4:D:637:LEU:HD23	1.94	0.68
7:M:1392:ILE:CG1	7:M:1437:LEU:HD12	2.22	0.68
7:M:1559:LEU:HD21	7:O:1642:LYS:CD	2.23	0.68
6:C:374:GLN:HA	6:C:374:GLN:NE2	2.09	0.68
4:J:793:LEU:HB3	6:L:439:ILE:HG22	1.72	0.67
3:1:494:ASN:HB3	3:1:512:ARG:CB	2.03	0.67
4:G:806:SER:OG	9:S:32:LEU:HA	1.93	0.67
5:K:322:ILE:HD12	5:K:322:ILE:O	1.92	0.67
4:D:793:LEU:HB3	6:F:439:ILE:HG22	1.72	0.67
9:Q:592:LYS:NZ	10:U:324:LYS:HD2	2.09	0.67
11:X:294:ILE:CA	11:X:361:ASN:HD21	2.06	0.67
6:C:371:LYS:N	6:C:371:LYS:HD2	2.09	0.67
7:M:1189:MET:HE3	8:N:249:ASP:HA	1.74	0.67
9:S:592:LYS:NZ	10:W:324:LYS:HD2	2.09	0.67
1:7:82:UNK:C	1:7:84:UNK:H	2.06	0.67
1:8:82:UNK:C	1:8:84:UNK:H	2.06	0.67
7:M:1188:THR:HB	8:N:248:GLN:HG3	1.75	0.67
7:M:1642:LYS:CD	7:O:1559:LEU:HD21	2.23	0.67
11:V:273:VAL:HB	11:V:356:VAL:HG23	1.23	0.67
11:X:289:SER:CA	11:X:294:ILE:HD11	2.02	0.67
2:0:517:LEU:O	2:0:517:LEU:HD22	1.94	0.67
8:N:306:VAL:HA	8:N:352:PHE:CE1	2.29	0.67
8:P:306:VAL:HA	8:P:352:PHE:CE1	2.30	0.67
4:D:636:THR:C	4:D:637:LEU:HD22	2.15	0.67
7:M:1429:ASP:CG	8:N:686:GLY:HA3	2.15	0.67
7:O:1188:THR:HB	8:P:248:GLN:HG3	1.75	0.67
5:B:323:LEU:CG	5:B:349:PRO:HG2	2.25	0.67
7:M:1382:TYR:HE2	8:N:748:HIS:HE2	1.33	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:413:LEU:HB2	6:I:373:PHE:HZ	1.45	0.67
11:X:273:VAL:HB	11:X:356:VAL:HG23	1.23	0.67
7:M:1562:ASP:CA	7:M:1580:VAL:HG13	2.23	0.66
8:N:225:ARG:O	8:N:228:ASN:CB	2.42	0.66
7:O:1562:ASP:CA	7:O:1580:VAL:HG13	2.23	0.66
8:P:227:ILE:HD11	8:P:255:GLU:HA	1.77	0.66
11:X:289:SER:CB	11:X:294:ILE:HD13	1.84	0.66
2:Y:516:LEU:HD12	2:Y:516:LEU:N	2.09	0.66
4:D:793:LEU:HB3	6:F:439:ILE:HG21	1.76	0.66
8:N:65:SER:H	8:N:83:VAL:HG21	1.60	0.66
3:1:922:LYS:HA	3:1:922:LYS:HE3	1.77	0.66
7:M:1382:TYR:CE1	8:N:748:HIS:CE1	2.82	0.66
11:V:355:TRP:CD1	11:V:400:ILE:CG2	2.78	0.66
8:P:273:LEU:HD13	8:P:328:ILE:CD1	2.24	0.66
9:T:675:VAL:HG22	9:T:728:PHE:CE2	2.11	0.66
3:Z:922:LYS:HE3	3:Z:922:LYS:HA	1.77	0.66
11:V:274:PHE:C	11:V:354:SER:O	2.34	0.66
4:J:793:LEU:HB3	6:L:439:ILE:HG21	1.76	0.66
5:K:371:GLN:O	5:K:375:ILE:HG13	1.96	0.66
7:O:1189:MET:CE	8:P:249:ASP:HA	2.23	0.66
10:W:266:ILE:HG12	10:W:336:ASN:CG	2.16	0.66
11:X:274:PHE:C	11:X:354:SER:O	2.34	0.66
1:7:76:UNK:O	9:R:429:THR:HG22	1.96	0.66
7:M:1429:ASP:O	7:M:1429:ASP:OD1	2.14	0.66
8:N:273:LEU:HD13	8:N:328:ILE:CD1	2.24	0.66
11:V:296:GLU:OE1	11:V:296:GLU:N	2.28	0.66
5:E:314:ASN:OD1	5:E:348:ILE:CD1	2.38	0.66
7:M:1580:VAL:HG23	7:M:1580:VAL:O	1.96	0.66
8:N:285:GLN:HG2	8:N:331:TYR:CE2	2.28	0.66
9:R:338:PHE:CZ	9:R:342:ARG:HD2	2.31	0.66
2:0:516:LEU:HA	2:0:537:LYS:HZ3	1.57	0.66
8:P:285:GLN:HG2	8:P:331:TYR:CE2	2.28	0.66
1:8:76:UNK:O	9:T:429:THR:HG22	1.96	0.66
6:C:369:LEU:N	6:C:369:LEU:HD23	2.11	0.66
8:N:267:ILE:CG2	8:N:271:LEU:HD11	2.26	0.66
3:1:493:ILE:CG2	3:1:494:ASN:N	2.36	0.66
7:O:1189:MET:H	8:P:248:GLN:CD	1.99	0.66
7:O:1580:VAL:HG23	7:O:1580:VAL:O	1.96	0.66
8:P:267:ILE:CG2	8:P:271:LEU:HD11	2.26	0.66
9:T:338:PHE:CZ	9:T:342:ARG:HD2	2.31	0.66
11:X:355:TRP:CD1	11:X:400:ILE:CG2	2.79	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:1019:ARG:HG3	9:R:246:ASN:HB2	1.77	0.66
9:R:675:VAL:HG22	9:R:728:PHE:CE2	2.11	0.66
2:0:1019:ARG:HG3	9:T:246:ASN:HB2	1.77	0.66
5:K:363:GLN:HG3	5:K:364:VAL:N	2.11	0.66
5:E:363:GLN:HG3	5:E:364:VAL:N	2.11	0.66
7:M:1189:MET:H	8:N:248:GLN:CD	1.99	0.66
5:K:371:GLN:HA	5:K:371:GLN:NE2	2.11	0.66
7:O:990:ILE:HB	7:O:999:LYS:NZ	2.11	0.66
10:W:304:LYS:HZ3	11:X:387:TYR:C	1.99	0.66
7:O:1560:GLY:CA	7:O:1580:VAL:CG2	2.73	0.66
11:X:294:ILE:HG22	11:X:361:ASN:ND2	2.11	0.66
7:M:335:ASP:H	7:M:771:ARG:NH2	1.94	0.65
7:M:1560:GLY:CA	7:M:1580:VAL:CG2	2.73	0.65
8:N:741:LYS:HA	8:N:744:LEU:HD23	1.75	0.65
4:A:800:HIS:ND1	9:Q:27:GLU:CB	2.58	0.65
9:R:435:TRP:CH2	9:R:474:PHE:CD1	2.84	0.65
7:O:335:ASP:H	7:O:771:ARG:NH2	1.94	0.65
9:T:435:TRP:CH2	9:T:474:PHE:CD1	2.84	0.65
7:M:1388:CYS:O	7:M:1392:ILE:HD12	1.95	0.65
5:K:317:ASN:HB2	5:K:348:ILE:CD1	2.24	0.65
7:M:1189:MET:HB3	8:N:248:GLN:C	2.17	0.65
7:O:990:ILE:HD11	7:O:996:LEU:HB2	1.78	0.65
7:O:1388:CYS:O	7:O:1392:ILE:HD12	1.95	0.65
9:Q:680:ASN:OD1	10:U:321:GLU:HB3	1.96	0.65
7:O:1189:MET:HB3	8:P:248:GLN:C	2.17	0.65
9:T:472:SER:O	9:T:473:ARG:HG2	1.97	0.65
10:W:248:TRP:HB2	11:X:346:LYS:O	1.97	0.65
10:U:248:TRP:HB2	11:V:346:LYS:O	1.97	0.65
10:U:322:LEU:HD12	10:U:325:SER:CB	2.27	0.65
3:1:1215:TYR:CB	3:1:1218:ILE:HG22	2.26	0.65
5:H:517:GLN:NE2	9:S:23:ASN:CB	2.60	0.65
6:L:353:LEU:HD11	6:L:369:LEU:HD12	1.77	0.65
9:S:680:ASN:OD1	10:W:321:GLU:HB3	1.96	0.65
1:8:76:UNK:CB	9:T:429:THR:OG1	2.45	0.65
5:B:323:LEU:CD1	5:B:338:ALA:C	2.50	0.65
7:O:1389:ILE:HG21	8:P:687:LYS:CB	2.27	0.65
10:W:304:LYS:NZ	11:X:387:TYR:C	2.50	0.65
10:W:322:LEU:HD12	10:W:325:SER:CB	2.27	0.65
3:Z:1215:TYR:HB2	3:Z:1218:ILE:HG12	1.77	0.65
8:N:216:TYR:N	8:N:220:PHE:CE1	2.65	0.65
9:R:472:SER:O	9:R:473:ARG:HG2	1.97	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:1174:LEU:C	3:Z:1177:VAL:HG12	2.15	0.64
3:Z:1191:LEU:CD1	3:Z:1215:TYR:HH	2.05	0.64
5:E:314:ASN:HD22	5:E:350:ILE:HG12	1.62	0.64
8:P:68:HIS:O	8:P:69:ASN:CB	2.45	0.64
11:V:298:PHE:CG	11:V:299:GLN:N	2.64	0.64
1:7:76:UNK:CB	9:R:429:THR:OG1	2.46	0.64
5:B:323:LEU:HG	5:B:342:LYS:HZ3	1.62	0.64
8:N:69:ASN:HB3	8:N:71:LEU:HG	1.78	0.64
4:D:636:THR:C	4:D:637:LEU:HD23	2.18	0.64
8:N:327:PHE:CD1	8:N:389:PHE:CD2	2.85	0.64
2:Y:517:LEU:O	2:Y:535:VAL:HG13	1.97	0.64
2:Y:1358:GLU:HB2	3:1:787:ALA:N	2.10	0.64
9:Q:596:ASP:OD1	9:Q:597:GLY:N	2.31	0.64
5:H:413:LEU:CB	6:I:373:PHE:CZ	2.56	0.64
5:K:322:ILE:HD13	5:K:323:LEU:HG	1.79	0.64
8:P:221:VAL:HG11	8:P:316:ILE:HG23	1.79	0.64
8:P:761:PHE:HZ	8:P:765:PHE:CE1	2.10	0.64
9:T:435:TRP:CH2	9:T:474:PHE:HE1	2.12	0.64
5:E:357:GLY:O	5:E:360:GLN:HG2	1.97	0.64
7:M:1380:ARG:H	7:M:1380:ARG:CD	2.08	0.64
8:N:1497:ASN:O	9:Q:146:LYS:CB	2.45	0.64
4:G:792:GLN:NE2	9:S:17:GLY:HA2	2.13	0.64
6:I:374:GLN:HA	6:I:374:GLN:NE2	2.12	0.64
7:O:444:THR:HG23	7:O:506:ASN:HD22	1.63	0.64
8:P:1497:ASN:O	9:S:146:LYS:CB	2.45	0.64
10:W:271:ALA:CB	10:W:283:ILE:HB	2.28	0.64
7:M:444:THR:HG23	7:M:506:ASN:HD22	1.63	0.64
7:M:1193:ARG:O	7:M:1194:LEU:C	2.35	0.64
8:N:216:TYR:N	8:N:220:PHE:HE1	1.95	0.64
8:N:761:PHE:HZ	8:N:765:PHE:CE1	2.10	0.64
9:R:435:TRP:CH2	9:R:474:PHE:HE1	2.12	0.64
9:R:577:ARG:HG3	9:R:623:ILE:HG23	1.79	0.64
10:W:280:PHE:HD2	10:W:282:VAL:HG13	1.61	0.64
1:7:76:UNK:C	9:R:429:THR:CG2	2.76	0.64
1:3:2:UNK:N	5:E:316:VAL:N	2.46	0.64
2:Y:1465:ILE:HG23	2:Y:1487:TYR:HB3	1.80	0.64
7:M:1393:ASN:HD21	8:N:687:LYS:NZ	1.95	0.64
2:0:1310:ASP:OD2	2:0:1311:PHE:CD2	2.49	0.64
7:O:1193:ARG:O	7:O:1194:LEU:C	2.35	0.64
7:O:1561:LEU:CA	7:O:1580:VAL:HG11	2.28	0.64
9:T:577:ARG:HG3	9:T:623:ILE:HG23	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:289:SER:HB3	11:X:294:ILE:HD11	0.66	0.64
1:8:76:UNK:C	9:T:429:THR:CG2	2.76	0.64
5:B:323:LEU:CD1	5:B:339:MET:CG	2.76	0.64
9:T:436:LEU:HD11	9:T:462:PHE:CE2	2.33	0.64
3:Z:1215:TYR:CB	3:Z:1218:ILE:CG1	2.73	0.63
7:M:1561:LEU:CA	7:M:1580:VAL:HG11	2.28	0.63
9:R:436:LEU:HD11	9:R:462:PHE:CE2	2.33	0.63
2:0:1465:ILE:HG23	2:0:1487:TYR:HB3	1.80	0.63
3:1:1199:VAL:O	3:1:1200:LEU:CG	2.46	0.63
3:1:922:LYS:HA	3:1:922:LYS:CE	2.29	0.63
5:K:517:GLN:CD	9:T:23:ASN:CB	2.64	0.63
7:O:384:MET:HG2	7:O:766:GLN:CD	2.12	0.63
10:W:271:ALA:HB2	10:W:283:ILE:HG22	1.79	0.63
3:Z:922:LYS:HA	3:Z:922:LYS:CE	2.29	0.63
7:M:333:GLU:O	7:M:771:ARG:NH2	2.31	0.63
8:N:249:ASP:OD1	8:N:835:LEU:HD21	1.97	0.63
9:R:675:VAL:CG2	9:R:728:PHE:CZ	2.78	0.63
2:0:1019:ARG:HB3	9:T:246:ASN:H	1.63	0.63
4:G:796:ILE:HG21	9:S:20:LYS:CB	2.28	0.63
7:O:333:GLU:O	7:O:771:ARG:NH2	2.31	0.63
10:W:266:ILE:HD11	10:W:336:ASN:HB2	1.80	0.63
1:3:4:UNK:CB	5:E:316:VAL:CG2	2.72	0.63
2:Y:1019:ARG:HB3	9:R:246:ASN:H	1.63	0.63
3:Z:493:ILE:HD12	3:Z:511:VAL:CG1	2.29	0.63
5:E:510:VAL:HG11	9:R:16:LYS:CB	2.28	0.63
8:N:744:LEU:HD11	8:N:745:HIS:CE1	2.32	0.63
11:V:274:PHE:CE1	11:V:383:GLY:O	2.52	0.63
3:1:493:ILE:HG21	3:1:512:ARG:O	1.97	0.63
4:G:810:ASN:CB	9:S:35:ALA:HB1	2.23	0.63
9:T:675:VAL:CG2	9:T:728:PHE:CZ	2.78	0.63
11:X:274:PHE:CE1	11:X:383:GLY:O	2.52	0.63
11:X:297:ASP:OD1	11:X:301:LEU:HG	1.98	0.63
5:E:380:LEU:HD11	6:F:314:TYR:CE2	2.34	0.63
7:M:1379:GLY:O	7:M:1383:GLN:NE2	2.31	0.63
2:0:1019:ARG:HB3	9:T:246:ASN:HB2	1.80	0.63
3:Z:1177:VAL:HG11	3:Z:1195:LEU:HD12	1.79	0.63
8:N:71:LEU:HB3	8:N:164:TYR:CE1	2.30	0.63
5:K:380:LEU:HD11	6:L:314:TYR:CE2	2.34	0.63
2:Y:516:LEU:HD12	2:Y:516:LEU:H	1.63	0.62
3:Z:1165:ASP:O	3:Z:1169:ILE:HG13	1.99	0.62
7:M:384:MET:HG2	7:M:766:GLN:CD	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:274:GLY:C	8:N:284:ILE:CB	2.67	0.62
9:R:671:ASP:N	9:R:671:ASP:OD1	2.28	0.62
7:O:1376:THR:HG21	7:O:1380:ARG:HB2	1.81	0.62
7:O:1379:GLY:O	7:O:1383:GLN:NE2	2.31	0.62
9:T:671:ASP:OD1	9:T:671:ASP:N	2.28	0.62
2:Y:1019:ARG:HB3	9:R:246:ASN:HB2	1.81	0.62
3:1:1165:ASP:O	3:1:1169:ILE:HG13	1.99	0.62
8:P:613:GLU:CB	8:P:617:TYR:CD2	2.81	0.62
3:Z:1209:CYS:O	3:Z:1213:LEU:CG	2.47	0.62
8:N:761:PHE:CG	8:N:761:PHE:O	2.52	0.62
11:V:273:VAL:C	11:V:356:VAL:H	2.02	0.62
6:I:371:LYS:N	6:I:371:LYS:HD2	2.14	0.62
7:M:1562:ASP:N	7:M:1580:VAL:HG13	2.13	0.62
8:N:613:GLU:CB	8:N:617:TYR:CD2	2.81	0.62
3:1:496:THR:O	3:1:498:ALA:N	2.33	0.62
3:1:1173:LEU:HD12	3:1:1195:LEU:HD13	1.80	0.62
8:P:274:GLY:C	8:P:284:ILE:CB	2.68	0.62
3:Z:1215:TYR:O	3:Z:1218:ILE:HG12	1.99	0.62
5:K:316:VAL:CG1	5:K:348:ILE:CG1	2.72	0.62
11:X:296:GLU:O	11:X:346:LYS:CG	2.42	0.62
5:E:364:VAL:O	5:E:367:GLU:HG2	1.99	0.62
7:M:1490:ARG:HH12	9:R:825:PRO:HA	1.64	0.62
9:Q:589:LEU:O	9:Q:603:VAL:HG22	2.00	0.62
7:O:1562:ASP:N	7:O:1580:VAL:HG13	2.13	0.62
8:P:761:PHE:CG	8:P:761:PHE:O	2.52	0.62
6:F:455:GLU:OE1	6:F:456:ARG:CD	2.39	0.62
2:0:1019:ARG:HB3	9:T:246:ASN:CB	2.30	0.62
9:T:407:TYR:CD1	9:T:428:VAL:CG1	2.83	0.62
11:X:273:VAL:C	11:X:356:VAL:H	2.03	0.62
5:E:316:VAL:O	5:E:348:ILE:HD12	1.98	0.62
8:N:277:THR:HG22	8:N:381:VAL:CG2	2.30	0.62
9:R:407:TYR:CD1	9:R:428:VAL:CG1	2.83	0.62
7:O:1490:ARG:HH12	9:T:825:PRO:HA	1.64	0.62
2:Y:1019:ARG:HB3	9:R:246:ASN:CB	2.30	0.62
3:Z:1191:LEU:CD2	3:Z:1213:LEU:CD2	2.76	0.62
4:D:673:GLY:HA3	5:E:315:LYS:HZ2	1.65	0.62
9:R:676:GLY:N	9:R:677:PRO:CD	2.63	0.62
6:L:371:LYS:HD3	6:L:371:LYS:H	1.65	0.62
8:P:277:THR:HG22	8:P:381:VAL:CG2	2.30	0.62
2:Y:1019:ARG:HB3	9:R:246:ASN:N	2.15	0.62
3:Z:1173:LEU:HD22	3:Z:1205:LEU:HD21	1.78	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:D:800:HIS:CE1	5:E:517:GLN:OE1	2.53	0.61
9:Q:601:PRO:CB	9:Q:605:GLU:HB2	2.16	0.61
9:T:676:GLY:N	9:T:677:PRO:CD	2.63	0.61
7:M:1379:GLY:HA3	7:M:1380:ARG:NH1	2.15	0.61
7:M:1389:ILE:HD13	7:M:1389:ILE:N	2.15	0.61
2:0:1019:ARG:HB3	9:T:246:ASN:N	2.15	0.61
6:L:434:THR:CA	6:L:438:ALA:HB2	2.13	0.61
9:T:159:PHE:HA	9:T:162:LEU:CB	2.30	0.61
11:X:296:GLU:OE1	11:X:296:GLU:N	2.33	0.61
3:Z:1173:LEU:HD21	3:Z:1205:LEU:CD2	2.29	0.61
3:Z:1213:LEU:HD12	3:Z:1215:TYR:H	1.65	0.61
3:1:1191:LEU:HD22	3:1:1215:TYR:CE2	2.34	0.61
7:O:1389:ILE:HD13	7:O:1389:ILE:N	2.15	0.61
3:Z:1174:LEU:CA	3:Z:1177:VAL:HG12	2.30	0.61
11:V:355:TRP:HZ2	11:V:401:ASP:C	2.04	0.61
3:1:1191:LEU:CD1	3:1:1215:TYR:OH	2.47	0.61
8:P:761:PHE:CD1	8:P:764:LYS:HD3	2.32	0.61
11:X:355:TRP:HZ2	11:X:401:ASP:C	2.04	0.61
1:8:80:UNK:CB	9:T:430:LEU:O	2.48	0.61
1:7:80:UNK:CB	9:R:430:LEU:O	2.48	0.61
3:Z:1174:LEU:HA	3:Z:1177:VAL:CG1	2.31	0.61
8:N:761:PHE:CD1	8:N:764:LYS:HD3	2.32	0.61
10:U:268:LEU:CA	10:U:283:ILE:CD1	1.74	0.61
3:1:1170:GLN:HA	3:1:1173:LEU:CD2	2.31	0.61
3:1:1199:VAL:O	3:1:1200:LEU:HG	2.00	0.61
4:D:637:LEU:HD22	4:D:637:LEU:N	2.14	0.61
4:J:803:ALA:HA	9:T:31:ASN:CB	2.31	0.61
7:O:336:LYS:HG2	7:O:771:ARG:HD3	1.81	0.61
3:Z:1213:LEU:CD1	3:Z:1215:TYR:N	2.63	0.61
4:D:793:LEU:CB	6:F:439:ILE:CG2	2.74	0.61
7:M:336:LYS:HG2	7:M:771:ARG:HD3	1.81	0.61
9:Q:573:HIS:CD2	9:Q:623:ILE:HD11	2.36	0.61
9:R:312:LYS:HE2	9:R:430:LEU:CD2	2.26	0.61
9:S:573:HIS:CD2	9:S:623:ILE:HD11	2.36	0.61
3:1:1170:GLN:OE1	3:1:1205:LEU:HD22	1.99	0.60
4:J:793:LEU:CB	6:L:439:ILE:CG2	2.74	0.60
7:O:1671:VAL:CG1	9:T:166:LYS:CA	2.69	0.60
9:T:680:ASN:HB2	9:T:683:THR:HG22	1.82	0.60
3:Z:1170:GLN:HA	3:Z:1173:LEU:CD2	2.31	0.60
7:M:1389:ILE:CG2	8:N:687:LYS:CD	2.79	0.60
5:K:317:ASN:CG	5:K:320:GLU:OE2	2.39	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:312:LYS:HE2	9:T:430:LEU:CD2	2.26	0.60
1:7:76:UNK:CA	9:R:429:THR:CG2	2.79	0.60
7:M:1378:ASP:O	7:M:1379:GLY:C	2.40	0.60
9:R:680:ASN:HB2	9:R:683:THR:HG22	1.82	0.60
11:V:271:ILE:HG22	11:V:271:ILE:O	2.01	0.60
5:K:361:ARG:O	5:K:365:GLN:HG3	2.01	0.60
11:X:271:ILE:HG22	11:X:271:ILE:O	2.01	0.60
11:X:361:ASN:C	11:X:361:ASN:OD1	2.39	0.60
2:Y:516:LEU:H	2:Y:516:LEU:CD1	2.15	0.60
7:O:1378:ASP:O	7:O:1379:GLY:C	2.40	0.60
11:X:355:TRP:HZ2	11:X:401:ASP:O	1.84	0.60
3:Z:1173:LEU:CD1	3:Z:1195:LEU:HD22	2.32	0.60
7:M:384:MET:CB	7:M:766:GLN:HE22	2.14	0.60
11:V:273:VAL:HG21	11:V:358:LEU:HG	1.82	0.60
11:V:355:TRP:HZ2	11:V:401:ASP:O	1.84	0.60
7:O:384:MET:CB	7:O:766:GLN:HE22	2.15	0.60
11:X:273:VAL:HG21	11:X:358:LEU:HG	1.81	0.60
1:8:76:UNK:CA	9:T:429:THR:CG2	2.79	0.60
5:E:436:MET:SD	6:F:370:ASP:HB3	2.41	0.60
9:Q:547:TYR:HB3	11:V:298:PHE:CD1	2.36	0.60
7:O:1392:ILE:HG22	7:O:1392:ILE:O	2.01	0.60
3:Z:1213:LEU:HD13	3:Z:1215:TYR:CD2	2.22	0.60
5:E:436:MET:SD	6:F:370:ASP:CB	2.90	0.60
8:N:350:ALA:O	8:N:354:GLU:HG2	2.01	0.60
8:P:350:ALA:O	8:P:354:GLU:HG2	2.01	0.60
3:Z:1210:ALA:HB1	3:Z:1218:ILE:HG13	1.84	0.60
5:B:323:LEU:HD12	5:B:339:MET:CA	1.95	0.60
7:M:1392:ILE:O	7:M:1392:ILE:HG22	2.01	0.60
7:O:1381:LEU:HG	7:O:1385:PHE:CE2	2.37	0.60
3:Z:1195:LEU:O	3:Z:1197:GLY:N	2.35	0.60
7:M:383:ASN:ND2	7:M:767:ILE:HG23	2.16	0.60
9:Q:601:PRO:HB3	9:Q:605:GLU:CD	2.22	0.60
7:O:383:ASN:ND2	7:O:767:ILE:HG23	2.16	0.60
1:3:2:UNK:C	5:E:316:VAL:HB	2.32	0.60
8:N:249:ASP:OD2	8:N:835:LEU:HG	2.01	0.60
10:U:284:LYS:HG2	10:U:284:LYS:O	2.02	0.60
3:1:1177:VAL:CG2	3:1:1215:TYR:OH	2.49	0.60
3:Z:1174:LEU:HA	3:Z:1195:LEU:HD13	1.84	0.59
2:0:1309:ASN:OD1	2:0:1310:ASP:N	2.35	0.59
3:1:494:ASN:O	3:1:511:VAL:HA	2.02	0.59
7:O:1376:THR:O	7:O:1380:ARG:NH2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:1213:LEU:CD1	3:Z:1215:TYR:CE2	2.84	0.59
8:N:327:PHE:CA	8:N:389:PHE:HE2	2.15	0.59
7:O:125:HIS:CG	7:O:126:GLU:H	2.19	0.59
2:Y:515:VAL:O	2:Y:537:LYS:NZ	2.34	0.59
2:Y:1309:ASN:OD1	2:Y:1310:ASP:N	2.35	0.59
7:M:125:HIS:CG	7:M:126:GLU:H	2.19	0.59
7:O:1189:MET:O	7:O:1189:MET:HE2	2.02	0.59
3:Z:1209:CYS:O	3:Z:1213:LEU:CD2	2.49	0.59
2:0:1310:ASP:CG	2:0:1311:PHE:CE2	2.74	0.59
4:J:665:TRP:CZ3	5:K:365:GLN:NE2	2.71	0.59
5:K:331:LEU:HD23	5:K:331:LEU:H	1.68	0.59
5:E:331:LEU:HD23	5:E:331:LEU:H	1.68	0.59
8:N:225:ARG:O	8:N:229:SER:N	2.35	0.59
4:D:670:VAL:HG12	5:E:315:LYS:HG3	1.85	0.59
10:U:313:TRP:HE1	10:U:358:LYS:H	1.50	0.59
7:O:245:ARG:H	7:O:245:ARG:HD3	1.67	0.59
7:M:245:ARG:H	7:M:245:ARG:HD3	1.68	0.59
7:M:1377:VAL:O	7:M:1377:VAL:HG12	2.03	0.59
9:R:282:PHE:CE1	9:R:342:ARG:CZ	2.85	0.59
11:V:274:PHE:HA	11:V:354:SER:O	2.02	0.59
3:1:1215:TYR:HB2	3:1:1218:ILE:HG21	1.83	0.59
10:W:313:TRP:HE1	10:W:358:LYS:H	1.50	0.59
3:Z:1177:VAL:CG2	3:Z:1215:TYR:OH	2.51	0.59
10:U:268:LEU:HD12	10:U:283:ILE:HG12	1.80	0.59
7:O:1382:TYR:HD2	8:P:748:HIS:HD1	1.44	0.59
9:T:282:PHE:CE1	9:T:342:ARG:CZ	2.85	0.59
10:W:304:LYS:HD3	11:X:387:TYR:O	2.03	0.59
7:M:384:MET:CA	7:M:766:GLN:OE1	2.41	0.59
8:N:327:PHE:HA	8:N:389:PHE:CE2	2.37	0.59
9:R:73:LEU:CB	9:S:72:LEU:CB	2.81	0.59
11:V:289:SER:HA	11:V:294:ILE:CD1	2.28	0.59
7:M:1389:ILE:HG21	8:N:687:LYS:CB	2.27	0.59
7:M:1561:LEU:CA	7:M:1580:VAL:HG21	2.30	0.59
8:N:1259:PHE:HZ	9:Q:133:ILE:CB	2.16	0.59
3:1:494:ASN:HB2	3:1:512:ARG:N	2.17	0.59
7:O:384:MET:CA	7:O:766:GLN:OE1	2.41	0.59
8:P:613:GLU:OE2	8:P:617:TYR:CG	2.55	0.59
11:X:274:PHE:HA	11:X:354:SER:O	2.03	0.59
1:8:70:UNK:CB	9:T:469:TYR:CZ	2.85	0.58
10:U:322:LEU:HD12	10:U:325:SER:HB2	1.84	0.58
6:I:376:LYS:HB2	6:I:376:LYS:NZ	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:N:613:GLU:OE2	8:N:617:TYR:CG	2.55	0.58
8:P:1259:PHE:HZ	9:S:133:ILE:CB	2.16	0.58
5:B:322:ILE:HD12	5:B:322:ILE:O	2.02	0.58
11:V:273:VAL:O	11:V:355:TRP:CA	2.51	0.58
7:O:1561:LEU:CA	7:O:1580:VAL:HG21	2.30	0.58
9:S:584:LYS:HE2	9:S:636:ARG:CD	2.32	0.58
10:W:271:ALA:CB	10:W:283:ILE:HG22	2.33	0.58
10:W:322:LEU:HD12	10:W:325:SER:HB2	1.85	0.58
9:Q:115:ILE:O	9:Q:120:GLU:CB	2.51	0.58
3:1:494:ASN:HB2	3:1:512:ARG:O	2.04	0.58
10:W:271:ALA:HB1	10:W:283:ILE:HB	1.84	0.58
11:X:273:VAL:O	11:X:355:TRP:CA	2.51	0.58
11:V:273:VAL:O	11:V:356:VAL:N	2.35	0.58
5:H:524:ASN:ND2	9:S:30:ASP:CB	2.67	0.58
3:Z:1185:GLU:OE2	3:Z:1188:ARG:HD2	2.03	0.58
8:P:613:GLU:HB3	8:P:617:TYR:CD2	2.39	0.58
10:W:330:GLU:HG3	10:W:330:GLU:O	2.03	0.58
5:E:517:GLN:HE21	9:R:24:GLU:C	1.95	0.58
8:N:56:ASN:HD22	8:N:144:ILE:HG12	1.68	0.58
8:N:613:GLU:HB3	8:N:617:TYR:CD2	2.39	0.58
4:G:809:ASP:OD1	9:S:35:ALA:O	2.22	0.58
8:P:56:ASN:HD22	8:P:144:ILE:HG12	1.68	0.58
8:P:529:LEU:CD2	8:P:531:ILE:CD1	2.79	0.58
3:Z:1130:ARG:NH2	3:Z:1198:ARG:HE	2.01	0.58
6:L:353:LEU:HD11	6:L:369:LEU:HD13	1.84	0.58
11:X:273:VAL:O	11:X:356:VAL:N	2.35	0.58
3:Z:407:ALA:HB1	3:Z:495:THR:HB	1.86	0.58
7:M:1389:ILE:CD1	8:N:686:GLY:O	2.51	0.58
9:R:339:TYR:HD1	9:R:342:ARG:HD3	1.69	0.58
7:O:1382:TYR:CE1	8:P:744:LEU:CD2	2.87	0.58
2:Y:1019:ARG:HG3	9:R:246:ASN:CB	2.33	0.58
5:E:314:ASN:OD1	5:E:316:VAL:O	2.21	0.58
5:H:322:ILE:CG2	5:H:335:TRP:CH2	2.83	0.58
7:O:1389:ILE:CD1	8:P:686:GLY:O	2.51	0.58
10:W:271:ALA:CB	10:W:283:ILE:CG2	2.82	0.58
11:X:296:GLU:O	11:X:346:LYS:CE	2.51	0.58
9:T:339:TYR:HD1	9:T:342:ARG:HD3	1.69	0.57
10:W:276:ILE:CG2	10:W:282:VAL:HG21	2.26	0.57
2:Y:443:GLY:CA	2:Y:519:THR:OG1	2.52	0.57
6:L:369:LEU:HD23	6:L:369:LEU:C	2.23	0.57
7:O:990:ILE:CD1	7:O:996:LEU:HB2	2.34	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1381:LEU:CG	7:O:1385:PHE:CE2	2.87	0.57
7:M:1392:ILE:HG21	7:M:1437:LEU:CB	2.34	0.57
3:1:917:GLU:CG	3:1:918:MET:H	1.95	0.57
3:Z:917:GLU:CG	3:Z:918:MET:H	1.95	0.57
7:M:335:ASP:N	7:M:771:ARG:NH2	2.53	0.57
8:N:225:ARG:C	8:N:228:ASN:HB2	2.23	0.57
2:0:1019:ARG:HG3	9:T:246:ASN:CB	2.33	0.57
8:P:286:SER:HB2	8:P:287:PRO:HD3	1.85	0.57
3:Z:1210:ALA:HA	3:Z:1218:ILE:HD11	1.86	0.57
5:B:323:LEU:CD1	5:B:339:MET:HG3	2.32	0.57
8:N:286:SER:HB2	8:N:287:PRO:HD3	1.85	0.57
7:O:335:ASP:N	7:O:771:ARG:NH2	2.53	0.57
5:B:323:LEU:CB	5:B:323:LEU:HG	2.35	0.57
7:M:383:ASN:O	7:M:766:GLN:HB2	2.03	0.57
7:O:1392:ILE:HG21	7:O:1437:LEU:CB	2.34	0.57
3:Z:1213:LEU:HD13	3:Z:1215:TYR:CZ	2.39	0.57
9:R:61:LYS:O	9:R:62:ALA:HB2	2.05	0.57
2:0:517:LEU:H	2:0:537:LYS:HZ2	1.52	0.57
3:1:599:LEU:HD23	3:1:599:LEU:H	1.70	0.57
5:K:380:LEU:HD22	6:L:314:TYR:CE2	2.33	0.57
7:O:384:MET:HG2	7:O:766:GLN:HE21	1.52	0.57
5:B:323:LEU:HD21	5:B:338:ALA:O	2.01	0.57
7:M:1395:PRO:HD2	7:M:1396:LEU:H	1.70	0.57
9:T:61:LYS:O	9:T:62:ALA:HB2	2.05	0.57
10:W:276:ILE:HG21	10:W:282:VAL:CG2	2.32	0.57
3:Z:599:LEU:HD23	3:Z:599:LEU:H	1.70	0.57
8:N:64:SER:HB3	8:N:73:SER:CB	2.31	0.57
8:N:65:SER:OG	8:N:83:VAL:CG1	2.39	0.57
7:O:383:ASN:O	7:O:766:GLN:HB2	2.03	0.57
7:O:1395:PRO:HD2	7:O:1396:LEU:H	1.70	0.57
4:D:673:GLY:HA3	5:E:315:LYS:HZ1	1.68	0.56
5:E:380:LEU:HD22	6:F:314:TYR:CE2	2.33	0.56
8:N:267:ILE:CG2	8:N:271:LEU:CD1	2.79	0.56
5:K:316:VAL:HG12	5:K:348:ILE:HG13	1.85	0.56
5:K:325:THR:O	5:K:326:LYS:HG2	2.05	0.56
8:P:68:HIS:O	8:P:69:ASN:CG	2.43	0.56
5:E:314:ASN:HD21	5:E:348:ILE:CG1	2.13	0.56
7:M:1391:GLY:C	7:M:1393:ASN:H	2.08	0.56
7:M:1579:ASN:ND2	9:T:173:LYS:O	2.38	0.56
9:Q:601:PRO:CB	9:Q:605:GLU:CB	2.80	0.56
3:1:1183:ILE:HG21	3:1:1213:LEU:CD1	2.35	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:L:353:LEU:CD1	6:L:369:LEU:HD12	2.33	0.56
6:L:371:LYS:H	6:L:371:LYS:CD	2.18	0.56
3:Z:1215:TYR:O	3:Z:1218:ILE:CG1	2.54	0.56
5:E:510:VAL:CG1	9:R:16:LYS:CB	2.83	0.56
6:F:394:ILE:CD1	9:R:40:GLY:O	2.52	0.56
7:M:335:ASP:OD1	7:M:857:GLY:HA3	2.05	0.56
7:M:384:MET:HG2	7:M:766:GLN:HE21	1.52	0.56
9:R:690:ARG:HG3	9:R:718:LEU:HD22	1.87	0.56
3:1:1210:ALA:CB	3:1:1218:ILE:HG23	2.34	0.56
5:K:371:GLN:HA	5:K:371:GLN:HE21	1.69	0.56
7:O:335:ASP:OD1	7:O:857:GLY:HA3	2.05	0.56
7:O:1385:PHE:HE1	7:O:1426:VAL:CG2	2.12	0.56
8:P:267:ILE:CG2	8:P:271:LEU:CD1	2.79	0.56
9:T:690:ARG:HG3	9:T:718:LEU:HD22	1.87	0.56
11:X:274:PHE:CB	11:X:355:TRP:CD2	2.80	0.56
1:7:76:UNK:HA	9:R:429:THR:HB	1.86	0.56
1:8:76:UNK:HA	9:T:429:THR:HB	1.86	0.56
5:K:380:LEU:HD21	6:L:314:TYR:CZ	2.40	0.56
1:7:76:UNK:C	9:R:429:THR:HG22	2.36	0.56
8:N:221:VAL:O	8:N:225:ARG:HG3	2.05	0.56
11:V:274:PHE:CB	11:V:355:TRP:CD2	2.81	0.56
4:J:778:LYS:H	5:K:473:ILE:HD12	1.69	0.56
7:O:1391:GLY:C	7:O:1393:ASN:H	2.08	0.56
9:S:584:LYS:CE	9:S:636:ARG:HD2	2.34	0.56
4:D:778:LYS:H	5:E:473:ILE:HD12	1.69	0.56
5:E:380:LEU:HD21	6:F:314:TYR:CZ	2.40	0.56
11:V:273:VAL:HG23	11:V:356:VAL:C	2.25	0.56
11:X:273:VAL:HG23	11:X:356:VAL:C	2.25	0.56
7:M:1392:ILE:HD12	7:M:1392:ILE:H	1.69	0.56
7:O:1392:ILE:HD12	7:O:1392:ILE:H	1.69	0.56
8:N:270:ILE:O	8:N:275:LEU:HB2	2.05	0.56
3:1:1191:LEU:HD11	3:1:1213:LEU:HB2	1.86	0.56
4:G:796:ILE:CG2	9:S:20:LYS:CB	2.83	0.56
8:P:270:ILE:O	8:P:275:LEU:HB2	2.06	0.56
1:8:76:UNK:C	9:T:429:THR:HG22	2.36	0.56
3:Z:789:ASP:OD2	2:0:1358:GLU:HA	2.06	0.56
7:M:1384:LEU:HD13	7:M:1412:TYR:CG	2.41	0.56
11:V:275:GLY:O	11:V:354:SER:CA	2.53	0.56
5:K:320:GLU:OE2	5:K:320:GLU:HA	2.06	0.56
7:O:1193:ARG:C	7:O:1195:PHE:N	2.59	0.56
11:X:275:GLY:O	11:X:354:SER:CA	2.53	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1193:ARG:C	7:M:1195:PHE:N	2.59	0.55
9:Q:588:VAL:O	9:Q:603:VAL:CG1	2.54	0.55
9:R:638:TYR:C	9:R:638:TYR:CD2	2.79	0.55
3:1:1183:ILE:CG2	3:1:1184:ASP:H	2.19	0.55
6:L:456:ARG:HE	9:T:61:LYS:CB	2.18	0.55
1:8:72:UNK:CB	9:T:426:PRO:CG	2.84	0.55
6:F:456:ARG:HE	9:R:61:LYS:CB	2.18	0.55
8:P:761:PHE:CE1	8:P:764:LYS:CD	2.58	0.55
8:N:277:THR:HG23	8:N:381:VAL:HG21	1.88	0.55
8:N:327:PHE:HA	8:N:389:PHE:HE2	1.71	0.55
9:R:672:GLN:CB	9:R:673:PRO:CD	2.73	0.55
3:1:1215:TYR:CB	3:1:1218:ILE:CG2	2.84	0.55
5:K:317:ASN:CB	5:K:348:ILE:HD11	2.35	0.55
7:O:1392:ILE:HG12	7:O:1437:LEU:CB	2.37	0.55
8:P:277:THR:HG23	8:P:381:VAL:HG21	1.88	0.55
9:T:638:TYR:C	9:T:638:TYR:CD2	2.79	0.55
5:E:360:GLN:C	5:E:363:GLN:HG2	2.26	0.55
7:M:1392:ILE:HG12	7:M:1437:LEU:CB	2.37	0.55
8:N:227:ILE:CD1	8:N:258:ILE:HG21	2.28	0.55
8:N:761:PHE:CE1	8:N:764:LYS:CD	2.58	0.55
7:O:1384:LEU:HD13	7:O:1412:TYR:CG	2.42	0.55
9:T:672:GLN:CB	9:T:673:PRO:CD	2.73	0.55
1:7:72:UNK:CB	9:R:426:PRO:HG3	2.37	0.55
3:Z:1213:LEU:CD1	3:Z:1215:TYR:H	2.20	0.55
6:C:371:LYS:HD2	6:C:371:LYS:H	1.70	0.55
7:M:1389:ILE:O	7:M:1393:ASN:HB2	2.07	0.55
2:0:163:GLU:HB3	2:0:186:ILE:HG21	1.87	0.55
5:K:360:GLN:C	5:K:363:GLN:HG2	2.26	0.55
9:T:518:ILE:HD11	9:T:535:ALA:HB2	1.89	0.55
9:R:518:ILE:HD11	9:R:535:ALA:HB2	1.89	0.55
2:Y:163:GLU:HB3	2:Y:186:ILE:HG21	1.87	0.55
3:Z:493:ILE:HD12	3:Z:511:VAL:HG12	1.87	0.55
8:N:613:GLU:OE1	8:N:617:TYR:CD1	2.58	0.55
8:P:613:GLU:OE1	8:P:617:TYR:CD1	2.58	0.55
9:S:599:ARG:NH2	9:S:605:GLU:OE1	2.40	0.55
9:T:301:ASN:HB3	9:T:345:LEU:HD13	1.87	0.55
10:U:268:LEU:CB	10:U:283:ILE:CD1	2.80	0.55
11:V:355:TRP:CZ2	11:V:401:ASP:N	2.75	0.55
7:O:1389:ILE:O	7:O:1393:ASN:HB2	2.07	0.55
7:O:1500:ASN:HD21	7:O:1551:SER:HB2	1.70	0.55
5:E:314:ASN:HD22	5:E:350:ILE:CG1	2.19	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:R:301:ASN:HB3	9:R:345:LEU:HD13	1.87	0.55
8:P:55:LEU:CD1	8:P:109:ARG:HE	2.19	0.55
10:W:252:ALA:HB3	10:W:345:TYR:CE1	2.42	0.55
7:M:1500:ASN:HD21	7:M:1551:SER:HB2	1.70	0.55
8:N:55:LEU:CD1	8:N:109:ARG:HE	2.19	0.55
10:U:252:ALA:HB3	10:U:345:TYR:CE1	2.42	0.55
3:1:928:LEU:HD11	3:1:957:LEU:HD23	1.89	0.55
9:T:35:ALA:O	9:T:39:LEU:N	2.35	0.55
3:Z:1199:VAL:O	3:Z:1200:LEU:CD2	2.49	0.54
4:D:765:LEU:HD23	5:E:460:TRP:CE2	2.42	0.54
4:J:765:LEU:HD23	5:K:460:TRP:CE2	2.42	0.54
3:Z:928:LEU:HD11	3:Z:957:LEU:HD23	1.89	0.54
4:D:636:THR:O	4:D:637:LEU:CD2	2.53	0.54
7:M:1189:MET:N	8:N:248:GLN:CD	2.60	0.54
8:N:274:GLY:O	8:N:284:ILE:CB	2.55	0.54
9:Q:601:PRO:HB3	9:Q:605:GLU:OE1	2.07	0.54
3:1:1169:ILE:HG22	3:1:1218:ILE:HD11	1.89	0.54
8:P:288:LEU:CD1	8:P:328:ILE:HG22	2.30	0.54
8:N:249:ASP:OD1	8:N:835:LEU:CD2	2.55	0.54
7:O:1189:MET:N	8:P:248:GLN:CD	2.60	0.54
8:P:274:GLY:O	8:P:284:ILE:CB	2.55	0.54
3:Z:787:ALA:N	2:0:1358:GLU:HB2	2.20	0.54
8:N:613:GLU:HB3	8:N:617:TYR:CE2	2.42	0.54
11:V:355:TRP:CE2	11:V:401:ASP:O	2.60	0.54
3:1:1191:LEU:HD12	3:1:1213:LEU:CD2	2.09	0.54
11:X:289:SER:HB2	11:X:300:VAL:HG21	1.90	0.54
11:X:355:TRP:CE2	11:X:401:ASP:O	2.60	0.54
5:E:457:ASN:HA	5:E:460:TRP:HD1	1.72	0.54
7:M:1376:THR:HG21	7:M:1415:ARG:HH21	1.72	0.54
8:N:288:LEU:CD1	8:N:328:ILE:HG22	2.30	0.54
9:Q:595:ARG:HD2	10:U:329:GLN:HE21	1.72	0.54
3:1:1198:ARG:HG3	3:1:1199:VAL:N	2.22	0.54
8:P:613:GLU:HB3	8:P:617:TYR:CE2	2.42	0.54
9:S:593:ILE:HG21	9:S:599:ARG:CA	2.37	0.54
11:X:355:TRP:CZ2	11:X:401:ASP:N	2.76	0.54
3:Z:1173:LEU:HD11	3:Z:1195:LEU:HD22	1.89	0.54
5:B:317:ASN:HD22	5:B:346:GLN:HB3	1.73	0.54
5:K:371:GLN:HE21	5:K:371:GLN:CA	2.18	0.54
5:E:316:VAL:O	5:E:348:ILE:CD1	2.56	0.54
9:Q:597:GLY:O	9:Q:598:ALA:HB3	2.07	0.54
2:0:989:GLN:HG2	2:0:1001:ILE:HD11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:584:LYS:CE	9:S:636:ARG:CD	2.85	0.54
1:8:77:UNK:CB	9:T:435:TRP:NE1	2.71	0.54
2:Y:989:GLN:HG2	2:Y:1001:ILE:HD11	1.89	0.54
7:M:1189:MET:HG2	8:N:248:GLN:CA	2.31	0.54
8:N:55:LEU:HD21	8:N:109:ARG:NH2	2.19	0.54
2:0:135:PHE:CE2	2:0:515:VAL:HG21	2.43	0.54
5:K:457:ASN:HA	5:K:460:TRP:HD1	1.72	0.54
8:P:68:HIS:O	8:P:69:ASN:HB2	2.07	0.54
1:7:74:UNK:HA	9:R:473:ARG:HG3	1.90	0.54
7:M:334:GLN:HA	7:M:334:GLN:NE2	2.22	0.54
7:M:1189:MET:HE3	8:N:252:TYR:CB	2.28	0.54
11:V:355:TRP:HZ2	11:V:401:ASP:CA	2.21	0.54
3:1:494:ASN:O	3:1:512:ARG:N	2.38	0.54
4:G:810:ASN:CG	9:S:35:ALA:CB	2.76	0.54
6:I:342:GLU:HB3	6:I:372:PHE:HE1	1.73	0.54
5:K:317:ASN:HD21	5:K:320:GLU:CD	2.10	0.54
1:7:77:UNK:CB	9:R:435:TRP:NE1	2.71	0.54
7:M:984:THR:O	7:M:988:SER:CB	2.55	0.54
2:0:1019:ARG:NH1	9:T:245:ALA:HA	2.17	0.54
7:O:1392:ILE:CD1	7:O:1437:LEU:CD1	2.79	0.54
9:Q:588:VAL:CG1	9:Q:603:VAL:HG11	2.38	0.53
7:O:334:GLN:HA	7:O:334:GLN:NE2	2.22	0.53
7:O:1189:MET:HG2	8:P:248:GLN:CA	2.31	0.53
10:W:252:ALA:HB3	10:W:345:TYR:CZ	2.44	0.53
10:W:262:ILE:HG13	10:W:336:ASN:CB	2.36	0.53
3:Z:140:ARG:HH22	3:Z:144:THR:H	1.56	0.53
3:Z:1234:ILE:HD13	3:Z:1282:VAL:HA	1.90	0.53
7:M:1392:ILE:CD1	7:M:1437:LEU:CD1	2.79	0.53
10:U:252:ALA:HB3	10:U:345:TYR:CZ	2.44	0.53
2:0:516:LEU:CB	2:0:537:LYS:HD3	2.39	0.53
3:1:1234:ILE:HD13	3:1:1282:VAL:HA	1.90	0.53
8:P:55:LEU:HD21	8:P:109:ARG:NH2	2.19	0.53
6:C:371:LYS:H	6:C:371:LYS:CD	2.20	0.53
3:1:918:MET:HA	3:1:918:MET:HE2	1.84	0.53
5:K:353:TYR:H	5:K:361:ARG:HH22	1.57	0.53
1:8:76:UNK:C	9:T:429:THR:HG21	2.38	0.53
2:Y:1019:ARG:NH1	9:R:245:ALA:HA	2.17	0.53
5:E:353:TYR:H	5:E:361:ARG:HH22	1.57	0.53
5:E:380:LEU:HD21	6:F:314:TYR:OH	2.07	0.53
3:1:140:ARG:HH22	3:1:144:THR:H	1.56	0.53
9:S:582:GLU:HA	11:X:302:ARG:NH1	2.23	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:X:273:VAL:CG1	11:X:356:VAL:HG23	2.15	0.53
1:7:76:UNK:C	9:R:429:THR:HG21	2.38	0.53
3:1:163:MET:HG3	3:1:568:LYS:HG3	1.90	0.53
5:K:317:ASN:HB2	5:K:348:ILE:HD11	1.90	0.53
5:K:380:LEU:HD21	6:L:314:TYR:OH	2.07	0.53
7:O:1378:ASP:O	7:O:1381:LEU:N	2.41	0.53
9:S:601:PRO:HB2	9:S:606:GLU:HG3	1.90	0.53
11:X:297:ASP:HB2	11:X:300:VAL:HG13	1.89	0.53
1:7:72:UNK:CA	9:R:426:PRO:CB	2.77	0.53
2:Y:517:LEU:CB	2:Y:537:LYS:HZ2	2.22	0.53
7:M:1071:ALA:HB3	7:M:1072:PRO:HD3	1.91	0.53
8:N:215:GLN:C	8:N:220:PHE:CE1	2.82	0.53
11:V:273:VAL:CG1	11:V:356:VAL:HG23	2.15	0.53
11:X:355:TRP:HZ2	11:X:401:ASP:CA	2.21	0.53
7:M:1378:ASP:O	7:M:1381:LEU:N	2.41	0.53
8:N:1497:ASN:HB3	9:Q:145:THR:O	2.08	0.53
2:0:135:PHE:HE2	2:0:515:VAL:HG21	1.72	0.53
3:1:1177:VAL:HG22	3:1:1215:TYR:OH	2.09	0.53
9:Q:594:GLY:HA2	10:U:324:LYS:CE	2.21	0.53
5:K:322:ILE:HD12	5:K:322:ILE:C	2.29	0.53
7:O:1071:ALA:HB3	7:O:1072:PRO:HD3	1.91	0.53
7:O:1185:ILE:HD12	7:O:1327:PHE:CD1	2.44	0.53
8:P:1497:ASN:HB3	9:S:145:THR:O	2.08	0.53
9:S:594:GLY:HA2	10:W:324:LYS:CE	2.21	0.53
3:Z:918:MET:HA	3:Z:918:MET:HE2	1.84	0.53
3:Z:1174:LEU:HD13	3:Z:1195:LEU:HB2	1.91	0.53
5:E:457:ASN:HA	5:E:460:TRP:CD1	2.44	0.53
7:M:1185:ILE:HD12	7:M:1327:PHE:CD1	2.44	0.53
9:R:432:ILE:HD11	9:R:477:TYR:CB	2.36	0.53
7:O:535:PHE:HA	7:O:622:GLN:HE22	1.73	0.53
2:Y:517:LEU:HB2	2:Y:537:LYS:NZ	2.24	0.53
3:Z:163:MET:HG3	3:Z:568:LYS:HG3	1.91	0.53
3:Z:917:GLU:CG	3:Z:918:MET:N	2.63	0.53
5:B:307:LYS:HA	5:B:331:LEU:HD22	1.91	0.53
7:M:535:PHE:HA	7:M:622:GLN:HE22	1.73	0.53
7:M:1189:MET:N	8:N:248:GLN:NE2	2.57	0.53
3:1:1215:TYR:HB2	3:1:1218:ILE:HG22	1.88	0.53
9:Q:72:LEU:CB	9:T:73:LEU:CB	2.87	0.52
3:1:1215:TYR:O	3:1:1218:ILE:CG2	2.54	0.52
5:H:307:LYS:HA	5:H:331:LEU:HD22	1.91	0.52
7:O:1189:MET:N	8:P:248:GLN:NE2	2.57	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:825:ILE:HD11	8:P:880:ASN:HD22	1.74	0.52
9:T:432:ILE:HD11	9:T:477:TYR:CB	2.37	0.52
5:B:413:LEU:HA	6:C:373:PHE:HE1	1.72	0.52
7:M:1490:ARG:HH12	9:R:825:PRO:CA	2.22	0.52
8:N:288:LEU:CD1	8:N:328:ILE:HG23	2.29	0.52
8:N:825:ILE:HD11	8:N:880:ASN:HD22	1.74	0.52
9:Q:594:GLY:N	10:U:324:LYS:HE2	2.19	0.52
11:V:273:VAL:HG11	11:V:356:VAL:HG21	1.89	0.52
5:K:457:ASN:HA	5:K:460:TRP:CD1	2.45	0.52
8:N:275:LEU:HD11	8:N:382:PHE:HB2	0.81	0.52
9:R:58:SER:C	9:R:60:ASN:H	2.11	0.52
7:O:1382:TYR:CZ	8:P:744:LEU:HD21	2.42	0.52
3:Z:186:ASN:ND2	3:Z:242:HIS:CD2	2.77	0.52
6:C:371:LYS:N	6:C:371:LYS:CD	2.73	0.52
10:U:266:ILE:HD11	10:U:336:ASN:HB2	1.92	0.52
11:V:273:VAL:HB	11:V:356:VAL:C	2.28	0.52
7:O:1490:ARG:HH12	9:T:825:PRO:CA	2.23	0.52
9:S:594:GLY:N	10:W:324:LYS:HE2	2.19	0.52
11:X:273:VAL:HB	11:X:356:VAL:C	2.28	0.52
4:D:806:SER:HB3	9:R:36:SER:CA	2.40	0.52
10:U:267:ILE:O	10:U:283:ILE:HD13	2.09	0.52
11:V:274:PHE:CE2	11:V:384:CYS:HA	2.45	0.52
5:K:456:THR:HB	5:K:460:TRP:HE1	1.75	0.52
7:O:1386:LYS:HZ3	8:P:683:ASP:CG	2.12	0.52
8:P:288:LEU:CD1	8:P:328:ILE:HG23	2.29	0.52
9:T:58:SER:C	9:T:60:ASN:H	2.11	0.52
11:X:274:PHE:CE2	11:X:384:CYS:HA	2.45	0.52
5:E:456:THR:HB	5:E:460:TRP:HE1	1.75	0.52
3:Z:1191:LEU:HD13	3:Z:1213:LEU:HD22	1.91	0.52
8:N:216:TYR:C	8:N:220:PHE:HD1	2.13	0.52
11:V:275:GLY:H	11:V:354:SER:C	2.13	0.52
3:1:186:ASN:ND2	3:1:242:HIS:CD2	2.77	0.52
6:L:371:LYS:N	6:L:371:LYS:CD	2.73	0.52
7:O:380:ALA:O	7:O:382:ASP:N	2.35	0.52
7:O:991:THR:H	7:O:995:VAL:HG11	1.75	0.52
7:O:1671:VAL:HB	9:T:162:LEU:O	2.10	0.52
9:S:680:ASN:CG	10:W:321:GLU:HB3	2.30	0.52
11:X:275:GLY:H	11:X:354:SER:C	2.13	0.52
5:E:364:VAL:HA	5:E:367:GLU:OE2	2.10	0.52
7:M:380:ALA:O	7:M:382:ASP:N	2.35	0.52
3:Z:1177:VAL:HG11	3:Z:1195:LEU:CD1	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:1177:VAL:HG23	3:Z:1215:TYR:OH	2.10	0.52
9:Q:680:ASN:CG	10:U:321:GLU:HB3	2.30	0.52
7:O:984:THR:C	7:O:988:SER:HB2	2.29	0.52
7:O:1189:MET:CG	7:O:1190:TYR:CD1	2.86	0.52
7:O:1376:THR:OG1	7:O:1415:ARG:NH2	2.43	0.52
8:P:1422:LEU:HB3	8:P:1468:VAL:HG11	1.90	0.52
11:X:273:VAL:O	11:X:355:TRP:HE3	1.91	0.52
2:Y:1465:ILE:HG12	2:Y:1487:TYR:CD2	2.45	0.52
7:O:1191:SER:OG	8:P:757:LYS:HB3	2.09	0.52
8:P:275:LEU:HD11	8:P:382:PHE:HB2	0.81	0.52
7:M:341:PHE:CE1	7:M:652:ALA:HB2	2.44	0.51
7:M:1191:SER:OG	8:N:757:LYS:HB3	2.09	0.51
8:N:1422:LEU:HB3	8:N:1468:VAL:HG11	1.90	0.51
11:V:273:VAL:O	11:V:355:TRP:HE3	1.91	0.51
2:0:1465:ILE:HG12	2:0:1487:TYR:CD2	2.45	0.51
3:1:493:ILE:HD13	3:1:513:LYS:HD3	1.85	0.51
5:E:373:ARG:HH22	6:F:304:LEU:HD22	1.75	0.51
7:M:1189:MET:CG	7:M:1190:TYR:CD1	2.86	0.51
7:M:1189:MET:HE2	7:M:1189:MET:O	2.10	0.51
7:M:1329:LEU:HD21	7:M:1380:ARG:NH2	2.24	0.51
10:U:322:LEU:HD12	10:U:325:SER:OG	2.10	0.51
5:K:318:GLU:OE2	5:K:345:PRO:HB2	2.09	0.51
5:K:373:ARG:HH22	6:L:304:LEU:HD22	1.75	0.51
9:S:589:LEU:HA	9:S:603:VAL:HG22	1.91	0.51
11:X:294:ILE:CG2	11:X:361:ASN:HD21	2.24	0.51
4:A:803:ALA:CA	9:Q:31:ASN:CB	2.89	0.51
5:B:312:VAL:HG21	5:B:361:ARG:HH21	1.74	0.51
8:N:212:TRP:HE1	8:N:269:THR:CG2	2.23	0.51
8:P:212:TRP:HE1	8:P:269:THR:CG2	2.23	0.51
10:W:276:ILE:H	10:W:283:ILE:CD1	2.19	0.51
10:W:322:LEU:HD12	10:W:325:SER:OG	2.11	0.51
9:R:339:TYR:HA	9:R:342:ARG:HD3	1.93	0.51
11:V:270:ALA:CB	11:V:357:LYS:HG3	2.38	0.51
6:I:376:LYS:NZ	6:I:376:LYS:CB	2.73	0.51
7:O:341:PHE:CE1	7:O:652:ALA:HB2	2.45	0.51
9:T:339:TYR:HA	9:T:342:ARG:HD3	1.93	0.51
3:Z:912:ALA:O	3:Z:916:PHE:CD2	2.63	0.51
8:N:1259:PHE:CZ	9:Q:133:ILE:CB	2.93	0.51
3:1:912:ALA:O	3:1:916:PHE:CD2	2.63	0.51
5:H:312:VAL:HG21	5:H:361:ARG:HH21	1.74	0.51
8:P:267:ILE:HG22	8:P:271:LEU:HD11	1.83	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1386:LYS:HZ3	8:N:683:ASP:CG	2.13	0.51
7:M:1585:PRO:CA	7:M:1659:ASN:HD21	2.16	0.51
11:V:274:PHE:CA	11:V:354:SER:O	2.59	0.51
3:1:1210:ALA:CB	3:1:1218:ILE:CG2	2.89	0.51
4:J:707:LEU:HD11	5:K:408:ILE:HD13	1.92	0.51
8:P:1259:PHE:CZ	9:S:133:ILE:CB	2.93	0.51
11:X:273:VAL:HG11	11:X:356:VAL:HG21	1.89	0.51
2:Y:1019:ARG:HD2	9:R:245:ALA:CA	2.38	0.51
11:X:270:ALA:CB	11:X:357:LYS:HG3	2.38	0.51
3:Z:1213:LEU:HD12	3:Z:1213:LEU:C	2.30	0.51
5:B:323:LEU:CA	5:B:349:PRO:HD2	2.40	0.51
3:1:493:ILE:HG21	3:1:513:LYS:HA	1.93	0.51
3:1:728:VAL:HG11	3:1:812:ILE:HD11	1.93	0.51
10:W:261:THR:C	10:W:263:ALA:H	2.14	0.51
1:4:5:UNK:CB	5:K:315:LYS:HB3	2.40	0.51
4:D:707:LEU:HD11	5:E:408:ILE:HD13	1.93	0.51
8:N:267:ILE:HG22	8:N:271:LEU:HD11	1.83	0.51
8:N:310:ILE:O	8:N:310:ILE:HG22	2.09	0.51
10:U:261:THR:C	10:U:263:ALA:H	2.14	0.51
2:0:516:LEU:CA	2:0:537:LYS:HZ2	2.16	0.51
11:X:274:PHE:CA	11:X:354:SER:O	2.59	0.51
3:Z:728:VAL:HG11	3:Z:812:ILE:HD11	1.93	0.51
4:D:793:LEU:HB2	6:F:439:ILE:HG21	1.93	0.51
5:E:316:VAL:HG13	5:E:348:ILE:CD1	2.40	0.51
4:J:793:LEU:HB2	6:L:439:ILE:HG21	1.93	0.51
7:O:1191:SER:OG	8:P:757:LYS:CB	2.58	0.51
8:P:310:ILE:O	8:P:310:ILE:HG22	2.10	0.51
9:S:504:VAL:HG13	9:S:538:LEU:HD23	1.93	0.51
11:X:289:SER:C	11:X:294:ILE:CD1	2.80	0.51
9:Q:504:VAL:HG13	9:Q:538:LEU:HD23	1.93	0.50
2:0:1019:ARG:HD2	9:T:245:ALA:CA	2.38	0.50
7:O:1585:PRO:CA	7:O:1659:ASN:HD21	2.16	0.50
7:M:1389:ILE:HG23	8:N:687:LYS:CG	2.26	0.50
11:V:355:TRP:HE1	11:V:400:ILE:C	2.15	0.50
8:P:613:GLU:OE2	8:P:617:TYR:CE2	2.64	0.50
10:W:276:ILE:N	10:W:283:ILE:CD1	2.69	0.50
1:4:5:UNK:HA	5:K:315:LYS:CD	2.39	0.50
8:N:613:GLU:OE2	8:N:617:TYR:CE2	2.64	0.50
9:Q:601:PRO:HA	9:Q:605:GLU:OE1	2.11	0.50
9:R:432:ILE:HD11	9:R:477:TYR:CD2	2.41	0.50
8:P:68:HIS:HB2	8:P:72:ARG:HB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:429:THR:CG2	9:T:434:ASP:HB3	2.31	0.50
11:X:355:TRP:HE1	11:X:400:ILE:C	2.15	0.50
7:M:1429:ASP:OD2	8:N:686:GLY:HA3	2.12	0.50
9:Q:595:ARG:O	9:Q:595:ARG:HG2	2.11	0.50
7:O:990:ILE:HG13	7:O:995:VAL:HG11	1.85	0.50
8:P:149:ILE:HG23	8:P:223:PHE:HD1	1.74	0.50
7:M:1191:SER:OG	8:N:757:LYS:CB	2.58	0.50
9:R:33:PRO:O	9:R:36:SER:CB	2.60	0.50
6:I:376:LYS:HB2	6:I:376:LYS:HZ2	1.77	0.50
7:O:1361:PHE:CZ	7:O:1412:TYR:CD1	3.00	0.50
2:Y:516:LEU:N	2:Y:516:LEU:CD1	2.73	0.50
3:Z:1213:LEU:HD22	3:Z:1215:TYR:HE2	1.48	0.50
7:M:1361:PHE:CZ	7:M:1412:TYR:CD1	3.00	0.50
9:Q:602:GLY:HA2	9:Q:606:GLU:OE2	2.12	0.50
9:Q:603:VAL:HG23	9:Q:604:ILE:N	2.26	0.50
11:V:274:PHE:CD2	11:V:355:TRP:CZ3	2.89	0.50
9:T:432:ILE:HD11	9:T:477:TYR:CD2	2.41	0.50
11:X:274:PHE:CD2	11:X:355:TRP:CZ3	2.88	0.50
7:M:1392:ILE:CG2	7:M:1436:LYS:C	2.79	0.50
9:R:429:THR:CG2	9:R:434:ASP:HB3	2.31	0.50
3:1:1183:ILE:CG2	3:1:1184:ASP:N	2.73	0.50
9:T:472:SER:C	9:T:473:ARG:HG2	2.31	0.50
3:Z:1210:ALA:CA	3:Z:1218:ILE:HD11	2.42	0.50
4:D:765:LEU:CD2	5:E:460:TRP:CE2	2.95	0.50
9:R:472:SER:O	9:R:473:ARG:CG	2.60	0.50
4:J:765:LEU:CD2	5:K:460:TRP:CE2	2.95	0.50
9:T:472:SER:O	9:T:473:ARG:CG	2.60	0.50
10:W:304:LYS:HZ3	11:X:388:SER:N	2.09	0.50
2:Y:1360:SER:HA	2:Y:1402:LEU:HD22	1.93	0.49
3:Z:1172:ASP:OD1	9:Q:754:ARG:HG2	2.11	0.49
8:N:309:ASN:OD1	8:N:315:PRO:HB3	2.12	0.49
9:R:472:SER:C	9:R:473:ARG:HG2	2.32	0.49
2:0:1360:SER:HA	2:0:1402:LEU:HD22	1.93	0.49
7:O:1392:ILE:CG2	7:O:1436:LYS:C	2.80	0.49
8:P:556:LEU:HG	8:P:556:LEU:O	2.11	0.49
11:X:273:VAL:HA	11:X:384:CYS:CB	2.42	0.49
11:X:273:VAL:HA	11:X:384:CYS:HB2	1.94	0.49
5:B:323:LEU:HG	5:B:349:PRO:CG	2.37	0.49
7:M:1372:THR:OG1	8:N:811:ASP:HB3	2.12	0.49
8:N:309:ASN:ND2	8:N:352:PHE:HE1	2.10	0.49
8:N:309:ASN:ND2	8:N:352:PHE:CE1	2.81	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
11:V:273:VAL:HA	11:V:384:CYS:CB	2.42	0.49
11:V:273:VAL:HA	11:V:384:CYS:HB2	1.94	0.49
2:0:1310:ASP:OD1	2:0:1311:PHE:N	2.46	0.49
3:1:1172:ASP:OD1	9:S:754:ARG:HG2	2.11	0.49
7:O:1382:TYR:CE1	8:P:744:LEU:HD21	2.48	0.49
8:P:309:ASN:ND2	8:P:352:PHE:CE1	2.81	0.49
8:P:309:ASN:OD1	8:P:315:PRO:HB3	2.13	0.49
1:7:72:UNK:CB	9:R:426:PRO:CD	2.90	0.49
4:D:807:LEU:HD13	5:E:523:LEU:HD23	1.95	0.49
6:L:374:GLN:HE21	6:L:374:GLN:H	1.56	0.49
8:P:309:ASN:ND2	8:P:352:PHE:HE1	2.10	0.49
9:T:429:THR:HG23	9:T:434:ASP:CG	2.33	0.49
11:X:274:PHE:C	11:X:274:PHE:CD1	2.85	0.49
5:E:322:ILE:HA	5:E:325:THR:HG23	1.95	0.49
7:M:1380:ARG:CD	7:M:1380:ARG:N	2.73	0.49
11:V:274:PHE:C	11:V:274:PHE:CD1	2.85	0.49
4:G:810:ASN:CB	9:S:35:ALA:HB3	2.24	0.49
4:J:807:LEU:HD13	5:K:523:LEU:HD23	1.95	0.49
7:O:1392:ILE:HG21	7:O:1437:LEU:HB2	1.93	0.49
9:S:584:LYS:HE2	9:S:639:ASP:OD2	2.12	0.49
9:T:684:ASN:OD1	9:T:685:PRO:HD2	2.12	0.49
10:W:271:ALA:CB	10:W:283:ILE:CB	2.91	0.49
5:B:323:LEU:CB	5:B:349:PRO:HD2	2.43	0.49
7:M:1372:THR:OG1	8:N:811:ASP:CB	2.60	0.49
7:M:1392:ILE:HG21	7:M:1437:LEU:HB2	1.93	0.49
9:R:429:THR:HG23	9:R:434:ASP:CG	2.33	0.49
3:1:408:LYS:HD3	3:1:497:CYS:HA	1.95	0.49
3:Z:495:THR:HG23	3:Z:510:CYS:O	2.13	0.49
7:M:1189:MET:CB	8:N:249:ASP:CA	2.72	0.49
9:Q:601:PRO:CB	9:Q:605:GLU:OE1	2.61	0.49
3:1:1210:ALA:HB1	3:1:1218:ILE:CG2	2.41	0.49
9:R:684:ASN:OD1	9:R:685:PRO:HD2	2.12	0.49
10:U:262:ILE:CG2	10:U:262:ILE:O	2.48	0.49
10:U:322:LEU:CD1	10:U:325:SER:CB	2.90	0.49
6:L:374:GLN:HE21	6:L:374:GLN:CA	2.23	0.49
7:O:1561:LEU:O	7:O:1580:VAL:CG1	2.55	0.49
9:S:448:ALA:HB1	9:S:456:ARG:HH12	1.78	0.49
11:X:294:ILE:O	11:X:301:LEU:HD11	2.13	0.49
3:Z:1213:LEU:HD13	3:Z:1215:TYR:CE2	2.46	0.49
7:M:1561:LEU:O	7:M:1580:VAL:CG1	2.55	0.49
9:Q:448:ALA:HB1	9:Q:456:ARG:HH12	1.78	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:1189:MET:CB	8:P:249:ASP:CA	2.72	0.49
7:O:1380:ARG:HD3	7:O:1415:ARG:HE	1.77	0.49
10:W:280:PHE:CD1	10:W:309:THR:HG21	2.47	0.49
10:W:322:LEU:CD1	10:W:325:SER:CB	2.91	0.49
2:Y:769:ARG:HH11	2:Y:773:ILE:CD1	2.26	0.49
7:M:1389:ILE:HD11	7:M:1429:ASP:OD2	2.13	0.49
9:R:282:PHE:CE1	9:R:342:ARG:NH2	2.80	0.49
9:R:676:GLY:N	9:R:677:PRO:HD2	2.27	0.49
2:0:769:ARG:HH11	2:0:773:ILE:CD1	2.26	0.49
11:X:297:ASP:OD2	11:X:301:LEU:CG	2.56	0.49
7:M:1189:MET:SD	7:M:1190:TYR:CD1	3.06	0.48
7:O:1189:MET:SD	7:O:1190:TYR:CD1	3.06	0.48
9:T:282:PHE:CE1	9:T:342:ARG:NH2	2.80	0.48
11:X:386:PRO:O	11:X:387:TYR:CG	2.66	0.48
3:Z:1191:LEU:HD22	3:Z:1213:LEU:HD22	1.88	0.48
6:C:369:LEU:N	6:C:369:LEU:CD2	2.74	0.48
5:E:315:LYS:O	5:E:315:LYS:HG2	2.13	0.48
9:R:338:PHE:O	9:R:342:ARG:HG3	2.13	0.48
11:V:401:ASP:N	11:V:401:ASP:OD1	2.46	0.48
6:I:342:GLU:HB3	6:I:372:PHE:CE1	2.49	0.48
5:K:325:THR:O	5:K:326:LYS:HD3	2.13	0.48
7:O:335:ASP:HA	7:O:771:ARG:NE	2.28	0.48
7:O:1374:LYS:CE	7:O:1418:SER:O	2.44	0.48
9:T:338:PHE:O	9:T:342:ARG:HG3	2.13	0.48
2:Y:761:LEU:HD21	2:Y:885:ALA:HB1	1.95	0.48
7:M:1585:PRO:HB3	7:M:1658:PRO:HG2	1.95	0.48
8:N:341:PHE:C	8:N:341:PHE:CD1	2.86	0.48
5:K:436:MET:SD	6:L:370:ASP:CB	3.00	0.48
6:L:374:GLN:O	6:L:377:ILE:HB	2.13	0.48
7:O:990:ILE:HA	7:O:995:VAL:HG11	1.95	0.48
7:O:1585:PRO:HB3	7:O:1658:PRO:HG2	1.95	0.48
9:T:676:GLY:N	9:T:677:PRO:HD2	2.27	0.48
11:X:401:ASP:N	11:X:401:ASP:OD1	2.46	0.48
1:3:2:UNK:N	5:E:316:VAL:CA	2.75	0.48
7:M:335:ASP:OD1	7:M:857:GLY:N	2.46	0.48
7:M:335:ASP:HA	7:M:771:ARG:NE	2.28	0.48
2:0:761:LEU:HD21	2:0:885:ALA:HB1	1.95	0.48
7:O:335:ASP:OD1	7:O:857:GLY:N	2.46	0.48
8:P:341:PHE:CD1	8:P:341:PHE:C	2.86	0.48
9:S:116:ILE:HA	9:S:120:GLU:CB	2.44	0.48
3:Z:1191:LEU:HD21	3:Z:1213:LEU:HD23	1.93	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1189:MET:N	8:N:248:GLN:HG3	2.10	0.48
8:N:71:LEU:HD12	8:N:71:LEU:C	2.33	0.48
9:R:670:LEU:HA	9:R:674:LEU:CD2	2.43	0.48
11:V:386:PRO:O	11:V:387:TYR:CG	2.67	0.48
9:T:339:TYR:HE1	9:T:342:ARG:HH11	1.30	0.48
7:M:335:ASP:OD1	7:M:856:GLU:O	2.32	0.48
7:M:1432:LEU:HD23	2:0:1425:LYS:NZ	2.28	0.48
2:0:515:VAL:HB	2:0:516:LEU:HD12	1.96	0.48
2:0:516:LEU:N	2:0:516:LEU:CD1	2.77	0.48
5:K:325:THR:O	5:K:326:LYS:CG	2.61	0.48
7:O:335:ASP:OD1	7:O:856:GLU:O	2.32	0.48
10:W:266:ILE:HG13	10:W:336:ASN:OD1	2.06	0.48
11:X:272:ILE:HG22	11:X:355:TRP:CZ3	2.49	0.48
11:X:294:ILE:HG22	11:X:361:ASN:HD21	1.76	0.48
4:D:655:PHE:HB2	5:E:355:PHE:CD1	2.49	0.48
8:N:215:GLN:C	8:N:220:PHE:HE1	2.15	0.48
8:N:327:PHE:CB	8:N:389:PHE:HE2	2.27	0.48
9:Q:603:VAL:CG2	9:Q:604:ILE:N	2.76	0.48
9:R:84:ASP:HA	9:S:73:LEU:CB	2.44	0.48
11:V:272:ILE:HG22	11:V:355:TRP:CZ3	2.49	0.48
4:J:655:PHE:HB2	5:K:355:PHE:CD1	2.49	0.48
7:O:1376:THR:CG2	7:O:1380:ARG:HB2	2.44	0.48
6:I:369:LEU:CA	6:I:373:PHE:HB2	2.44	0.48
6:L:353:LEU:CD1	6:L:369:LEU:CD1	2.89	0.48
9:T:433:GLU:H	9:T:433:GLU:HG3	1.40	0.48
9:T:670:LEU:HA	9:T:674:LEU:CD2	2.44	0.48
1:8:72:UNK:C	9:T:426:PRO:HB3	2.43	0.48
7:M:1561:LEU:H	7:M:1580:VAL:HB	1.71	0.48
8:N:309:ASN:C	8:N:311:VAL:H	2.15	0.48
9:S:592:LYS:O	9:S:600:ILE:HB	2.14	0.48
10:W:271:ALA:HB2	10:W:283:ILE:CG2	2.43	0.48
2:Y:1465:ILE:CG2	2:Y:1484:ILE:HA	2.43	0.48
3:Z:977:GLY:HA3	3:Z:979:GLN:HE21	1.78	0.48
8:N:226:ASN:O	8:N:229:SER:HB3	2.14	0.48
8:N:273:LEU:HB3	8:N:328:ILE:HD11	1.96	0.48
9:R:500:GLU:O	9:R:504:VAL:HG23	2.14	0.48
2:0:1465:ILE:CG2	2:0:1484:ILE:HA	2.43	0.48
3:1:977:GLY:HA3	3:1:979:GLN:HE21	1.78	0.48
8:P:273:LEU:HB3	8:P:328:ILE:HD11	1.96	0.48
9:T:500:GLU:O	9:T:504:VAL:HG23	2.14	0.48
1:7:72:UNK:CB	9:R:426:PRO:HD3	2.43	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:1308:PHE:CE1	2:Y:1313:VAL:HG23	2.49	0.47
5:B:323:LEU:HD11	5:B:338:ALA:O	2.11	0.47
9:R:339:TYR:HE1	9:R:342:ARG:HH11	1.30	0.47
10:U:322:LEU:CD1	10:U:325:SER:HB2	2.44	0.47
8:P:309:ASN:C	8:P:311:VAL:H	2.16	0.47
1:8:72:UNK:HA	9:T:426:PRO:HB3	1.89	0.47
4:A:665:TRP:HE1	5:B:369:VAL:HG11	1.78	0.47
5:B:323:LEU:CG	5:B:335:TRP:CZ3	2.97	0.47
2:0:1308:PHE:CE1	2:0:1313:VAL:HG23	2.49	0.47
4:G:665:TRP:HE1	5:H:369:VAL:HG11	1.78	0.47
5:K:325:THR:C	5:K:326:LYS:HG2	2.34	0.47
7:O:1561:LEU:H	7:O:1580:VAL:HB	1.71	0.47
7:M:687:TYR:CE1	7:M:746:LYS:HE2	2.49	0.47
9:R:414:LEU:HD13	9:R:441:MET:HG3	1.95	0.47
9:R:433:GLU:H	9:R:433:GLU:HG3	1.40	0.47
7:O:1189:MET:N	8:P:248:GLN:HG3	2.11	0.47
10:W:322:LEU:CD1	10:W:325:SER:HB2	2.44	0.47
9:Q:772:PRO:HB3	9:Q:828:THR:HG21	1.96	0.47
3:1:493:ILE:CD1	3:1:513:LYS:CD	2.81	0.47
5:K:459:LEU:HD21	6:L:395:GLU:HG2	1.96	0.47
9:S:547:TYR:O	11:X:298:PHE:CB	2.60	0.47
2:Y:1358:GLU:HA	3:1:789:ASP:OD2	2.15	0.47
9:Q:681:SER:HB3	10:U:322:LEU:HD22	1.95	0.47
6:I:371:LYS:N	6:I:371:LYS:CD	2.77	0.47
8:P:289:TYR:HB3	8:P:290:MET:H	1.47	0.47
9:S:593:ILE:HG21	9:S:598:ALA:O	2.14	0.47
9:S:772:PRO:HB3	9:S:828:THR:HG21	1.96	0.47
5:E:459:LEU:HD21	6:F:395:GLU:HG2	1.96	0.47
8:N:55:LEU:HD11	8:N:109:ARG:NE	2.26	0.47
9:Q:641:ILE:HG23	9:Q:653:VAL:HG13	1.95	0.47
11:V:293:HIS:C	11:V:361:ASN:HD21	2.14	0.47
8:P:63:THR:O	8:P:82:ASN:OD1	2.32	0.47
9:S:681:SER:HB3	10:W:322:LEU:HD22	1.95	0.47
9:T:414:LEU:HD13	9:T:441:MET:HG3	1.95	0.47
11:X:275:GLY:H	11:X:354:SER:CB	2.11	0.47
7:M:1490:ARG:HH22	9:R:825:PRO:HA	1.80	0.47
8:N:271:LEU:HD21	8:N:378:VAL:CG2	2.44	0.47
8:N:1506:LEU:HA	8:N:1509:GLN:HE21	1.80	0.47
11:V:286:GLU:N	11:V:300:VAL:CG2	2.78	0.47
11:V:286:GLU:N	11:V:300:VAL:HG21	2.30	0.47
3:1:1183:ILE:HG21	3:1:1213:LEU:HD11	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:O:687:TYR:CE1	7:O:746:LYS:HE2	2.49	0.47
7:O:1490:ARG:HH22	9:T:825:PRO:HA	1.80	0.47
7:O:1585:PRO:HB3	7:O:1659:ASN:OD1	2.14	0.47
8:P:55:LEU:HD11	8:P:109:ARG:NE	2.26	0.47
8:P:271:LEU:HD21	8:P:378:VAL:CG2	2.44	0.47
3:Z:407:ALA:CB	3:Z:495:THR:HB	2.44	0.47
7:M:383:ASN:HB3	7:M:767:ILE:HG12	1.97	0.47
8:N:316:ILE:HB	8:N:317:PHE:H	1.62	0.47
11:V:275:GLY:H	11:V:354:SER:CB	2.11	0.47
4:G:792:GLN:HE22	9:S:17:GLY:HA2	1.77	0.47
5:K:316:VAL:O	5:K:348:ILE:CG1	2.54	0.47
7:O:383:ASN:HB3	7:O:767:ILE:HG12	1.97	0.47
8:P:1506:LEU:HA	8:P:1509:GLN:HE21	1.80	0.47
9:S:641:ILE:HG23	9:S:653:VAL:HG13	1.95	0.47
3:Z:1213:LEU:CD1	3:Z:1215:TYR:CB	2.82	0.47
7:M:1585:PRO:HB3	7:M:1659:ASN:OD1	2.14	0.47
8:N:289:TYR:HB3	8:N:290:MET:H	1.47	0.47
8:P:316:ILE:HB	8:P:317:PHE:H	1.62	0.47
7:M:1189:MET:O	7:M:1190:TYR:HB3	2.14	0.46
8:N:249:ASP:OD2	8:N:835:LEU:CD1	2.63	0.46
7:M:384:MET:CB	7:M:766:GLN:NE2	2.77	0.46
7:M:1395:PRO:CD	7:M:1396:LEU:H	2.28	0.46
8:N:56:ASN:HD22	8:N:144:ILE:CG1	2.26	0.46
4:G:810:ASN:CG	9:S:35:ALA:HB2	2.36	0.46
7:O:1189:MET:O	7:O:1190:TYR:HB3	2.14	0.46
7:O:1385:PHE:CZ	7:O:1429:ASP:OD2	2.68	0.46
7:M:1584:ASN:HA	7:M:1585:PRO:HD3	1.76	0.46
9:R:301:ASN:HB3	9:R:345:LEU:CD1	2.46	0.46
4:J:665:TRP:CE3	5:K:365:GLN:NE2	2.83	0.46
7:O:384:MET:CB	7:O:766:GLN:NE2	2.77	0.46
7:O:1385:PHE:CE1	7:O:1429:ASP:OD2	2.68	0.46
7:O:1395:PRO:CD	7:O:1396:LEU:H	2.28	0.46
8:P:56:ASN:HD22	8:P:144:ILE:CG1	2.26	0.46
8:P:286:SER:H	8:P:287:PRO:HD2	1.81	0.46
4:A:806:SER:HB2	9:Q:35:ALA:HB1	1.97	0.46
5:B:331:LEU:HD23	5:B:331:LEU:H	1.79	0.46
5:E:539:ASN:H	5:E:539:ASN:ND2	2.14	0.46
7:M:335:ASP:OD1	7:M:857:GLY:CA	2.64	0.46
8:N:60:GLN:HB3	8:N:61:ASN:H	1.52	0.46
8:N:613:GLU:HG3	8:N:617:TYR:CD1	2.42	0.46
5:K:539:ASN:H	5:K:539:ASN:ND2	2.14	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:335:ASP:OD2	7:M:774:ARG:HD3	2.16	0.46
3:1:1213:LEU:HD23	3:1:1215:TYR:CE1	2.50	0.46
5:H:331:LEU:HD23	5:H:331:LEU:H	1.79	0.46
5:K:322:ILE:CD1	5:K:323:LEU:HG	2.43	0.46
8:P:613:GLU:HG3	8:P:617:TYR:CD1	2.42	0.46
9:S:603:VAL:HG23	9:S:604:ILE:N	2.31	0.46
9:T:301:ASN:HB3	9:T:345:LEU:CD1	2.46	0.46
3:Z:1174:LEU:O	3:Z:1177:VAL:HG13	2.12	0.46
9:R:678:ASP:HA	9:R:687:LEU:HG	1.97	0.46
3:1:1199:VAL:C	3:1:1200:LEU:HG	2.36	0.46
7:O:335:ASP:OD2	7:O:774:ARG:HD3	2.16	0.46
7:O:335:ASP:OD1	7:O:857:GLY:CA	2.64	0.46
8:P:825:ILE:O	8:P:825:ILE:HG22	2.15	0.46
9:T:435:TRP:CZ3	9:T:474:PHE:HE1	2.34	0.46
9:T:678:ASP:HA	9:T:687:LEU:HG	1.97	0.46
10:W:280:PHE:CE1	10:W:309:THR:CG2	2.99	0.46
11:X:294:ILE:O	11:X:294:ILE:HG13	2.15	0.46
3:Z:225:ALA:CB	3:Z:263:ILE:HD11	2.45	0.46
3:Z:1191:LEU:HD11	3:Z:1213:LEU:CB	2.46	0.46
5:B:317:ASN:ND2	5:B:346:GLN:HB3	2.29	0.46
5:E:314:ASN:OD1	5:E:348:ILE:N	2.48	0.46
8:N:74:THR:O	8:N:77:ASN:HB2	2.16	0.46
9:R:435:TRP:CZ3	9:R:474:PHE:HE1	2.34	0.46
11:V:355:TRP:HE1	11:V:400:ILE:CB	2.11	0.46
2:0:515:VAL:O	2:0:537:LYS:NZ	2.25	0.46
3:1:225:ALA:CB	3:1:263:ILE:HD11	2.45	0.46
3:1:1224:LYS:HB2	3:1:1276:THR:HG22	1.98	0.46
3:Z:1224:LYS:HB2	3:Z:1276:THR:HG22	1.98	0.46
8:N:286:SER:H	8:N:287:PRO:HD2	1.81	0.46
8:N:825:ILE:O	8:N:825:ILE:HG22	2.15	0.46
2:0:1183:LEU:HB2	2:0:1184:PRO:HD3	1.98	0.46
7:O:1392:ILE:HD11	7:O:1437:LEU:CD1	2.39	0.46
9:S:641:ILE:HG22	9:S:645:GLN:HE21	1.80	0.46
9:T:676:GLY:O	9:T:679:ASP:HB2	2.15	0.46
3:Z:1215:TYR:CB	3:Z:1218:ILE:HD11	2.27	0.46
7:M:1392:ILE:HD11	7:M:1437:LEU:CD1	2.39	0.46
9:Q:641:ILE:HG22	9:Q:645:GLN:HE21	1.80	0.46
3:1:264:ILE:HG22	3:1:345:LEU:HD13	1.97	0.46
7:O:1584:ASN:HA	7:O:1585:PRO:HD3	1.76	0.46
8:P:288:LEU:HD22	8:P:295:PHE:HD1	1.81	0.46
11:X:296:GLU:O	11:X:346:LYS:CD	2.64	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:Y:1183:LEU:HB2	2:Y:1184:PRO:HD3	1.98	0.46
9:R:676:GLY:O	9:R:679:ASP:HB2	2.15	0.46
3:1:1191:LEU:HD11	3:1:1213:LEU:HB3	1.95	0.46
7:O:1189:MET:HB3	8:P:248:GLN:CD	2.35	0.46
8:P:60:GLN:HB3	8:P:61:ASN:H	1.52	0.46
11:X:355:TRP:HE1	11:X:400:ILE:CB	2.11	0.46
3:Z:264:ILE:HG22	3:Z:345:LEU:HD13	1.97	0.45
3:Z:1269:LEU:HD11	3:Z:1311:PHE:CE1	2.51	0.45
7:M:1490:ARG:HH12	9:R:825:PRO:CB	2.29	0.45
8:N:288:LEU:HD22	8:N:295:PHE:HD1	1.81	0.45
9:Q:207:ILE:HD11	11:V:398:CYS:HB3	1.99	0.45
3:1:1269:LEU:HD11	3:1:1311:PHE:CE1	2.51	0.45
7:O:1391:GLY:O	7:O:1393:ASN:N	2.43	0.45
2:Y:517:LEU:HB3	2:Y:537:LYS:HZ2	1.80	0.45
5:E:380:LEU:HD13	6:F:314:TYR:CE2	2.51	0.45
7:M:1185:ILE:HG22	7:M:1194:LEU:HB2	1.96	0.45
7:M:1189:MET:HB3	8:N:248:GLN:CD	2.35	0.45
7:M:1385:PHE:CZ	7:M:1426:VAL:HG22	2.51	0.45
3:1:957:LEU:HG	3:1:957:LEU:O	2.16	0.45
3:1:1183:ILE:HG21	3:1:1213:LEU:HD13	1.96	0.45
7:O:1490:ARG:HH12	9:T:825:PRO:CB	2.29	0.45
3:Z:1146:SER:CA	9:R:447:ASP:OD1	2.58	0.45
3:Z:1185:GLU:HA	3:Z:1188:ARG:HB3	1.98	0.45
4:D:637:LEU:CD2	4:D:637:LEU:N	2.78	0.45
7:M:335:ASP:H	7:M:771:ARG:HH21	1.63	0.45
6:I:374:GLN:HE21	6:I:374:GLN:CA	2.20	0.45
4:J:806:SER:OG	9:T:31:ASN:O	2.32	0.45
5:K:371:GLN:NE2	5:K:371:GLN:CA	2.77	0.45
7:O:1185:ILE:HG22	7:O:1194:LEU:HB2	1.96	0.45
11:X:355:TRP:CD1	11:X:400:ILE:CG1	2.97	0.45
7:M:1189:MET:CA	8:N:248:GLN:HE21	2.30	0.45
7:M:1389:ILE:CG2	8:N:687:LYS:HE2	2.47	0.45
9:Q:548:SER:HB2	11:V:349:ILE:HB	1.97	0.45
11:V:355:TRP:HZ2	11:V:401:ASP:N	2.13	0.45
3:1:1146:SER:CA	9:T:447:ASP:OD1	2.58	0.45
5:K:380:LEU:HD13	6:L:314:TYR:CE2	2.51	0.45
7:O:1189:MET:CA	8:P:248:GLN:HE21	2.30	0.45
8:P:286:SER:CB	8:P:287:PRO:HD3	2.47	0.45
9:S:207:ILE:HD11	11:X:398:CYS:HB3	1.99	0.45
9:S:548:SER:HB2	11:X:349:ILE:HB	1.97	0.45
11:X:275:GLY:CA	11:X:354:SER:HB2	2.47	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:Z:957:LEU:HG	3:Z:957:LEU:O	2.16	0.45
7:M:331:ILE:H	7:M:331:ILE:HG12	1.35	0.45
8:N:286:SER:CB	8:N:287:PRO:HD3	2.47	0.45
11:V:275:GLY:CA	11:V:354:SER:HB2	2.47	0.45
11:V:355:TRP:CD1	11:V:400:ILE:CG1	2.97	0.45
7:O:335:ASP:H	7:O:771:ARG:HH21	1.63	0.45
7:O:336:LYS:HD2	7:O:339:GLU:OE1	2.17	0.45
1:4:4:UNK:N	5:K:316:VAL:HG23	2.31	0.45
4:D:810:ASN:OD1	9:R:35:ALA:O	2.34	0.45
7:M:336:LYS:HD2	7:M:339:GLU:OE1	2.17	0.45
7:M:1391:GLY:O	7:M:1393:ASN:N	2.44	0.45
8:N:309:ASN:C	8:N:311:VAL:N	2.70	0.45
11:V:294:ILE:CG1	11:V:361:ASN:OD1	2.61	0.45
2:0:613:GLY:H	2:0:635:GLU:HB2	1.80	0.45
5:K:373:ARG:HH21	6:L:307:SER:CB	2.29	0.45
7:O:1185:ILE:HG13	7:O:1185:ILE:O	2.16	0.45
9:S:547:TYR:CB	11:X:298:PHE:HB2	2.42	0.45
10:W:321:GLU:HB2	11:X:293:HIS:HE2	1.71	0.45
2:Y:613:GLY:H	2:Y:635:GLU:HB2	1.80	0.45
2:Y:1272:GLN:HE22	2:Y:1301:ILE:HA	1.80	0.45
2:Y:1484:ILE:H	2:Y:1484:ILE:HG13	1.53	0.45
3:Z:917:GLU:CB	3:Z:957:LEU:HD13	2.30	0.45
3:Z:1177:VAL:HG21	3:Z:1215:TYR:OH	2.17	0.45
7:M:1189:MET:SD	8:N:252:TYR:HB2	2.56	0.45
7:M:1381:LEU:HB3	7:M:1385:PHE:HE2	1.82	0.45
9:R:787:HIS:O	9:R:787:HIS:CG	2.70	0.45
10:U:262:ILE:CG2	10:U:265:SER:HG	1.89	0.45
6:I:371:LYS:CD	6:I:371:LYS:H	2.30	0.45
8:P:309:ASN:C	8:P:311:VAL:N	2.70	0.45
9:T:787:HIS:O	9:T:787:HIS:CG	2.70	0.45
10:W:262:ILE:O	10:W:266:ILE:HG13	2.17	0.45
5:B:323:LEU:HD13	5:B:339:MET:HG2	1.94	0.45
5:E:363:GLN:CG	5:E:364:VAL:N	2.79	0.45
7:M:1185:ILE:O	7:M:1185:ILE:HG13	2.16	0.45
9:Q:620:LEU:HD22	9:Q:647:ALA:HA	1.98	0.45
11:V:285:ILE:CG2	11:V:300:VAL:HG11	2.47	0.45
2:0:1272:GLN:HE22	2:0:1301:ILE:HA	1.80	0.45
5:K:363:GLN:CG	5:K:364:VAL:N	2.79	0.45
7:O:1189:MET:SD	8:P:252:TYR:HB2	2.56	0.45
7:O:1385:PHE:CE2	7:O:1429:ASP:OD2	2.70	0.45
7:O:1561:LEU:N	7:O:1580:VAL:CG1	2.68	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:186:LYS:HG2	8:P:190:GLN:HE21	1.82	0.45
8:P:286:SER:N	8:P:287:PRO:CD	2.79	0.45
8:P:286:SER:N	8:P:287:PRO:HD2	2.31	0.45
9:S:620:LEU:HD22	9:S:647:ALA:HA	1.98	0.45
10:W:252:ALA:CB	10:W:345:TYR:CE1	3.00	0.45
10:W:276:ILE:CA	10:W:283:ILE:HD11	2.47	0.45
1:8:74:UNK:CB	9:T:473:ARG:HE	2.30	0.45
5:E:380:LEU:CG	6:F:314:TYR:HE2	2.25	0.45
8:N:186:LYS:HG2	8:N:190:GLN:HE21	1.82	0.45
8:N:286:SER:N	8:N:287:PRO:CD	2.79	0.45
8:N:286:SER:N	8:N:287:PRO:HD2	2.32	0.45
9:Q:593:ILE:CG2	9:Q:600:ILE:CG1	2.94	0.45
5:K:380:LEU:CG	6:L:314:TYR:HE2	2.25	0.45
7:O:1189:MET:CE	8:P:252:TYR:HB2	2.47	0.45
7:O:1385:PHE:CD1	7:O:1429:ASP:OD2	2.70	0.45
7:M:336:LYS:HE2	7:M:771:ARG:HD3	1.98	0.45
7:M:690:GLU:H	7:M:690:GLU:CD	2.20	0.45
7:M:1189:MET:CE	8:N:252:TYR:HB2	2.47	0.45
7:M:1389:ILE:HG13	8:N:687:LYS:HA	1.98	0.45
10:U:248:TRP:CD1	10:U:248:TRP:O	2.70	0.45
10:U:252:ALA:CB	10:U:345:TYR:CE1	3.00	0.45
10:U:262:ILE:O	10:U:266:ILE:HG13	2.17	0.45
3:1:917:GLU:CB	3:1:957:LEU:HD13	2.30	0.45
7:O:336:LYS:HE2	7:O:771:ARG:HD3	1.98	0.45
3:Z:1262:LEU:HD21	3:Z:1306:SER:HB2	1.99	0.44
8:N:1293:ILE:HD13	8:N:1307:PHE:HB2	1.99	0.44
2:0:1484:ILE:H	2:0:1484:ILE:HG13	1.53	0.44
3:1:1215:TYR:HB3	3:1:1218:ILE:HG22	1.96	0.44
7:O:331:ILE:H	7:O:331:ILE:HG12	1.35	0.44
7:O:690:GLU:H	7:O:690:GLU:CD	2.20	0.44
7:O:1389:ILE:HG13	8:P:687:LYS:HA	1.98	0.44
2:Y:519:THR:HG23	2:Y:533:SER:OG	2.17	0.44
7:M:1561:LEU:N	7:M:1580:VAL:CG1	2.68	0.44
8:N:72:ARG:HA	8:N:75:ILE:HD12	2.00	0.44
9:R:740:GLU:HA	9:R:747:PHE:CE2	2.53	0.44
10:U:321:GLU:HB2	11:V:293:HIS:HE2	1.71	0.44
3:1:1262:LEU:HD21	3:1:1306:SER:HB2	1.99	0.44
7:O:1584:ASN:HA	7:O:1584:ASN:HD22	1.55	0.44
10:W:248:TRP:O	10:W:248:TRP:CD1	2.71	0.44
5:B:325:THR:HG22	5:B:335:TRP:CZ2	2.51	0.44
3:1:492:TYR:HD1	3:1:509:THR:HG21	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:1:918:MET:HB3	3:1:919:ILE:H	1.51	0.44
3:1:1173:LEU:CD1	3:1:1195:LEU:CD2	2.90	0.44
5:K:325:THR:O	5:K:326:LYS:CD	2.65	0.44
5:K:373:ARG:HA	5:K:376:LEU:HG	1.99	0.44
7:O:384:MET:SD	7:O:760:ILE:HA	2.57	0.44
8:P:1293:ILE:HD13	8:P:1307:PHE:HB2	1.99	0.44
2:Y:1471:ILE:HD13	2:Y:1471:ILE:HA	1.91	0.44
3:Z:1210:ALA:CB	3:Z:1218:ILE:CG1	2.95	0.44
7:M:1374:LYS:HE3	7:M:1419:ASP:HA	1.99	0.44
11:V:273:VAL:O	11:V:355:TRP:CB	2.66	0.44
11:V:273:VAL:O	11:V:355:TRP:CE3	2.68	0.44
11:V:394:GLN:O	11:V:398:CYS:N	2.51	0.44
2:0:1019:ARG:CB	9:T:246:ASN:H	2.29	0.44
2:0:1306:GLU:O	2:0:1310:ASP:OD1	2.35	0.44
8:P:266:THR:O	8:P:270:ILE:HB	2.18	0.44
11:X:273:VAL:O	11:X:355:TRP:CE3	2.68	0.44
11:X:355:TRP:HZ2	11:X:401:ASP:N	2.14	0.44
2:Y:1019:ARG:CB	9:R:246:ASN:H	2.29	0.44
7:M:384:MET:SD	7:M:760:ILE:HA	2.57	0.44
7:M:1189:MET:HE1	8:N:252:TYR:CB	2.48	0.44
7:M:1247:ARG:HG2	7:M:1247:ARG:HH11	1.81	0.44
8:N:266:THR:O	8:N:270:ILE:HB	2.18	0.44
9:R:160:GLY:O	9:R:163:ILE:CB	2.66	0.44
9:R:674:LEU:HD21	9:R:724:ARG:HB3	1.99	0.44
10:U:321:GLU:CB	11:V:293:HIS:NE2	2.62	0.44
7:O:1381:LEU:CD1	7:O:1426:VAL:HG23	2.47	0.44
11:X:270:ALA:HB1	11:X:271:ILE:H	1.60	0.44
11:X:273:VAL:O	11:X:355:TRP:CB	2.66	0.44
11:X:355:TRP:CD1	11:X:400:ILE:HD12	2.49	0.44
11:X:394:GLN:O	11:X:398:CYS:N	2.51	0.44
3:Z:408:LYS:HD3	3:Z:497:CYS:HA	2.00	0.44
7:M:1584:ASN:HA	7:M:1584:ASN:HD22	1.55	0.44
9:R:435:TRP:CZ2	9:R:474:PHE:HD1	2.35	0.44
11:V:282:ASN:HB2	11:V:300:VAL:HB	2.00	0.44
11:V:355:TRP:CD1	11:V:400:ILE:HD12	2.50	0.44
2:0:1471:ILE:HD13	2:0:1471:ILE:HA	1.90	0.44
7:O:1190:TYR:CG	7:O:1190:TYR:O	2.70	0.44
9:T:435:TRP:CZ2	9:T:474:PHE:HD1	2.35	0.44
9:T:674:LEU:HD21	9:T:724:ARG:HB3	1.99	0.44
9:T:740:GLU:HA	9:T:747:PHE:CE2	2.53	0.44
10:W:266:ILE:HA	10:W:336:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:W:321:GLU:CB	11:X:293:HIS:NE2	2.62	0.44
2:Y:516:LEU:HD21	2:Y:577:PHE:CZ	2.53	0.44
7:M:1190:TYR:CG	7:M:1190:TYR:O	2.70	0.44
8:N:185:LEU:HB3	8:N:257:LEU:HD22	1.99	0.44
9:R:670:LEU:HA	9:R:674:LEU:HD23	1.99	0.44
3:1:1127:LEU:HB2	3:1:1197:GLY:O	2.17	0.44
7:O:1247:ARG:HG2	7:O:1247:ARG:HH11	1.82	0.44
7:O:1382:TYR:CG	8:P:748:HIS:CE1	2.66	0.44
11:V:282:ASN:HD22	11:V:299:GLN:CB	2.31	0.44
5:K:317:ASN:CB	5:K:348:ILE:CD1	2.92	0.44
8:P:185:LEU:HB3	8:P:257:LEU:HD22	1.99	0.44
6:F:456:ARG:HH21	9:R:61:LYS:HA	1.82	0.44
7:M:1559:LEU:CD2	7:O:1642:LYS:CD	2.90	0.44
7:M:1585:PRO:O	7:M:1594:GLY:C	2.56	0.44
9:Q:127:THR:O	9:Q:131:GLU:N	2.31	0.44
9:R:339:TYR:CD1	9:R:342:ARG:HD3	2.52	0.44
3:1:493:ILE:HB	3:1:511:VAL:CG1	2.48	0.44
3:1:1173:LEU:CD1	3:1:1195:LEU:HD13	2.47	0.44
9:T:339:TYR:CD1	9:T:342:ARG:HD3	2.52	0.44
3:Z:918:MET:HB3	3:Z:919:ILE:H	1.51	0.43
6:C:374:GLN:HE21	6:C:374:GLN:CA	2.15	0.43
7:M:1479:LEU:HB3	7:M:1485:LEU:HB2	2.00	0.43
8:N:69:ASN:HD22	8:N:69:ASN:HA	1.52	0.43
9:R:674:LEU:HD13	9:R:674:LEU:HA	1.75	0.43
11:V:274:PHE:CZ	11:V:383:GLY:O	2.71	0.43
9:S:716:LEU:HD23	9:S:767:ILE:CD1	2.48	0.43
11:X:274:PHE:CZ	11:X:383:GLY:O	2.71	0.43
3:Z:493:ILE:HB	3:Z:494:ASN:H	1.54	0.43
5:E:294:LYS:H	5:E:294:LYS:HD3	1.83	0.43
8:N:249:ASP:OD2	8:N:835:LEU:CG	2.64	0.43
9:Q:716:LEU:HD23	9:Q:767:ILE:CD1	2.48	0.43
2:0:516:LEU:HA	2:0:537:LYS:CE	2.45	0.43
4:J:821:ILE:HD11	5:K:534:VAL:CG2	2.48	0.43
6:L:456:ARG:HH21	9:T:61:LYS:HA	1.82	0.43
7:O:1479:LEU:HB3	7:O:1485:LEU:HB2	2.00	0.43
9:S:603:VAL:HG23	9:S:604:ILE:HG13	1.99	0.43
9:T:670:LEU:HA	9:T:674:LEU:HD23	2.00	0.43
9:T:674:LEU:HD13	9:T:674:LEU:HA	1.75	0.43
3:Z:1191:LEU:HD11	3:Z:1213:LEU:HB2	2.01	0.43
5:E:314:ASN:CG	5:E:348:ILE:CD1	2.86	0.43
5:E:364:VAL:O	5:E:367:GLU:CG	2.66	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:M:1381:LEU:C	7:M:1385:PHE:CD2	2.92	0.43
8:N:305:ASP:OD1	8:N:352:PHE:CZ	2.71	0.43
11:V:270:ALA:HB1	11:V:271:ILE:H	1.60	0.43
3:1:1177:VAL:CG2	3:1:1215:TYR:CE2	2.82	0.43
5:K:294:LYS:HD3	5:K:294:LYS:H	1.83	0.43
5:K:322:ILE:C	5:K:322:ILE:CD1	2.87	0.43
7:O:1585:PRO:O	7:O:1594:GLY:C	2.56	0.43
8:P:305:ASP:OD1	8:P:352:PHE:CZ	2.71	0.43
4:D:821:ILE:HD11	5:E:534:VAL:CG2	2.48	0.43
7:M:1189:MET:HB3	8:N:248:GLN:NE2	2.33	0.43
7:O:1189:MET:HB3	8:P:248:GLN:NE2	2.33	0.43
8:N:222:GLU:HA	8:N:222:GLU:OE1	2.18	0.43
8:N:226:ASN:C	8:N:229:SER:H	2.20	0.43
7:O:380:ALA:C	7:O:382:ASP:H	2.20	0.43
7:O:1385:PHE:CD2	7:O:1429:ASP:OD2	2.72	0.43
11:X:386:PRO:O	11:X:387:TYR:CD2	2.71	0.43
2:Y:181:ARG:HD2	2:Y:192:LEU:HB3	2.00	0.43
5:B:323:LEU:CD1	5:B:338:ALA:O	2.65	0.43
10:U:304:LYS:N	11:V:271:ILE:CG1	2.78	0.43
11:V:298:PHE:CE2	11:V:299:GLN:HB2	2.54	0.43
2:0:181:ARG:HD2	2:0:192:LEU:HB3	2.01	0.43
8:N:227:ILE:HG13	8:N:258:ILE:HD13	2.00	0.43
9:R:577:ARG:HD3	9:R:623:ILE:HA	2.01	0.43
11:V:386:PRO:O	11:V:387:TYR:CD2	2.71	0.43
3:1:1305:GLY:HA3	3:1:1345:TRP:CD2	2.53	0.43
7:O:125:HIS:CG	7:O:126:GLU:N	2.86	0.43
2:Y:683:LEU:HD22	2:Y:773:ILE:HA	2.01	0.43
3:Z:225:ALA:HB2	3:Z:263:ILE:HD11	2.01	0.43
3:Z:1305:GLY:HA3	3:Z:1345:TRP:CD2	2.53	0.43
5:E:314:ASN:ND2	5:E:348:ILE:O	2.52	0.43
7:M:125:HIS:CG	7:M:126:GLU:N	2.86	0.43
7:M:380:ALA:C	7:M:382:ASP:H	2.20	0.43
8:N:225:ARG:O	8:N:228:ASN:C	2.57	0.43
2:0:683:LEU:HD22	2:0:773:ILE:HA	2.01	0.43
3:1:919:ILE:HB	3:1:920:ASP:H	1.58	0.43
5:K:316:VAL:HG13	5:K:317:ASN:CG	2.39	0.43
7:O:1380:ARG:CD	7:O:1415:ARG:HE	2.32	0.43
9:T:577:ARG:HD3	9:T:623:ILE:HA	2.01	0.43
3:Z:420:LEU:HD22	3:Z:433:TYR:HB3	2.01	0.43
3:1:494:ASN:N	3:1:494:ASN:HD22	2.17	0.43
3:1:1199:VAL:HG12	3:1:1200:LEU:N	2.34	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:H:318:GLU:OE1	5:H:318:GLU:HA	2.19	0.43
7:O:126:GLU:HA	7:O:131:TYR:CD2	2.54	0.43
9:T:359:ASN:OD1	11:X:368:ARG:NE	2.52	0.43
11:X:378:ARG:HD3	11:X:378:ARG:HA	1.92	0.43
3:Z:770:ARG:HB3	3:Z:771:PRO:HD3	2.01	0.43
5:B:323:LEU:CD2	5:B:338:ALA:O	2.62	0.43
7:M:1555:VAL:HG21	7:M:1561:LEU:HD11	2.00	0.43
9:R:359:ASN:OD1	11:V:368:ARG:NE	2.52	0.43
3:1:225:ALA:HB2	3:1:263:ILE:HD11	2.01	0.43
3:1:420:LEU:HD22	3:1:433:TYR:HB3	2.01	0.43
3:1:770:ARG:HB3	3:1:771:PRO:HD3	2.01	0.43
6:I:371:LYS:HD2	6:I:371:LYS:H	1.83	0.43
4:J:702:ARG:NE	4:J:702:ARG:HA	2.34	0.43
10:W:266:ILE:CD1	10:W:336:ASN:HB2	2.49	0.43
2:Y:829:ILE:H	2:Y:831:LYS:HG2	1.84	0.42
4:D:765:LEU:CD2	5:E:460:TRP:CZ2	2.96	0.42
8:N:744:LEU:HD12	8:N:744:LEU:C	2.40	0.42
3:1:1173:LEU:HD13	3:1:1195:LEU:HD22	1.98	0.42
3:1:1184:ASP:CB	3:1:1187:TYR:CD2	2.88	0.42
4:J:765:LEU:CD2	5:K:460:TRP:CZ2	2.96	0.42
8:P:1357:CYS:SG	9:T:453:VAL:CB	3.07	0.42
9:S:601:PRO:HB2	9:S:606:GLU:CG	2.49	0.42
11:X:273:VAL:HB	11:X:356:VAL:CA	2.48	0.42
11:X:274:PHE:HA	11:X:354:SER:C	2.39	0.42
3:Z:494:ASN:HB2	3:Z:512:ARG:CB	2.49	0.42
3:Z:919:ILE:HB	3:Z:920:ASP:H	1.58	0.42
4:D:702:ARG:NE	4:D:702:ARG:HA	2.34	0.42
9:R:301:ASN:CB	9:R:345:LEU:HD13	2.48	0.42
11:V:273:VAL:HB	11:V:356:VAL:CA	2.48	0.42
11:V:274:PHE:HA	11:V:354:SER:C	2.39	0.42
2:0:829:ILE:H	2:0:831:LYS:HG2	1.84	0.42
7:O:1555:VAL:HG21	7:O:1561:LEU:HD11	2.00	0.42
8:P:174:VAL:HG21	8:P:242:TYR:CD2	2.53	0.42
1:4:2:UNK:CB	5:K:314:ASN:OD1	2.66	0.42
5:E:435:LYS:HA	5:E:438:SER:HB2	2.01	0.42
7:M:126:GLU:HA	7:M:131:TYR:CD2	2.55	0.42
8:N:808:THR:O	8:N:872:ASN:HB2	2.20	0.42
8:N:1357:CYS:SG	9:R:453:VAL:CB	3.07	0.42
9:R:58:SER:C	9:R:60:ASN:N	2.73	0.42
10:U:321:GLU:OE2	10:U:321:GLU:HA	2.20	0.42
11:V:294:ILE:HA	11:V:361:ASN:ND2	2.35	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:K:435:LYS:HA	5:K:438:SER:HB2	2.01	0.42
7:O:1500:ASN:HD21	7:O:1551:SER:CB	2.32	0.42
8:P:808:THR:O	8:P:872:ASN:HB2	2.20	0.42
9:T:301:ASN:CB	9:T:345:LEU:HD13	2.48	0.42
4:A:803:ALA:HA	9:Q:31:ASN:CB	2.50	0.42
7:M:995:VAL:HG12	7:M:999:LYS:HZ3	1.85	0.42
7:M:1500:ASN:HD21	7:M:1551:SER:CB	2.33	0.42
7:M:1642:LYS:CD	7:O:1559:LEU:CD2	2.91	0.42
8:N:174:VAL:HG21	8:N:242:TYR:CD2	2.54	0.42
8:N:225:ARG:O	8:N:228:ASN:CA	2.67	0.42
8:N:1107:GLU:O	8:N:1111:HIS:CE1	2.72	0.42
5:K:317:ASN:CB	5:K:348:ILE:HG12	2.30	0.42
6:L:433:LYS:CB	9:T:51:ARG:CB	2.97	0.42
9:T:58:SER:C	9:T:60:ASN:N	2.73	0.42
10:W:321:GLU:OE2	10:W:321:GLU:HA	2.20	0.42
11:X:271:ILE:HD13	11:X:386:PRO:HB3	2.01	0.42
4:A:809:ASP:CG	9:Q:36:SER:CB	2.88	0.42
7:M:800:ILE:HD12	7:M:800:ILE:H	1.83	0.42
9:R:432:ILE:CD1	9:R:477:TYR:CG	2.80	0.42
10:U:266:ILE:CD1	10:U:336:ASN:HB2	2.50	0.42
11:V:271:ILE:HD13	11:V:386:PRO:HB3	2.01	0.42
11:V:282:ASN:HD22	11:V:299:GLN:HB2	1.83	0.42
11:V:378:ARG:HD3	11:V:378:ARG:HA	1.93	0.42
6:L:374:GLN:CA	6:L:374:GLN:NE2	2.83	0.42
8:P:1107:GLU:O	8:P:1111:HIS:CE1	2.73	0.42
3:Z:412:ILE:HG23	3:Z:415:CYS:HB2	2.02	0.42
4:D:812:THR:HA	4:D:815:GLU:HG2	2.02	0.42
7:M:381:THR:CB	7:M:703:TYR:HB3	2.50	0.42
8:N:635:ILE:HG21	8:N:671:LEU:HD13	2.01	0.42
2:0:1313:VAL:H	2:0:1314:PRO:HD2	1.85	0.42
3:1:412:ILE:HG23	3:1:415:CYS:HB2	2.02	0.42
3:1:1169:ILE:HG22	3:1:1218:ILE:CD1	2.49	0.42
7:O:331:ILE:HG13	7:O:491:SER:HB2	2.00	0.42
7:O:800:ILE:H	7:O:800:ILE:HD12	1.83	0.42
7:O:1385:PHE:CG	7:O:1429:ASP:OD2	2.73	0.42
2:Y:1313:VAL:H	2:Y:1314:PRO:HD2	1.85	0.42
3:Z:1210:ALA:HB1	3:Z:1218:ILE:CG1	2.48	0.42
5:B:317:ASN:HB3	5:B:346:GLN:CG	2.43	0.42
6:F:433:LYS:O	6:F:441:SER:OG	2.30	0.42
7:M:331:ILE:HG13	7:M:491:SER:HB2	2.00	0.42
9:Q:595:ARG:HD2	10:U:329:GLN:NE2	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:J:812:THR:HA	4:J:815:GLU:HG2	2.02	0.42
7:O:381:THR:CB	7:O:703:TYR:HB3	2.50	0.42
8:P:221:VAL:O	8:P:225:ARG:HG3	2.19	0.42
8:P:635:ILE:HG21	8:P:671:LEU:HD13	2.01	0.42
9:S:547:TYR:O	11:X:298:PHE:CD2	2.73	0.42
9:S:584:LYS:CE	9:S:636:ARG:HD3	2.48	0.42
7:M:1393:ASN:ND2	8:N:687:LYS:NZ	2.64	0.42
2:0:518:GLU:HA	2:0:518:GLU:OE2	2.18	0.42
2:0:832:VAL:HG12	2:0:834:ILE:H	1.84	0.42
7:O:985:GLN:HA	7:O:988:SER:CB	2.36	0.42
9:T:631:ALA:HA	9:T:636:ARG:HH21	1.83	0.42
2:Y:832:VAL:HG12	2:Y:834:ILE:H	1.84	0.42
5:B:320:GLU:HB2	5:B:348:ILE:HD11	2.01	0.42
7:M:831:ILE:HD13	7:M:831:ILE:HG21	1.85	0.42
7:M:1642:LYS:HD2	7:O:1559:LEU:HD21	2.02	0.42
9:Q:601:PRO:O	9:Q:606:GLU:HG3	2.19	0.42
9:R:394:TYR:CE2	9:R:419:ASP:HB2	2.55	0.42
9:R:631:ALA:HA	9:R:636:ARG:HH21	1.83	0.42
10:U:321:GLU:CG	11:V:293:HIS:CD2	2.88	0.42
7:O:1193:ARG:C	7:O:1195:PHE:H	2.21	0.42
2:Y:517:LEU:CB	2:Y:537:LYS:NZ	2.82	0.42
6:F:394:ILE:CG1	9:R:40:GLY:O	2.68	0.42
7:M:1329:LEU:HD23	7:M:1380:ARG:NH2	2.30	0.42
9:R:670:LEU:H	9:R:670:LEU:HG	1.61	0.42
5:H:322:ILE:HG22	5:H:335:TRP:CZ2	2.53	0.42
6:I:352:VAL:HG23	6:L:292:HIS:CE1	2.55	0.42
6:I:369:LEU:N	6:I:373:PHE:HB2	2.35	0.42
7:O:1490:ARG:NH1	9:T:825:PRO:HA	2.33	0.42
7:O:1652:LYS:HA	7:O:1652:LYS:HE3	2.01	0.42
8:P:270:ILE:HD13	8:P:270:ILE:HA	1.75	0.42
9:T:432:ILE:CD1	9:T:477:TYR:CG	2.80	0.42
3:Z:914:GLN:O	3:Z:917:GLU:HG2	2.19	0.41
6:C:352:VAL:HG23	6:F:292:HIS:CE1	2.55	0.41
7:M:1490:ARG:NH1	9:R:825:PRO:HA	2.33	0.41
8:N:220:PHE:CD2	8:N:265:PHE:CZ	3.08	0.41
8:N:273:LEU:HB3	8:N:328:ILE:CD1	2.50	0.41
9:Q:589:LEU:HA	9:Q:603:VAL:HG22	1.98	0.41
3:1:214:PHE:CG	3:1:221:LEU:HD11	2.55	0.41
5:K:318:GLU:HA	5:K:346:GLN:N	2.33	0.41
7:O:1189:MET:HE1	8:P:252:TYR:CG	2.54	0.41
8:P:273:LEU:HB3	8:P:328:ILE:CD1	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:T:394:TYR:CE2	9:T:419:ASP:HB2	2.55	0.41
10:W:253:ILE:H	10:W:318:TYR:HD2	1.68	0.41
11:X:289:SER:C	11:X:294:ILE:HD11	2.39	0.41
3:Z:214:PHE:CG	3:Z:221:LEU:HD11	2.55	0.41
6:F:353:LEU:HD11	6:F:369:LEU:HD12	2.02	0.41
7:M:1385:PHE:CZ	7:M:1426:VAL:CG2	3.03	0.41
7:M:1652:LYS:HA	7:M:1652:LYS:HE3	2.01	0.41
8:N:741:LYS:C	8:N:744:LEU:HG	2.32	0.41
9:Q:588:VAL:CG2	10:U:248:TRP:HZ3	2.33	0.41
2:0:518:GLU:HB3	2:0:536:ILE:HB	2.01	0.41
2:0:1020:ASN:HD22	9:T:248:THR:N	2.18	0.41
7:O:341:PHE:CE2	7:O:652:ALA:HB2	2.44	0.41
7:O:1671:VAL:CG1	9:T:166:LYS:HA	2.50	0.41
11:X:293:HIS:O	11:X:361:ASN:ND2	2.53	0.41
2:Y:1020:ASN:HD22	9:R:248:THR:N	2.18	0.41
7:M:341:PHE:CE2	7:M:652:ALA:HB2	2.44	0.41
7:M:1193:ARG:C	7:M:1195:PHE:H	2.21	0.41
7:M:1619:ASN:HA	9:R:634:ASP:O	2.21	0.41
8:N:274:GLY:HA2	8:N:284:ILE:C	2.40	0.41
8:N:327:PHE:HB3	8:N:389:PHE:HE2	1.85	0.41
9:Q:73:LEU:CB	9:T:84:ASP:HA	2.50	0.41
9:Q:573:HIS:CG	9:Q:623:ILE:HD11	2.55	0.41
10:U:253:ILE:H	10:U:318:TYR:HD2	1.68	0.41
11:V:295:MET:C	11:V:297:ASP:H	2.24	0.41
3:1:914:GLN:O	3:1:917:GLU:HG2	2.19	0.41
3:1:1170:GLN:CD	3:1:1205:LEU:HD22	2.41	0.41
7:O:1381:LEU:HD21	7:O:1425:LYS:CB	2.50	0.41
9:S:588:VAL:CG2	10:W:248:TRP:HZ3	2.33	0.41
8:N:270:ILE:HD13	8:N:270:ILE:HA	1.75	0.41
8:N:1339:PHE:CE2	8:N:1343:VAL:HG21	2.56	0.41
7:O:831:ILE:HD13	7:O:831:ILE:HG21	1.85	0.41
8:P:274:GLY:HA2	8:P:284:ILE:C	2.40	0.41
9:S:573:HIS:CG	9:S:623:ILE:HD11	2.55	0.41
9:T:99:ASN:C	9:T:101:PRO:N	2.73	0.41
7:M:1389:ILE:HD11	8:N:686:GLY:O	2.20	0.41
9:R:99:ASN:C	9:R:101:PRO:N	2.73	0.41
3:1:1195:LEU:C	3:1:1197:GLY:H	2.23	0.41
3:1:1210:ALA:HB2	3:1:1218:ILE:CG2	2.51	0.41
7:O:1385:PHE:CZ	7:O:1426:VAL:CG2	3.04	0.41
7:O:1389:ILE:HD11	8:P:686:GLY:O	2.20	0.41
8:P:1339:PHE:CE2	8:P:1343:VAL:HG21	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:S:673:PRO:HA	9:S:728:PHE:CE2	2.55	0.41
3:Z:1176:LEU:HD13	3:Z:1217:GLU:CD	2.41	0.41
7:M:444:THR:HG23	7:M:506:ASN:ND2	2.31	0.41
7:M:1190:TYR:HD2	8:N:758:TYR:O	2.04	0.41
9:Q:673:PRO:HA	9:Q:728:PHE:CE2	2.55	0.41
3:1:1176:LEU:HD13	3:1:1217:GLU:CD	2.41	0.41
3:1:1194:LYS:CE	3:1:1208:ASP:O	2.68	0.41
7:O:1619:ASN:HA	9:T:634:ASP:O	2.21	0.41
9:S:589:LEU:HD23	9:S:603:VAL:HG21	2.01	0.41
9:T:670:LEU:H	9:T:670:LEU:HG	1.61	0.41
3:Z:919:ILE:HD13	3:Z:919:ILE:N	2.36	0.41
5:B:323:LEU:CG	5:B:335:TRP:CH2	3.04	0.41
7:M:1381:LEU:HD12	7:M:1426:VAL:HG23	2.03	0.41
7:O:444:THR:HG23	7:O:506:ASN:ND2	2.31	0.41
7:O:1190:TYR:HD2	8:P:758:TYR:O	2.04	0.41
8:P:271:LEU:HD21	8:P:378:VAL:HG21	2.03	0.41
2:Y:1005:ARG:O	2:Y:1009:HIS:CD2	2.74	0.41
7:M:523:ARG:O	7:M:527:TYR:CD2	2.74	0.41
7:M:1381:LEU:C	7:M:1385:PHE:HD2	2.20	0.41
3:1:495:THR:HA	3:1:510:CYS:O	2.21	0.41
3:1:919:ILE:HD13	3:1:919:ILE:N	2.36	0.41
5:H:321:ALA:HA	5:H:348:ILE:HG12	2.02	0.41
6:I:372:PHE:CE2	6:I:376:LYS:HD3	2.55	0.41
5:K:457:ASN:CA	5:K:460:TRP:HD1	2.32	0.41
7:O:523:ARG:O	7:O:527:TYR:CD2	2.74	0.41
1:4:2:UNK:HA	5:K:314:ASN:OD1	2.16	0.41
2:Y:120:VAL:HG12	2:Y:122:ASP:H	1.86	0.41
2:Y:1140:LYS:HA	2:Y:1140:LYS:HD3	1.89	0.41
2:Y:1425:LYS:NZ	7:O:1432:LEU:HD23	2.35	0.41
5:B:295:CYS:O	6:C:280:LEU:HD11	2.20	0.41
5:B:322:ILE:HD12	5:B:322:ILE:C	2.41	0.41
5:E:314:ASN:ND2	5:E:348:ILE:CD1	2.83	0.41
5:E:457:ASN:CA	5:E:460:TRP:HD1	2.32	0.41
7:M:771:ARG:HH21	7:M:856:GLU:HB3	1.86	0.41
8:N:271:LEU:HD21	8:N:378:VAL:HG21	2.03	0.41
9:R:337:ILE:HD13	9:R:337:ILE:HG21	1.89	0.41
2:0:1005:ARG:O	2:0:1009:HIS:CD2	2.74	0.41
2:0:1140:LYS:HA	2:0:1140:LYS:HD3	1.90	0.41
5:H:295:CYS:O	6:I:280:LEU:HD11	2.20	0.41
5:H:322:ILE:CG2	5:H:335:TRP:CZ2	3.04	0.41
7:O:771:ARG:HH21	7:O:856:GLU:HB3	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:P:221:VAL:HG12	8:P:225:ARG:HE	1.86	0.41
9:S:564:GLU:OE2	9:S:612:HIS:CD2	2.74	0.41
10:W:271:ALA:HB2	10:W:283:ILE:CB	2.51	0.41
3:Z:492:TYR:CD1	3:Z:492:TYR:N	2.89	0.41
4:D:819:ASN:H	4:D:819:ASN:ND2	2.19	0.41
8:N:225:ARG:HA	8:N:228:ASN:HB2	2.02	0.41
8:N:276:ASN:HB2	8:N:280:ALA:HB2	2.02	0.41
8:N:327:PHE:CB	8:N:389:PHE:CE2	3.04	0.41
9:Q:564:GLU:OE2	9:Q:612:HIS:CD2	2.74	0.41
11:V:355:TRP:CD1	11:V:400:ILE:HD13	2.34	0.41
3:1:182:LEU:HD12	3:1:194:ILE:CD1	2.50	0.41
5:K:370:ALA:HB2	5:K:373:ARG:HD2	2.02	0.41
10:W:282:VAL:HG23	10:W:283:ILE:HD13	1.98	0.41
3:Z:182:LEU:HD12	3:Z:194:ILE:CD1	2.51	0.40
7:M:43:LYS:HD3	7:M:79:ASP:HA	2.03	0.40
11:V:282:ASN:HB2	11:V:300:VAL:CA	2.51	0.40
3:1:1191:LEU:HD22	3:1:1215:TYR:HE2	1.83	0.40
6:L:369:LEU:C	6:L:369:LEU:CD2	2.89	0.40
7:O:1380:ARG:HD2	7:O:1415:ARG:HD3	2.03	0.40
9:T:432:ILE:HD11	9:T:477:TYR:CD1	2.50	0.40
7:M:1189:MET:SD	7:M:1190:TYR:HD1	2.44	0.40
7:M:1391:GLY:C	7:M:1393:ASN:N	2.73	0.40
8:N:741:LYS:O	8:N:744:LEU:CD1	2.70	0.40
2:0:120:VAL:HG12	2:0:122:ASP:H	1.86	0.40
4:J:803:ALA:CA	9:T:31:ASN:CB	2.98	0.40
4:J:819:ASN:H	4:J:819:ASN:ND2	2.20	0.40
7:O:43:LYS:HD3	7:O:79:ASP:HA	2.03	0.40
7:O:1189:MET:SD	7:O:1190:TYR:HD1	2.44	0.40
8:P:276:ASN:HB2	8:P:280:ALA:HB2	2.03	0.40
2:Y:1186:LEU:HB3	2:Y:1200:LEU:HD13	2.03	0.40
3:Z:344:GLN:OE1	3:Z:497:CYS:CB	2.57	0.40
3:Z:968:LEU:HA	3:Z:968:LEU:HD23	1.84	0.40
5:B:323:LEU:CB	5:B:335:TRP:CZ3	3.01	0.40
9:R:435:TRP:CZ2	9:R:474:PHE:CD1	3.09	0.40
2:0:1310:ASP:OD2	2:0:1311:PHE:CZ	2.66	0.40
3:1:1192:THR:O	3:1:1196:ASN:HB2	2.21	0.40
5:K:324:TYR:HB2	5:K:335:TRP:CZ3	2.55	0.40
7:O:1391:GLY:C	7:O:1393:ASN:N	2.73	0.40
7:O:1671:VAL:HG12	9:T:166:LYS:HA	2.02	0.40
9:T:337:ILE:HD13	9:T:337:ILE:HG21	1.89	0.40
9:T:435:TRP:CZ2	9:T:474:PHE:CD1	3.09	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:B:540:LYS:NZ	6:C:467:LEU:HD22	2.37	0.40
9:R:432:ILE:HD11	9:R:477:TYR:CD1	2.50	0.40
3:1:494:ASN:ND2	3:1:512:ARG:O	2.51	0.40
4:G:752:ASP:OD1	4:G:755:LEU:HD22	2.21	0.40
6:L:371:LYS:H	6:L:371:LYS:CE	2.34	0.40
1:7:78:UNK:CB	9:R:473:ARG:HD2	2.51	0.40
1:8:78:UNK:CB	9:T:473:ARG:HD2	2.51	0.40
2:Y:433:ASN:HB3	2:Y:449:ASN:HD22	1.86	0.40
2:Y:517:LEU:HB2	2:Y:537:LYS:HZ2	1.83	0.40
4:A:752:ASP:OD1	4:A:755:LEU:HD22	2.21	0.40
8:N:255:GLU:O	8:N:258:ILE:HG13	2.21	0.40
2:0:433:ASN:HB3	2:0:449:ASN:HD22	1.86	0.40
2:0:1186:LEU:HB3	2:0:1200:LEU:HD13	2.04	0.40
3:1:494:ASN:C	3:1:512:ARG:H	2.25	0.40
5:H:540:LYS:NZ	6:I:467:LEU:HD22	2.37	0.40
7:O:1385:PHE:CZ	7:O:1426:VAL:HG22	2.51	0.40
8:P:1438:ILE:HD13	8:P:1438:ILE:HA	1.91	0.40
11:X:355:TRP:CD1	11:X:400:ILE:HD13	2.34	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
2	0	1244/1502 (83%)	1144 (92%)	65 (5%)	35 (3%)	5 30
2	Y	1244/1502 (83%)	1143 (92%)	66 (5%)	35 (3%)	5 30
3	1	1152/1391 (83%)	1077 (94%)	51 (4%)	24 (2%)	7 36
3	Z	1152/1391 (83%)	1080 (94%)	50 (4%)	22 (2%)	8 38
4	A	157/823 (19%)	151 (96%)	3 (2%)	3 (2%)	8 38
4	D	163/823 (20%)	153 (94%)	4 (2%)	6 (4%)	3 24

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
4	G	157/823 (19%)	151 (96%)	3 (2%)	3 (2%)	8	38
4	J	163/823 (20%)	153 (94%)	6 (4%)	4 (2%)	5	32
5	B	211/541 (39%)	178 (84%)	22 (10%)	11 (5%)	2	19
5	E	211/541 (39%)	194 (92%)	12 (6%)	5 (2%)	6	33
5	H	211/541 (39%)	180 (85%)	21 (10%)	10 (5%)	2	21
5	K	211/541 (39%)	192 (91%)	13 (6%)	6 (3%)	5	30
6	C	160/472 (34%)	150 (94%)	9 (6%)	1 (1%)	25	66
6	F	167/472 (35%)	159 (95%)	7 (4%)	1 (1%)	25	66
6	I	160/472 (34%)	150 (94%)	9 (6%)	1 (1%)	25	66
6	L	167/472 (35%)	156 (93%)	8 (5%)	3 (2%)	8	40
7	M	1655/1683 (98%)	1536 (93%)	80 (5%)	39 (2%)	6	33
7	O	1655/1683 (98%)	1533 (93%)	78 (5%)	44 (3%)	5	31
8	N	1636/1655 (99%)	1524 (93%)	86 (5%)	26 (2%)	9	44
8	P	1639/1655 (99%)	1524 (93%)	87 (5%)	28 (2%)	9	42
9	Q	785/839 (94%)	717 (91%)	55 (7%)	13 (2%)	9	42
9	R	796/839 (95%)	715 (90%)	54 (7%)	27 (3%)	3	26
9	S	785/839 (94%)	722 (92%)	51 (6%)	12 (2%)	10	46
9	T	797/839 (95%)	719 (90%)	51 (6%)	27 (3%)	3	26
10	U	90/475 (19%)	67 (74%)	18 (20%)	5 (6%)	2	18
10	W	90/475 (19%)	67 (74%)	17 (19%)	6 (7%)	1	15
11	V	86/528 (16%)	70 (81%)	14 (16%)	2 (2%)	6	34
11	X	86/528 (16%)	71 (83%)	13 (15%)	2 (2%)	6	34
All	All	17030/25168 (68%)	15676 (92%)	953 (6%)	401 (2%)	9	33

All (401) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
2	Y	129	SER
2	Y	250	ALA
2	Y	289	SER
2	Y	356	ILE
2	Y	409	ALA
2	Y	431	ASN
2	Y	471	SER

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Mol	Chain	Res	Type
2	Y	690	ASN
2	Y	766	LEU
2	Y	830	SER
2	Y	870	ALA
2	Y	1223	SER
2	Y	1380	ASP
3	Z	79	HIS
3	Z	115	ASP
3	Z	414	MET
3	Z	1230	ASP
5	B	291	GLN
5	B	309	ARG
5	B	346	GLN
5	B	434	GLU
4	D	637	LEU
4	D	639	ASP
4	D	776	PHE
7	M	360	LEU
7	M	519	ASP
7	M	1194	LEU
7	M	1260	ASN
7	M	1392	ILE
7	M	1568	VAL
7	M	1591	ASP
8	N	68	HIS
8	N	1429	HIS
9	Q	33	PRO
9	Q	73	LEU
9	Q	681	SER
9	R	46	ILE
9	R	101	PRO
9	R	154	GLU
9	R	434	ASP
9	R	520	SER
9	R	549	ASP
9	R	795	GLN
10	U	356	LEU
11	V	272	ILE
2	0	129	SER
2	0	250	ALA
2	0	289	SER
2	0	356	ILE

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Mol	Chain	Res	Type
2	0	409	ALA
2	0	431	ASN
2	0	471	SER
2	0	690	ASN
2	0	766	LEU
2	0	830	SER
2	0	870	ALA
2	0	1223	SER
2	0	1380	ASP
3	1	79	HIS
3	1	115	ASP
3	1	414	MET
3	1	497	CYS
3	1	1230	ASP
5	H	291	GLN
5	H	309	ARG
5	H	346	GLN
5	H	434	GLU
4	J	639	ASP
4	J	776	PHE
7	O	360	LEU
7	O	519	ASP
7	O	1194	LEU
7	O	1260	ASN
7	O	1375	GLY
7	O	1378	ASP
7	O	1392	ILE
7	O	1558	ASP
7	O	1568	VAL
7	O	1591	ASP
8	P	68	HIS
8	P	69	ASN
8	P	1429	HIS
9	S	73	LEU
9	S	681	SER
9	T	41	SER
9	T	46	ILE
9	T	101	PRO
9	T	154	GLU
9	T	434	ASP
9	T	520	SER
9	T	549	ASP

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Mol	Chain	Res	Type
9	T	795	GLN
10	W	356	LEU
11	X	272	ILE
2	Y	408	ARG
2	Y	871	ASN
2	Y	920	GLU
2	Y	1154	ASP
2	Y	1288	ALA
3	Z	85	LEU
3	Z	361	SER
3	Z	497	CYS
3	Z	652	ASN
3	Z	919	ILE
3	Z	1301	SER
4	A	744	ALA
4	A	752	ASP
5	B	299	TRP
5	B	305	LYS
5	B	355	PHE
4	D	754	ASN
5	E	299	TRP
5	E	317	ASN
7	M	205	ALA
7	M	373	SER
7	M	378	ALA
7	M	381	THR
7	M	670	LYS
7	M	678	LEU
7	M	742	GLN
7	M	957	ALA
7	M	1036	PRO
7	M	1214	SER
7	M	1379	GLY
7	M	1505	HIS
7	M	1558	ASP
8	N	316	ILE
8	N	487	SER
8	N	608	ILE
8	N	614	ILE
9	Q	45	SER
9	Q	269	ASN
9	Q	562	LEU

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Mol	Chain	Res	Type
9	R	85	ALA
9	R	155	VAL
9	R	169	VAL
9	R	473	ARG
9	R	612	HIS
10	U	262	ILE
2	0	408	ARG
2	0	871	ASN
2	0	920	GLU
2	0	1154	ASP
2	0	1288	ALA
3	1	85	LEU
3	1	361	SER
3	1	652	ASN
3	1	919	ILE
3	1	1301	SER
4	G	744	ALA
4	G	752	ASP
5	H	299	TRP
5	H	305	LYS
5	H	355	PHE
4	J	754	ASN
5	K	299	TRP
7	O	205	ALA
7	O	373	SER
7	O	378	ALA
7	O	381	THR
7	O	670	LYS
7	O	678	LEU
7	O	742	GLN
7	O	957	ALA
7	O	989	SER
7	O	1036	PRO
7	O	1214	SER
7	O	1379	GLY
7	O	1505	HIS
8	P	316	ILE
8	P	487	SER
8	P	608	ILE
8	P	614	ILE
9	S	34	SER
9	S	45	SER

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Mol	Chain	Res	Type
9	S	269	ASN
9	S	562	LEU
9	T	85	ALA
9	T	155	VAL
9	T	473	ARG
9	T	612	HIS
10	W	262	ILE
10	W	283	ILE
2	Y	384	GLU
2	Y	519	THR
2	Y	522	ALA
2	Y	761	LEU
2	Y	1300	LYS
3	Z	351	ARG
3	Z	493	ILE
3	Z	920	ASP
3	Z	1026	SER
3	Z	1052	ASN
3	Z	1255	SER
5	B	298	SER
5	B	327	PRO
4	D	633	ASP
4	D	755	LEU
7	M	20	PHE
7	M	62	SER
7	M	136	LYS
7	M	366	ILE
7	M	368	SER
7	M	379	SER
7	M	1190	TYR
7	M	1581	THR
8	N	92	SER
8	N	236	THR
8	N	315	PRO
8	N	485	SER
8	N	978	SER
8	N	1435	ASP
8	N	1574	LYS
9	Q	204	GLU
9	R	62	ALA
9	R	105	GLU
9	R	324	ASN

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Mol	Chain	Res	Type
9	R	419	ASP
9	R	472	SER
9	R	533	ARG
9	R	545	PHE
10	U	354	ALA
2	0	384	GLU
2	0	522	ALA
2	0	761	LEU
2	0	1300	LYS
3	1	351	ARG
3	1	920	ASP
3	1	1026	SER
3	1	1052	ASN
3	1	1255	SER
5	H	298	SER
4	J	755	LEU
5	K	317	ASN
6	L	436	LEU
6	L	437	ALA
7	O	20	PHE
7	O	62	SER
7	O	136	LYS
7	O	366	ILE
7	O	368	SER
7	O	379	SER
7	O	1190	TYR
8	P	92	SER
8	P	236	THR
8	P	315	PRO
8	P	485	SER
8	P	978	SER
8	P	1435	ASP
8	P	1574	LYS
9	S	204	GLU
9	T	62	ALA
9	T	105	GLU
9	T	324	ASN
9	T	419	ASP
9	T	472	SER
9	T	533	ARG
9	T	545	PHE
10	W	354	ALA

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Mol	Chain	Res	Type
2	Y	304	TRP
2	Y	305	PHE
2	Y	764	VAL
2	Y	865	ALA
2	Y	1088	PHE
2	Y	1287	SER
2	Y	1313	VAL
3	Z	498	ALA
3	Z	575	ARG
3	Z	1253	VAL
5	B	307	LYS
6	C	300	ASP
5	E	295	CYS
5	E	422	LEU
7	M	304	THR
7	M	1191	SER
7	M	1263	SER
7	M	1656	SER
8	N	86	ASP
8	N	94	ASP
8	N	123	ASP
8	N	273	LEU
8	N	545	GLN
9	Q	232	PHE
9	Q	405	ASP
9	Q	475	SER
9	R	39	LEU
9	R	102	LYS
2	0	304	TRP
2	0	305	PHE
2	0	764	VAL
2	0	865	ALA
2	0	1088	PHE
2	0	1287	SER
2	0	1313	VAL
3	1	493	ILE
3	1	498	ALA
3	1	575	ARG
3	1	1196	ASN
3	1	1253	VAL
5	H	307	LYS
6	I	300	ASP

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Mol	Chain	Res	Type
5	K	295	CYS
5	K	325	THR
5	K	422	LEU
7	O	304	THR
7	O	1191	SER
7	O	1263	SER
7	O	1581	THR
7	O	1656	SER
8	P	86	ASP
8	P	94	ASP
8	P	123	ASP
8	P	273	LEU
8	P	545	GLN
9	S	232	PHE
9	S	405	ASP
9	S	475	SER
9	T	102	LYS
9	T	169	VAL
2	Y	538	SER
3	Z	113	ASN
3	Z	403	ALA
4	A	705	ASP
5	B	344	SER
5	E	344	SER
6	F	352	VAL
7	M	267	SER
7	M	385	SER
7	M	1129	ASN
7	M	1585	PRO
8	N	120	PRO
8	N	278	SER
8	N	293	GLU
8	N	581	THR
9	Q	447	ASP
9	R	44	VAL
9	R	59	LYS
9	R	825	PRO
10	U	261	THR
11	V	347	TYR
2	0	538	SER
3	1	113	ASN
3	1	403	ALA

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Mol	Chain	Res	Type
3	1	1214	ASP
4	G	705	ASP
5	H	344	SER
5	K	344	SER
6	L	352	VAL
7	O	267	SER
7	O	385	SER
7	O	1129	ASN
7	O	1585	PRO
8	P	120	PRO
8	P	278	SER
8	P	293	GLU
8	P	581	THR
9	S	447	ASP
9	T	44	VAL
9	T	59	LYS
9	T	825	PRO
10	W	261	THR
11	X	347	TYR
2	Y	303	ASP
7	M	1654	ASN
8	N	290	MET
8	N	337	SER
8	N	1377	ASN
9	Q	601	PRO
9	R	521	SER
9	R	674	LEU
10	U	320	SER
2	0	303	ASP
2	0	1312	ALA
7	O	988	SER
7	O	1377	VAL
7	O	1654	ASN
8	P	290	MET
8	P	337	SER
8	P	1377	ASN
9	T	521	SER
9	T	674	LEU
10	W	320	SER
7	M	1395	PRO
7	O	1395	PRO
2	Y	765	ILE

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Mol	Chain	Res	Type
9	R	685	PRO
2	0	765	ILE
9	T	685	PRO
2	Y	468	PRO
9	Q	46	ILE
2	0	119	PRO
2	0	468	PRO
9	S	46	ILE
2	Y	119	PRO
7	M	1192	VAL
8	N	1583	VAL
7	O	1192	VAL
8	P	1583	VAL
8	P	227	ILE
3	Z	504	PRO
3	1	504	PRO

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
2	0	1130/1353 (84%)	1091 (96%)	39 (4%)	36 59
2	Y	1130/1353 (84%)	1091 (96%)	39 (4%)	36 59
3	1	1051/1250 (84%)	1026 (98%)	25 (2%)	49 69
3	Z	1051/1250 (84%)	1027 (98%)	24 (2%)	50 70
4	A	154/674 (23%)	147 (96%)	7 (4%)	27 52
4	D	154/674 (23%)	144 (94%)	10 (6%)	17 42
4	G	154/674 (23%)	147 (96%)	7 (4%)	27 52
4	J	155/674 (23%)	145 (94%)	10 (6%)	17 42
5	B	196/439 (45%)	178 (91%)	18 (9%)	9 29
5	E	196/439 (45%)	186 (95%)	10 (5%)	24 49
5	H	196/439 (45%)	180 (92%)	16 (8%)	11 34

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
5	K	196/439 (45%)	182 (93%)	14 (7%)	14	39
6	C	155/377 (41%)	150 (97%)	5 (3%)	39	61
6	F	155/377 (41%)	151 (97%)	4 (3%)	46	66
6	I	155/377 (41%)	150 (97%)	5 (3%)	39	61
6	L	155/377 (41%)	150 (97%)	5 (3%)	39	61
7	M	1518/1538 (99%)	1456 (96%)	62 (4%)	30	55
7	O	1518/1538 (99%)	1458 (96%)	60 (4%)	31	55
8	N	1538/1557 (99%)	1470 (96%)	68 (4%)	28	53
8	P	1539/1557 (99%)	1474 (96%)	65 (4%)	30	54
9	Q	590/762 (77%)	573 (97%)	17 (3%)	42	64
9	R	582/762 (76%)	560 (96%)	22 (4%)	33	57
9	S	590/762 (77%)	573 (97%)	17 (3%)	42	64
9	T	582/762 (76%)	560 (96%)	22 (4%)	33	57
10	U	80/421 (19%)	72 (90%)	8 (10%)	7	26
10	W	80/421 (19%)	70 (88%)	10 (12%)	4	19
11	V	77/477 (16%)	69 (90%)	8 (10%)	7	25
11	X	77/477 (16%)	68 (88%)	9 (12%)	5	21
All	All	15154/22200 (68%)	14548 (96%)	606 (4%)	35	55

All (606) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	Y	86	MET
2	Y	95	MET
2	Y	101	LEU
2	Y	113	HIS
2	Y	124	ARG
2	Y	185	THR
2	Y	201	TYR
2	Y	207	MET
2	Y	223	THR
2	Y	251	THR
2	Y	298	TYR
2	Y	311	LYS
2	Y	361	ILE
2	Y	377	ILE

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Mol	Chain	Res	Type
2	Y	391	MET
2	Y	441	VAL
2	Y	468	PRO
2	Y	503	GLU
2	Y	520	THR
2	Y	524	THR
2	Y	571	THR
2	Y	618	THR
2	Y	665	ASN
2	Y	761	LEU
2	Y	955	PRO
2	Y	973	ARG
2	Y	1018	LEU
2	Y	1070	ILE
2	Y	1129	ASN
2	Y	1130	GLN
2	Y	1133	ILE
2	Y	1171	GLU
2	Y	1184	PRO
2	Y	1252	LYS
2	Y	1254	ARG
2	Y	1304	THR
2	Y	1436	THR
2	Y	1484	ILE
2	Y	1488	VAL
3	Z	301	LYS
3	Z	369	THR
3	Z	414	MET
3	Z	441	ARG
3	Z	512	ARG
3	Z	536	HIS
3	Z	575	ARG
3	Z	582	THR
3	Z	599	LEU
3	Z	662	LEU
3	Z	664	PHE
3	Z	727	ARG
3	Z	740	MET
3	Z	918	MET
3	Z	919	ILE
3	Z	920	ASP
3	Z	922	LYS

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Mol	Chain	Res	Type
3	Z	978	ASN
3	Z	1082	PRO
3	Z	1136	ARG
3	Z	1274	LYS
3	Z	1277	ARG
3	Z	1299	LYS
3	Z	1338	LEU
4	A	655	PHE
4	A	695	GLN
4	A	704	GLN
4	A	714	PHE
4	A	794	ILE
4	A	795	LYS
4	A	816	LYS
5	B	287	GLN
5	B	299	TRP
5	B	309	ARG
5	B	315	LYS
5	B	317	ASN
5	B	323	LEU
5	B	345	PRO
5	B	392	LEU
5	B	394	THR
5	B	436	MET
5	B	446	ARG
5	B	460	TRP
5	B	462	ARG
5	B	465	ILE
5	B	471	LYS
5	B	518	ARG
5	B	523	LEU
5	B	529	LYS
6	C	304	LEU
6	C	307	SER
6	C	448	THR
6	C	451	MET
6	C	462	GLN
4	D	645	THR
4	D	657	GLN
4	D	688	HIS
4	D	690	GLN
4	D	695	GLN

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Mol	Chain	Res	Type
4	D	705	ASP
4	D	765	LEU
4	D	776	PHE
4	D	794	ILE
4	D	795	LYS
5	E	293	LEU
5	E	294	LYS
5	E	304	THR
5	E	331	LEU
5	E	392	LEU
5	E	417	THR
5	E	435	LYS
5	E	446	ARG
5	E	455	LYS
5	E	463	LEU
6	F	374	GLN
6	F	439	ILE
6	F	456	ARG
6	F	457	ILE
7	M	7	PRO
7	M	38	ASN
7	M	101	ASN
7	M	180	LYS
7	M	245	ARG
7	M	295	ARG
7	M	303	LYS
7	M	331	ILE
7	M	333	GLU
7	M	340	LEU
7	M	363	ASP
7	M	364	GLU
7	M	451	THR
7	M	515	SER
7	M	572	PHE
7	M	573	ASN
7	M	590	ILE
7	M	602	ASN
7	M	683	SER
7	M	689	SER
7	M	697	THR
7	M	800	ILE
7	M	826	PRO

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Mol	Chain	Res	Type
7	M	852	SER
7	M	879	GLN
7	M	910	ARG
7	M	990	ILE
7	M	991	THR
7	M	1013	TYR
7	M	1015	ARG
7	M	1036	PRO
7	M	1118	ARG
7	M	1129	ASN
7	M	1186	SER
7	M	1189	MET
7	M	1225	GLN
7	M	1227	THR
7	M	1241	LYS
7	M	1323	THR
7	M	1348	THR
7	M	1378	ASP
7	M	1380	ARG
7	M	1386	LYS
7	M	1387	THR
7	M	1390	GLN
7	M	1396	LEU
7	M	1418	SER
7	M	1435	LYS
7	M	1436	LYS
7	M	1527	ARG
7	M	1532	ARG
7	M	1573	SER
7	M	1576	LEU
7	M	1577	LYS
7	M	1581	THR
7	M	1582	LEU
7	M	1583	ASP
7	M	1584	ASN
7	M	1589	ASP
7	M	1595	VAL
7	M	1635	ARG
7	M	1652	LYS
8	N	15	PHE
8	N	20	ASN
8	N	55	LEU

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Mol	Chain	Res	Type
8	N	59	ARG
8	N	61	ASN
8	N	62	VAL
8	N	63	THR
8	N	64	SER
8	N	69	ASN
8	N	78	LEU
8	N	202	THR
8	N	233	SER
8	N	270	ILE
8	N	275	LEU
8	N	277	THR
8	N	285	GLN
8	N	289	TYR
8	N	291	ASP
8	N	292	THR
8	N	293	GLU
8	N	299	ASN
8	N	305	ASP
8	N	308	THR
8	N	311	VAL
8	N	313	GLU
8	N	316	ILE
8	N	336	GLN
8	N	340	SER
8	N	376	THR
8	N	508	PRO
8	N	536	GLN
8	N	538	GLN
8	N	560	ASN
8	N	602	VAL
8	N	615	LEU
8	N	620	ASN
8	N	647	GLN
8	N	729	HIS
8	N	745	HIS
8	N	755	ASN
8	N	789	GLN
8	N	803	LEU
8	N	827	PRO
8	N	862	ARG
8	N	955	PHE

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Mol	Chain	Res	Type
8	N	958	THR
8	N	965	ASP
8	N	980	LYS
8	N	991	LYS
8	N	1061	THR
8	N	1149	ARG
8	N	1176	PRO
8	N	1184	LYS
8	N	1188	THR
8	N	1216	LYS
8	N	1270	LYS
8	N	1349	TYR
8	N	1356	LEU
8	N	1369	THR
8	N	1411	SER
8	N	1441	GLN
8	N	1527	LYS
8	N	1574	LYS
8	N	1597	ARG
8	N	1630	GLU
8	N	1631	SER
8	N	1633	ARG
8	N	1653	LYS
9	Q	211	LYS
9	Q	220	PHE
9	Q	249	ARG
9	Q	325	LEU
9	Q	419	ASP
9	Q	496	TYR
9	Q	524	LEU
9	Q	562	LEU
9	Q	580	VAL
9	Q	592	LYS
9	Q	593	ILE
9	Q	609	PRO
9	Q	629	ARG
9	Q	703	SER
9	Q	721	SER
9	Q	798	THR
9	Q	822	TYR
9	R	205	ASN
9	R	372	LYS

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Mol	Chain	Res	Type
9	R	421	SER
9	R	428	VAL
9	R	432	ILE
9	R	433	GLU
9	R	434	ASP
9	R	496	TYR
9	R	520	SER
9	R	526	LYS
9	R	567	THR
9	R	614	ARG
9	R	670	LEU
9	R	671	ASP
9	R	672	GLN
9	R	674	LEU
9	R	678	ASP
9	R	680	ASN
9	R	683	THR
9	R	684	ASN
9	R	799	LYS
9	R	823	ARG
10	U	253	ILE
10	U	260	GLU
10	U	273	PHE
10	U	309	THR
10	U	317	THR
10	U	320	SER
10	U	324	LYS
10	U	338	THR
11	V	272	ILE
11	V	273	VAL
11	V	295	MET
11	V	354	SER
11	V	376	ILE
11	V	385	ILE
11	V	399	LYS
11	V	401	ASP
2	0	86	MET
2	0	95	MET
2	0	101	LEU
2	0	113	HIS
2	0	124	ARG
2	0	185	THR

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Mol	Chain	Res	Type
2	0	201	TYR
2	0	207	MET
2	0	223	THR
2	0	251	THR
2	0	298	TYR
2	0	311	LYS
2	0	361	ILE
2	0	377	ILE
2	0	391	MET
2	0	441	VAL
2	0	468	PRO
2	0	503	GLU
2	0	516	LEU
2	0	524	THR
2	0	571	THR
2	0	618	THR
2	0	665	ASN
2	0	761	LEU
2	0	955	PRO
2	0	973	ARG
2	0	1018	LEU
2	0	1070	ILE
2	0	1129	ASN
2	0	1130	GLN
2	0	1133	ILE
2	0	1171	GLU
2	0	1184	PRO
2	0	1252	LYS
2	0	1254	ARG
2	0	1304	THR
2	0	1436	THR
2	0	1484	ILE
2	0	1488	VAL
3	1	301	LYS
3	1	369	THR
3	1	414	MET
3	1	441	ARG
3	1	512	ARG
3	1	536	HIS
3	1	575	ARG
3	1	582	THR
3	1	599	LEU

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Mol	Chain	Res	Type
3	1	662	LEU
3	1	664	PHE
3	1	727	ARG
3	1	740	MET
3	1	918	MET
3	1	919	ILE
3	1	920	ASP
3	1	922	LYS
3	1	978	ASN
3	1	1082	PRO
3	1	1136	ARG
3	1	1198	ARG
3	1	1274	LYS
3	1	1277	ARG
3	1	1299	LYS
3	1	1338	LEU
4	G	655	PHE
4	G	695	GLN
4	G	704	GLN
4	G	714	PHE
4	G	794	ILE
4	G	795	LYS
4	G	816	LYS
5	H	287	GLN
5	H	299	TRP
5	H	309	ARG
5	H	315	LYS
5	H	345	PRO
5	H	392	LEU
5	H	394	THR
5	H	436	MET
5	H	446	ARG
5	H	460	TRP
5	H	462	ARG
5	H	465	ILE
5	H	471	LYS
5	H	518	ARG
5	H	523	LEU
5	H	529	LYS
6	I	304	LEU
6	I	307	SER
6	I	448	THR

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Mol	Chain	Res	Type
6	I	451	MET
6	I	462	GLN
4	J	645	THR
4	J	657	GLN
4	J	688	HIS
4	J	690	GLN
4	J	695	GLN
4	J	705	ASP
4	J	765	LEU
4	J	776	PHE
4	J	794	ILE
4	J	795	LYS
5	K	293	LEU
5	K	294	LYS
5	K	304	THR
5	K	316	VAL
5	K	319	THR
5	K	323	LEU
5	K	331	LEU
5	K	371	GLN
5	K	392	LEU
5	K	417	THR
5	K	435	LYS
5	K	446	ARG
5	K	455	LYS
5	K	463	LEU
6	L	371	LYS
6	L	374	GLN
6	L	439	ILE
6	L	456	ARG
6	L	457	ILE
7	O	7	PRO
7	O	38	ASN
7	O	101	ASN
7	O	180	LYS
7	O	245	ARG
7	O	295	ARG
7	O	303	LYS
7	O	331	ILE
7	O	333	GLU
7	O	340	LEU
7	O	363	ASP

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Mol	Chain	Res	Type
7	O	451	THR
7	O	515	SER
7	O	572	PHE
7	O	573	ASN
7	O	590	ILE
7	O	602	ASN
7	O	683	SER
7	O	689	SER
7	O	697	THR
7	O	800	ILE
7	O	826	PRO
7	O	852	SER
7	O	879	GLN
7	O	910	ARG
7	O	991	THR
7	O	1013	TYR
7	O	1015	ARG
7	O	1036	PRO
7	O	1118	ARG
7	O	1129	ASN
7	O	1186	SER
7	O	1189	MET
7	O	1225	GLN
7	O	1227	THR
7	O	1241	LYS
7	O	1323	THR
7	O	1348	THR
7	O	1378	ASP
7	O	1382	TYR
7	O	1386	LYS
7	O	1387	THR
7	O	1390	GLN
7	O	1396	LEU
7	O	1418	SER
7	O	1435	LYS
7	O	1436	LYS
7	O	1527	ARG
7	O	1532	ARG
7	O	1573	SER
7	O	1576	LEU
7	O	1577	LYS
7	O	1581	THR

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Mol	Chain	Res	Type
7	O	1582	LEU
7	O	1583	ASP
7	O	1584	ASN
7	O	1589	ASP
7	O	1595	VAL
7	O	1635	ARG
7	O	1652	LYS
8	P	15	PHE
8	P	20	ASN
8	P	55	LEU
8	P	59	ARG
8	P	61	ASN
8	P	62	VAL
8	P	78	LEU
8	P	202	THR
8	P	233	SER
8	P	270	ILE
8	P	275	LEU
8	P	277	THR
8	P	285	GLN
8	P	289	TYR
8	P	291	ASP
8	P	292	THR
8	P	293	GLU
8	P	299	ASN
8	P	305	ASP
8	P	308	THR
8	P	311	VAL
8	P	313	GLU
8	P	316	ILE
8	P	336	GLN
8	P	340	SER
8	P	376	THR
8	P	508	PRO
8	P	536	GLN
8	P	538	GLN
8	P	560	ASN
8	P	602	VAL
8	P	615	LEU
8	P	620	ASN
8	P	647	GLN
8	P	729	HIS

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Mol	Chain	Res	Type
8	P	745	HIS
8	P	755	ASN
8	P	789	GLN
8	P	803	LEU
8	P	827	PRO
8	P	862	ARG
8	P	955	PHE
8	P	958	THR
8	P	965	ASP
8	P	980	LYS
8	P	991	LYS
8	P	1061	THR
8	P	1149	ARG
8	P	1176	PRO
8	P	1184	LYS
8	P	1188	THR
8	P	1216	LYS
8	P	1270	LYS
8	P	1349	TYR
8	P	1356	LEU
8	P	1369	THR
8	P	1411	SER
8	P	1441	GLN
8	P	1527	LYS
8	P	1574	LYS
8	P	1597	ARG
8	P	1630	GLU
8	P	1631	SER
8	P	1633	ARG
8	P	1653	LYS
9	S	211	LYS
9	S	220	PHE
9	S	249	ARG
9	S	325	LEU
9	S	419	ASP
9	S	496	TYR
9	S	524	LEU
9	S	562	LEU
9	S	580	VAL
9	S	592	LYS
9	S	593	ILE
9	S	609	PRO

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Mol	Chain	Res	Type
9	S	629	ARG
9	S	703	SER
9	S	721	SER
9	S	798	THR
9	S	822	TYR
9	T	205	ASN
9	T	372	LYS
9	T	421	SER
9	T	428	VAL
9	T	432	ILE
9	T	433	GLU
9	T	434	ASP
9	T	496	TYR
9	T	520	SER
9	T	526	LYS
9	T	567	THR
9	T	614	ARG
9	T	670	LEU
9	T	671	ASP
9	T	672	GLN
9	T	674	LEU
9	T	678	ASP
9	T	680	ASN
9	T	683	THR
9	T	684	ASN
9	T	799	LYS
9	T	823	ARG
10	W	253	ILE
10	W	260	GLU
10	W	262	ILE
10	W	273	PHE
10	W	283	ILE
10	W	309	THR
10	W	317	THR
10	W	320	SER
10	W	324	LYS
10	W	338	THR
11	X	272	ILE
11	X	273	VAL
11	X	295	MET
11	X	300	VAL
11	X	354	SER

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Mol	Chain	Res	Type
11	X	376	ILE
11	X	385	ILE
11	X	399	LYS
11	X	401	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (216) such sidechains are listed below:

Mol	Chain	Res	Type
2	Y	573	GLN
2	Y	574	HIS
2	Y	665	ASN
2	Y	1009	HIS
2	Y	1020	ASN
2	Y	1086	ASN
2	Y	1158	HIS
2	Y	1160	HIS
2	Y	1240	ASN
2	Y	1263	GLN
2	Y	1272	GLN
2	Y	1369	ASN
2	Y	1377	ASN
2	Y	1481	ASN
3	Z	186	ASN
3	Z	242	HIS
3	Z	349	GLN
3	Z	417	ASN
3	Z	494	ASN
3	Z	656	HIS
3	Z	909	HIS
3	Z	914	GLN
3	Z	978	ASN
3	Z	979	GLN
3	Z	1056	HIS
3	Z	1258	GLN
3	Z	1267	ASN
3	Z	1387	HIS
4	A	654	HIS
4	A	749	GLN
4	A	800	HIS
5	B	317	ASN
5	B	368	ASN
6	C	287	GLN

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Mol	Chain	Res	Type
6	C	374	GLN
6	C	462	GLN
4	D	800	HIS
4	D	810	ASN
4	D	819	ASN
5	E	314	ASN
5	E	457	ASN
5	E	517	GLN
5	E	539	ASN
6	F	275	GLN
6	F	293	HIS
6	F	399	ASN
7	M	45	ASN
7	M	115	GLN
7	M	122	ASN
7	M	132	GLN
7	M	163	ASN
7	M	195	GLN
7	M	334	GLN
7	M	411	ASN
7	M	426	GLN
7	M	506	ASN
7	M	711	GLN
7	M	720	HIS
7	M	842	ASN
7	M	1021	HIS
7	M	1030	ASN
7	M	1202	ASN
7	M	1285	HIS
7	M	1311	GLN
7	M	1393	ASN
7	M	1468	ASN
7	M	1584	ASN
8	N	56	ASN
8	N	69	ASN
8	N	80	GLN
8	N	162	HIS
8	N	190	GLN
8	N	248	GLN
8	N	356	HIS
8	N	534	GLN
8	N	539	GLN

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Mol	Chain	Res	Type
8	N	748	HIS
8	N	804	GLN
8	N	979	ASN
8	N	999	GLN
8	N	1111	HIS
8	N	1174	ASN
8	N	1198	ASN
8	N	1232	HIS
8	N	1377	ASN
8	N	1462	ASN
8	N	1497	ASN
8	N	1509	GLN
9	Q	303	ASN
9	Q	397	HIS
9	Q	573	HIS
9	Q	612	HIS
9	Q	719	ASN
9	Q	770	ASN
9	Q	802	GLN
9	Q	812	GLN
9	R	450	ASN
9	R	463	GLN
9	R	505	HIS
9	R	540	ASN
9	R	680	ASN
9	R	707	HIS
9	R	719	ASN
9	R	773	ASN
9	R	821	GLN
10	U	329	GLN
10	U	336	ASN
11	V	293	HIS
2	0	573	GLN
2	0	574	HIS
2	0	665	ASN
2	0	1009	HIS
2	0	1020	ASN
2	0	1086	ASN
2	0	1158	HIS
2	0	1160	HIS
2	0	1240	ASN
2	0	1263	GLN

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Mol	Chain	Res	Type
2	0	1272	GLN
2	0	1369	ASN
2	0	1377	ASN
2	0	1481	ASN
3	1	186	ASN
3	1	242	HIS
3	1	349	GLN
3	1	417	ASN
3	1	494	ASN
3	1	656	HIS
3	1	909	HIS
3	1	914	GLN
3	1	978	ASN
3	1	979	GLN
3	1	1056	HIS
3	1	1258	GLN
3	1	1267	ASN
3	1	1387	HIS
4	G	654	HIS
4	G	749	GLN
4	G	792	GLN
4	G	800	HIS
5	H	368	ASN
5	H	517	GLN
6	I	287	GLN
6	I	374	GLN
6	I	462	GLN
4	J	810	ASN
4	J	819	ASN
5	K	317	ASN
5	K	365	GLN
5	K	371	GLN
5	K	457	ASN
5	K	517	GLN
5	K	539	ASN
6	L	275	GLN
6	L	293	HIS
6	L	374	GLN
6	L	399	ASN
7	O	45	ASN
7	O	115	GLN
7	O	122	ASN

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Mol	Chain	Res	Type
7	O	132	GLN
7	O	163	ASN
7	O	195	GLN
7	O	334	GLN
7	O	411	ASN
7	O	426	GLN
7	O	506	ASN
7	O	711	GLN
7	O	720	HIS
7	O	842	ASN
7	O	1021	HIS
7	O	1030	ASN
7	O	1202	ASN
7	O	1285	HIS
7	O	1311	GLN
7	O	1468	ASN
7	O	1584	ASN
8	P	56	ASN
8	P	69	ASN
8	P	80	GLN
8	P	190	GLN
8	P	248	GLN
8	P	356	HIS
8	P	539	GLN
8	P	748	HIS
8	P	804	GLN
8	P	979	ASN
8	P	999	GLN
8	P	1111	HIS
8	P	1174	ASN
8	P	1198	ASN
8	P	1232	HIS
8	P	1377	ASN
8	P	1462	ASN
8	P	1497	ASN
8	P	1509	GLN
9	S	303	ASN
9	S	397	HIS
9	S	573	HIS
9	S	612	HIS
9	S	719	ASN
9	S	770	ASN

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Mol	Chain	Res	Type
9	S	802	GLN
9	S	812	GLN
9	T	450	ASN
9	T	463	GLN
9	T	505	HIS
9	T	540	ASN
9	T	680	ASN
9	T	707	HIS
9	T	719	ASN
9	T	773	ASN
9	T	821	GLN
11	X	282	ASN
11	X	293	HIS
11	X	361	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

The following chains have linkage breaks:

Mol	Chain	Number of breaks
9	S	1
9	Q	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	S	101:PRO	C	114:LYS	N	33.71
1	Q	101:PRO	C	114:LYS	N	32.23

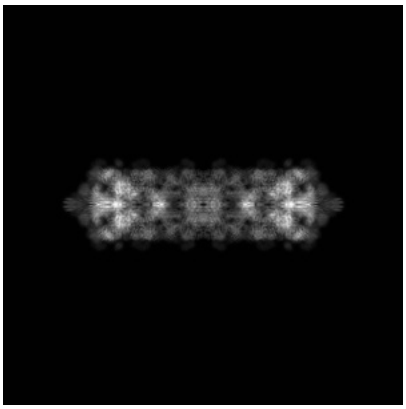
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-41300. These allow visual inspection of the internal detail of the map and identification of artifacts.

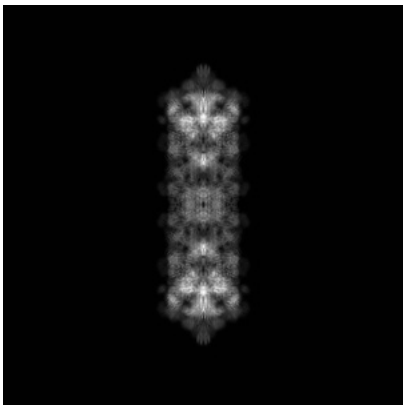
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

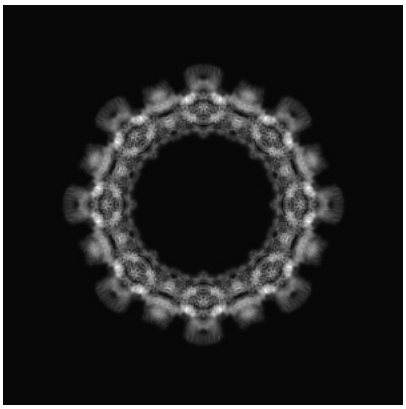
6.1.1 Primary map



X

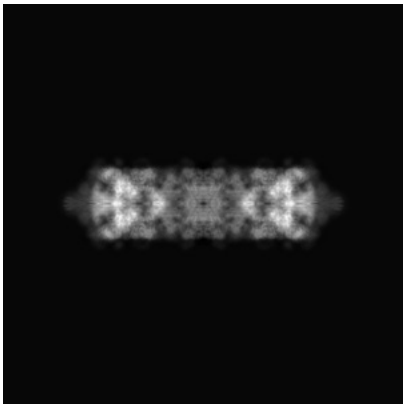


Y

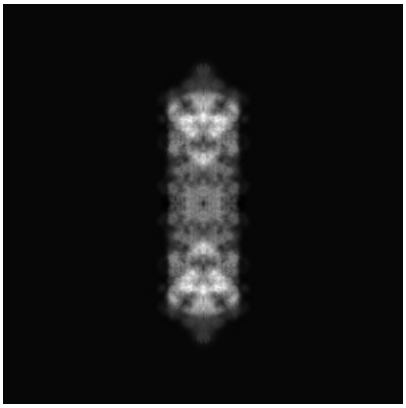


Z

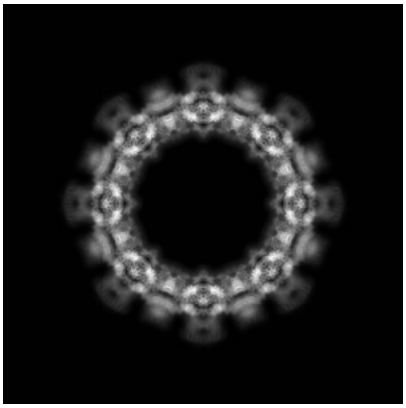
6.1.2 Raw map



X



Y

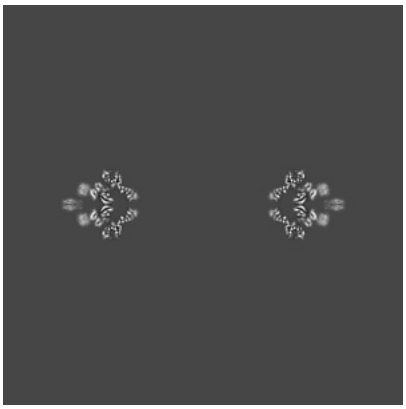


Z

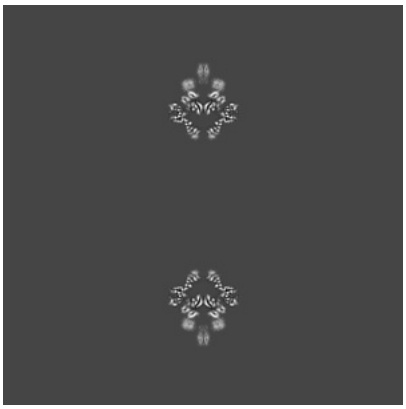
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map



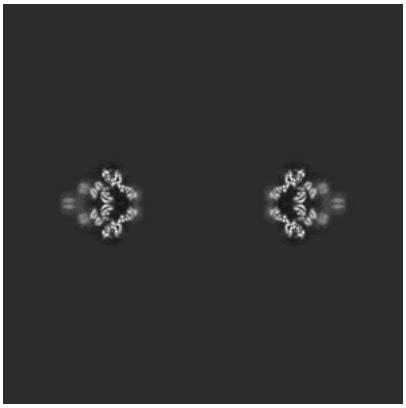
X Index: 240



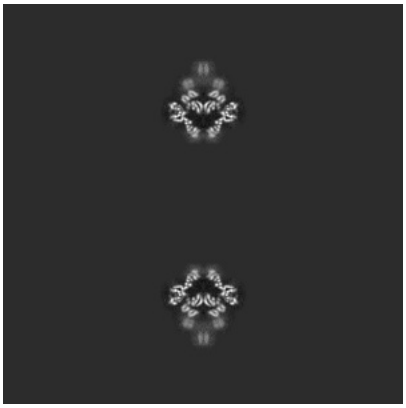
Y Index: 240

Z Index: 240

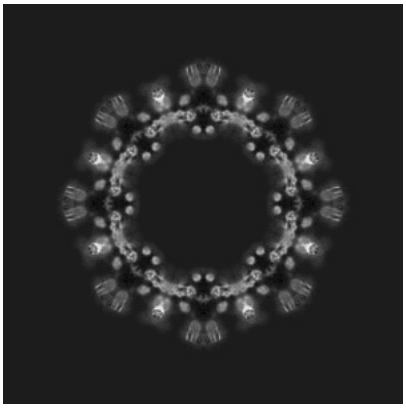
6.2.2 Raw map



X Index: 240



Y Index: 240

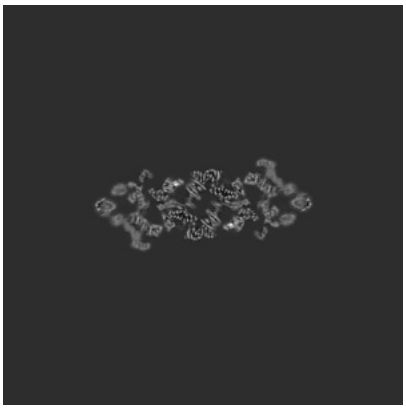


Z Index: 240

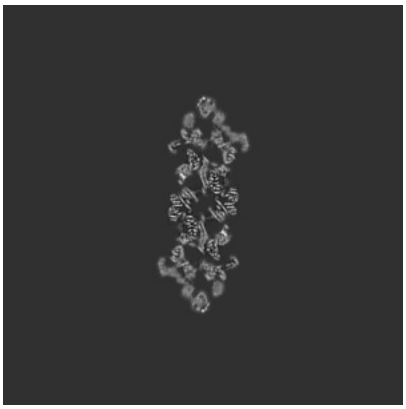
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

6.3.1 Primary map



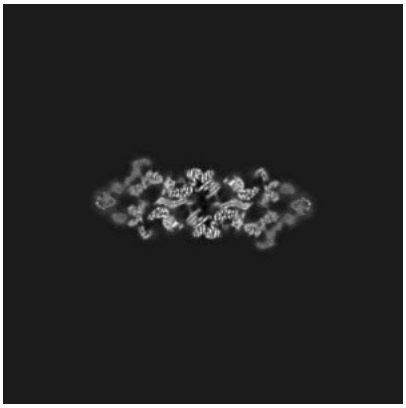
X Index: 139



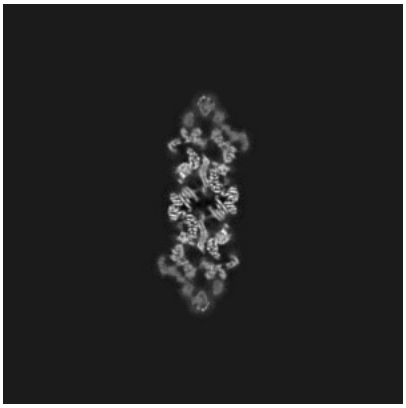
Y Index: 340

Z Index: 238

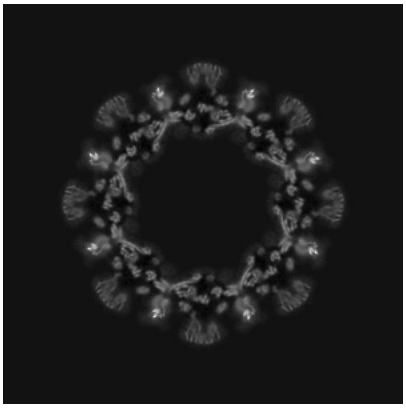
6.3.2 Raw map



X Index: 340



Y Index: 340

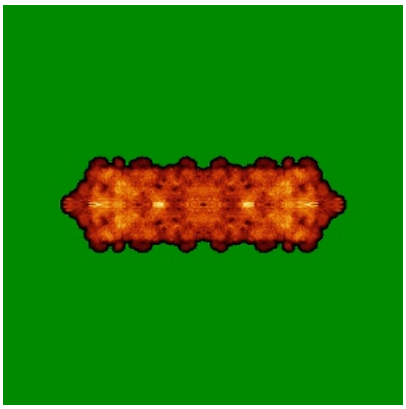


Z Index: 242

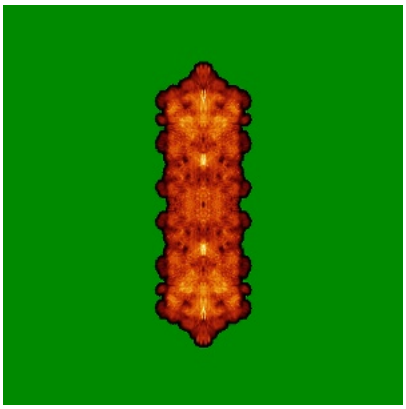
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal standard-deviation projections (False-color) (i)

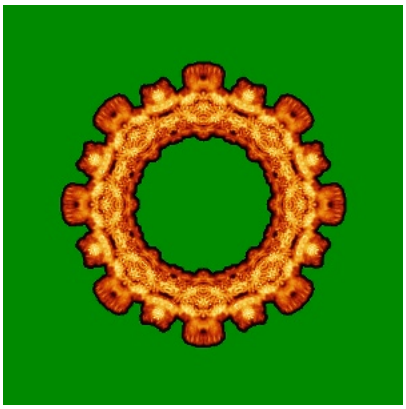
6.4.1 Primary map



X

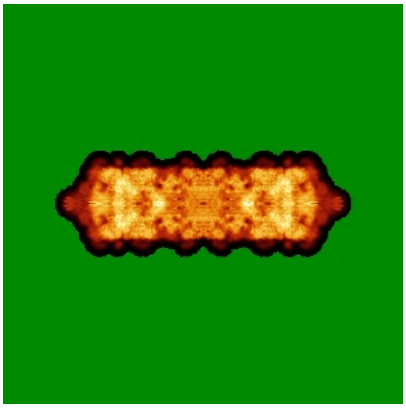


Y

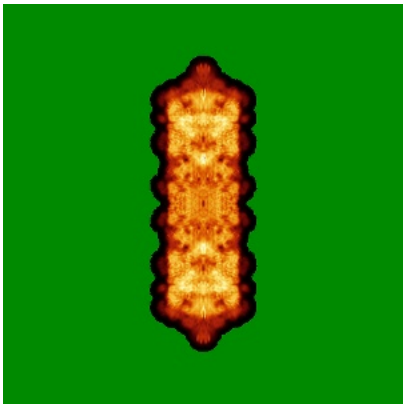


Z

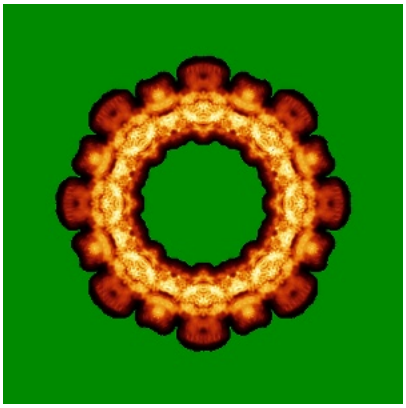
6.4.2 Raw map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

6.5.1 Primary map

X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.65. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map

X Y Z

These images show the 3D surface of the raw map. The raw map's contour level was selected so that its surface encloses the same volume as the primary map does at its recommended contour level.

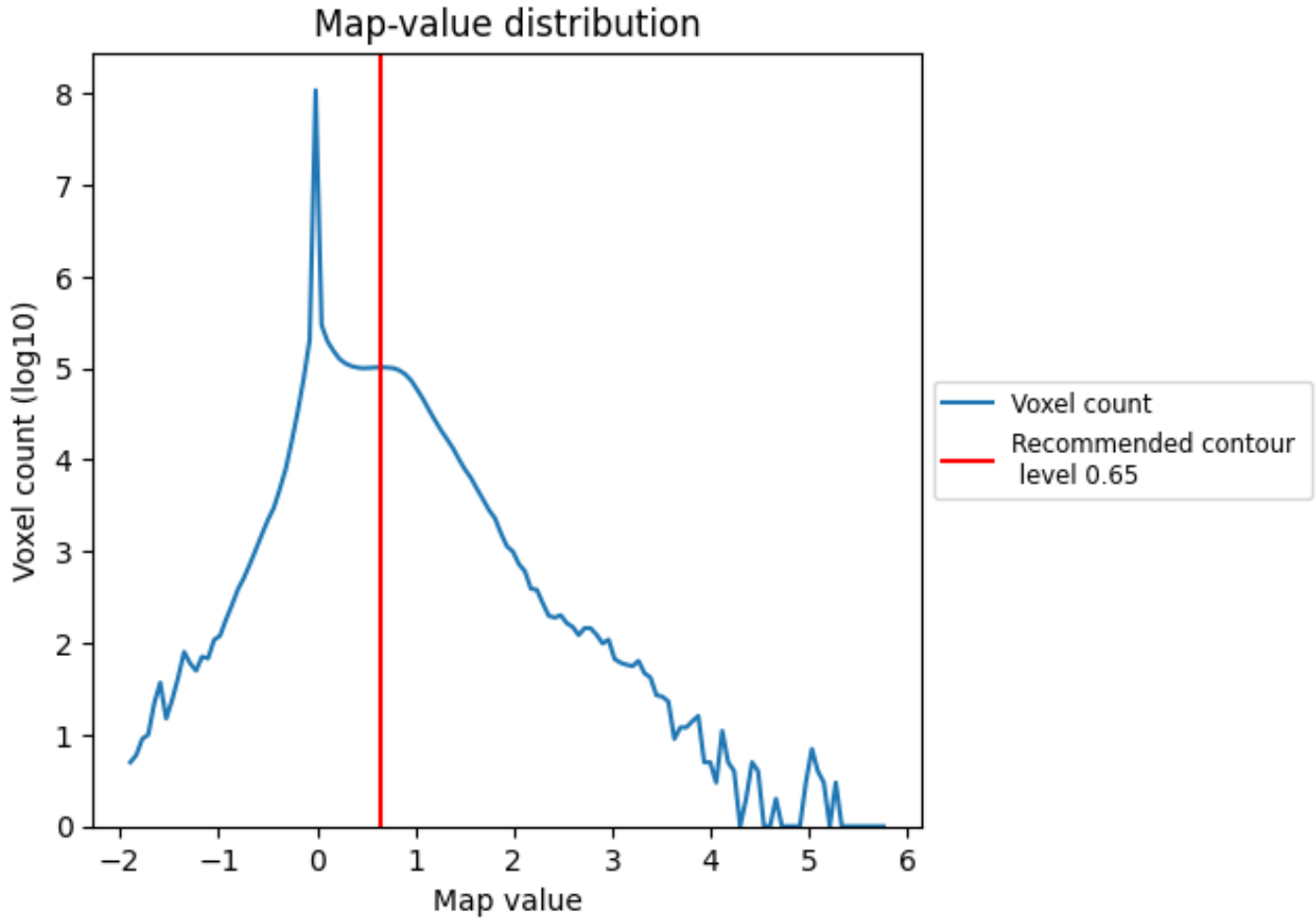
6.6 Mask visualisation (i)

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

7 Map analysis

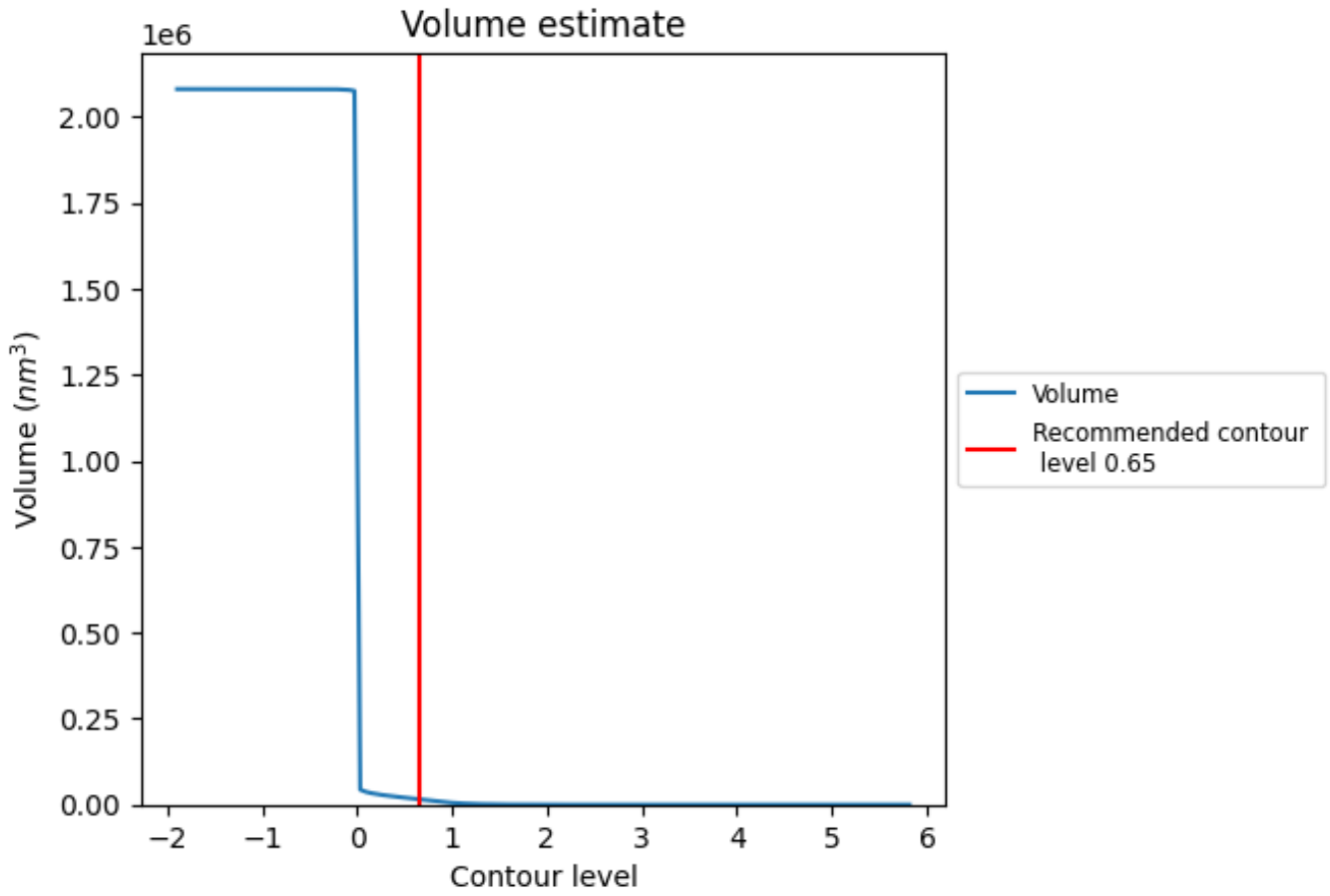
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

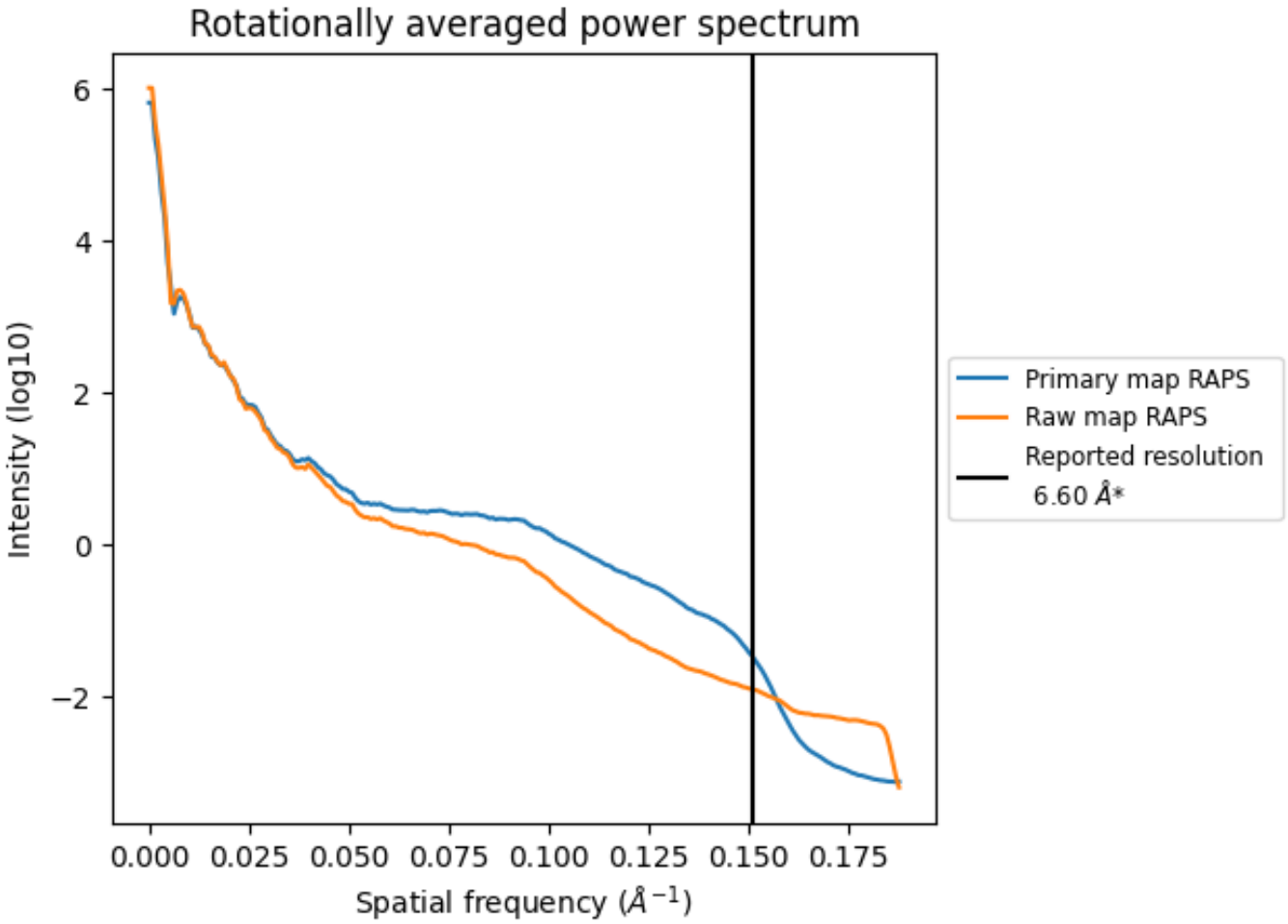
7.2 Volume estimate



The volume at the recommended contour level is 15598 nm^3; this corresponds to an approximate mass of 14090 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)

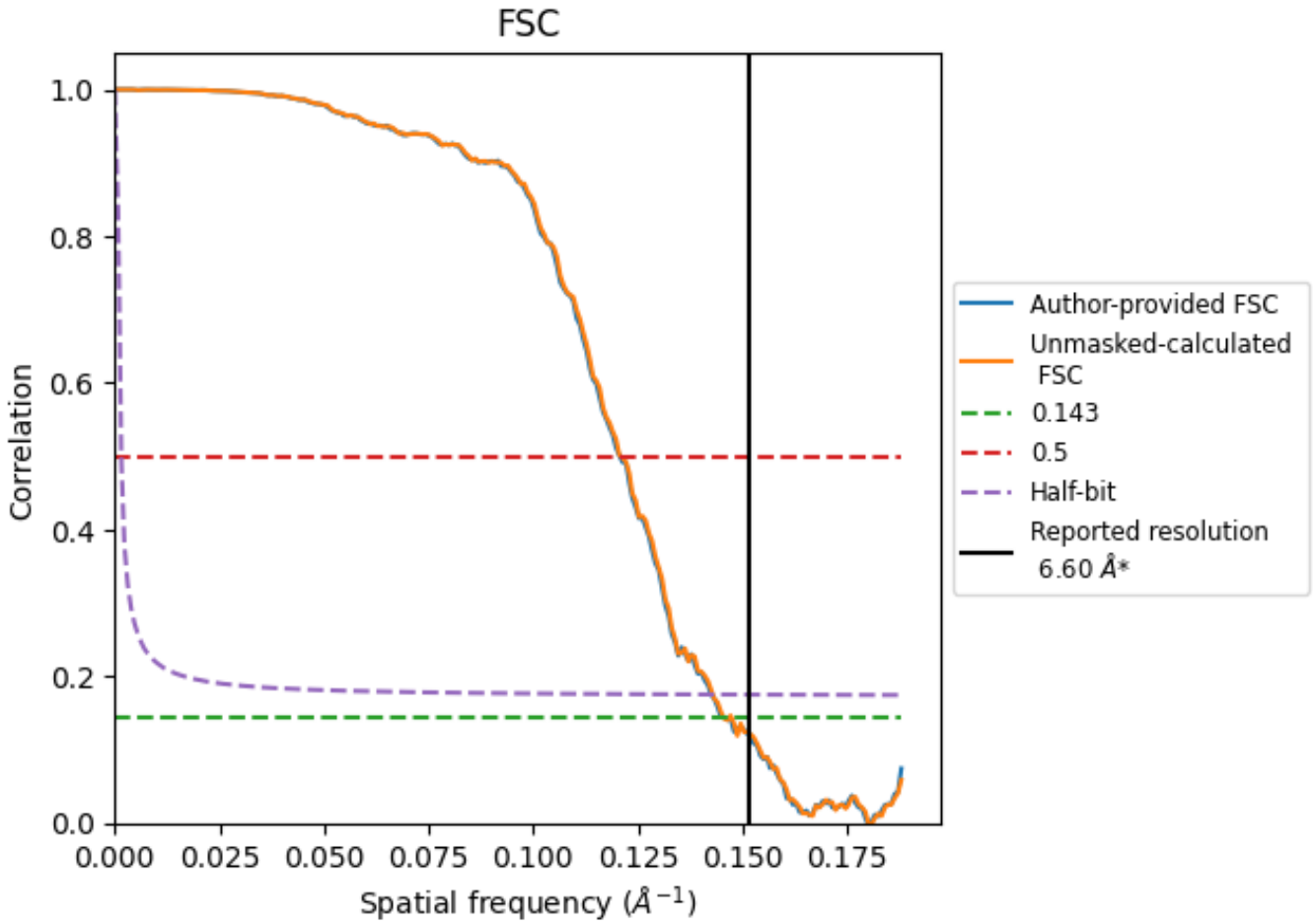


*Reported resolution corresponds to spatial frequency of 0.152 Å^{-1}

8 Fourier-Shell correlation

Fourier-Shell Correlation (FSC) is the most commonly used method to estimate the resolution of single-particle and subtomogram-averaged maps. The shape of the curve depends on the imposed symmetry, mask and whether or not the two 3D reconstructions used were processed from a common reference. The reported resolution is shown as a black line. A curve is displayed for the half-bit criterion in addition to lines showing the 0.143 gold standard cut-off and 0.5 cut-off.

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.152 Å^{-1}

8.2 Resolution estimates (i)

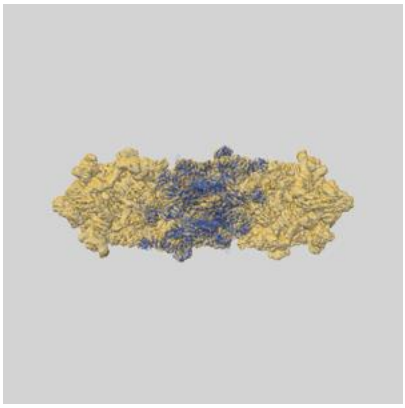
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	6.60	-	-
Author-provided FSC curve	6.86	8.29	7.02
Unmasked-calculated*	6.87	8.27	6.99

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

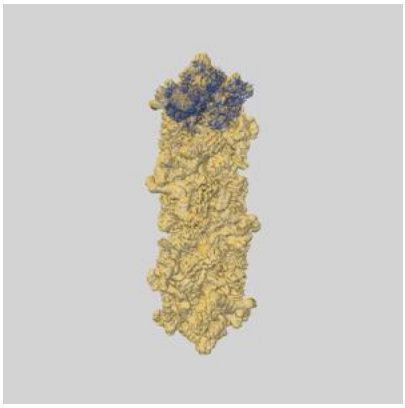
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-41300 and PDB model 8TJ5. Per-residue inclusion information can be found in section 3 on page 9.

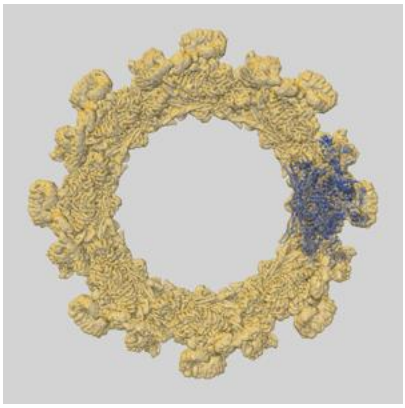
9.1 Map-model overlay



X



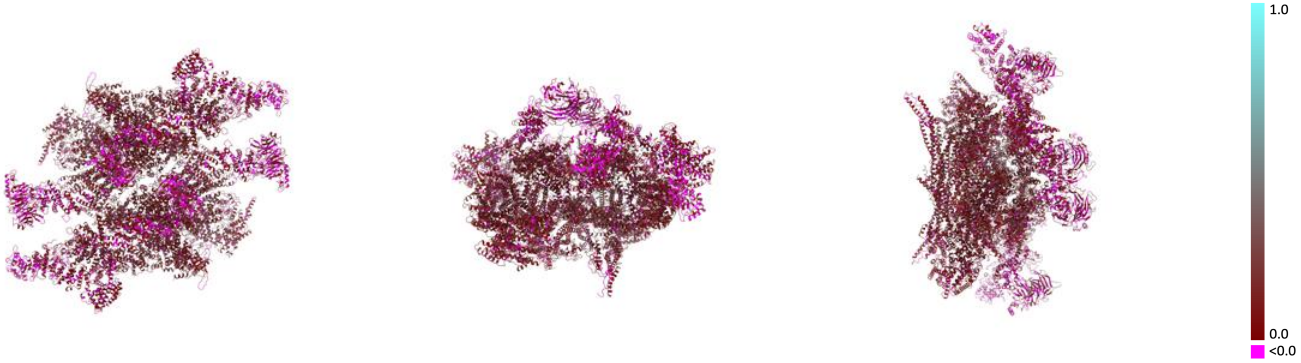
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.65 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.

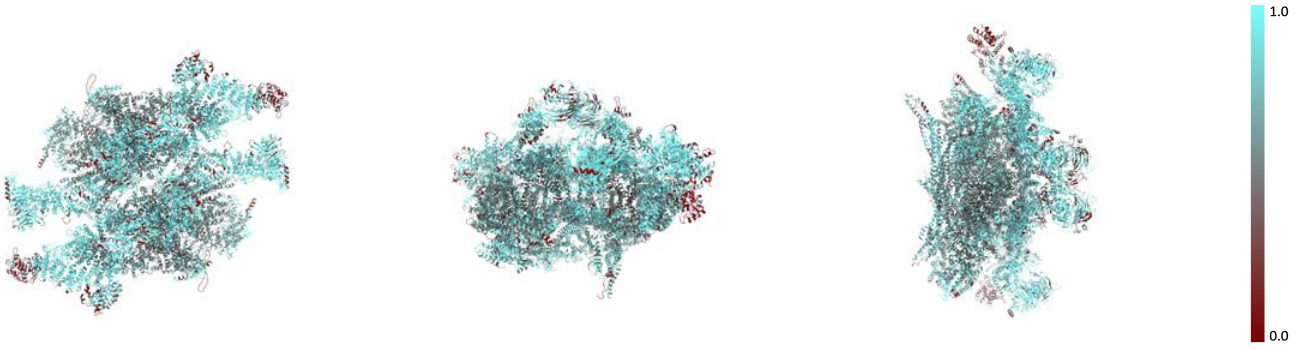
9.2 Q-score mapped to coordinate model (i)



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.

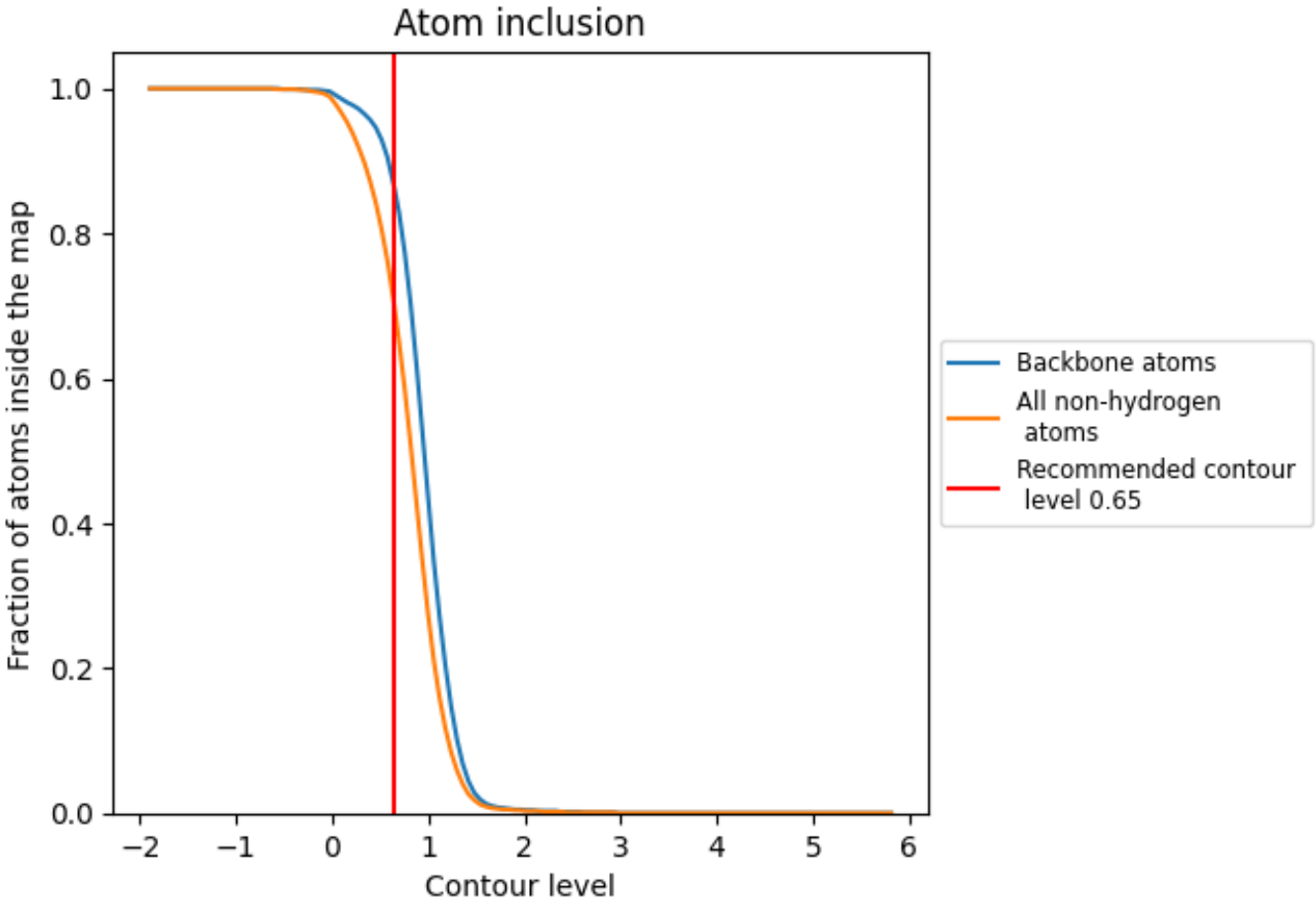
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.65).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 70% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary

The table lists the average atom inclusion at the recommended contour level (0.65) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6970	0.1130
0	0.8040	0.0850
1	0.7170	0.0560
3	0.8380	0.2750
4	0.8500	0.2630
7	0.8940	0.1740
8	0.9180	0.1870
A	0.7000	0.1480
B	0.6510	0.1110
C	0.6650	0.1440
D	0.7470	0.1580
E	0.7510	0.1430
F	0.7260	0.1430
G	0.7030	0.1500
H	0.6510	0.1100
I	0.6750	0.1400
J	0.7490	0.1560
K	0.7580	0.1440
L	0.7310	0.1430
M	0.6160	0.1320
N	0.6170	0.1340
O	0.6190	0.1330
P	0.6160	0.1350
Q	0.6710	0.0820
R	0.8020	0.1440
S	0.6720	0.0830
T	0.8060	0.1430
U	0.9020	0.0800
V	0.9080	0.0570
W	0.8960	0.0860
X	0.9240	0.0660
Y	0.8030	0.0880
Z	0.7140	0.0560
a	0.2500	0.1860
b	0.6290	0.2290

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Chain	Atom inclusion	Q-score
c	0.4590	0.1280
d	0.7460	0.2710
e	0.8270	0.2490
f	0.2750	0.2220
g	0.6400	0.2240
h	0.5650	0.2270
i	0.6820	0.2670
j	0.7030	0.2170
k	0.5540	0.2590
l	0.6000	0.2420
m	0.7360	0.2080
n	0.7360	0.1930