Full wwPDB EM Validation Report ⓘ

Mar 6, 2026 – 04:39 PM UTC

PDB ID	:	7N84 / pdb_00007n84
EMDB ID	:	EMD-24231
Title	:	Double nuclear outer ring from the isolated yeast NPC
Authors	:	Akey, C.W.; Rout, M.P.; Ouch, C.; Echeverria, I.; Fernandez-Martinez, J.; Nudelman, I.
Deposited on	:	2021-06-13
Resolution	:	11.60 Å(reported)

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

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

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

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

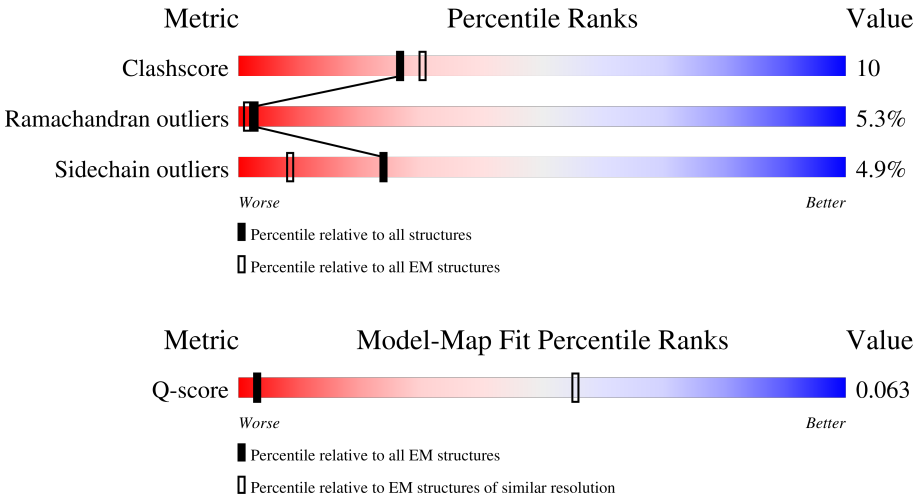
EMDB validation analysis	:	0.0.1.dev132
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance

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

The reported resolution of this entry is 11.60 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)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	94 (11.10 - 12.10)

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	X	1655	6% 26% 33% 8% 31%
2	Y	63	100%
2	Z	63	100%
3	a	1037	40% 44% 11%

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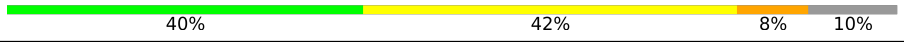
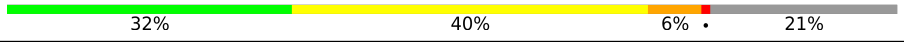
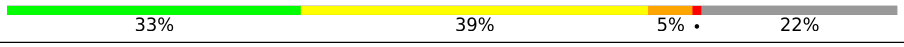
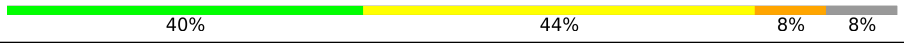
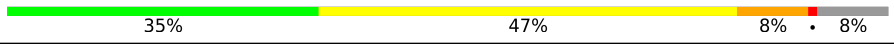
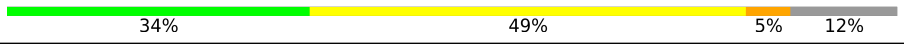
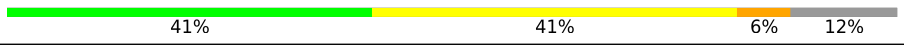
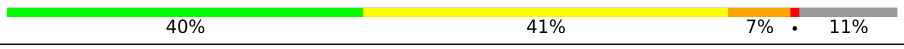
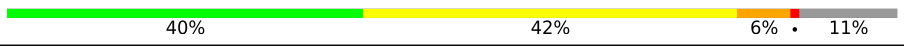
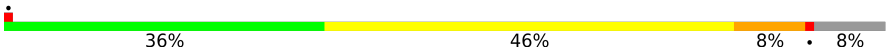
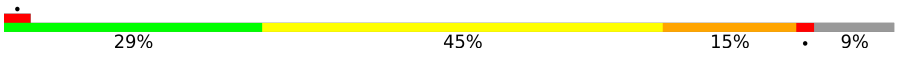
Mol	Chain	Length	Quality of chain
3	l	1037	
4	b	744	
4	m	744	
5	c	712	
5	n	712	
6	d	297	
6	o	297	
7	e	349	
7	p	349	
8	f	726	
8	q	726	
9	g	1157	
9	r	1157	

2 Entry composition

There are 9 unique types of molecules in this entry. The entry contains 83142 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 Nucleoporin NUP188.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	X	1137	9208	6035	1455	1700	18	0	0

- Molecule 2 is a protein called unknown.

Mol	Chain	Residues	Atoms				AltConf	Trace
			Total	C	N	O		
2	Y	63	315	189	63	63	0	0
2	Z	63	Total	C	N	O	0	0
			315	189	63	63		

- Molecule 3 is a protein called Nucleoporin NUP120.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	a	1006	8279	5346	1334	1566	33	0	0
3	l	1006	Total	C	N	O	S	0	0
			8279	5346	1334	1566	33		

- Molecule 4 is a protein called Nucleoporin NUP85.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	b	675	5424	3493	863	1038	30	0	0
4	m	670	Total	C	N	O	S	0	0
			5384	3468	857	1031	28		

- Molecule 5 is a protein called Nucleoporin 145c.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	c	559	4520	2884	750	869	17	0	0

Continued on next page...

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Mol	Chain	Residues	Atoms					AltConf	Trace
5	n	557	Total	C	N	O	S	0	0
			4505	2873	748	867	17		

- Molecule 6 is a protein called Protein transport protein SEC13.

Mol	Chain	Residues	Atoms					AltConf	Trace
6	d	274	Total	C	N	O	S	0	0
			2160	1379	369	409	3		
6	o	274	Total	C	N	O	S	0	0
			2160	1379	369	409	3		

- Molecule 7 is a protein called Nucleoporin SEH1.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	e	307	Total	C	N	O	S	0	0
			2438	1543	422	462	11		
7	p	307	Total	C	N	O	S	0	0
			2438	1543	422	462	11		

- Molecule 8 is a protein called Nucleoporin NUP84.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	f	649	Total	C	N	O	S	0	0
			5261	3370	866	1011	14		
8	q	648	Total	C	N	O	S	0	0
			5254	3365	865	1010	14		

- Molecule 9 is a protein called Nucleoporin NUP133.

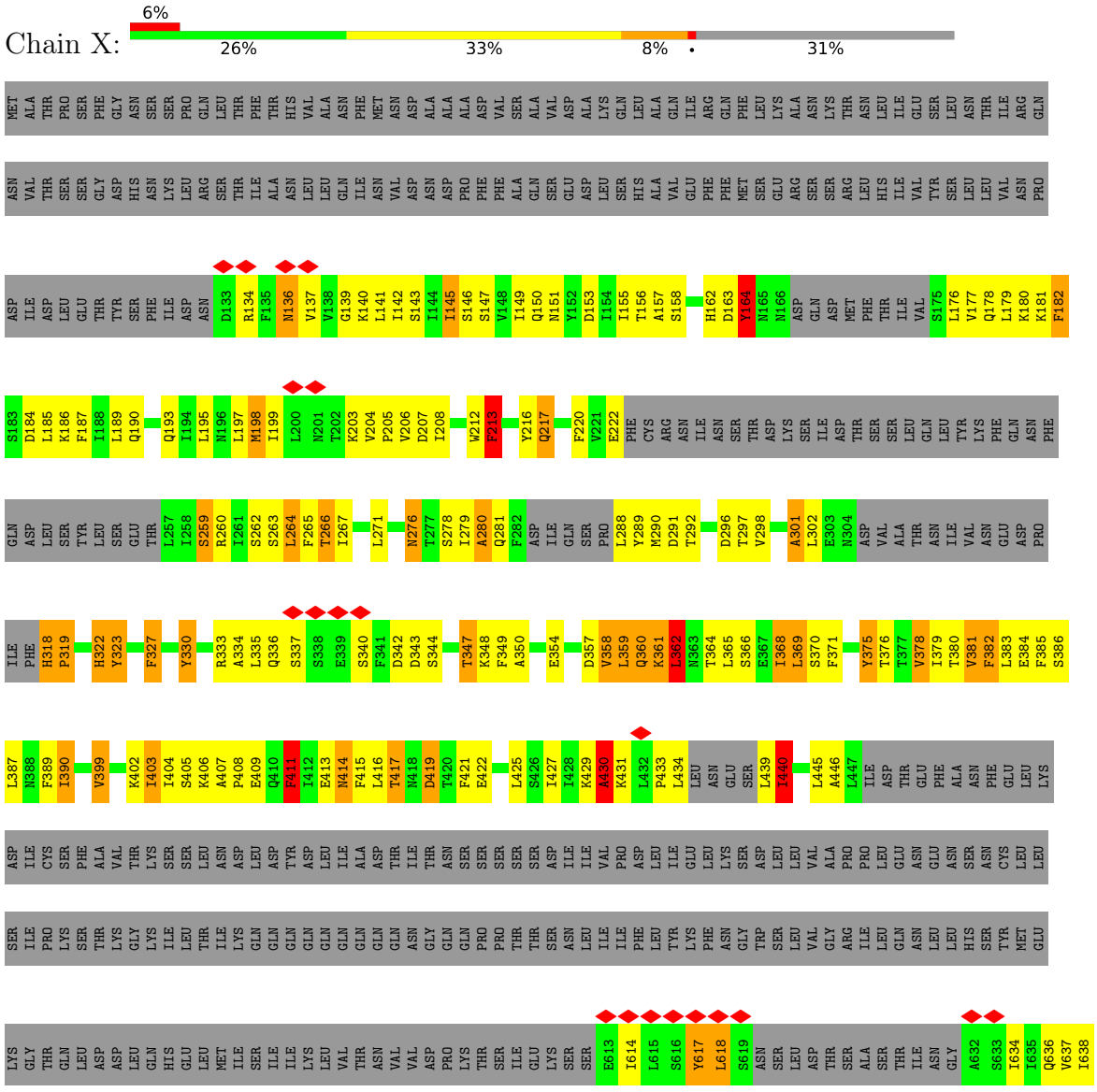
Mol	Chain	Residues	Atoms					AltConf	Trace
9	g	1062	Total	C	N	O	S	0	0
			8627	5541	1393	1664	29		
9	r	1056	Total	C	N	O	S	0	0
			8575	5511	1381	1654	29		

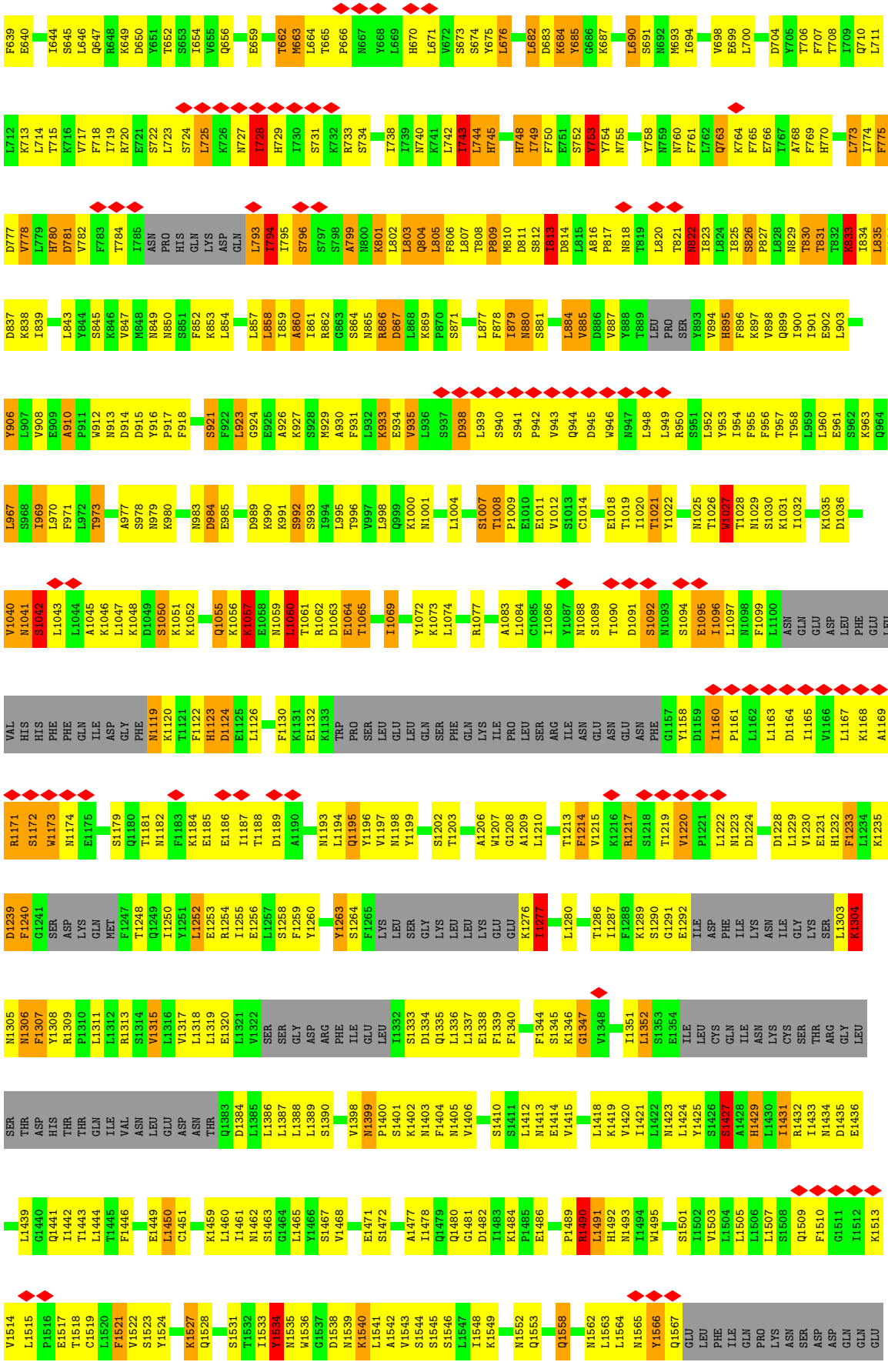
3 Residue-property plots (i)

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: Nucleoporin NUP188

Chain X:

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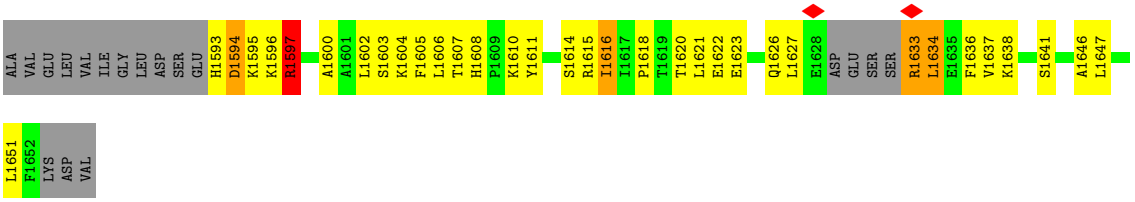
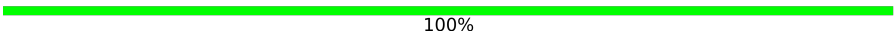
L712 K713 L714 T715 K716 V717 F718 I719 R720 E721 S722 L723 S724 L725 K726 N727 T728 H729 T730 S731 K732 R733 S734 T738 T739 N740 K741 L742 T743 L744 H745 H748 I749 F750 E751 S752 Y753 Y754 N755 Y758 N759 N760 F761 L762 Q763 K764 F765 E766 I767 A768 F769 H770 L773 I774 F775 Y776
D777 V778 L779 H780 D781 V782 F783 T784 I785 ASN PRO HIS GLN LYS ASP GLN L793 I794 I795 S796 S797 S798 A799 N800 K801 L802 L803 Q804 L805 F806 L807 T808 P809 M810 D811 S812 I813 D814 L815 A816 P817 N818 T819 L820 T821 N822 I823 L824 I825 S826 P827 L828 N829 T830 T831 T832 K833 I834 L835 G836
D837 K838 I839 L843 Y844 S845 K846 V847 N848 N849 N850 S851 F852 K853 L854 L857 L858 I859 A860 I861 R862 G863 S864 N865 R866 D867 L868 K869 P870 S871 L877 F878 I879 N880 S881 L884 V885 D886 V887 Y888 T889 LEU PRO SER Y893 V894 H895 F896 K897 V898 Q899 I900 I901 E902 L903
Y906 L907 V908 E909 A910 P911 W912 N913 D914 D915 Y916 P917 F918 S921 F922 L923 G924 E925 A926 K927 S928 M929 A930 F931 L932 K933 E934 V935 L936 S937 D938 L939 S940 S941 P942 V943 Q944 D945 W946 N947 L948 L949 R950 S951 L952 Y953 I954 F955 F956 T957 T958 L959 L960 E961 S962 K963 Q964 D965 G966
L967 S968 I969 L970 F971 L972 T973 A977 S978 N979 K980 N983 D984 E985 D989 K990 K991 S992 S993 I994 L995 T996 V997 L998 Q999 K1000 N1001 L1004 S1007 T1008 P1009 E1010 E1011 V1012 S1013 C1014 E1018 T1019 I1020 T1021 Y1022 N1025 T1026 W1027 T1028 N1029 S1030 K1031 I1032 K1035 D1036
V1040 N1041 S1042 L1043 L1044 A1045 K1046 L1047 K1048 D1049 S1050 K1051 K1052 Q1055 K1056 K1057 E1058 N1059 L1060 T1061 R1062 D1063 E1064 T1065 I1069 Y1072 K1073 L1074 R1077 A1083 L1084 C1085 I1086 Y1087 N1088 S1089 T1090 D1091 S1092 N1093 S1094 E1095 I1096 L1097 N1098 F1099 L1100 ASN GLN GLU GLU ASP LEU PHE GLU LEU
VAL HIS HIS PHE PHE GLN ILE ASP GLY PHE N1119 K1120 T1121 F1122 H1123 D1124 E1125 L1126 F1130 K1131 E1132 K1133 TRP PRO SER LEU GLU LEU GLN SER PHE GLN LYS ILE PRO LEU SER ARG ILE ASN GLU ASN GLU ASN PHE G1157 Y1158 D1159 I1160 P1161 L1162 L1163 D1164 I1165 V1166 L1167 K1168 A1169 D1170
R1171 S1172 W1173 N1174 E1175 S1179 Q1180 T1181 N1182 F1183 K1184 E1185 E1186 I1187 T1188 D1189 A1190 N1193 L1194 Q1195 Y1196 V1197 N1198 Y1199 S1202 T1203 A1206 W1207 G1208 A1209 L1210 T1213 F1214 V1215 K1216 R1217 S1218 T1219 V1220 P1221 L1222 N1223 D1224 D1228 L1229 V1230 E1231 H1232 F1233 L1234 K1235 L1236 N1237 I1238
D1239 F1240 G1241 SER ASP LYS GLN MET F1247 T1248 Q1249 I1250 Y1251 L1252 E1253 R1254 I1255 E1256 L1257 S1258 F1259 Y1260 Y1263 S1264 F1265 LYS LEU SER GLY LYS LEU LEU LYS GLU GLU K1276 I1277 L1280 T1286 I1287 F1288 K1289 S1290 G1291 E1292 ILE ASP PHE ILE LYS ASN ILE GLY LYS SER L1303 K1304
N1305 N1306 F1307 Y1308 R1309 P1310 L1311 L1312 R1313 S1314 V1315 L1316 V1317 L1318 L1319 E1320 L1321 V1322 SER SER GLY ASP ARG PHE ILE GLU LEU I1332 S1333 D1334 Q1335 L1336 L1337 E1338 F1339 F1340 F1344 S1345 K1346 G1347 V1348 I1351 L1352 S1353 E1354 ILE LEU CYS GLN ILE ASN LYS CYS SER THR ARG GLY LEU
SER THR ASP HIS THR THR GLN ILE VAL ASN LEU GLU ASP ASN THR Q1383 D1384 L1385 L1386 L1387 L1388 L1389 S1390 V1398 N1399 P1400 S1401 K1402 N1403 F1404 N1405 V1406 S1410 S1411 L1412 N1413 E1414 V1415 L1418 K1419 V1420 I1421 L1422 N1423 L1424 Y1425 S1426 S1427 A1428 H1429 L1430 T1431 R1432 I1433 N1434 D1435 E1436
L1439 G1440 Q1441 I1442 T1443 L1444 T1445 F1446 E1449 L1450 C1451 K1459 L1460 I1461 N1462 S1463 G1464 L1465 Y1466 S1467 V1468 E1471 S1472 A1477 I1478 Q1479 Q1480 G1481 D1482 I1483 K1484 P1485 E1486 P1489 R1490 L1491 H1492 N1493 I1494 W1495 S1501 I1502 V1503 L1504 L1505 L1506 L1507 S1508 Q1509 F1510 G1511 I1512 K1513
V1514 L1515 P1516 E1517 T1518 C1519 L1520 F1521 V1522 S1523 Y1524 K1527 Q1528 S1531 T1532 I1533 Y1534 N1535 W1536 G1537 D1538 N1539 K1540 L1541 A1542 V1543 S1544 S1545 S1546 L1547 T1548 K1549 N1552 Q1553 Q1558 N1562 L1563 L1564 N1565 Y1566 Q1567 GLU LEU PHE ILE GLN PRO LYS ASN SER ASP ASP GLN GLN GLU



• Molecule 2: unknown

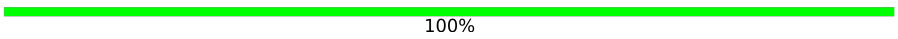
Chain Y:



There are no outlier residues recorded for this chain.

• Molecule 2: unknown

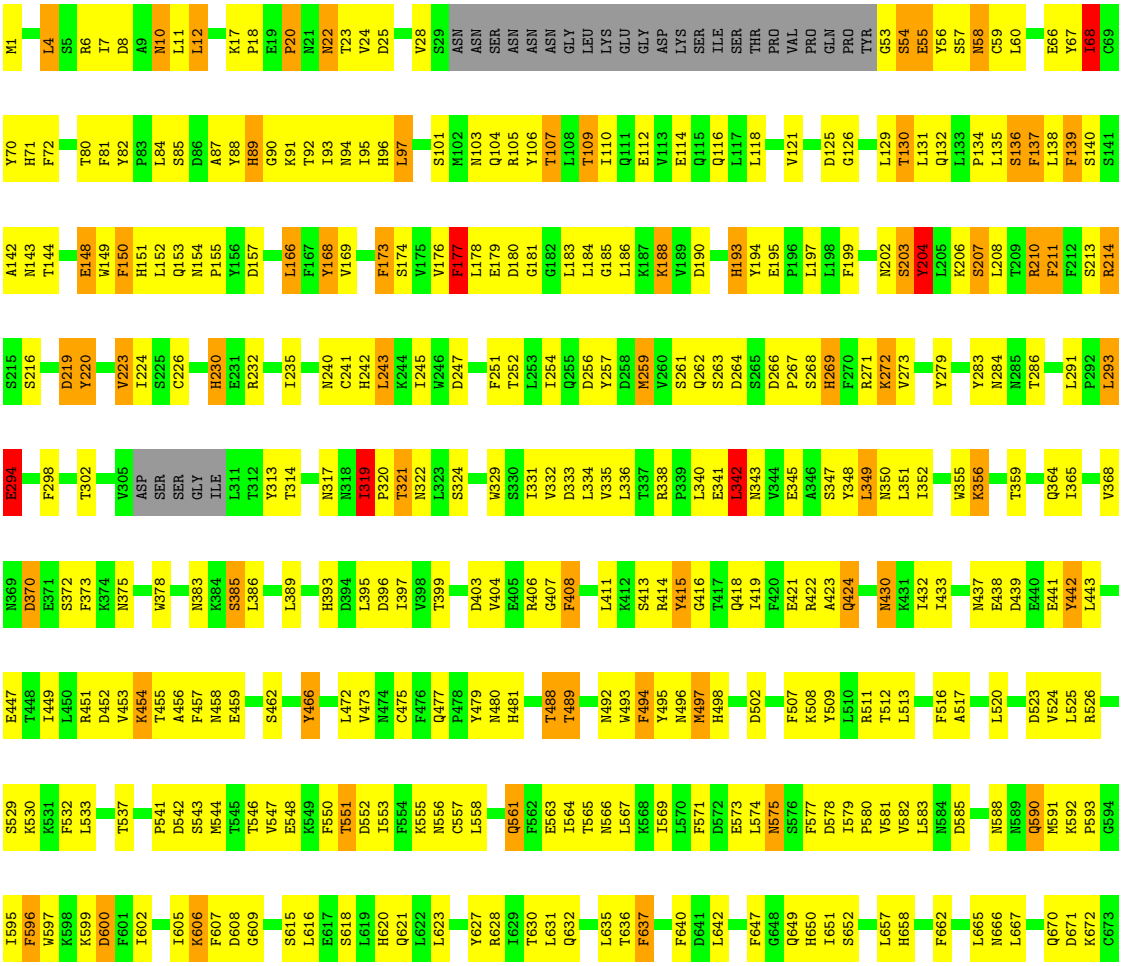
Chain Z:

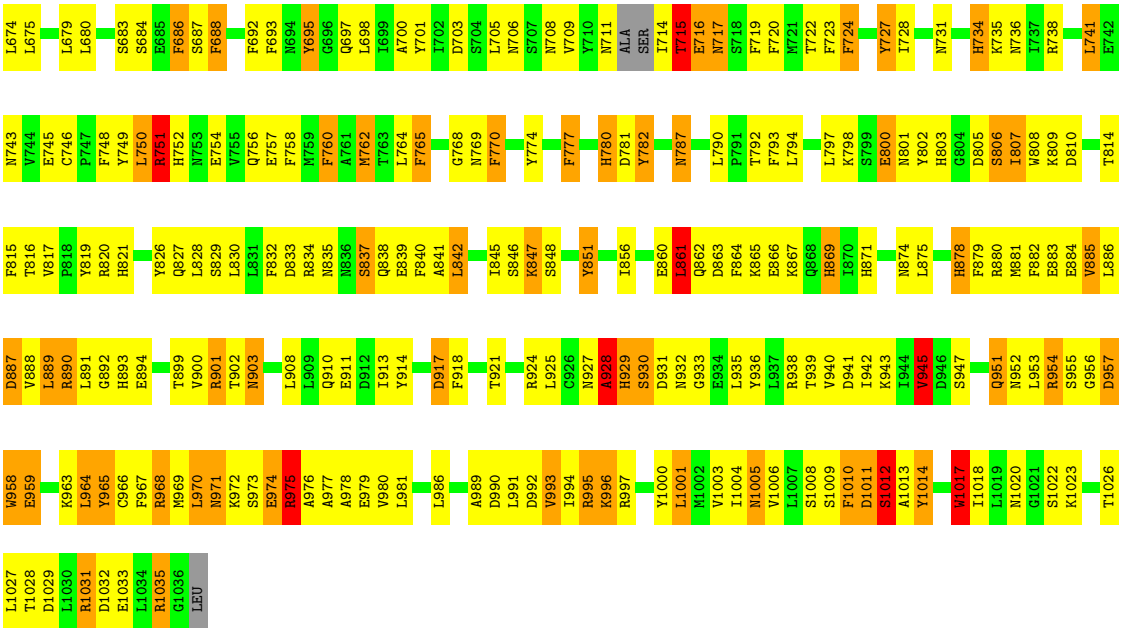


There are no outlier residues recorded for this chain.

• Molecule 3: Nucleoporin NUP120

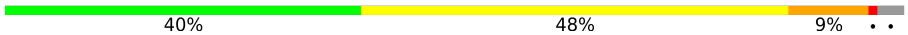
Chain a:

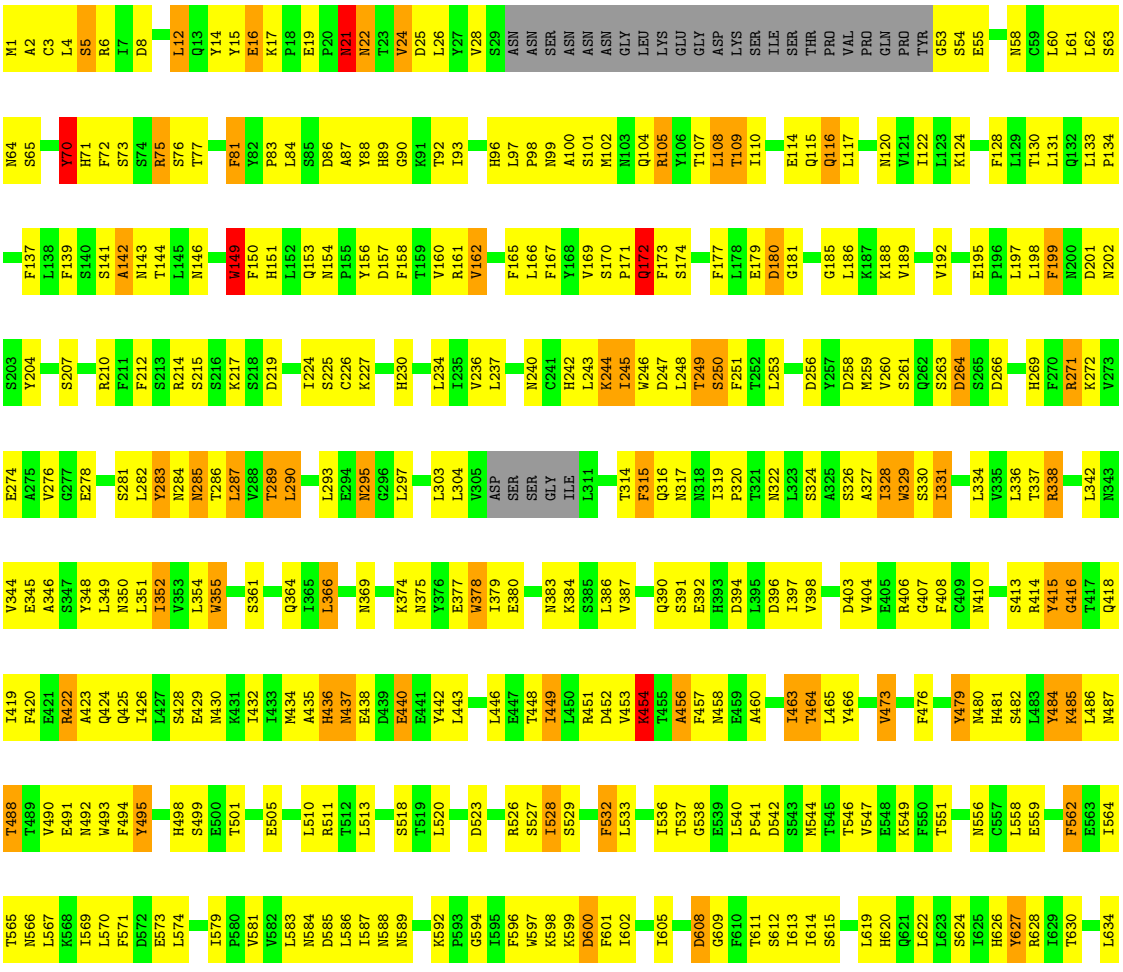


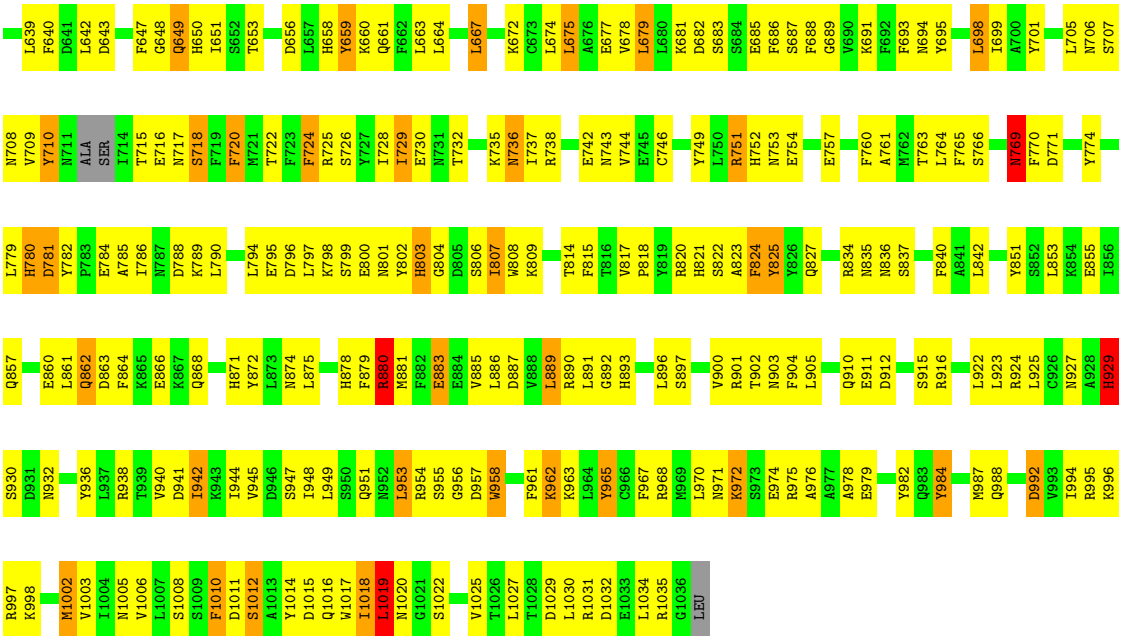


• Molecule 3: Nucleoporin NUP120

Chain l:

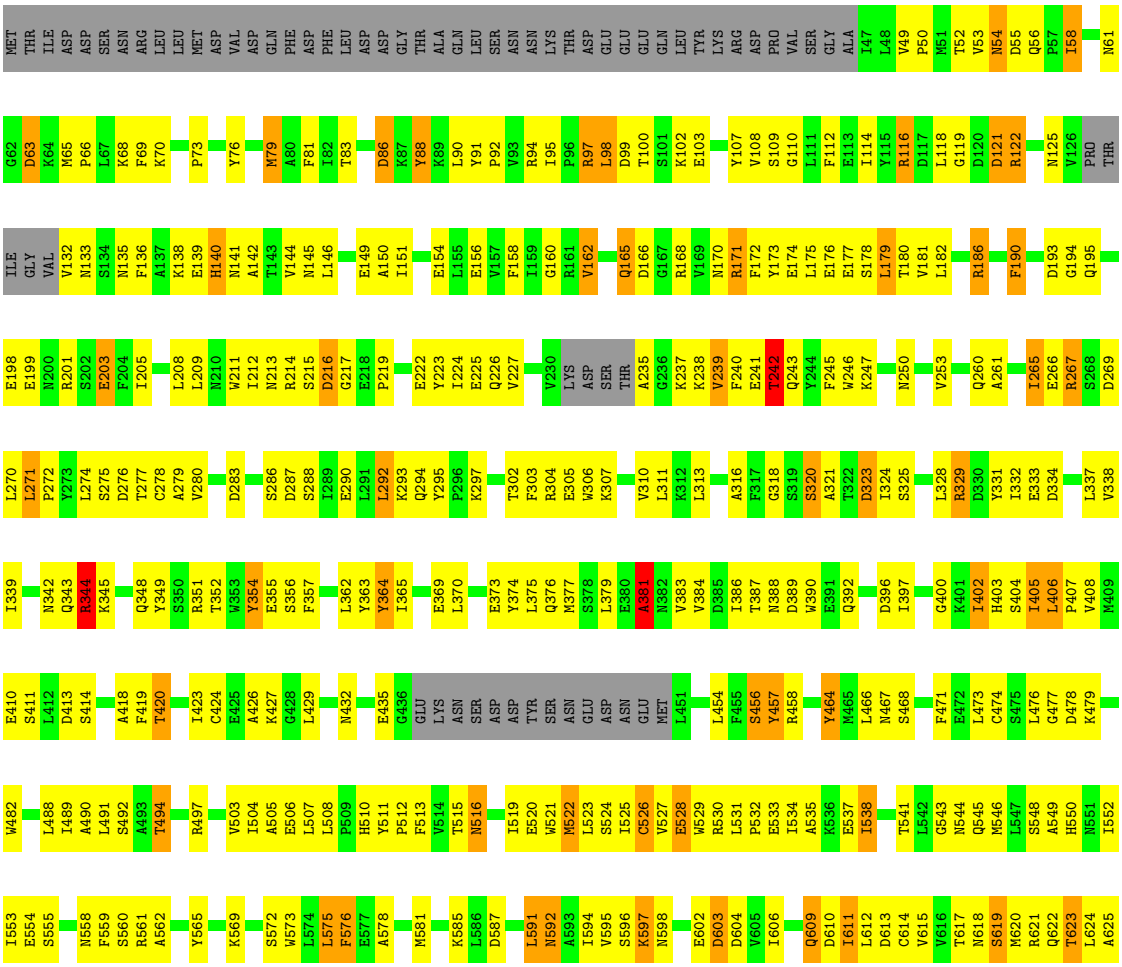


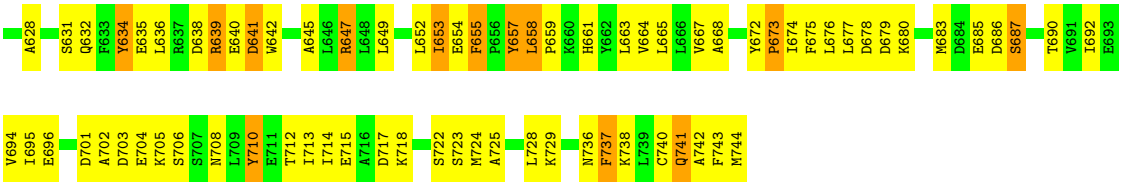




• Molecule 4: Nucleoporin NUP85

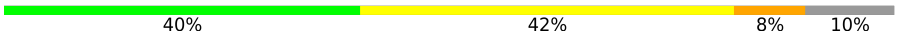
Chain b:

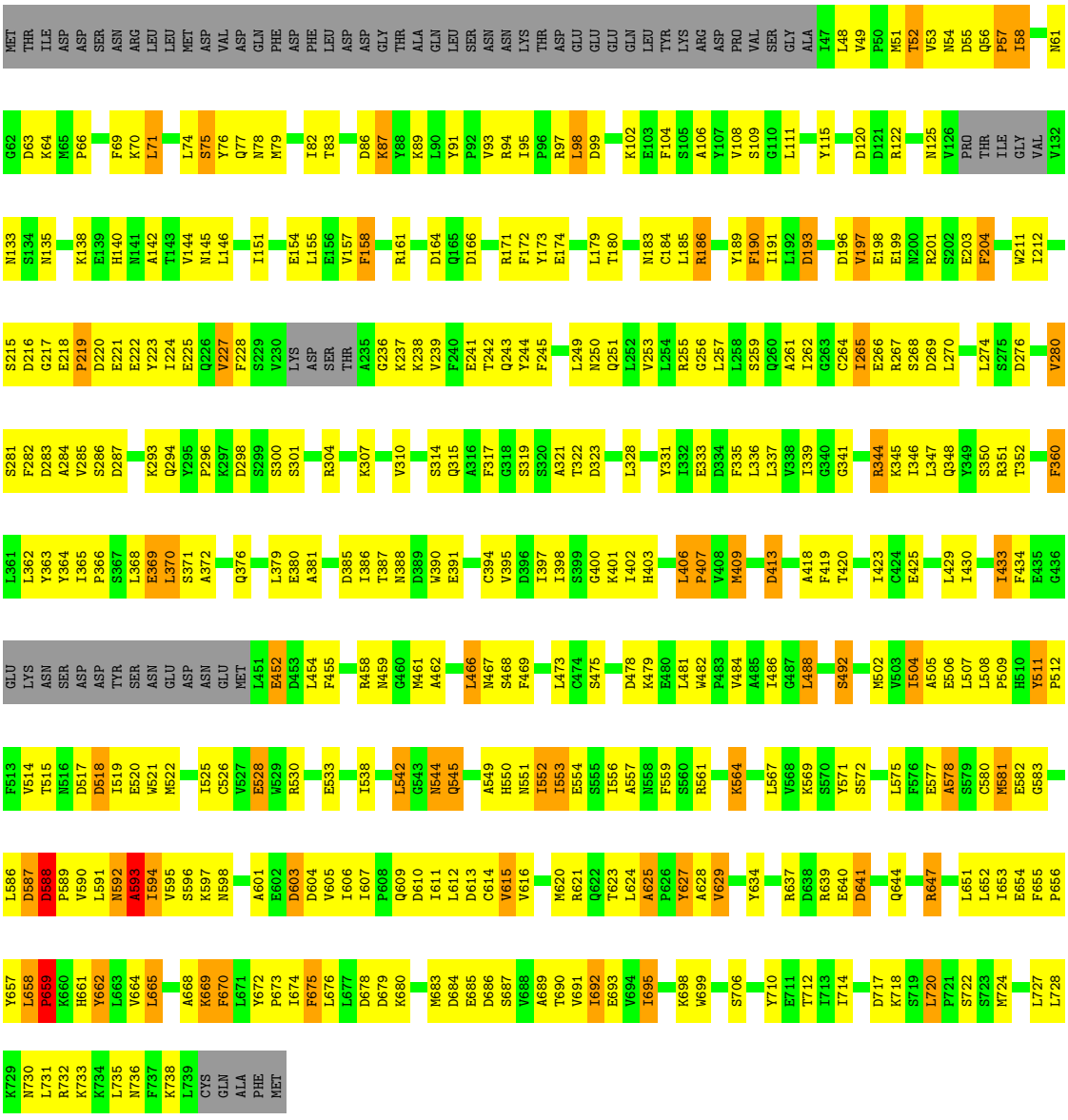




• Molecule 4: Nucleoporin NUP85

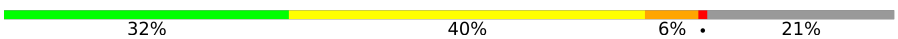
Chain m:

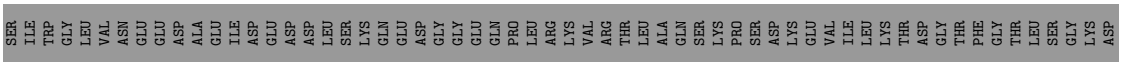


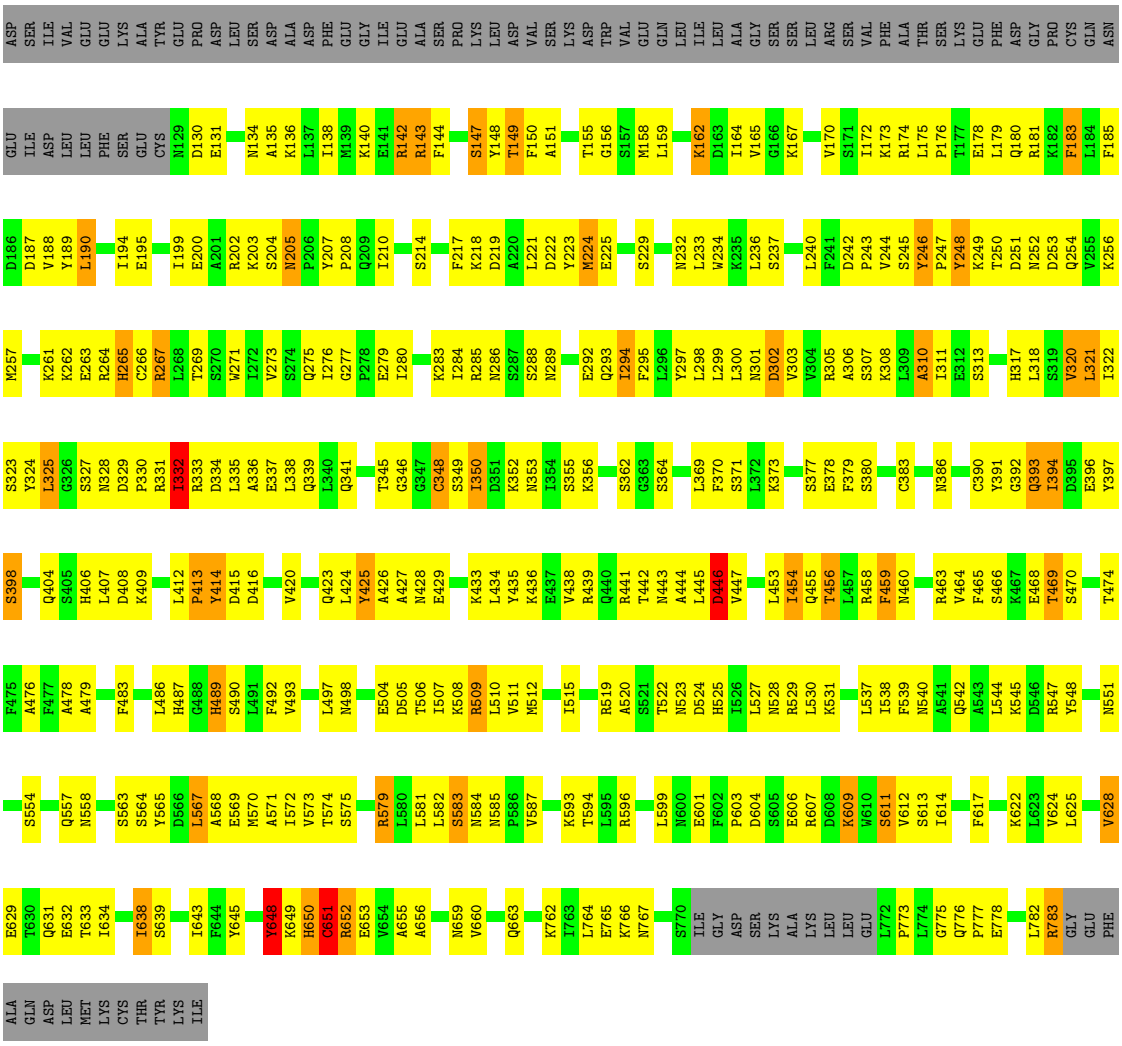


• Molecule 5: Nucleoporin 145c

Chain c:

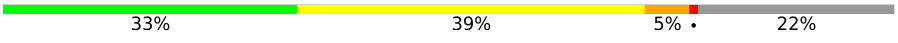


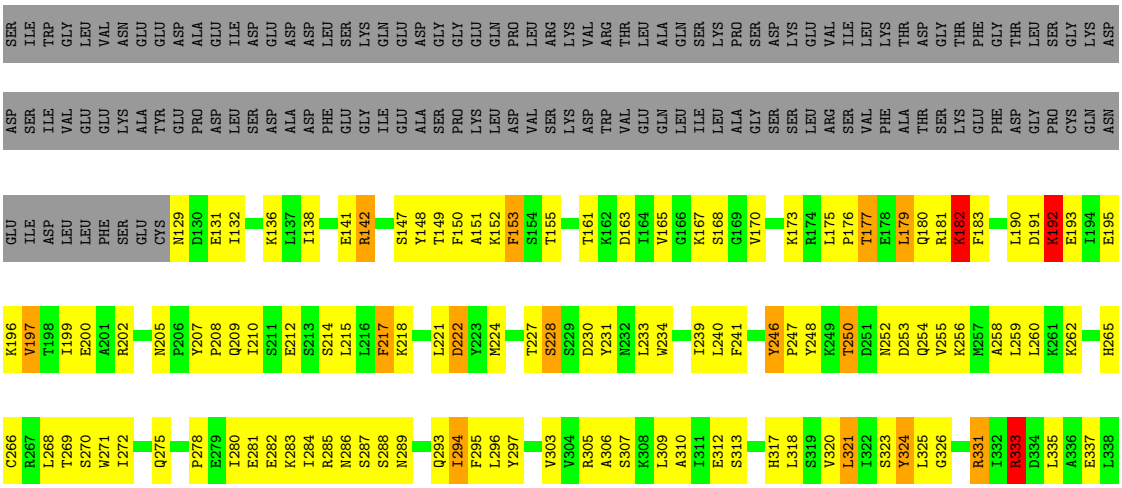


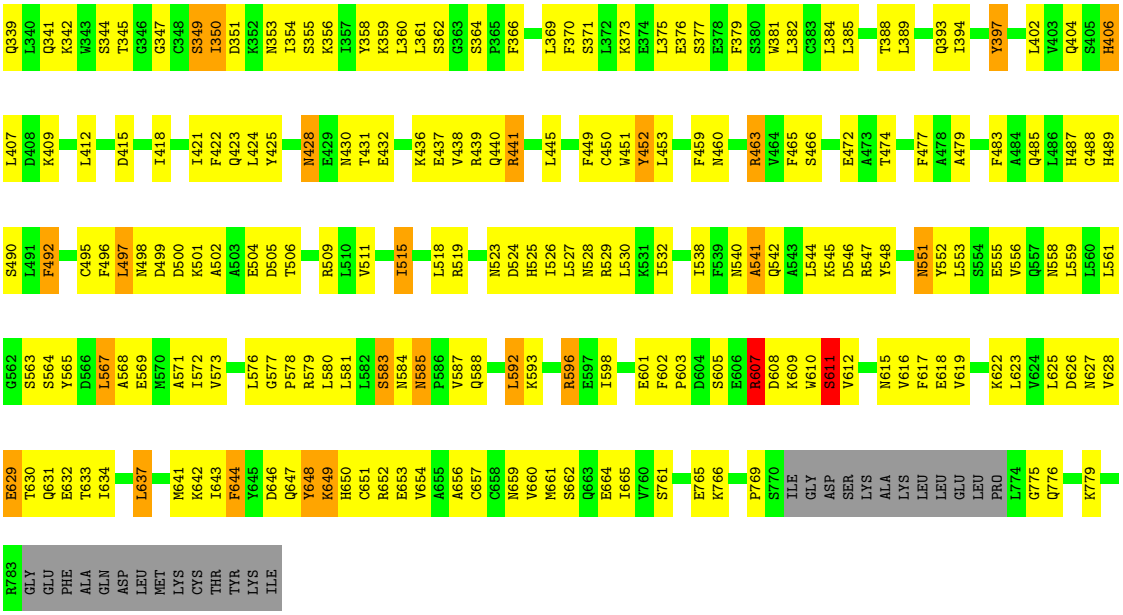


• Molecule 5: Nucleoporin 145c

Chain n:

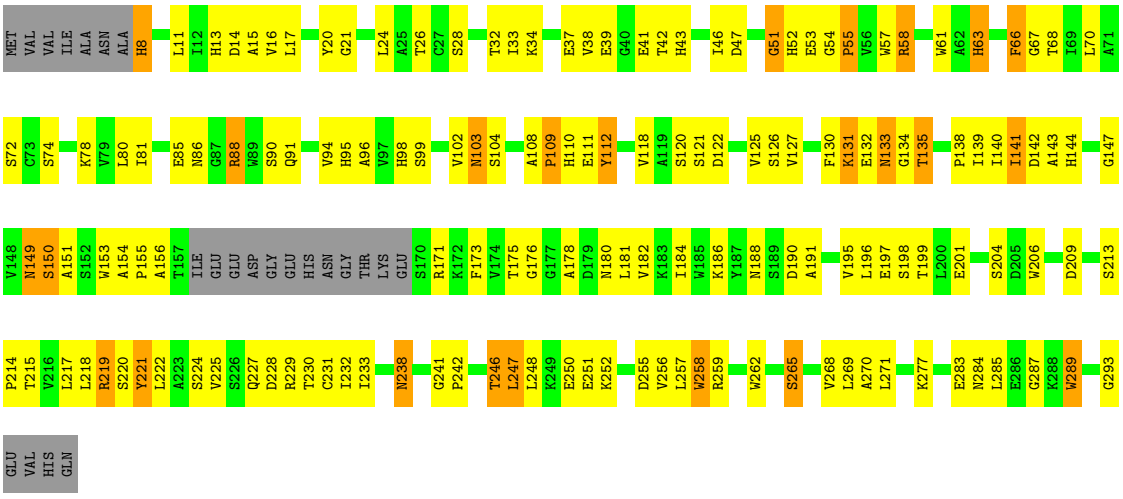






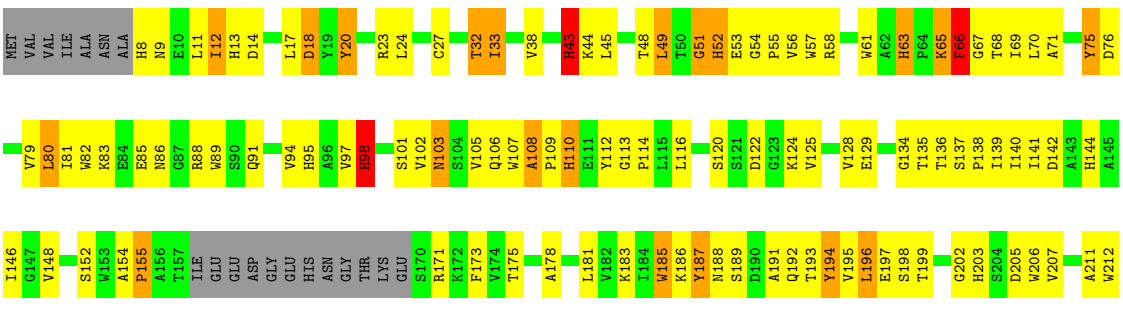
• Molecule 6: Protein transport protein SEC13

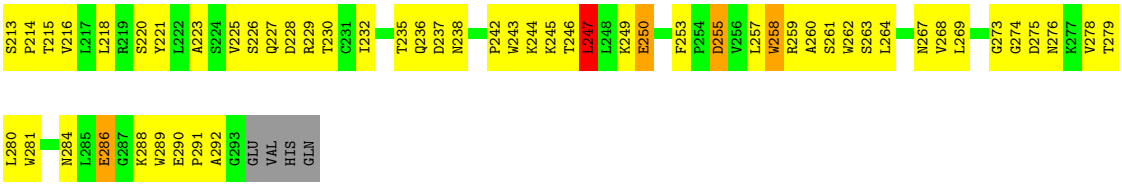
Chain d:



• Molecule 6: Protein transport protein SEC13

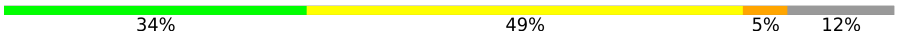
Chain o:

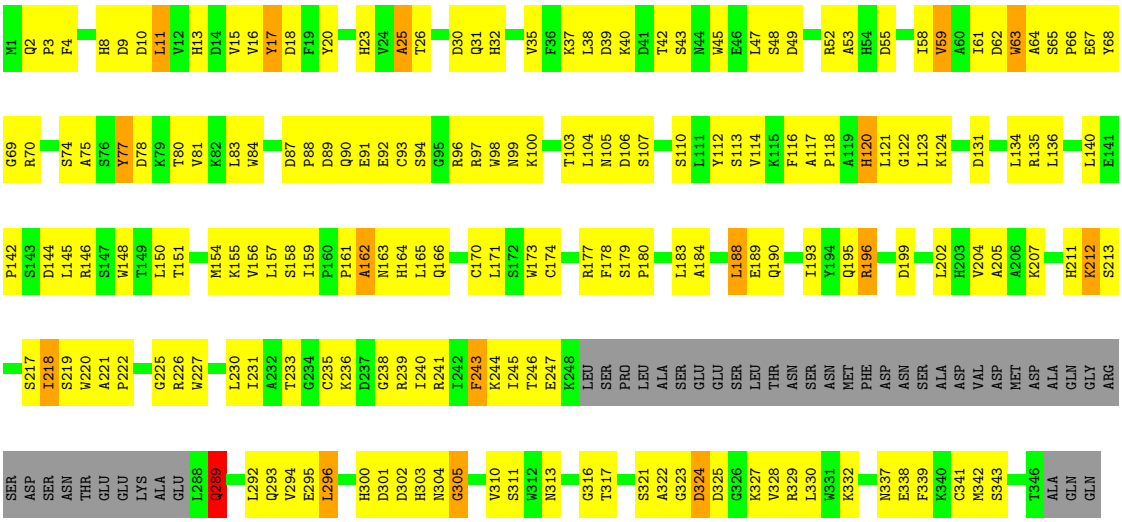




• Molecule 7: Nucleoporin SEH1

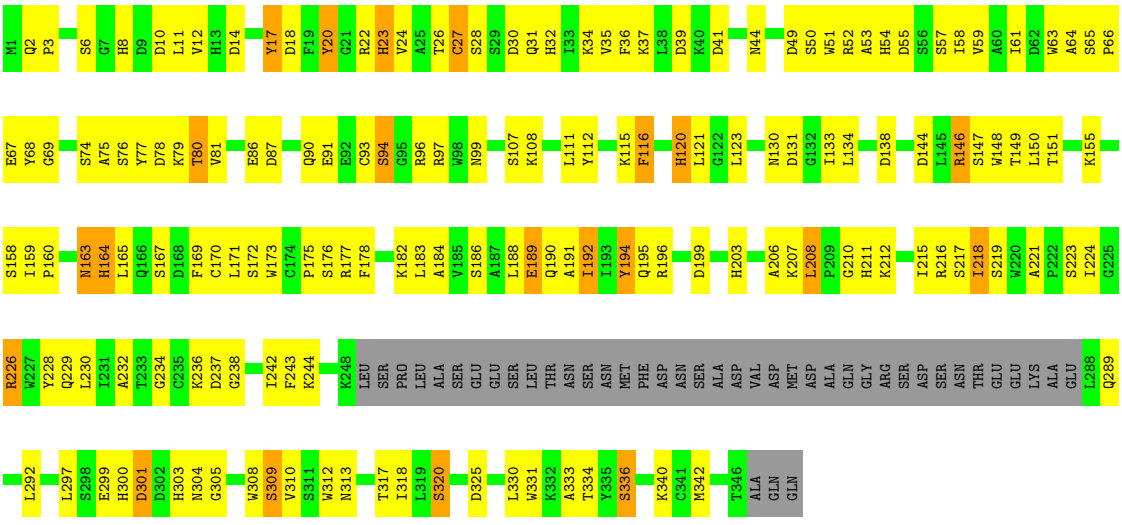
Chain e:





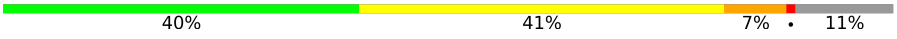
• Molecule 7: Nucleoporin SEH1

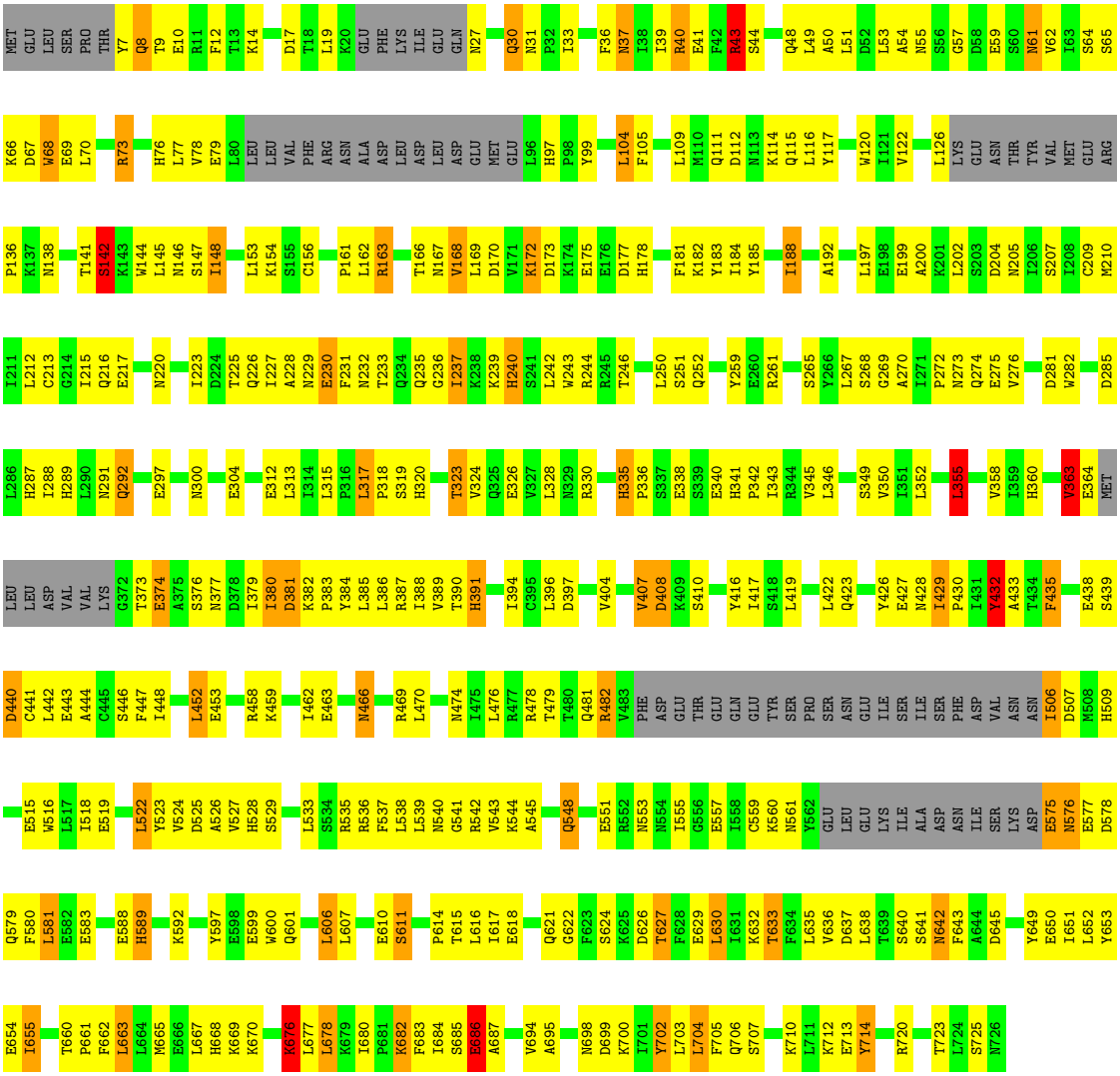
Chain p:



• Molecule 8: Nucleoporin NUP84

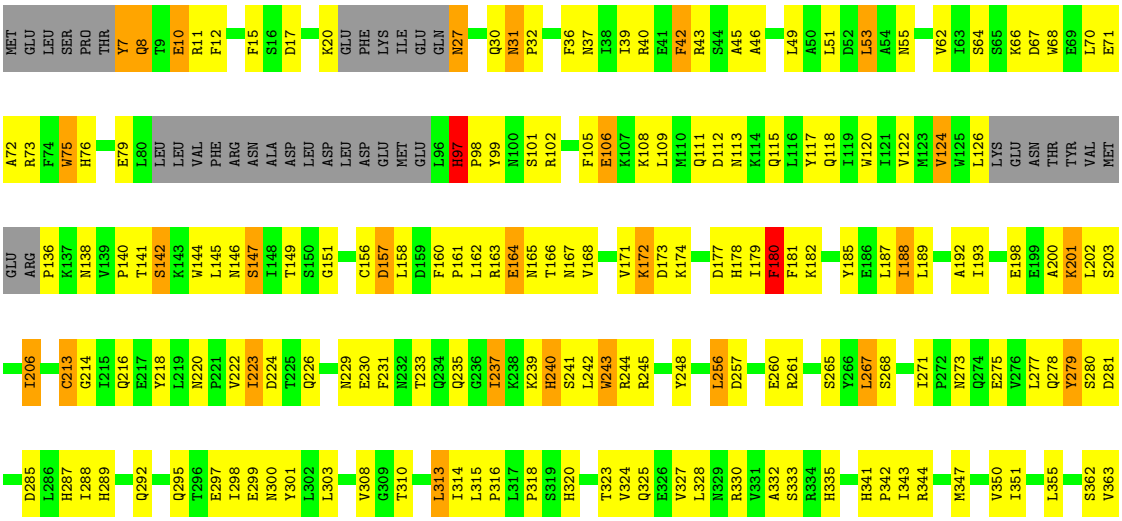
Chain f:

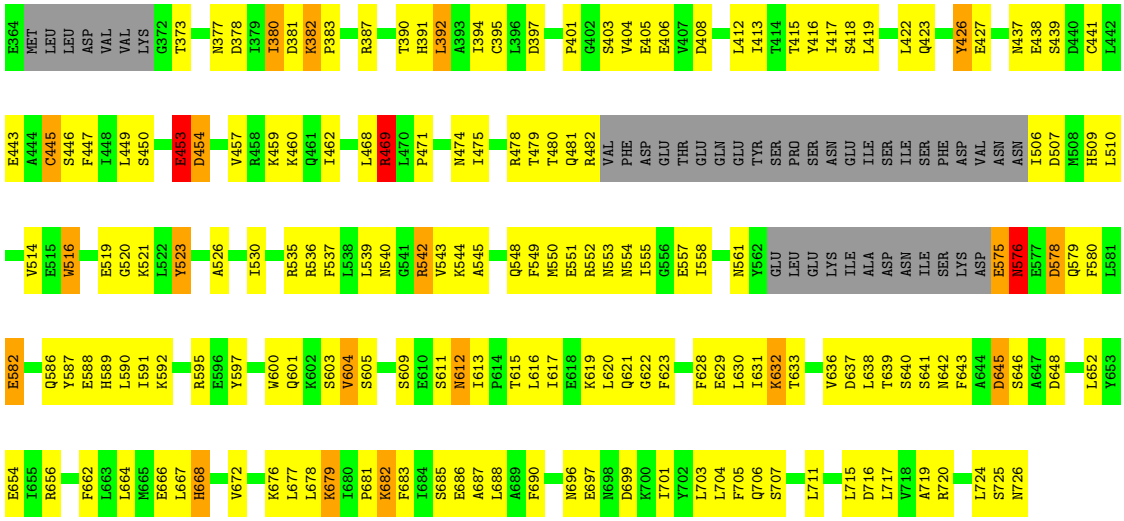




• Molecule 8: Nucleoporin NUP84

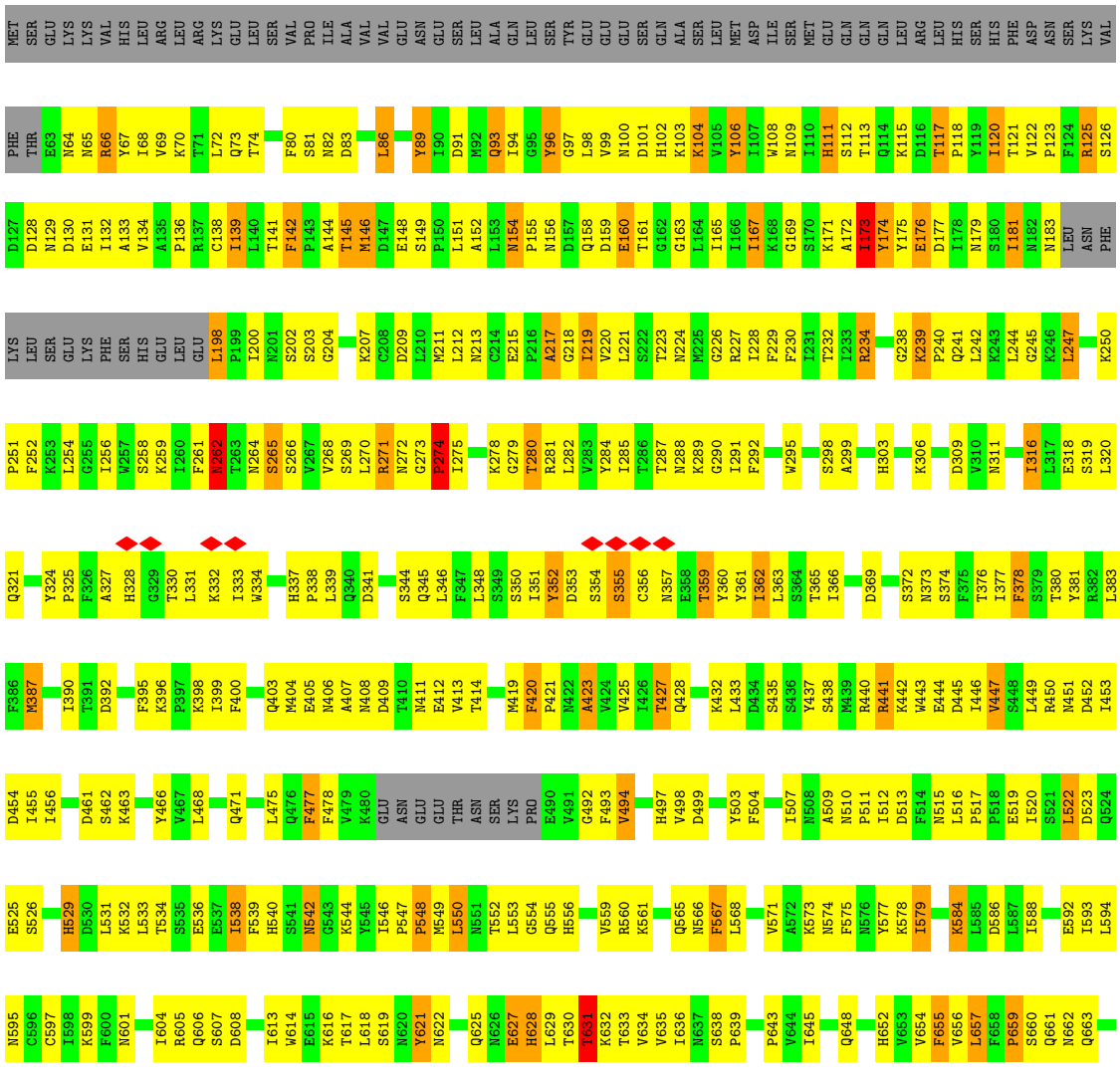
Chain q:

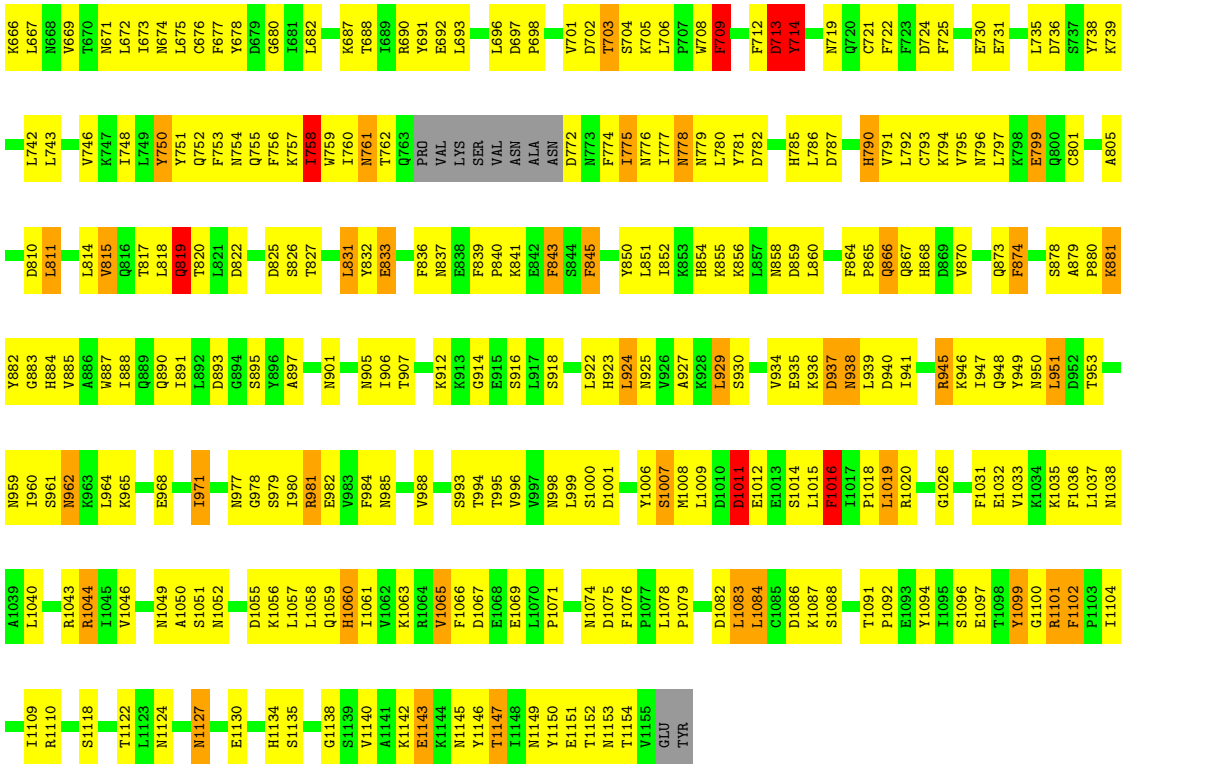




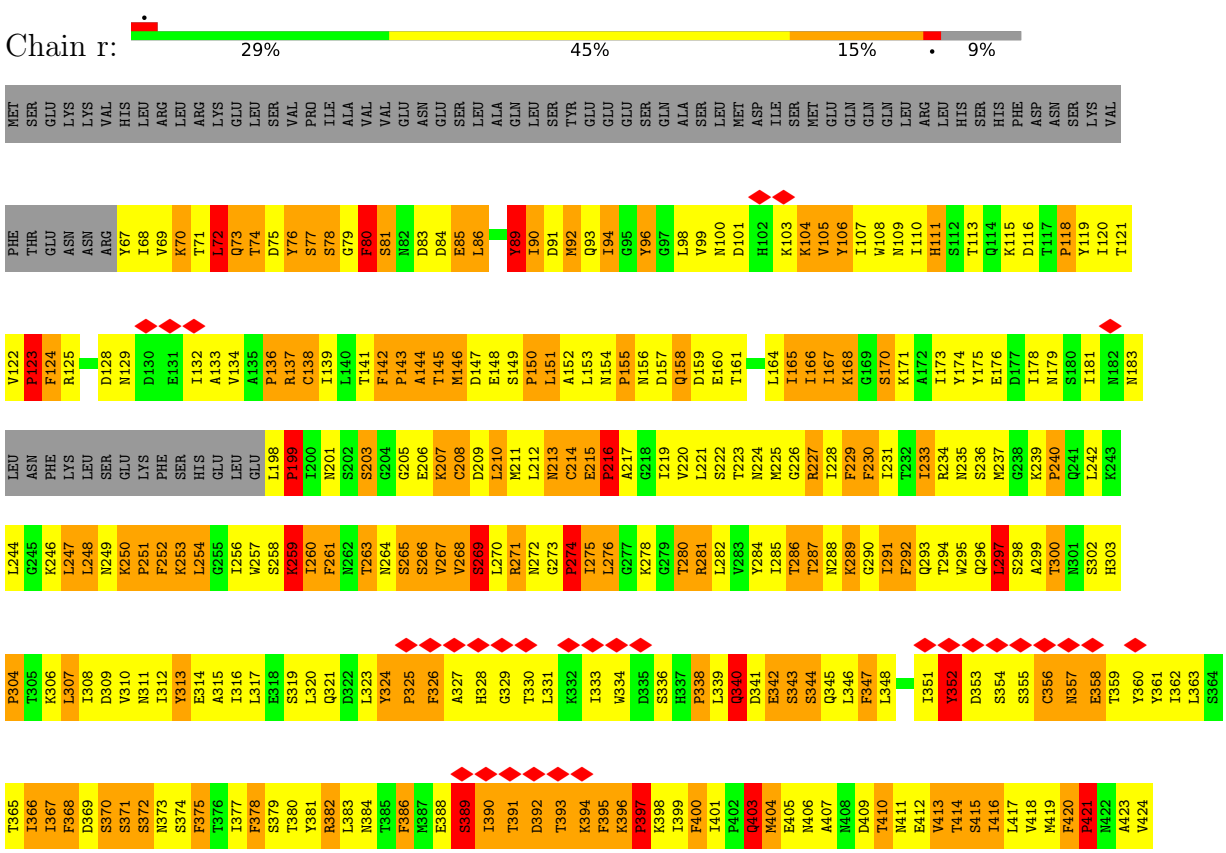
• Molecule 9: Nucleoporin NUP133

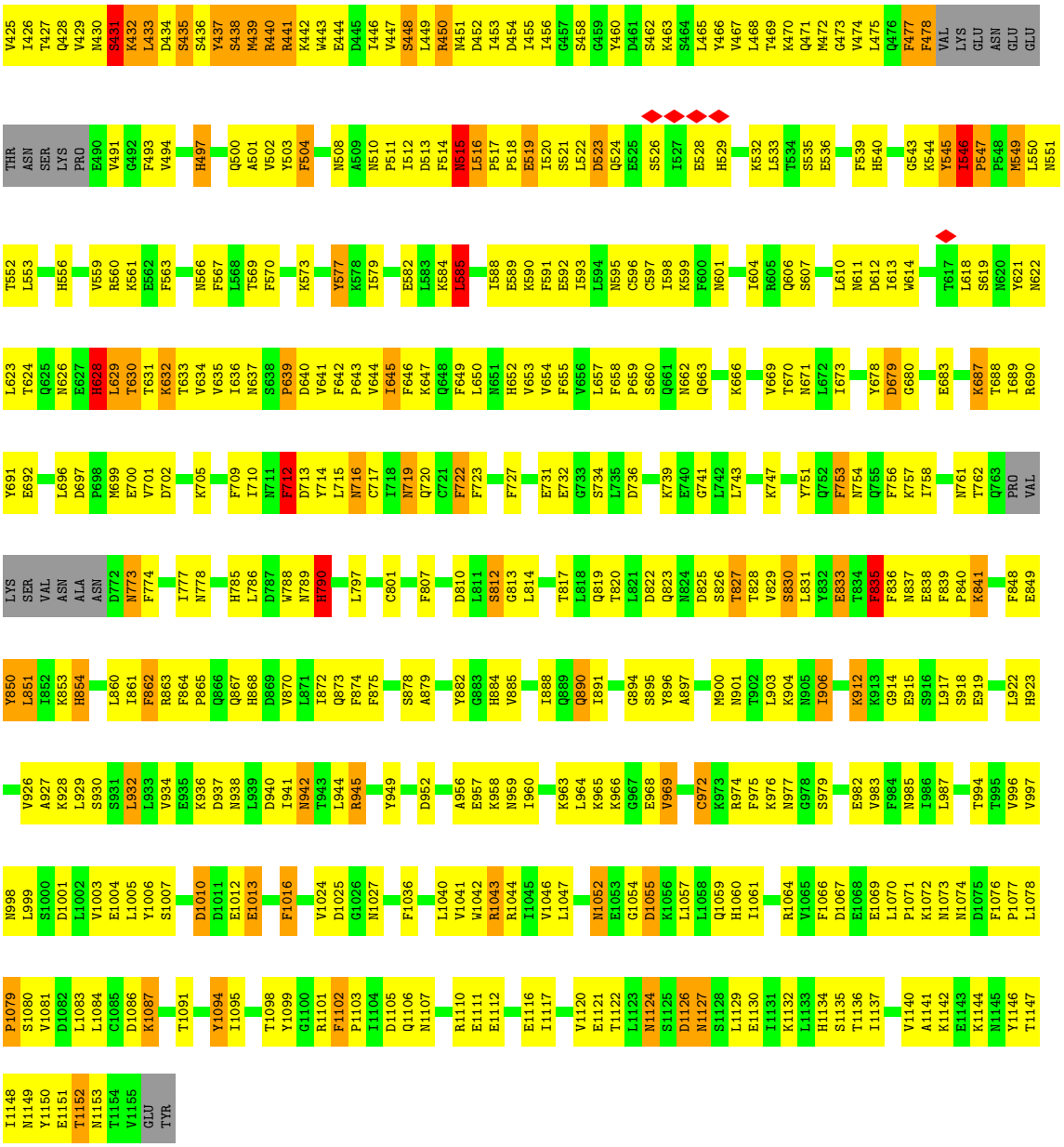
Chain g:





• Molecule 9: Nucleoporin NUP133




V425 I426 T427 Q428 V429 N430 S431 K432 L433 D434 S435 S436 Y437 S438 M439 R440 R441 K442 W443 E444 D445 I446 V447 S448 L449 R450 N451 D452 I453 D454 I455 I456 G457 S458 G459 Y460 D461 S462 K463 S464 L465 Y466 V467 L468 T469 K470 Q471 M472 G473 V474 L475 Q476 F477 F478 VAL LYS GLU ASN GLU GLU
THR ASN SER LYS PRO E490 V491 G492 F493 V494 H497 Q500 A501 V502 Y503 F504 N508 A509 N510 P511 I512 D513 F514 N515 L516 P517 P518 E519 I520 S521 L522 D523 Q524 E525 S526 I527 E528 H529 K532 L533 T534 S535 E536 F539 H540 G543 K544 Y545 I546 P547 P548 M549 L550 N551
T552 L553 H556 V559 R560 K561 E562 F563 N566 F567 L568 T569 F570 K573 Y577 K578 I579 E582 L583 K584 L585 I588 E589 K590 F591 E592 I593 L594 N595 C596 C597 I598 K599 F600 N601 I604 R605 Q606 S607 L610 N611 D612 I613 W614 T617 L618 S619 N620 Y621 N622
L623 T624 Q625 N626 E627 H628 L629 T630 T631 K632 T633 V634 V635 I636 N637 S638 P639 D640 V641 F642 P643 V644 I645 F646 K647 Q648 F649 L650 N651 H652 V653 V654 F655 V656 L657 F658 P659 S660 Q661 N662 Q663 K666 V669 T670 N671 L672 I673 Y678 D679 G680 E683 K687 T688 I689 R690
Y691 E692 L696 D697 P698 M699 E700 V701 D702 K705 F709 I710 N711 F712 D713 Y714 L715 N716 C717 I718 N719 Q720 C721 F722 F723 F727 E731 E732 G733 S734 L735 D736 K739 E740 G741 L742 L743 K747 Y751 Q752 F753 N754 Q755 F756 K757 I758 N761 T762 Q763 PRO VAL
LYS SER VAL ASN ALA ASN D772 N773 F774 I777 N778 H785 L786 D787 W788 N789 H790 L797 C801 F807 D810 L811 S812 G813 L814 T817 L818 Q819 T820 L821 D822 Q823 N824 D825 S826 T827 T828 V829 S830 L831 Y832 E833 T834 F835 F836 N837 E838 F839 P840 K841 F848 E849
Y850 L851 I852 K853 H854 L860 I861 F862 R863 F864 P865 Q866 Q867 H868 D869 V870 L871 I872 Q873 F874 F875 S878 A879 Y882 G883 H884 V885 I888 Q889 Q890 I891 G894 S895 Y896 A897 M900 N901 T902 L903 K904 N905 I906 K912 K913 G914 E915 S916 L917 S918 E919 L922 H923
V926 A927 K928 L929 S930 S931 L932 L933 V934 E935 K936 D937 N938 L939 D940 I941 N942 T943 L944 R945 Y949 D952 A956 E957 K958 N959 I960 K963 L964 K965 K966 G967 E968 V969 C972 K973 R974 F975 K976 N977 G978 S979 E982 V983 F984 N985 I986 L987 T994 T995 V996 V997
N998 L999 S1000 D1001 L1002 V1003 E1004 L1005 Y1006 S1007 D1010 D1011 E1012 E1013 F1016 V1024 D1025 G1026 N1027 F1036 L1040 V1041 W1042 R1043 R1044 I1045 V1046 L1047 N1052 E1053 G1054 D1055 K1056 L1057 L1058 Q1059 H1060 I1061 R1064 V1065 F1066 D1067 E1068 E1069 L1070 P1071 K1072 N1073 N1074 D1075 F1076 P1077 L1078
P1079 S1080 V1081 D1082 L1083 L1084 C1085 D1086 K1087 T1091 Y1094 I1095 T1098 Y1099 G1100 R1101 F1102 P1103 I1104 D1105 Q1106 N1107 R1110 E1111 E1112 E1116 I1117 V1120 E1121 T1122 L1123 N1124 S1125 D1126 N1127 S1128 L1129 E1130 I1131 K1132 L1133 H1134 S1135 T1136 I1137 V1140 A1141 K1142 E1143 K1144 N1145 Y1146 T1147
I1148 N1149 Y1150 E1151 T1152 N1153 T1154 V1155 GLU TYR

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C1	Depositor
Number of particles used	45000	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	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)	3800	Depositor
Magnification	37651	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.130	Depositor
Minimum map value	-0.019	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.006	Depositor
Recommended contour level	0.01	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
1	X	2.22	278/9370 (3.0%)	2.51	665/12670 (5.2%)
3	a	2.24	284/8464 (3.4%)	2.39	507/11469 (4.4%)
3	l	2.30	281/8461 (3.3%)	2.43	532/11460 (4.6%)
4	b	2.21	189/5533 (3.4%)	2.39	359/7493 (4.8%)
4	m	2.23	177/5492 (3.2%)	2.37	295/7440 (4.0%)
5	c	2.23	160/4600 (3.5%)	2.41	289/6211 (4.7%)
5	n	2.24	155/4584 (3.4%)	2.41	290/6188 (4.7%)
6	d	2.33	88/2220 (4.0%)	2.36	130/3028 (4.3%)
6	o	2.31	95/2220 (4.3%)	2.40	140/3028 (4.6%)
7	e	2.31	113/2499 (4.5%)	2.35	139/3388 (4.1%)
7	p	2.23	93/2499 (3.7%)	2.33	121/3388 (3.6%)
8	f	2.17	164/5359 (3.1%)	2.41	337/7258 (4.6%)
8	q	2.22	164/5352 (3.1%)	2.42	350/7248 (4.8%)
9	g	2.21	286/8806 (3.2%)	2.41	530/11936 (4.4%)
9	r	4.09	203/8755 (2.3%)	3.33	664/11870 (5.6%)
All	All	2.50	2730/84214 (3.2%)	2.52	5348/114075 (4.7%)

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	X	7	51
3	a	0	71
3	l	1	50
4	b	0	30
4	m	0	29
5	c	0	27
5	n	0	28
6	d	0	5
6	o	0	11
7	e	0	9

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Mol	Chain	#Chirality outliers	#Planarity outliers
7	p	0	12
8	f	1	15
8	q	1	19
9	g	0	54
9	r	0	33
All	All	10	444

All (2730) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	251	PRO	N-CD	123.92	3.21	1.47
9	r	150	PRO	N-CD	123.39	3.20	1.47
9	r	155	PRO	N-CD	122.51	3.19	1.47
9	r	325	PRO	N-CD	121.67	3.18	1.47
9	r	304	PRO	N-CD	119.28	3.14	1.47
9	r	274	PRO	N-CD	118.85	3.14	1.47
9	r	199	PRO	N-CD	58.17	2.29	1.47
9	r	118	PRO	N-CD	56.79	2.27	1.47
9	r	143	PRO	N-CD	53.47	2.22	1.47
9	r	240	PRO	N-CD	53.26	2.22	1.47
9	r	421	PRO	N-CD	52.97	2.21	1.47
9	r	136	PRO	N-CD	52.74	2.21	1.47
9	r	397	PRO	N-CD	49.78	2.17	1.47
9	r	123	PRO	N-CD	49.56	2.17	1.47
9	r	216	PRO	N-CD	43.70	2.08	1.47
9	r	338	PRO	N-CD	43.49	2.08	1.47
3	l	415	TYR	CA-CB	-42.99	1.11	1.53
3	l	416	GLY	CA-C	-35.49	1.01	1.51
1	X	794	ILE	CA-CB	-32.66	1.10	1.54
1	X	1059	ASN	N-CA	-32.39	1.05	1.45
1	X	1304	LYS	CA-CB	-24.27	1.12	1.53
1	X	1060	LEU	CA-CB	-23.70	1.13	1.53
1	X	1277	ILE	CA-CB	-22.29	1.24	1.54
8	f	576	ASN	CA-CB	-20.12	1.19	1.53
8	q	482	ARG	N-CA	-13.97	1.19	1.46
1	X	1303	LEU	N-CA	-13.13	1.21	1.46
1	X	793	LEU	N-CA	-12.65	1.22	1.46
9	g	211	MET	CA-C	-12.26	1.37	1.52
4	b	712	THR	C-N	12.02	1.45	1.33
5	n	208	PRO	C-N	11.83	1.43	1.33
3	a	734	HIS	CA-C	-11.79	1.36	1.52
9	r	138	CYS	CB-SG	-11.77	1.42	1.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	356	CYS	CB-SG	-11.77	1.42	1.81
9	r	214	CYS	CB-SG	-11.76	1.42	1.81
9	r	208	CYS	CB-SG	-11.72	1.42	1.81
8	q	576	ASN	CA-CB	-11.49	1.34	1.53
6	d	28	SER	CA-CB	11.42	1.68	1.54
1	X	1231	GLU	CA-C	-11.31	1.38	1.52
9	g	65	ASN	CA-C	-11.04	1.45	1.52
4	b	83	THR	CA-C	-10.95	1.42	1.53
3	l	266	ASP	C-N	10.86	1.44	1.33
6	o	211	ALA	CA-C	-10.75	1.39	1.53
3	a	386	LEU	C-N	10.74	1.45	1.34
4	m	49	VAL	CA-CB	-10.69	1.46	1.54
3	a	929	HIS	ND1-CE1	10.54	1.43	1.32
6	d	269	LEU	CA-C	-10.44	1.39	1.52
7	p	175	PRO	CA-C	-10.34	1.41	1.52
3	l	185	GLY	CA-C	-10.26	1.42	1.52
8	f	579	GLN	CA-C	-10.10	1.40	1.52
3	a	992	ASP	N-CA	-10.10	1.34	1.46
3	l	243	LEU	CA-CB	10.05	1.66	1.53
6	o	214	PRO	N-CA	-10.03	1.39	1.47
1	X	1276	LYS	N-CA	-9.96	1.27	1.46
4	m	620	MET	C-N	9.95	1.47	1.33
7	e	184	ALA	CA-C	-9.90	1.39	1.52
8	f	652	LEU	CA-C	-9.88	1.40	1.52
3	a	746	CYS	CA-C	-9.81	1.43	1.52
3	a	151	HIS	ND1-CE1	9.80	1.42	1.32
5	n	652	ARG	NE-CZ	9.80	1.43	1.33
1	X	1091	ASP	CA-C	-9.68	1.42	1.53
4	b	261	ALA	CA-C	-9.61	1.43	1.53
4	m	508	LEU	N-CA	-9.53	1.37	1.46
3	l	199	PHE	C-N	9.52	1.46	1.33
9	r	1153	ASN	C-N	9.50	1.47	1.33
3	a	537	THR	CA-C	-9.49	1.40	1.52
5	c	465	PHE	N-CA	-9.49	1.34	1.46
6	d	21	GLY	CA-C	-9.46	1.38	1.51
6	o	114	PRO	CA-C	-9.43	1.43	1.53
9	r	822	ASP	CA-CB	9.41	1.65	1.53
7	e	189	GLU	N-CA	-9.31	1.39	1.47
9	r	934	VAL	CA-C	-9.31	1.41	1.52
9	g	352	TYR	CA-C	-9.30	1.41	1.52
3	a	581	VAL	N-CA	-9.29	1.34	1.46
5	c	251	ASP	C-N	9.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	l	179	GLU	N-CA	-9.26	1.34	1.46
4	b	68	LYS	CA-C	-9.21	1.41	1.52
6	d	118	VAL	CA-C	9.19	1.63	1.52
7	e	11	LEU	CA-CB	9.19	1.67	1.53
1	X	1608	HIS	ND1-CE1	9.14	1.41	1.32
3	l	149	TRP	CA-C	-9.09	1.40	1.52
3	a	716	GLU	N-CA	-9.07	1.34	1.46
4	b	90	LEU	CA-C	-9.04	1.42	1.52
3	a	835	ASN	N-CA	-8.99	1.35	1.46
9	g	64	ASN	N-CA	-8.99	1.34	1.46
4	m	259	SER	CA-C	-8.99	1.41	1.52
9	g	262	ASN	CA-CB	8.97	1.67	1.53
8	q	260	GLU	CA-C	-8.97	1.43	1.52
9	g	1016	PHE	C-N	8.95	1.43	1.33
9	r	660	SER	CA-C	-8.94	1.40	1.52
7	e	118	PRO	CA-CB	8.92	1.65	1.53
8	q	37	ASN	C-N	8.90	1.43	1.34
3	a	758	PHE	N-CA	-8.88	1.35	1.46
7	p	147	SER	CA-C	-8.87	1.43	1.53
6	o	154	ALA	C-N	8.87	1.41	1.33
5	c	487	HIS	N-CA	-8.84	1.35	1.46
9	r	895	SER	CA-C	-8.81	1.42	1.53
9	g	337	HIS	CA-CB	8.80	1.63	1.53
9	g	965	LYS	CA-C	-8.79	1.40	1.52
1	X	833	LYS	N-CA	-8.77	1.35	1.46
3	l	116	GLN	CA-C	-8.76	1.41	1.52
4	m	267	ARG	NE-CZ	8.75	1.42	1.33
9	g	234	ARG	NE-CZ	8.73	1.42	1.33
5	c	392	GLY	C-N	8.71	1.45	1.33
7	p	3	PRO	C-N	8.69	1.45	1.33
9	g	337	HIS	ND1-CE1	8.68	1.41	1.32
5	n	253	ASP	CA-C	-8.67	1.41	1.52
7	p	52	ARG	CA-C	-8.67	1.42	1.52
4	b	552	ILE	CA-C	-8.67	1.43	1.52
4	b	171	ARG	CD-NE	8.63	1.58	1.46
1	X	1059	ASN	CA-CB	8.62	1.70	1.53
8	f	145	LEU	CA-C	-8.61	1.44	1.52
3	l	319	ILE	N-CA	8.60	1.53	1.46
3	l	529	SER	N-CA	-8.59	1.36	1.46
3	a	899	THR	CA-C	-8.58	1.41	1.53
5	n	333	ARG	NE-CZ	8.56	1.42	1.33
9	r	838	GLU	N-CA	-8.53	1.35	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	l	979	GLU	C-N	8.52	1.42	1.33
3	l	154	ASN	CA-CB	8.51	1.63	1.53
3	l	949	LEU	CA-C	-8.50	1.42	1.52
1	X	992	SER	N-CA	-8.50	1.35	1.46
5	n	765	GLU	N-CA	-8.48	1.36	1.46
8	q	589	HIS	ND1-CE1	8.48	1.41	1.32
5	c	585	ASN	C-N	8.48	1.40	1.33
9	g	1079	PRO	CA-C	-8.45	1.42	1.52
3	a	415	TYR	CA-C	-8.45	1.41	1.52
6	d	232	ILE	N-CA	-8.44	1.36	1.46
3	l	742	GLU	CA-C	-8.43	1.45	1.52
9	g	83	ASP	CA-CB	8.39	1.59	1.53
9	g	360	TYR	CA-C	-8.38	1.42	1.52
5	n	585	ASN	N-CA	-8.37	1.37	1.45
9	g	851	LEU	CA-C	-8.36	1.43	1.53
4	b	351	ARG	C-N	8.36	1.43	1.33
4	b	655	PHE	N-CA	8.36	1.51	1.46
1	X	1482	ASP	CA-C	-8.35	1.42	1.52
6	o	258	TRP	NE1-CE2	8.32	1.46	1.37
9	g	428	GLN	C-N	8.29	1.43	1.33
9	g	268	VAL	CA-CB	-8.29	1.46	1.55
4	m	692	ILE	N-CA	-8.28	1.36	1.46
9	r	700	GLU	C-N	8.28	1.44	1.34
5	c	624	VAL	N-CA	-8.28	1.38	1.46
3	l	342	LEU	N-CA	-8.27	1.35	1.45
7	e	84	TRP	CA-C	-8.27	1.42	1.52
3	a	319	ILE	CA-C	-8.26	1.45	1.53
3	a	151	HIS	CA-C	-8.26	1.42	1.52
5	n	532	ILE	CA-C	8.24	1.61	1.52
9	g	571	VAL	CA-C	-8.24	1.43	1.52
5	c	764	LEU	CA-CB	8.23	1.67	1.53
3	l	602	ILE	CA-C	-8.22	1.42	1.52
5	n	377	SER	CA-CB	8.22	1.65	1.54
3	l	162	VAL	CA-C	-8.21	1.46	1.52
1	X	1433	ILE	CA-C	-8.19	1.42	1.52
4	b	545	GLN	CA-CB	8.19	1.66	1.53
8	q	278	GLN	CA-C	-8.19	1.41	1.52
7	e	145	LEU	N-CA	-8.19	1.36	1.46
9	g	400	PHE	C-N	8.19	1.42	1.33
3	a	692	PHE	CA-CB	8.18	1.65	1.53
4	b	702	ALA	CA-C	-8.18	1.41	1.52
3	l	647	PHE	CA-C	-8.18	1.42	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	n	540	ASN	CA-CB	8.17	1.66	1.53
7	p	123	LEU	CA-CB	8.15	1.63	1.52
8	q	330	ARG	NE-CZ	8.15	1.42	1.33
6	o	197	GLU	CA-C	-8.14	1.42	1.52
6	o	292	ALA	CA-C	8.13	1.60	1.52
3	a	658	HIS	ND1-CE1	8.13	1.40	1.32
1	X	1533	ILE	CA-CB	-8.12	1.45	1.54
6	o	116	LEU	CA-C	-8.12	1.42	1.52
1	X	1011	GLU	CA-C	8.12	1.64	1.52
3	l	892	GLY	N-CA	-8.12	1.38	1.45
3	l	1018	ILE	N-CA	8.12	1.56	1.46
4	m	400	GLY	CA-C	-8.10	1.40	1.51
8	q	589	HIS	CE1-NE2	-8.09	1.24	1.32
3	l	154	ASN	CA-C	-8.08	1.43	1.52
4	m	146	LEU	C-N	8.07	1.45	1.33
3	l	378	TRP	CA-C	-8.07	1.42	1.52
9	g	822	ASP	CA-C	-8.06	1.42	1.52
8	q	453	GLU	CA-CB	-8.06	1.47	1.54
4	m	672	TYR	N-CA	-8.06	1.39	1.46
3	l	492	ASN	CA-C	-8.05	1.41	1.52
4	b	715	GLU	C-N	8.03	1.44	1.33
3	a	481	HIS	CE1-NE2	-8.00	1.24	1.32
9	r	1141	ALA	CA-CB	7.99	1.66	1.53
4	b	529	TRP	N-CA	-7.98	1.36	1.46
9	g	73	GLN	C-N	7.98	1.43	1.33
8	q	288	ILE	C-N	7.97	1.43	1.33
1	X	1486	GLU	CA-C	-7.96	1.42	1.52
8	f	462	ILE	C-O	-7.96	1.14	1.24
8	f	640	SER	N-CA	-7.96	1.38	1.46
5	n	214	SER	CA-C	7.96	1.63	1.52
8	f	17	ASP	CA-CB	7.96	1.66	1.53
3	l	482	SER	CA-C	-7.96	1.43	1.53
3	l	585	ASP	C-N	7.95	1.43	1.33
8	f	282	TRP	CA-C	-7.95	1.42	1.52
8	q	725	SER	C-N	7.95	1.44	1.33
1	X	1048	LYS	CA-CB	7.95	1.63	1.53
9	g	411	ASN	CA-CB	7.92	1.59	1.53
6	o	155	PRO	CA-C	-7.92	1.45	1.52
8	f	506	ILE	CB-CG1	7.91	1.69	1.53
5	n	625	LEU	N-CA	7.90	1.55	1.46
8	q	237	ILE	CA-C	-7.90	1.43	1.52
3	a	176	VAL	CA-C	-7.89	1.43	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	611	SER	CA-C	-7.89	1.42	1.52
3	l	259	MET	N-CA	-7.87	1.37	1.46
5	c	587	VAL	CA-CB	7.86	1.65	1.54
3	a	139	PHE	N-CA	-7.86	1.36	1.46
4	m	253	VAL	N-CA	-7.85	1.36	1.46
7	p	22	ARG	NE-CZ	7.85	1.41	1.33
9	g	461	ASP	N-CA	-7.84	1.36	1.46
5	n	618	GLU	C-N	7.84	1.43	1.33
5	n	153	PHE	CA-C	-7.84	1.42	1.52
9	g	529	HIS	ND1-CE1	7.83	1.40	1.32
6	d	150	SER	CA-C	-7.82	1.43	1.52
6	d	143	ALA	CA-C	-7.82	1.44	1.52
8	q	378	ASP	CA-CB	7.82	1.66	1.53
5	n	662	SER	CA-C	-7.81	1.43	1.52
9	r	1016	PHE	CA-CB	7.80	1.66	1.53
9	r	535	SER	C-N	7.80	1.44	1.33
6	d	28	SER	C-O	-7.80	1.18	1.24
8	q	439	SER	N-CA	-7.80	1.37	1.46
9	r	1012	GLU	C-N	7.79	1.44	1.33
6	o	79	VAL	CA-C	-7.78	1.44	1.52
9	g	452	ASP	CA-C	7.77	1.63	1.53
9	g	923	HIS	CA-CB	7.77	1.65	1.53
3	l	26	LEU	CA-C	-7.76	1.42	1.52
8	q	716	ASP	N-CA	7.74	1.55	1.46
1	X	1336	LEU	CA-C	-7.73	1.42	1.52
8	q	289	HIS	ND1-CE1	7.73	1.40	1.32
9	r	841	LYS	CA-C	7.72	1.63	1.52
5	c	583	SER	N-CA	-7.72	1.39	1.46
3	a	94	ASN	CA-CB	7.71	1.64	1.53
6	d	118	VAL	CA-CB	-7.71	1.44	1.54
8	f	684	ILE	CA-CB	-7.71	1.45	1.54
4	m	661	HIS	ND1-CE1	7.71	1.40	1.32
3	a	650	HIS	ND1-CE1	7.71	1.40	1.32
3	l	736	ASN	CA-C	-7.70	1.42	1.52
6	d	258	TRP	C-N	7.70	1.44	1.33
4	m	508	LEU	CA-CB	7.70	1.63	1.53
1	X	1123	HIS	ND1-CE1	7.69	1.40	1.32
6	d	171	ARG	NE-CZ	7.68	1.41	1.33
4	b	613	ASP	CA-CB	7.68	1.63	1.53
9	r	997	VAL	C-N	7.67	1.44	1.33
6	o	128	VAL	CA-CB	-7.67	1.44	1.54
5	n	266	CYS	N-CA	-7.65	1.37	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	m	433	ILE	C-N	7.65	1.43	1.33
7	p	144	ASP	CA-CB	7.64	1.63	1.53
5	c	334	ASP	N-CA	-7.64	1.37	1.46
4	b	379	LEU	C-N	7.64	1.44	1.33
9	r	937	ASP	N-CA	-7.64	1.36	1.46
9	g	822	ASP	C-N	7.63	1.44	1.33
1	X	344	SER	CA-C	-7.63	1.42	1.52
9	g	471	GLN	CA-CB	7.63	1.64	1.53
3	a	372	SER	N-CA	-7.62	1.36	1.46
8	q	392	LEU	CA-C	-7.62	1.42	1.52
4	b	345	LYS	CA-C	7.62	1.63	1.52
4	b	139	GLU	CA-C	-7.62	1.42	1.52
7	p	305	GLY	CA-C	-7.61	1.44	1.51
6	d	86	ASN	C-N	7.61	1.41	1.33
1	X	1277	ILE	CA-C	-7.60	1.43	1.52
7	e	178	PHE	CA-CB	7.60	1.64	1.53
4	m	486	ILE	C-N	7.59	1.43	1.33
3	l	374	LYS	C-N	7.59	1.43	1.33
5	c	245	SER	CA-CB	7.59	1.64	1.53
5	n	653	GLU	CA-C	-7.59	1.43	1.52
9	r	304	PRO	C-N	7.58	1.44	1.33
6	d	38	VAL	CA-C	-7.56	1.44	1.53
9	g	592	GLU	C-N	7.56	1.43	1.33
3	l	779	LEU	N-CA	-7.55	1.35	1.46
1	X	1549	LYS	C-N	7.55	1.43	1.33
6	d	231	CYS	CA-C	-7.55	1.43	1.52
6	o	45	LEU	CA-C	-7.54	1.42	1.52
6	o	289	TRP	N-CA	-7.54	1.36	1.46
7	e	301	ASP	CA-C	-7.54	1.43	1.52
6	o	148	VAL	CA-CB	-7.54	1.45	1.54
9	g	560	ARG	C-N	7.53	1.43	1.33
9	g	1091	THR	C-N	7.53	1.43	1.34
3	l	76	SER	N-CA	-7.53	1.36	1.46
5	c	519	ARG	NE-CZ	7.53	1.41	1.33
9	r	936	LYS	C-N	7.51	1.43	1.33
8	f	579	GLN	N-CA	-7.51	1.37	1.46
5	n	394	ILE	CA-C	7.51	1.62	1.52
1	X	1047	LEU	N-CA	-7.50	1.36	1.46
7	e	171	LEU	CA-C	-7.50	1.43	1.52
9	g	1101	ARG	CD-NE	7.50	1.56	1.46
5	n	170	VAL	CA-C	-7.50	1.43	1.52
6	d	78	LYS	N-CA	-7.49	1.36	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	l	266	ASP	CA-C	7.49	1.63	1.53
3	a	60	LEU	CA-C	-7.47	1.43	1.52
5	n	637	LEU	CA-CB	7.46	1.65	1.53
3	a	526	ARG	CD-NE	7.46	1.56	1.46
5	c	390	CYS	CA-C	-7.46	1.42	1.52
9	r	1060	HIS	CA-CB	7.46	1.65	1.53
5	c	631	GLN	CA-CB	7.44	1.63	1.53
8	q	328	LEU	C-N	7.44	1.44	1.34
3	l	22	ASN	CA-CB	7.43	1.66	1.53
9	r	213	ASN	C-O	-7.43	1.15	1.24
8	q	536	ARG	CD-NE	7.43	1.56	1.46
1	X	733	ARG	NE-CZ	7.42	1.41	1.33
9	r	438	SER	C-N	-7.42	1.23	1.33
7	e	158	SER	C-N	7.42	1.38	1.33
3	a	55	GLU	CA-C	-7.42	1.42	1.52
4	m	215	SER	CA-C	7.42	1.58	1.52
6	d	126	SER	CA-C	-7.42	1.44	1.52
8	q	415	THR	C-N	7.41	1.43	1.33
3	l	272	LYS	CA-C	-7.41	1.43	1.52
1	X	336	GLN	CA-C	-7.41	1.43	1.52
9	g	513	ASP	C-N	7.40	1.44	1.34
3	a	722	THR	CA-C	-7.40	1.45	1.52
5	c	242	ASP	CA-C	7.39	1.60	1.52
3	l	866	GLU	C-N	7.39	1.44	1.33
3	l	202	ASN	CA-C	-7.39	1.42	1.52
7	e	177	ARG	CZ-NH2	7.39	1.43	1.33
1	X	1219	THR	C-N	7.38	1.39	1.33
3	a	208	LEU	CA-C	-7.38	1.43	1.52
7	e	218	ILE	CA-C	-7.38	1.44	1.52
9	g	250	LYS	CA-C	7.38	1.61	1.52
9	r	1036	PHE	CA-C	-7.38	1.42	1.52
3	a	177	PHE	C-N	7.38	1.43	1.33
6	d	130	PHE	C-N	7.38	1.44	1.33
7	e	196	ARG	NE-CZ	7.38	1.41	1.33
1	X	343	ASP	N-CA	-7.37	1.38	1.46
5	c	547	ARG	CD-NE	7.36	1.56	1.46
3	l	61	LEU	CA-CB	7.35	1.63	1.53
5	n	648	TYR	CA-C	-7.35	1.44	1.52
3	l	133	LEU	CA-C	7.35	1.61	1.52
8	q	315	LEU	CA-C	7.35	1.58	1.52
3	l	766	SER	N-CA	-7.35	1.37	1.46
3	l	75	ARG	CA-CB	7.34	1.65	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	m	253	VAL	CA-CB	-7.34	1.45	1.54
9	g	221	LEU	CA-CB	7.34	1.62	1.53
4	b	125	ASN	N-CA	-7.34	1.37	1.46
7	e	4	PHE	CA-CB	7.34	1.66	1.53
8	q	509	HIS	ND1-CE1	7.33	1.39	1.32
9	g	981	ARG	NE-CZ	7.33	1.41	1.33
7	e	47	LEU	C-N	7.33	1.43	1.33
3	a	561	GLN	CA-CB	7.32	1.66	1.53
5	n	165	VAL	CA-C	7.32	1.62	1.53
9	r	1047	LEU	CA-C	7.31	1.62	1.52
3	l	227	LYS	N-CA	-7.29	1.37	1.46
3	l	383	ASN	CA-CB	7.29	1.63	1.53
9	g	517	PRO	CA-C	-7.28	1.45	1.52
5	n	650	HIS	CA-C	-7.26	1.43	1.52
9	g	1153	ASN	CA-C	-7.26	1.43	1.52
1	X	1608	HIS	CA-C	-7.26	1.45	1.52
1	X	1468	VAL	C-N	7.25	1.43	1.33
3	a	901	ARG	CA-CB	7.25	1.62	1.53
3	a	874	ASN	CA-C	-7.25	1.43	1.52
1	X	827	PRO	N-CA	-7.23	1.38	1.47
9	r	1146	TYR	CA-C	-7.23	1.43	1.52
7	p	77	TYR	CZ-OH	7.23	1.53	1.38
3	l	955	SER	C-N	7.22	1.43	1.32
5	c	142	ARG	CD-NE	7.22	1.56	1.46
5	c	269	THR	N-CA	-7.22	1.37	1.46
7	e	330	LEU	CA-C	-7.22	1.43	1.52
3	l	579	ILE	CA-C	-7.22	1.45	1.52
3	a	1	MET	C-N	7.22	1.43	1.33
8	q	355	LEU	C-N	7.21	1.43	1.33
9	g	272	ASN	CA-CB	7.21	1.64	1.53
3	a	827	GLN	CA-CB	7.21	1.64	1.53
7	e	322	ALA	CA-CB	7.20	1.64	1.53
6	o	186	LYS	CA-CB	7.20	1.64	1.53
1	X	1594	ASP	N-CA	-7.20	1.40	1.47
8	f	205	ASN	CA-C	-7.20	1.44	1.52
6	o	195	VAL	CA-C	-7.20	1.43	1.52
3	l	911	GLU	N-CA	-7.20	1.37	1.46
7	p	238	GLY	C-N	7.20	1.43	1.33
4	m	294	GLN	CA-CB	7.19	1.63	1.53
4	m	364	TYR	C-N	7.19	1.39	1.33
6	o	81	ILE	CA-C	-7.19	1.46	1.53
5	n	766	LYS	CA-C	-7.19	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	f	522	LEU	CA-C	-7.18	1.43	1.52
3	a	72	PHE	C-N	7.18	1.43	1.33
8	f	97	HIS	CA-C	7.17	1.60	1.52
9	r	952	ASP	CA-CB	7.17	1.65	1.53
8	q	245	ARG	CZ-NH1	7.17	1.42	1.32
1	X	1442	ILE	CA-CB	-7.17	1.46	1.54
3	a	136	SER	CA-CB	7.17	1.65	1.53
1	X	446	ALA	C-N	7.16	1.43	1.33
3	a	494	PHE	CA-CB	7.16	1.65	1.53
3	l	963	LYS	CA-CB	7.16	1.64	1.54
9	g	333	ILE	CA-C	-7.15	1.43	1.52
7	e	163	ASN	C-N	7.15	1.43	1.33
6	o	225	VAL	N-CA	7.15	1.54	1.46
1	X	670	HIS	ND1-CE1	7.14	1.39	1.32
3	a	842	LEU	CA-C	-7.14	1.43	1.52
3	a	419	ILE	CA-C	-7.13	1.43	1.52
4	b	723	SER	C-N	7.13	1.43	1.33
6	o	198	SER	CA-C	-7.13	1.44	1.52
9	g	673	ILE	CA-CB	-7.13	1.46	1.54
9	r	529	HIS	ND1-CE1	7.13	1.39	1.32
1	X	763	GLN	N-CA	-7.12	1.37	1.45
5	n	527	LEU	C-N	7.12	1.44	1.33
3	a	989	ALA	CA-C	-7.12	1.44	1.52
4	m	335	PHE	CA-CB	7.12	1.65	1.53
5	n	359	LYS	N-CA	-7.12	1.37	1.46
5	n	587	VAL	CA-C	-7.11	1.43	1.52
9	g	1097	GLU	CA-CB	7.10	1.64	1.54
7	p	170	CYS	CA-C	-7.10	1.44	1.52
4	m	692	ILE	C-N	7.10	1.43	1.33
8	f	702	TYR	N-CA	-7.09	1.37	1.46
9	r	1146	TYR	C-N	7.09	1.43	1.33
8	f	54	ALA	C-N	7.09	1.43	1.33
5	c	349	SER	N-CA	-7.08	1.37	1.46
9	r	884	HIS	ND1-CE1	7.08	1.39	1.32
8	q	136	PRO	C-N	7.08	1.43	1.33
3	l	165	PHE	CA-CB	7.08	1.65	1.53
3	a	834	ARG	CD-NE	7.07	1.56	1.46
7	p	226	ARG	CA-C	-7.07	1.43	1.52
3	a	414	ARG	CA-C	-7.07	1.43	1.52
3	l	929	HIS	ND1-CE1	7.06	1.39	1.32
9	g	1060	HIS	CE1-NE2	7.06	1.39	1.32
5	n	761	SER	N-CA	-7.06	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	636	LEU	N-CA	-7.05	1.38	1.46
7	p	50	SER	CA-C	-7.05	1.46	1.53
9	g	395	PHE	N-CA	-7.05	1.37	1.46
3	a	226	CYS	C-N	7.05	1.43	1.33
8	q	439	SER	C-N	7.05	1.43	1.33
5	c	453	LEU	CA-CB	7.04	1.64	1.53
4	b	573	TRP	CA-CB	7.04	1.65	1.53
8	q	526	ALA	N-CA	-7.03	1.37	1.46
6	d	72	SER	CA-C	-7.03	1.45	1.52
1	X	749	ILE	N-CA	7.02	1.55	1.46
9	g	677	PHE	CA-C	-7.02	1.43	1.52
3	a	834	ARG	C-N	7.01	1.43	1.33
8	f	77	LEU	C-N	7.01	1.42	1.33
9	g	1149	ASN	CA-C	-7.01	1.44	1.52
9	g	787	ASP	CA-C	-7.01	1.43	1.52
1	X	849	ASN	N-CA	-7.00	1.37	1.46
8	f	397	ASP	CA-C	-7.00	1.43	1.52
8	q	267	LEU	CA-C	-7.00	1.42	1.52
3	l	226	CYS	CA-C	-6.99	1.43	1.52
1	X	1603	SER	CA-C	-6.99	1.43	1.52
3	a	1012	SER	N-CA	6.99	1.55	1.46
9	g	594	LEU	N-CA	-6.99	1.38	1.46
7	p	10	ASP	CA-C	-6.98	1.43	1.52
3	l	569	ILE	C-N	6.98	1.42	1.33
3	l	871	HIS	ND1-CE1	6.98	1.39	1.32
7	e	104	LEU	CA-C	-6.98	1.45	1.53
3	l	589	ASN	CA-C	-6.98	1.45	1.52
3	l	890	ARG	CD-NE	6.97	1.56	1.46
8	q	53	LEU	CA-CB	6.97	1.65	1.53
1	X	278	SER	CA-C	-6.97	1.43	1.52
6	d	33	ILE	CA-CB	6.97	1.62	1.53
7	p	108	LYS	CA-C	-6.96	1.44	1.52
3	l	71	HIS	ND1-CE1	6.96	1.39	1.32
3	a	242	HIS	ND1-CE1	6.96	1.39	1.32
9	g	344	SER	C-N	6.96	1.44	1.33
8	q	180	PHE	C-N	6.95	1.43	1.34
9	r	650	LEU	C-N	6.95	1.43	1.33
7	p	151	THR	CA-C	-6.95	1.45	1.52
9	g	462	SER	CA-CB	6.94	1.64	1.53
3	a	104	GLN	CA-C	-6.94	1.43	1.52
4	m	236	GLY	N-CA	6.94	1.55	1.45
6	o	185	TRP	NE1-CE2	6.94	1.45	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1434	ASN	CA-C	-6.93	1.43	1.52
6	d	63	HIS	CA-CB	-6.93	1.43	1.53
5	n	509	ARG	N-CA	-6.93	1.37	1.46
5	n	596	ARG	NE-CZ	6.93	1.40	1.33
5	c	777	PRO	C-N	6.92	1.43	1.33
3	a	87	ALA	N-CA	-6.92	1.38	1.46
3	l	115	GLN	N-CA	-6.91	1.37	1.46
9	r	1137	ILE	CA-CB	6.91	1.63	1.54
3	l	242	HIS	ND1-CE1	6.91	1.39	1.32
9	r	329	GLY	C-N	-6.91	1.25	1.33
9	g	756	PHE	C-N	6.91	1.43	1.34
6	d	8	HIS	ND1-CE1	6.91	1.39	1.32
1	X	966	GLY	CA-C	-6.90	1.42	1.51
5	c	321	LEU	C-N	6.90	1.42	1.33
4	m	479	LYS	C-N	6.90	1.43	1.33
9	r	1127	ASN	CA-C	-6.90	1.44	1.52
9	g	1007	SER	CA-C	6.89	1.62	1.52
9	g	1135	SER	N-CA	-6.89	1.37	1.46
5	n	406	HIS	ND1-CE1	6.89	1.39	1.32
8	q	167	ASN	CA-CB	6.89	1.64	1.53
8	q	720	ARG	N-CA	-6.89	1.37	1.46
5	c	337	GLU	CA-CB	6.88	1.64	1.53
4	b	418	ALA	CA-C	-6.88	1.44	1.52
8	f	439	SER	CA-CB	6.88	1.62	1.53
5	c	428	ASN	CA-C	-6.88	1.43	1.52
9	r	105	VAL	N-CA	-6.88	1.38	1.46
7	e	144	ASP	CA-C	-6.87	1.44	1.52
4	m	363	TYR	N-CA	-6.87	1.36	1.46
6	o	227	GLN	CA-C	-6.87	1.42	1.52
8	f	705	PHE	C-N	6.87	1.43	1.33
5	c	214	SER	C-O	-6.87	1.14	1.24
3	l	785	ALA	C-N	-6.87	1.24	1.33
9	g	345	GLN	CA-C	-6.87	1.43	1.52
8	f	685	SER	N-CA	6.86	1.54	1.46
7	e	90	GLN	CA-CB	6.86	1.65	1.53
7	p	146	ARG	CA-C	-6.86	1.44	1.52
3	a	193	HIS	CE1-NE2	-6.86	1.25	1.32
7	p	35	VAL	CA-C	-6.85	1.45	1.52
6	o	242	PRO	CA-C	-6.85	1.44	1.52
4	m	481	LEU	CA-CB	6.85	1.63	1.53
3	l	271	ARG	CA-C	-6.84	1.43	1.52
1	X	995	LEU	C-N	6.84	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	g	91	ASP	C-N	6.84	1.43	1.33
4	m	486	ILE	CA-C	-6.84	1.44	1.52
9	g	672	LEU	C-N	6.84	1.42	1.34
3	a	595	ILE	CA-C	-6.83	1.45	1.52
6	o	203	HIS	ND1-CE1	6.83	1.39	1.32
9	r	511	PRO	CA-C	-6.83	1.42	1.52
5	c	369	LEU	N-CA	-6.82	1.37	1.46
5	c	545	LYS	CA-C	-6.82	1.43	1.52
3	a	422	ARG	CZ-NH1	6.82	1.42	1.32
3	l	630	THR	CA-C	6.82	1.61	1.52
9	g	254	LEU	CA-CB	6.82	1.62	1.53
3	l	5	SER	CA-C	-6.81	1.44	1.52
3	a	579	ILE	CB-CG1	6.81	1.67	1.53
4	m	641	ASP	C-N	6.81	1.44	1.33
9	r	497	HIS	ND1-CE1	6.81	1.39	1.32
4	m	672	TYR	CA-CB	6.81	1.62	1.53
6	d	63	HIS	ND1-CE1	6.80	1.39	1.32
6	o	195	VAL	CA-CB	-6.80	1.45	1.54
7	e	124	LYS	N-CA	-6.80	1.37	1.46
7	e	244	LYS	CA-CB	6.80	1.61	1.52
1	X	1543	VAL	N-CA	-6.79	1.38	1.46
7	e	161	PRO	N-CA	-6.79	1.39	1.47
5	c	180	GLN	CA-CB	6.79	1.62	1.53
3	a	735	LYS	CA-CB	6.79	1.64	1.53
5	n	240	LEU	C-N	6.79	1.43	1.33
8	q	168	VAL	C-O	-6.79	1.16	1.24
7	e	96	ARG	NE-CZ	6.79	1.40	1.33
8	f	383	PRO	C-N	6.78	1.42	1.33
8	q	301	TYR	CA-CB	6.78	1.64	1.53
1	X	913	ASN	CA-CB	6.77	1.63	1.53
3	a	230	HIS	C-N	6.77	1.43	1.33
3	a	878	HIS	ND1-CE1	6.77	1.39	1.32
5	n	581	LEU	CA-C	-6.77	1.45	1.53
9	r	874	PHE	C-N	6.77	1.41	1.33
5	n	214	SER	C-N	6.77	1.43	1.33
7	e	161	PRO	CA-CB	-6.77	1.44	1.53
4	m	613	ASP	CA-C	-6.77	1.43	1.52
3	l	481	HIS	ND1-CE1	6.76	1.39	1.32
4	m	676	LEU	C-N	6.76	1.42	1.33
3	a	257	TYR	CA-C	-6.76	1.44	1.52
8	f	112	ASP	CA-C	-6.76	1.44	1.52
9	g	660	SER	CA-C	-6.76	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	748	HIS	ND1-CE1	6.76	1.39	1.32
3	a	508	LYS	N-CA	-6.76	1.37	1.46
8	q	318	PRO	C-N	6.75	1.41	1.33
8	q	552	ARG	NE-CZ	6.75	1.40	1.33
3	l	893	HIS	C-N	6.75	1.46	1.34
8	f	583	GLU	C-N	6.75	1.42	1.33
4	m	339	ILE	C-N	6.75	1.42	1.33
4	m	612	LEU	CA-C	-6.75	1.46	1.53
7	e	316	GLY	CA-C	-6.74	1.44	1.51
9	r	982	GLU	C-N	6.74	1.42	1.33
9	r	1105	ASP	CA-C	-6.74	1.44	1.52
4	b	562	ALA	CA-CB	6.73	1.63	1.53
3	l	324	SER	CA-C	-6.73	1.43	1.52
4	b	649	LEU	N-CA	-6.73	1.38	1.46
4	m	242	THR	C-N	6.73	1.42	1.33
3	a	143	ASN	N-CA	-6.72	1.38	1.45
5	c	243	PRO	CA-C	6.72	1.59	1.52
7	e	329	ARG	CD-NE	6.72	1.55	1.46
4	b	86	ASP	CA-CB	6.72	1.64	1.53
5	n	190	LEU	C-N	6.72	1.43	1.34
8	f	660	THR	CA-C	6.72	1.60	1.52
9	g	230	PHE	CA-CB	6.72	1.61	1.53
5	c	497	LEU	N-CA	-6.71	1.37	1.46
9	r	642	PHE	CA-CB	6.71	1.62	1.53
5	n	228	SER	CA-C	-6.71	1.43	1.52
3	a	341	GLU	CA-C	-6.71	1.44	1.52
4	b	108	VAL	CA-CB	6.71	1.63	1.54
7	p	232	ALA	N-CA	-6.71	1.37	1.45
9	r	1144	LYS	C-N	6.71	1.43	1.33
3	a	845	ILE	N-CA	6.70	1.52	1.46
7	e	116	PHE	C-N	6.69	1.44	1.33
4	m	482	TRP	CA-CB	6.69	1.64	1.53
3	l	100	ALA	C-N	6.69	1.42	1.33
8	q	299	GLU	CA-CB	6.69	1.64	1.53
3	l	406	ARG	NE-CZ	6.69	1.40	1.33
1	X	639	PHE	C-O	-6.68	1.16	1.24
3	l	695	TYR	CA-C	-6.68	1.44	1.52
8	q	630	LEU	CA-C	-6.68	1.44	1.52
5	c	311	ILE	N-CA	-6.68	1.37	1.46
3	l	938	ARG	NE-CZ	6.68	1.40	1.33
5	c	583	SER	C-N	6.67	1.42	1.33
8	q	681	PRO	C-N	6.67	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	343	ASP	CA-C	-6.67	1.44	1.52
9	g	1038	ASN	C-N	6.67	1.42	1.33
7	p	184	ALA	CA-CB	6.67	1.62	1.53
9	r	751	TYR	CA-C	6.67	1.61	1.52
1	X	1073	LYS	CA-C	-6.67	1.44	1.52
3	a	517	ALA	CA-C	-6.67	1.44	1.52
5	c	393	GLN	CA-C	-6.67	1.43	1.52
1	X	322	HIS	C-N	6.66	1.43	1.33
1	X	368	ILE	CA-CB	6.66	1.63	1.54
4	b	510	HIS	CG-CD2	6.66	1.43	1.35
3	a	652	SER	CA-CB	6.66	1.63	1.53
5	n	331	ARG	C-N	6.66	1.42	1.33
9	r	833	GLU	C-N	6.66	1.42	1.33
9	r	546	ILE	C-N	6.66	1.41	1.33
7	p	310	VAL	CA-C	-6.66	1.44	1.52
1	X	943	VAL	C-O	-6.65	1.17	1.24
3	l	314	THR	CA-C	-6.65	1.44	1.52
3	l	133	LEU	CA-CB	6.65	1.61	1.53
8	q	178	HIS	ND1-CE1	6.65	1.39	1.32
3	a	599	LYS	CA-CB	6.65	1.62	1.53
5	c	324	TYR	CA-C	-6.64	1.45	1.53
3	a	953	LEU	CA-CB	6.64	1.63	1.53
4	b	526	CYS	N-CA	-6.64	1.37	1.46
4	b	95	ILE	CA-C	-6.63	1.47	1.53
3	l	615	SER	CA-C	6.63	1.62	1.52
1	X	768	ALA	N-CA	-6.63	1.38	1.46
7	p	97	ARG	NE-CZ	6.63	1.40	1.33
1	X	362	LEU	C-N	6.63	1.43	1.33
7	e	97	ARG	N-CA	-6.63	1.37	1.46
6	o	124	LYS	N-CA	-6.63	1.37	1.45
3	a	152	LEU	CA-CB	-6.62	1.43	1.53
1	X	186	LYS	C-O	-6.62	1.16	1.24
4	b	466	LEU	N-CA	-6.62	1.38	1.46
3	a	291	LEU	CA-C	-6.62	1.47	1.52
8	f	386	LEU	CA-CB	6.62	1.63	1.53
7	p	51	TRP	CA-C	-6.62	1.44	1.52
9	r	106	TYR	CA-C	-6.62	1.44	1.52
7	p	216	ARG	CA-C	-6.62	1.43	1.52
8	q	223	ILE	CA-C	6.62	1.61	1.52
4	b	690	THR	C-N	6.61	1.42	1.33
3	a	481	HIS	CG-ND1	6.61	1.45	1.38
8	q	629	GLU	CA-C	-6.61	1.44	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	452	ASP	CA-C	-6.61	1.44	1.52
7	p	20	TYR	CA-CB	6.61	1.64	1.53
8	f	318	PRO	C-N	6.61	1.42	1.33
5	c	464	VAL	N-CA	-6.60	1.38	1.46
5	n	161	THR	N-CA	-6.60	1.38	1.46
3	a	71	HIS	ND1-CE1	6.60	1.39	1.32
9	g	442	LYS	N-CA	6.60	1.54	1.46
1	X	912	TRP	N-CA	-6.60	1.37	1.46
3	a	407	GLY	N-CA	-6.60	1.37	1.45
8	f	649	TYR	CA-C	-6.60	1.43	1.52
3	a	148	GLU	CA-CB	6.59	1.63	1.53
1	X	421	PHE	CA-CB	6.59	1.64	1.53
3	a	125	ASP	N-CA	-6.59	1.38	1.46
7	e	166	GLN	CA-C	6.59	1.61	1.52
8	f	482	ARG	C-O	-6.59	1.15	1.23
3	l	1025	VAL	N-CA	6.59	1.52	1.46
8	f	523	TYR	N-CA	6.59	1.52	1.47
3	l	864	PHE	C-N	6.59	1.43	1.33
1	X	837	ASP	CA-C	-6.59	1.44	1.52
8	f	452	LEU	C-N	6.59	1.43	1.33
4	m	454	LEU	CA-C	-6.59	1.44	1.52
9	g	66	ARG	NE-CZ	6.58	1.40	1.33
8	f	109	LEU	CA-C	6.58	1.61	1.52
5	c	544	LEU	CA-C	-6.58	1.44	1.52
3	a	368	VAL	C-O	-6.58	1.17	1.24
5	c	519	ARG	CA-CB	6.58	1.65	1.53
4	m	345	LYS	C-N	6.58	1.42	1.34
9	r	1024	VAL	C-N	6.58	1.42	1.33
8	f	448	ILE	N-CA	-6.58	1.38	1.46
4	b	529	TRP	C-N	6.58	1.42	1.33
3	a	375	ASN	CA-CB	6.57	1.63	1.53
9	g	432	LYS	N-CA	-6.57	1.37	1.46
4	b	227	VAL	CA-CB	-6.57	1.46	1.54
3	a	439	ASP	N-CA	-6.57	1.37	1.45
9	g	390	ILE	N-CA	-6.57	1.38	1.46
8	q	271	ILE	N-CA	-6.57	1.40	1.47
8	q	423	GLN	C-O	6.56	1.31	1.24
1	X	663	MET	CA-C	-6.56	1.44	1.52
4	b	403	HIS	CG-CD2	6.56	1.43	1.35
6	o	171	ARG	CD-NE	6.56	1.55	1.46
8	q	229	ASN	CA-C	6.55	1.62	1.52
3	a	356	LYS	N-CA	-6.55	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	525	HIS	ND1-CE1	6.55	1.39	1.32
6	o	262	TRP	CA-C	-6.55	1.44	1.52
8	f	319	SER	C-N	6.55	1.41	1.33
9	r	666	LYS	CA-CB	6.55	1.63	1.53
3	l	237	LEU	CA-C	-6.55	1.44	1.52
3	a	792	THR	CA-C	-6.54	1.44	1.52
4	b	225	GLU	CA-CB	6.54	1.63	1.53
9	r	659	PRO	CA-C	-6.54	1.44	1.52
9	g	556	HIS	ND1-CE1	6.54	1.39	1.32
7	p	237	ASP	C-N	6.54	1.41	1.33
9	g	204	GLY	CA-C	-6.54	1.45	1.52
6	o	107	TRP	CA-C	-6.54	1.44	1.52
1	X	390	ILE	CA-C	6.54	1.58	1.52
8	f	725	SER	C-N	6.54	1.42	1.33
8	f	226	GLN	N-CA	-6.54	1.37	1.46
3	a	592	LYS	N-CA	-6.53	1.38	1.46
7	e	75	ALA	N-CA	-6.53	1.38	1.46
8	q	536	ARG	CA-CB	6.53	1.64	1.53
5	c	174	ARG	CA-C	-6.53	1.45	1.52
9	g	66	ARG	CA-C	-6.53	1.44	1.52
6	d	52	HIS	CB-CG	6.53	1.59	1.50
5	n	353	ASN	C-N	6.53	1.42	1.33
5	n	661	MET	N-CA	-6.53	1.38	1.46
3	a	635	LEU	C-N	6.53	1.42	1.33
9	g	1099	TYR	CA-C	-6.53	1.44	1.52
3	a	930	SER	N-CA	-6.52	1.39	1.46
4	b	680	LYS	C-O	-6.52	1.15	1.23
3	a	979	GLU	C-N	6.52	1.40	1.33
5	c	275	GLN	C-O	6.52	1.32	1.23
3	l	944	ILE	CA-CB	6.52	1.63	1.54
6	o	17	LEU	CA-C	-6.52	1.44	1.52
3	l	818	PRO	CA-CB	6.52	1.63	1.53
5	n	646	ASP	CA-C	6.51	1.61	1.52
1	X	1069	ILE	CA-CB	-6.51	1.45	1.54
3	a	195	GLU	CA-C	-6.51	1.45	1.52
1	X	1060	LEU	C-N	6.51	1.42	1.33
3	a	1009	SER	CA-C	-6.51	1.44	1.52
9	r	111	HIS	CA-CB	6.51	1.61	1.52
7	e	64	ALA	N-CA	-6.50	1.38	1.45
6	o	279	THR	C-N	6.50	1.42	1.33
5	c	289	ASN	C-N	6.50	1.43	1.34
4	m	611	ILE	C-N	6.50	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1042	SER	N-CA	6.50	1.54	1.46
5	n	499	ASP	CA-C	6.49	1.61	1.52
8	q	678	LEU	CA-C	-6.49	1.44	1.52
9	g	1087	LYS	CA-CB	6.49	1.62	1.53
3	a	256	ASP	CA-CB	6.49	1.62	1.53
1	X	1047	LEU	C-N	6.49	1.42	1.33
7	e	10	ASP	N-CA	-6.49	1.37	1.45
8	q	243	TRP	CZ2-CH2	6.49	1.49	1.37
5	n	176	PRO	N-CA	-6.48	1.39	1.47
7	e	107	SER	CA-C	-6.48	1.45	1.52
8	q	188	ILE	CA-CB	-6.48	1.45	1.54
8	q	575	GLU	N-CA	6.48	1.58	1.46
9	g	836	PHE	CA-CB	6.48	1.62	1.53
9	r	788	TRP	NE1-CE2	6.48	1.44	1.37
6	o	144	HIS	ND1-CE1	6.48	1.39	1.32
6	d	277	LYS	C-N	6.47	1.42	1.33
8	f	725	SER	CA-CB	6.47	1.64	1.53
5	n	441	ARG	N-CA	-6.47	1.37	1.45
9	r	1107	ASN	N-CA	-6.47	1.38	1.46
1	X	343	ASP	C-N	6.47	1.42	1.33
6	d	67	GLY	N-CA	-6.47	1.36	1.45
4	b	302	THR	C-N	6.47	1.43	1.33
9	r	1095	ILE	C-N	6.46	1.44	1.33
5	n	563	SER	CA-C	-6.46	1.46	1.53
1	X	1014	CYS	C-N	6.46	1.42	1.33
1	X	1646	ALA	C-N	6.46	1.41	1.33
1	X	728	ILE	N-CA	-6.46	1.38	1.46
3	a	66	GLU	CA-C	6.46	1.60	1.52
4	b	140	HIS	CB-CG	6.46	1.59	1.50
8	f	526	ALA	CA-C	-6.46	1.44	1.52
3	a	688	PHE	CA-CB	6.45	1.63	1.53
4	m	607	ILE	CA-C	6.45	1.58	1.52
5	n	659	ASN	CA-C	-6.45	1.44	1.52
1	X	301	ALA	CA-CB	6.45	1.63	1.53
4	b	456	SER	CA-C	-6.45	1.44	1.52
8	f	240	HIS	ND1-CE1	6.45	1.39	1.32
3	l	361	SER	CA-CB	6.45	1.64	1.53
3	l	541	PRO	CA-CB	6.45	1.62	1.53
8	f	440	ASP	CA-C	-6.45	1.44	1.52
4	b	215	SER	CA-C	-6.45	1.43	1.52
1	X	1345	SER	CA-C	-6.44	1.44	1.52
4	b	725	ALA	CA-CB	-6.44	1.46	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	n	558	ASN	CA-CB	6.44	1.63	1.53
3	l	911	GLU	CA-CB	6.44	1.64	1.53
7	e	77	TYR	C-N	6.44	1.42	1.33
1	X	1390	SER	CA-CB	6.43	1.63	1.53
5	c	217	PHE	C-N	6.43	1.42	1.33
3	a	966	CYS	CA-C	-6.43	1.44	1.53
5	n	379	PHE	C-N	6.43	1.42	1.33
6	o	80	LEU	CA-C	6.42	1.60	1.52
6	o	110	HIS	CB-CG	6.42	1.59	1.50
5	c	294	ILE	N-CA	-6.42	1.39	1.46
5	n	627	ASN	C-N	6.42	1.42	1.33
1	X	869	LYS	C-N	-6.42	1.26	1.34
6	o	51	GLY	C-N	6.42	1.41	1.33
1	X	1513	LYS	C-N	6.42	1.40	1.33
8	f	651	ILE	CA-C	-6.41	1.46	1.53
3	a	313	TYR	N-CA	-6.41	1.38	1.46
7	e	321	SER	CA-C	-6.41	1.46	1.53
8	f	172	LYS	CA-CB	6.41	1.64	1.53
5	n	222	ASP	CA-C	-6.41	1.44	1.52
9	g	151	LEU	CA-C	-6.41	1.44	1.52
4	m	620	MET	CG-SD	6.41	1.96	1.80
6	d	204	SER	CA-CB	6.41	1.64	1.53
3	a	458	ASN	N-CA	-6.41	1.38	1.46
1	X	1233	PHE	C-N	6.40	1.43	1.33
5	c	221	LEU	N-CA	-6.40	1.38	1.46
7	e	311	SER	N-CA	-6.40	1.38	1.45
8	f	235	GLN	N-CA	6.40	1.53	1.46
9	r	573	LYS	CA-C	6.40	1.61	1.52
8	f	317	LEU	CA-CB	6.40	1.62	1.53
1	X	1050	SER	N-CA	-6.39	1.38	1.46
1	X	1052	LYS	N-CA	-6.39	1.38	1.46
1	X	664	LEU	CA-CB	6.39	1.64	1.53
6	d	214	PRO	CA-C	-6.39	1.47	1.53
3	l	14	TYR	N-CA	-6.39	1.38	1.46
4	b	513	PHE	CA-CB	6.39	1.64	1.53
3	l	289	THR	CA-C	-6.38	1.44	1.53
1	X	1436	GLU	CA-C	-6.38	1.45	1.52
6	d	268	VAL	CA-C	-6.38	1.45	1.52
3	a	808	TRP	CA-C	-6.38	1.44	1.52
3	l	278	GLU	C-N	6.38	1.43	1.33
3	a	1027	LEU	C-N	6.38	1.42	1.33
4	b	525	ILE	N-CA	-6.38	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	317	HIS	ND1-CE1	6.38	1.39	1.32
5	c	199	ILE	N-CA	6.37	1.54	1.46
8	f	223	ILE	CA-C	-6.37	1.46	1.52
9	g	288	ASN	CA-C	6.37	1.61	1.52
3	l	256	ASP	C-N	6.37	1.42	1.33
9	g	724	ASP	CA-CB	6.37	1.63	1.53
5	n	423	GLN	N-CA	-6.37	1.38	1.46
9	r	556	HIS	ND1-CE1	6.36	1.39	1.32
3	a	782	TYR	CA-CB	6.36	1.61	1.52
3	a	930	SER	CA-C	-6.36	1.44	1.53
8	f	185	TYR	CA-CB	6.36	1.63	1.53
8	q	383	PRO	N-CA	-6.36	1.39	1.47
9	g	1134	HIS	CE1-NE2	-6.36	1.26	1.32
7	p	292	LEU	N-CA	-6.36	1.37	1.45
8	f	229	ASN	CA-CB	6.35	1.62	1.54
4	m	522	MET	C-O	-6.34	1.15	1.24
3	a	964	LEU	C-N	6.34	1.42	1.33
8	f	714	TYR	CA-CB	6.34	1.63	1.53
9	g	227	ARG	NE-CZ	6.34	1.40	1.33
9	g	423	ALA	CA-C	-6.34	1.44	1.52
1	X	1255	ILE	CA-C	-6.34	1.44	1.52
4	b	654	GLU	CA-C	-6.34	1.46	1.53
4	b	678	ASP	CA-C	-6.33	1.44	1.52
4	b	528	GLU	N-CA	-6.33	1.38	1.46
8	f	630	LEU	C-N	6.33	1.40	1.33
9	g	561	LYS	CA-CB	6.33	1.63	1.53
7	e	25	ALA	CA-CB	6.33	1.61	1.52
3	l	968	ARG	NE-CZ	6.33	1.40	1.33
4	b	609	GLN	N-CA	-6.33	1.38	1.46
5	c	594	THR	CA-C	6.33	1.61	1.52
7	e	142	PRO	N-CA	-6.33	1.39	1.47
5	n	278	PRO	C-N	6.33	1.42	1.34
1	X	417	THR	CA-CB	6.32	1.64	1.53
3	l	122	ILE	CA-C	-6.32	1.45	1.52
7	p	292	LEU	CA-C	-6.32	1.45	1.52
1	X	1429	HIS	CA-CB	6.32	1.64	1.53
6	d	80	LEU	C-N	6.32	1.42	1.33
8	f	466	ASN	C-N	6.32	1.43	1.33
3	l	345	GLU	CA-CB	6.31	1.63	1.53
4	b	549	ALA	CA-CB	6.31	1.57	1.53
5	c	511	VAL	N-CA	-6.31	1.38	1.46
4	m	732	ARG	NE-CZ	6.31	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	869	HIS	CB-CG	6.30	1.58	1.50
9	g	440	ARG	CA-C	-6.30	1.44	1.53
1	X	1605	PHE	CA-CB	6.30	1.63	1.53
8	q	616	LEU	C-N	6.30	1.41	1.33
9	g	456	ILE	CA-CB	6.30	1.62	1.54
9	r	502	VAL	C-N	6.30	1.42	1.33
4	m	243	GLN	CA-C	-6.30	1.44	1.52
5	n	260	LEU	C-O	-6.30	1.16	1.24
6	o	20	TYR	CA-C	-6.30	1.43	1.52
7	e	295	GLU	CA-C	-6.30	1.45	1.52
9	g	1074	ASN	CA-C	-6.30	1.45	1.52
7	e	303	HIS	N-CA	-6.29	1.38	1.46
3	l	319	ILE	CA-C	-6.29	1.47	1.52
4	m	319	SER	N-CA	-6.29	1.38	1.46
8	q	705	PHE	CA-C	-6.29	1.45	1.52
4	b	717	ASP	CA-C	-6.29	1.46	1.52
9	g	395	PHE	C-O	-6.29	1.16	1.24
3	a	181	GLY	CA-C	-6.29	1.43	1.51
7	p	206	ALA	N-CA	-6.29	1.38	1.46
9	g	525	GLU	CA-CB	6.29	1.63	1.53
3	l	551	THR	C-N	6.29	1.42	1.33
3	a	968	ARG	NE-CZ	6.28	1.40	1.33
7	e	292	LEU	CB-CG	6.28	1.66	1.53
3	l	706	ASN	CA-C	6.28	1.60	1.52
3	a	628	ARG	NE-CZ	6.28	1.40	1.33
3	a	958	TRP	NE1-CE2	-6.28	1.30	1.37
9	r	528	GLU	C-N	6.28	1.42	1.33
5	n	449	PHE	CA-CB	6.27	1.63	1.53
9	g	1109	ILE	CA-CB	6.27	1.62	1.54
3	l	422	ARG	NE-CZ	6.27	1.40	1.33
3	a	18	PRO	C-O	-6.27	1.16	1.24
9	g	122	VAL	CA-CB	-6.27	1.47	1.53
3	a	279	TYR	CA-C	6.27	1.61	1.52
7	e	151	THR	C-N	6.27	1.41	1.33
4	b	400	GLY	C-N	6.26	1.41	1.33
4	m	352	THR	N-CA	6.26	1.53	1.46
8	q	514	VAL	CA-C	6.26	1.60	1.53
8	f	62	VAL	CA-CB	-6.26	1.46	1.54
9	g	1083	LEU	N-CA	-6.26	1.38	1.46
6	o	229	ARG	CA-CB	6.26	1.62	1.53
3	a	1033	GLU	N-CA	-6.26	1.38	1.46
9	g	131	GLU	N-CA	-6.26	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	l	329	TRP	C-N	6.26	1.41	1.33
3	a	105	ARG	CZ-NH1	6.26	1.41	1.32
7	p	303	HIS	ND1-CE1	6.26	1.38	1.32
9	r	741	GLY	CA-C	-6.25	1.45	1.52
4	b	214	ARG	CD-NE	6.25	1.55	1.46
6	o	24	LEU	CA-C	-6.25	1.44	1.52
9	r	714	TYR	CA-C	-6.25	1.44	1.52
1	X	1553	GLN	C-O	-6.25	1.16	1.24
9	g	289	LYS	CA-C	-6.25	1.44	1.52
9	g	1102	PHE	CA-C	6.25	1.58	1.52
4	b	179	LEU	CA-CB	6.25	1.63	1.53
4	b	209	LEU	CA-CB	6.25	1.63	1.53
4	b	246	TRP	CA-CB	6.25	1.61	1.53
5	c	446	ASP	CA-CB	6.25	1.63	1.53
8	f	660	THR	C-N	6.25	1.41	1.34
9	g	519	GLU	N-CA	-6.25	1.38	1.46
9	g	851	LEU	CA-CB	6.24	1.61	1.53
4	m	83	THR	CA-C	6.24	1.60	1.53
8	q	308	VAL	CA-CB	-6.24	1.47	1.54
7	e	87	ASP	C-N	6.24	1.39	1.33
9	g	754	ASN	CA-C	-6.23	1.45	1.52
8	q	240	HIS	CA-C	-6.23	1.44	1.52
5	c	454	ILE	CA-CB	-6.23	1.47	1.54
7	e	120	HIS	CA-C	-6.23	1.44	1.52
1	X	1167	LEU	CA-CB	6.22	1.63	1.53
3	a	411	LEU	CA-CB	6.22	1.63	1.53
9	r	644	VAL	CA-CB	-6.22	1.47	1.54
9	g	172	ALA	N-CA	6.22	1.54	1.46
5	n	288	SER	C-N	6.22	1.41	1.33
8	q	164	GLU	N-CA	-6.22	1.38	1.46
1	X	1593	HIS	N-CA	6.22	1.58	1.46
3	a	59	CYS	CA-C	-6.22	1.45	1.53
6	d	135	THR	CA-C	-6.22	1.45	1.52
7	e	202	LEU	N-CA	-6.22	1.38	1.45
3	l	117	LEU	N-CA	-6.22	1.38	1.46
8	q	609	SER	CA-C	-6.22	1.45	1.52
1	X	162	HIS	ND1-CE1	6.21	1.38	1.32
3	a	150	PHE	CA-C	-6.21	1.45	1.52
3	l	153	GLN	C-N	6.21	1.39	1.33
6	d	221	TYR	CA-C	-6.21	1.45	1.52
3	l	1018	ILE	CA-CB	-6.21	1.48	1.54
3	a	204	TYR	CA-CB	6.21	1.63	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	181	VAL	CA-CB	-6.21	1.45	1.54
4	m	122	ARG	NE-CZ	6.21	1.39	1.33
7	e	124	LYS	CA-CB	6.21	1.64	1.53
4	m	680	LYS	N-CA	-6.20	1.38	1.46
5	n	779	LYS	N-CA	-6.20	1.38	1.46
9	r	875	PHE	CA-CB	6.20	1.57	1.53
9	g	1052	ASN	CA-C	-6.20	1.45	1.52
3	l	600	ASP	CA-C	-6.20	1.44	1.52
4	m	98	LEU	CA-CB	6.20	1.64	1.53
8	q	51	LEU	C-N	6.20	1.42	1.33
1	X	1233	PHE	CA-CB	6.20	1.63	1.53
4	m	647	ARG	CD-NE	6.20	1.54	1.46
1	X	1264	SER	C-N	6.20	1.42	1.33
8	f	61	ASN	N-CA	-6.20	1.37	1.46
9	g	525	GLU	N-CA	6.20	1.53	1.46
5	n	651	CYS	C-N	6.20	1.41	1.33
3	l	883	GLU	CA-CB	6.19	1.61	1.53
3	a	214	ARG	N-CA	-6.19	1.38	1.46
3	a	865	LYS	C-N	6.19	1.41	1.33
9	g	743	LEU	CA-CB	6.19	1.61	1.53
3	a	605	ILE	N-CA	-6.19	1.39	1.46
3	l	53	GLY	N-CA	6.19	1.55	1.45
3	l	134	PRO	CA-C	-6.18	1.45	1.52
7	p	160	PRO	CA-C	-6.18	1.46	1.52
8	q	138	ASN	N-CA	-6.18	1.38	1.46
6	o	243	TRP	CA-CB	6.18	1.62	1.52
7	e	131	ASP	CA-CB	6.18	1.63	1.53
9	g	988	VAL	CA-CB	-6.18	1.47	1.54
5	n	459	PHE	CA-CB	6.18	1.64	1.53
4	b	193	ASP	CA-C	-6.18	1.44	1.52
9	g	221	LEU	CA-C	-6.18	1.45	1.53
1	X	162	HIS	CB-CG	6.17	1.58	1.50
1	X	718	PHE	C-N	6.17	1.41	1.33
1	X	369	LEU	N-CA	-6.17	1.38	1.45
1	X	1402	LYS	CA-C	-6.17	1.44	1.52
3	a	81	PHE	CA-C	-6.17	1.45	1.52
3	a	978	ALA	C-N	6.16	1.42	1.33
5	c	444	ALA	N-CA	-6.16	1.40	1.46
6	d	241	GLY	C-N	6.16	1.41	1.33
9	r	1043	ARG	NE-CZ	6.16	1.39	1.33
7	p	75	ALA	C-N	6.16	1.40	1.33
4	b	50	PRO	CA-C	6.16	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	966	LYS	CA-C	-6.16	1.45	1.52
4	m	452	GLU	CA-C	-6.16	1.45	1.52
9	r	1057	LEU	N-CA	-6.15	1.39	1.46
1	X	1194	LEU	N-CA	-6.15	1.39	1.46
7	p	96	ARG	CA-C	-6.15	1.45	1.53
1	X	182	PHE	N-CA	-6.15	1.38	1.46
9	g	652	HIS	ND1-CE1	6.15	1.38	1.32
3	l	338	ARG	CA-CB	6.15	1.62	1.53
8	q	510	LEU	CA-C	-6.15	1.44	1.52
4	b	375	LEU	CB-CG	6.15	1.65	1.53
8	q	418	SER	CA-CB	6.15	1.63	1.53
3	l	210	ARG	NE-CZ	6.14	1.39	1.33
8	q	120	TRP	NE1-CE2	-6.14	1.30	1.37
1	X	650	ASP	C-N	6.14	1.42	1.33
8	f	539	LEU	N-CA	-6.14	1.37	1.46
1	X	711	LEU	CA-CB	6.14	1.62	1.53
4	m	144	VAL	N-CA	-6.14	1.38	1.46
3	a	597	TRP	CA-C	-6.14	1.45	1.52
6	o	63	HIS	CA-C	6.13	1.59	1.53
1	X	1181	THR	C-N	6.13	1.42	1.33
7	e	35	VAL	N-CA	-6.13	1.39	1.46
4	m	87	LYS	CA-C	-6.13	1.45	1.52
6	d	173	PHE	C-N	6.13	1.40	1.33
4	m	597	LYS	C-N	6.13	1.42	1.33
8	q	285	ASP	C-N	6.13	1.42	1.33
9	r	1060	HIS	C-N	6.13	1.41	1.33
3	l	215	SER	CA-CB	6.12	1.63	1.53
4	b	634	TYR	CA-C	-6.12	1.44	1.52
8	f	197	LEU	N-CA	-6.12	1.39	1.46
9	g	320	LEU	N-CA	6.12	1.53	1.46
9	g	1060	HIS	C-N	6.12	1.41	1.33
3	l	116	GLN	N-CA	-6.12	1.38	1.46
9	r	591	PHE	CA-C	-6.12	1.44	1.52
9	r	1069	GLU	CA-C	-6.12	1.47	1.53
8	f	699	ASP	CA-CB	6.12	1.62	1.54
8	q	601	GLN	CA-CB	6.12	1.63	1.53
4	m	506	GLU	N-CA	-6.12	1.39	1.46
8	f	326	GLU	CA-C	-6.12	1.44	1.52
4	b	550	HIS	CA-CB	6.11	1.63	1.53
5	n	602	PHE	CA-C	-6.11	1.44	1.52
7	p	23	HIS	ND1-CE1	6.11	1.38	1.32
8	q	554	ASN	CA-CB	6.11	1.63	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	280	THR	C-N	6.11	1.42	1.33
7	p	224	ILE	N-CA	-6.11	1.39	1.46
4	b	645	ALA	CA-C	-6.11	1.44	1.52
3	a	578	ASP	CA-CB	6.11	1.60	1.52
5	c	613	SER	N-CA	-6.11	1.40	1.46
6	o	244	LYS	CA-CB	6.11	1.61	1.53
1	X	683	ASP	N-CA	6.11	1.53	1.46
5	c	244	VAL	C-O	6.11	1.31	1.24
9	g	359	THR	N-CA	6.11	1.53	1.46
7	e	310	VAL	C-N	6.10	1.41	1.33
4	b	683	MET	C-N	6.10	1.42	1.33
9	r	646	PHE	CA-CB	6.10	1.62	1.53
9	g	442	LYS	C-N	6.10	1.42	1.33
5	n	607	ARG	NE-CZ	6.10	1.39	1.33
8	f	381	ASP	N-CA	-6.10	1.39	1.46
3	l	945	VAL	CA-CB	-6.10	1.46	1.54
9	g	74	THR	N-CA	-6.09	1.38	1.46
9	g	918	SER	N-CA	6.09	1.54	1.46
3	l	410	ASN	CA-CB	6.09	1.62	1.53
3	a	10	ASN	CA-C	-6.09	1.45	1.52
3	a	252	THR	N-CA	-6.09	1.38	1.45
3	a	84	LEU	CA-C	-6.09	1.44	1.52
1	X	1414	GLU	C-O	6.09	1.31	1.24
3	a	509	TYR	CA-C	-6.09	1.45	1.52
3	l	903	ASN	CA-CB	6.08	1.62	1.53
5	n	295	PHE	CA-CB	6.08	1.62	1.53
9	r	723	PHE	CA-CB	6.08	1.62	1.53
9	r	1044	ARG	C-N	6.08	1.41	1.33
5	c	336	ALA	C-N	6.08	1.42	1.33
3	l	322	ASN	CA-CB	6.08	1.63	1.53
4	m	287	ASP	CA-CB	6.08	1.64	1.53
5	n	202	ARG	CD-NE	6.08	1.54	1.46
6	o	281	TRP	C-N	6.08	1.41	1.33
5	c	155	THR	CA-C	-6.08	1.44	1.52
9	g	450	ARG	NE-CZ	6.07	1.39	1.33
8	f	275	GLU	CA-CB	6.07	1.61	1.53
8	f	636	VAL	N-CA	-6.07	1.39	1.46
4	m	221	GLU	CA-C	-6.07	1.44	1.52
9	g	1037	LEU	C-N	6.07	1.41	1.33
8	q	315	LEU	CA-CB	6.07	1.62	1.53
9	g	72	LEU	CA-CB	6.07	1.63	1.53
9	g	104	LYS	N-CA	-6.06	1.38	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	g	619	SER	CA-CB	6.06	1.62	1.53
4	m	605	VAL	C-N	6.06	1.41	1.33
5	c	320	VAL	C-O	6.06	1.30	1.23
7	p	190	GLN	CA-CB	6.06	1.62	1.53
3	a	213	SER	C-N	6.05	1.41	1.33
7	e	103	THR	N-CA	-6.05	1.39	1.46
7	e	150	LEU	CA-C	-6.05	1.44	1.52
4	m	594	ILE	CB-CG1	6.05	1.65	1.53
8	q	178	HIS	CB-CG	6.05	1.58	1.50
8	q	443	GLU	CA-CB	6.05	1.63	1.53
1	X	184	ASP	C-N	6.05	1.41	1.33
3	l	230	HIS	ND1-CE1	6.05	1.38	1.32
1	X	1553	GLN	N-CA	-6.05	1.39	1.46
4	b	520	GLU	N-CA	-6.05	1.38	1.46
6	d	90	SER	CA-C	-6.05	1.45	1.52
4	m	82	ILE	N-CA	-6.05	1.39	1.46
8	q	303	LEU	CA-C	6.05	1.61	1.52
3	a	404	VAL	CA-CB	-6.05	1.47	1.54
8	f	147	SER	CA-C	-6.04	1.45	1.52
9	g	722	PHE	CA-C	-6.04	1.44	1.52
5	n	266	CYS	C-N	6.04	1.42	1.34
1	X	302	LEU	CA-C	6.04	1.60	1.53
1	X	337	SER	CA-CB	6.04	1.62	1.53
3	a	994	ILE	CA-C	-6.04	1.45	1.52
8	f	655	ILE	N-CA	6.04	1.54	1.46
9	g	918	SER	CA-C	6.04	1.61	1.52
4	m	690	THR	C-N	6.04	1.41	1.33
6	d	204	SER	C-N	6.04	1.41	1.33
3	l	485	LYS	CA-C	-6.04	1.45	1.52
3	l	108	LEU	CA-C	-6.04	1.45	1.52
3	a	93	ILE	CA-C	-6.04	1.45	1.52
9	g	224	ASN	CA-C	-6.04	1.43	1.52
7	p	53	ALA	CA-C	-6.04	1.44	1.52
3	a	969	MET	CA-C	-6.03	1.44	1.52
4	b	511	TYR	N-CA	-6.03	1.41	1.46
1	X	1309	ARG	CD-NE	6.03	1.54	1.46
8	f	12	PHE	N-CA	-6.03	1.38	1.46
3	a	155	PRO	CA-CB	6.03	1.62	1.53
6	d	52	HIS	ND1-CE1	6.03	1.38	1.32
4	b	585	LYS	CA-CB	6.03	1.60	1.52
7	e	61	ILE	CA-C	-6.03	1.45	1.52
8	f	244	ARG	NE-CZ	6.03	1.39	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	179	LEU	CA-C	-6.03	1.45	1.52
4	m	419	PHE	C-N	6.03	1.41	1.33
3	a	939	THR	C-O	-6.02	1.17	1.24
7	e	165	LEU	CA-C	6.02	1.60	1.52
4	m	339	ILE	N-CA	-6.02	1.39	1.46
5	n	303	VAL	CA-C	-6.02	1.46	1.52
3	a	393	HIS	ND1-CE1	6.02	1.38	1.32
4	b	145	ASN	CA-CB	6.02	1.62	1.53
9	g	672	LEU	N-CA	-6.02	1.39	1.46
9	g	1055	ASP	CA-C	-6.02	1.44	1.52
4	m	640	GLU	CA-C	-6.02	1.45	1.52
6	o	253	PHE	C-N	6.02	1.41	1.33
8	q	285	ASP	CA-C	-6.02	1.45	1.52
7	p	192	ILE	C-N	6.01	1.39	1.33
9	g	398	LYS	CA-C	-6.01	1.45	1.52
1	X	376	THR	CA-C	-6.01	1.43	1.52
3	a	118	LEU	N-CA	-6.01	1.39	1.46
4	m	714	ILE	C-N	6.01	1.42	1.33
1	X	952	LEU	C-O	-6.01	1.16	1.24
8	q	289	HIS	N-CA	-6.01	1.39	1.46
3	l	473	VAL	N-CA	-6.01	1.38	1.46
8	f	638	LEU	C-N	6.01	1.41	1.33
3	l	351	LEU	CA-CB	6.01	1.60	1.52
8	q	679	LYS	N-CA	-6.01	1.39	1.46
5	c	261	LYS	N-CA	-6.00	1.39	1.46
8	f	19	LEU	CA-C	-6.00	1.45	1.53
8	q	422	LEU	CA-CB	6.00	1.63	1.53
7	p	223	SER	CA-CB	6.00	1.61	1.53
8	q	118	GLN	CA-CB	6.00	1.62	1.53
9	g	98	LEU	CA-C	-6.00	1.45	1.52
3	l	1018	ILE	CA-C	-6.00	1.44	1.53
4	m	347	LEU	CA-C	-6.00	1.45	1.53
8	f	383	PRO	N-CA	-6.00	1.39	1.47
7	e	40	LYS	C-N	5.99	1.42	1.33
9	g	636	ILE	CA-CB	5.99	1.61	1.54
3	l	942	ILE	C-N	5.99	1.42	1.33
8	q	703	LEU	CA-C	-5.99	1.44	1.52
4	m	276	ASP	CA-CB	5.99	1.63	1.53
4	m	70	LYS	CA-C	-5.99	1.45	1.52
1	X	1228	ASP	CA-C	-5.99	1.44	1.52
8	f	723	THR	C-N	5.99	1.41	1.33
9	g	97	GLY	CA-C	-5.99	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	d	242	PRO	CA-C	-5.99	1.47	1.53
1	X	1620	THR	CA-C	-5.98	1.45	1.53
7	e	211	HIS	CA-C	-5.98	1.45	1.52
9	g	1060	HIS	CG-CD2	5.98	1.42	1.35
4	m	215	SER	N-CA	-5.98	1.40	1.46
9	g	560	ARG	CD-NE	5.98	1.54	1.46
4	b	402	ILE	CA-C	-5.98	1.45	1.52
5	n	611	SER	CA-C	-5.98	1.44	1.52
3	a	28	VAL	C-N	5.97	1.41	1.33
3	a	351	LEU	N-CA	-5.97	1.38	1.46
3	a	493	TRP	NE1-CE2	-5.97	1.30	1.37
3	l	380	GLU	CA-CB	5.97	1.63	1.53
7	p	194	TYR	CZ-OH	5.97	1.50	1.38
3	l	331	ILE	C-O	-5.97	1.15	1.23
8	q	235	GLN	N-CA	-5.97	1.38	1.45
5	c	466	SER	CA-CB	5.96	1.63	1.53
9	r	519	GLU	N-CA	-5.96	1.38	1.46
9	g	1043	ARG	CZ-NH1	5.96	1.41	1.32
8	q	412	LEU	CA-CB	5.96	1.63	1.53
9	g	271	ARG	CA-C	-5.96	1.45	1.52
9	g	559	VAL	CA-C	-5.96	1.43	1.52
4	m	720	LEU	CA-C	-5.96	1.45	1.52
7	e	195	GLN	CA-C	-5.96	1.45	1.52
9	r	998	ASN	CA-CB	5.96	1.61	1.53
4	m	564	LYS	C-N	5.96	1.40	1.33
5	c	341	GLN	CA-C	-5.95	1.44	1.52
5	n	439	ARG	CA-C	5.95	1.61	1.52
7	p	87	ASP	C-N	-5.95	1.28	1.33
9	r	645	ILE	CA-CB	5.95	1.62	1.54
3	a	809	LYS	CA-CB	5.95	1.64	1.53
3	a	867	LYS	CA-CB	5.95	1.62	1.53
9	g	363	LEU	CA-CB	5.95	1.60	1.52
9	g	129	ASN	CA-C	-5.95	1.46	1.53
3	l	2	ALA	CA-C	5.95	1.59	1.52
4	b	511	TYR	CA-CB	5.95	1.61	1.53
9	g	93	GLN	CA-CB	5.95	1.63	1.53
5	n	581	LEU	C-N	5.95	1.42	1.33
3	a	860	GLU	N-CA	-5.95	1.39	1.46
5	c	493	VAL	CA-CB	-5.95	1.45	1.54
9	r	885	VAL	CA-CB	-5.95	1.47	1.54
9	g	549	MET	CA-C	-5.94	1.44	1.52
9	g	1100	GLY	C-N	5.94	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	512	ILE	CA-C	-5.94	1.45	1.52
4	m	109	SER	CA-CB	5.94	1.62	1.53
5	n	151	ALA	C-N	5.94	1.41	1.33
4	m	224	ILE	N-CA	-5.94	1.39	1.46
4	b	195	GLN	CA-C	-5.94	1.45	1.53
8	f	611	SER	C-N	5.94	1.42	1.33
3	l	592	LYS	CA-CB	5.94	1.60	1.53
1	X	714	LEU	C-N	5.93	1.41	1.33
3	a	210	ARG	NE-CZ	5.93	1.39	1.33
8	f	67	ASP	CA-CB	5.93	1.62	1.53
8	f	199	GLU	CA-C	-5.93	1.45	1.52
8	q	117	TYR	CA-CB	5.93	1.62	1.53
8	q	446	SER	CA-CB	5.93	1.62	1.53
3	a	143	ASN	CA-C	-5.93	1.45	1.52
9	g	515	ASN	N-CA	-5.93	1.38	1.46
3	l	893	HIS	CA-C	-5.93	1.44	1.52
6	o	57	TRP	CA-C	-5.93	1.47	1.53
3	a	174	SER	CA-C	-5.92	1.45	1.53
5	n	269	THR	CA-C	-5.92	1.44	1.52
9	g	318	GLU	C-N	5.92	1.42	1.33
9	g	1020	ARG	CD-NE	5.92	1.54	1.46
8	q	185	TYR	CA-CB	5.92	1.63	1.53
1	X	134	ARG	CA-C	5.92	1.60	1.52
6	d	104	SER	C-N	5.92	1.41	1.33
8	q	656	ARG	CA-C	-5.92	1.45	1.52
8	q	168	VAL	CA-C	-5.92	1.45	1.52
3	l	821	HIS	ND1-CE1	5.92	1.38	1.32
1	X	763	GLN	CA-C	5.92	1.59	1.52
8	f	636	VAL	CA-CB	-5.91	1.49	1.55
3	l	195	GLU	CA-C	-5.91	1.46	1.52
8	q	454	ASP	CA-C	-5.91	1.46	1.53
9	g	895	SER	CA-C	-5.91	1.45	1.52
3	l	972	LYS	CA-C	-5.91	1.44	1.52
3	l	1035	ARG	CZ-NH1	5.91	1.41	1.32
3	a	25	ASP	CA-CB	5.91	1.60	1.53
7	e	243	PHE	N-CA	-5.91	1.39	1.46
4	b	585	LYS	C-N	5.91	1.42	1.33
3	l	64	ASN	N-CA	5.91	1.53	1.46
4	m	592	ASN	CA-C	-5.91	1.47	1.53
9	r	919	GLU	N-CA	-5.91	1.38	1.46
9	r	1102	PHE	CA-C	-5.91	1.46	1.53
5	c	243	PRO	C-N	5.91	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	507	ILE	N-CA	-5.91	1.39	1.46
8	f	668	HIS	N-CA	-5.91	1.38	1.46
5	n	572	ILE	CA-CB	5.91	1.61	1.54
9	r	1043	ARG	CA-C	-5.91	1.45	1.52
5	c	286	ASN	C-N	5.90	1.41	1.33
8	f	49	LEU	N-CA	5.90	1.53	1.46
7	p	167	SER	CA-C	-5.90	1.45	1.52
6	d	238	ASN	CA-CB	5.90	1.66	1.54
3	l	15	TYR	N-CA	-5.90	1.39	1.46
3	l	150	PHE	CA-CB	5.90	1.62	1.53
8	f	391	HIS	ND1-CE1	5.90	1.38	1.32
6	o	142	ASP	CA-CB	5.90	1.61	1.53
6	d	270	ALA	CA-C	-5.90	1.45	1.52
3	l	656	ASP	C-N	5.90	1.41	1.33
3	l	423	ALA	CA-C	-5.89	1.44	1.52
9	r	1061	ILE	CA-C	-5.89	1.44	1.52
6	d	55	PRO	N-CA	-5.89	1.39	1.47
6	d	57	TRP	CA-C	-5.89	1.47	1.52
8	f	320	HIS	CB-CG	5.89	1.58	1.50
3	l	369	ASN	CA-C	-5.89	1.44	1.52
9	r	720	GLN	C-N	5.89	1.42	1.34
4	b	375	LEU	CA-CB	5.89	1.63	1.53
1	X	1338	GLU	C-N	5.89	1.41	1.33
1	X	1513	LYS	CA-C	-5.89	1.44	1.52
4	m	598	ASN	CA-C	-5.89	1.44	1.52
9	r	801	CYS	N-CA	-5.89	1.39	1.46
3	a	414	ARG	CD-NE	5.88	1.54	1.46
7	e	289	GLN	CA-C	5.88	1.60	1.52
8	f	114	LYS	CA-CB	5.88	1.63	1.53
9	r	865	PRO	N-CA	-5.88	1.39	1.47
9	r	1072	LYS	CA-C	-5.88	1.45	1.52
9	g	275	ILE	CA-CB	-5.88	1.46	1.54
5	n	313	SER	C-N	5.88	1.42	1.33
3	a	475	CYS	C-N	5.88	1.41	1.33
4	m	190	PHE	CA-C	-5.88	1.46	1.53
1	X	364	THR	CA-C	-5.87	1.45	1.53
9	r	944	LEU	C-N	5.87	1.41	1.33
7	e	193	ILE	N-CA	-5.87	1.38	1.46
9	g	593	ILE	N-CA	-5.87	1.39	1.46
9	g	762	THR	N-CA	-5.87	1.39	1.46
7	p	97	ARG	CD-NE	5.87	1.54	1.46
8	q	404	VAL	N-CA	-5.87	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	830	SER	C-N	5.87	1.42	1.33
1	X	733	ARG	CA-C	-5.87	1.44	1.52
9	g	203	SER	N-CA	-5.87	1.38	1.46
3	a	352	ILE	CA-C	-5.87	1.47	1.52
5	c	244	VAL	C-N	5.87	1.42	1.33
3	a	683	SER	CA-C	-5.87	1.45	1.52
7	e	164	HIS	ND1-CE1	5.87	1.38	1.32
4	m	577	GLU	N-CA	-5.87	1.38	1.46
6	o	215	THR	CA-C	5.87	1.61	1.53
8	f	285	ASP	CA-C	-5.86	1.45	1.52
9	g	414	THR	N-CA	5.86	1.53	1.46
4	b	575	LEU	N-CA	-5.86	1.38	1.45
6	o	178	ALA	CA-C	-5.86	1.45	1.52
5	c	529	ARG	CA-C	-5.86	1.46	1.53
4	m	733	LYS	CA-C	-5.86	1.44	1.52
1	X	1189	ASP	CA-CB	5.86	1.62	1.53
4	b	135	ASN	C-N	5.86	1.41	1.33
4	b	176	GLU	N-CA	5.86	1.53	1.46
9	g	1071	PRO	C-N	5.86	1.41	1.33
8	q	75	TRP	CZ2-CH2	5.86	1.48	1.37
4	m	86	ASP	CA-CB	5.85	1.63	1.53
8	q	241	SER	C-N	5.85	1.42	1.33
4	b	476	LEU	C-N	5.85	1.41	1.33
5	c	244	VAL	CA-CB	-5.85	1.48	1.54
3	l	749	TYR	CA-CB	5.85	1.61	1.53
3	a	121	VAL	C-N	-5.85	1.27	1.33
9	g	163	GLY	CA-C	-5.85	1.45	1.51
9	r	976	LYS	C-N	5.85	1.41	1.33
3	a	54	SER	N-CA	-5.84	1.39	1.46
1	X	1132	GLU	C-N	5.84	1.41	1.33
4	b	569	LYS	CA-C	-5.84	1.44	1.52
3	l	484	TYR	N-CA	-5.84	1.39	1.46
6	d	138	PRO	CA-C	-5.84	1.46	1.52
8	q	688	LEU	N-CA	5.84	1.53	1.46
1	X	430	ALA	CA-C	-5.84	1.45	1.52
3	a	787	ASN	N-CA	-5.84	1.38	1.46
3	l	822	SER	C-N	5.83	1.42	1.33
4	m	269	ASP	CA-C	-5.83	1.45	1.52
9	r	1047	LEU	CA-CB	5.83	1.62	1.53
9	g	573	LYS	C-N	5.83	1.41	1.33
9	g	357	ASN	CA-C	-5.83	1.46	1.53
9	g	523	ASP	N-CA	-5.83	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	g	882	TYR	CA-C	-5.83	1.45	1.52
8	q	171	VAL	C-N	5.83	1.41	1.33
4	m	157	VAL	C-N	5.82	1.42	1.33
8	q	330	ARG	CD-NE	5.82	1.54	1.46
9	r	532	LYS	N-CA	-5.82	1.39	1.46
5	c	327	SER	N-CA	-5.82	1.38	1.46
9	r	632	LYS	C-N	5.82	1.42	1.33
3	a	866	GLU	C-N	5.82	1.41	1.33
6	d	195	VAL	CA-C	-5.82	1.46	1.52
3	a	284	ASN	CA-CB	5.82	1.63	1.53
4	b	119	GLY	C-N	5.82	1.41	1.33
6	o	55	PRO	N-CA	-5.82	1.40	1.47
3	l	997	ARG	CD-NE	5.81	1.54	1.46
1	X	1651	LEU	CA-CB	5.81	1.62	1.53
3	l	290	LEU	CA-C	-5.81	1.45	1.52
4	b	413	ASP	C-N	5.81	1.42	1.34
4	b	639	ARG	CD-NE	5.81	1.54	1.46
5	c	629	GLU	N-CA	-5.81	1.39	1.46
8	f	105	PHE	CA-CB	5.81	1.62	1.53
5	n	650	HIS	CB-CG	5.81	1.58	1.50
9	r	517	PRO	CA-C	-5.81	1.46	1.52
8	q	576	ASN	CA-C	-5.81	1.45	1.52
1	X	1465	LEU	CA-C	-5.80	1.46	1.52
4	b	168	ARG	CD-NE	5.80	1.54	1.46
8	q	327	VAL	N-CA	-5.80	1.38	1.46
9	g	453	ILE	CA-CB	-5.80	1.47	1.54
5	n	437	GLU	CA-CB	5.80	1.62	1.53
6	o	95	HIS	C-N	5.80	1.41	1.33
1	X	153	ASP	CA-CB	5.80	1.61	1.53
9	g	145	THR	C-N	5.80	1.41	1.33
1	X	1171	ARG	CA-C	-5.80	1.45	1.52
9	r	1079	PRO	CA-C	-5.80	1.44	1.52
1	X	971	PHE	CA-C	-5.80	1.45	1.52
3	l	608	ASP	CA-CB	5.80	1.61	1.53
3	l	956	GLY	CA-C	-5.80	1.44	1.52
7	p	74	SER	N-CA	-5.80	1.38	1.46
4	m	627	TYR	CA-CB	5.79	1.63	1.53
4	m	651	LEU	CA-CB	5.79	1.62	1.53
9	r	636	ILE	CA-C	-5.79	1.46	1.52
5	n	199	ILE	CA-C	5.79	1.59	1.52
1	X	1425	TYR	C-N	5.79	1.41	1.33
3	a	150	PHE	N-CA	-5.79	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	q	335	HIS	N-CA	-5.79	1.39	1.46
9	g	914	GLY	N-CA	5.79	1.49	1.44
4	b	267	ARG	CA-CB	5.79	1.61	1.53
5	c	380	SER	N-CA	5.79	1.52	1.45
4	m	220	ASP	CA-C	-5.79	1.45	1.52
8	f	680	ILE	N-CA	5.78	1.51	1.46
1	X	399	VAL	C-N	5.78	1.41	1.33
4	b	121	ASP	N-CA	-5.78	1.36	1.46
3	l	594	GLY	CA-C	5.78	1.60	1.51
3	a	403	ASP	N-CA	5.78	1.49	1.46
5	c	350	ILE	CA-CB	-5.78	1.47	1.54
9	g	1049	ASN	CA-C	-5.78	1.44	1.52
9	r	585	LEU	N-CA	-5.78	1.39	1.46
4	m	530	ARG	NE-CZ	5.78	1.39	1.33
7	p	243	PHE	N-CA	-5.78	1.39	1.46
8	q	40	ARG	NE-CZ	5.78	1.39	1.33
1	X	946	TRP	CA-C	-5.78	1.45	1.52
1	X	748	HIS	CA-C	-5.78	1.45	1.52
4	b	151	ILE	N-CA	-5.78	1.38	1.46
8	q	301	TYR	N-CA	-5.77	1.39	1.46
8	f	444	ALA	CA-CB	-5.77	1.43	1.53
3	l	271	ARG	CZ-NH1	5.77	1.40	1.32
3	a	1022	SER	N-CA	-5.77	1.38	1.45
8	f	507	ASP	C-N	5.77	1.41	1.33
9	g	927	ALA	CA-CB	-5.77	1.43	1.53
3	l	225	SER	N-CA	-5.77	1.38	1.46
8	f	251	SER	C-N	5.77	1.39	1.33
9	g	281	ARG	CD-NE	5.77	1.54	1.46
3	l	897	SER	N-CA	-5.77	1.42	1.47
1	X	822	ASN	CA-C	-5.76	1.45	1.52
8	f	441	CYS	N-CA	-5.76	1.38	1.46
3	a	263	SER	C-N	5.76	1.41	1.33
4	m	79	MET	CA-CB	5.76	1.64	1.53
4	b	467	ASN	CA-C	5.76	1.60	1.52
5	n	629	GLU	CA-C	-5.76	1.45	1.52
6	o	289	TRP	CA-C	-5.75	1.45	1.52
1	X	1317	VAL	C-N	5.75	1.41	1.34
3	a	1005	ASN	CA-CB	5.75	1.61	1.53
5	c	581	LEU	C-N	5.75	1.41	1.33
3	l	260	VAL	CA-CB	-5.75	1.47	1.54
4	m	587	ASP	CA-CB	5.75	1.63	1.53
3	a	135	LEU	CA-CB	5.75	1.60	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1351	ILE	CA-C	-5.75	1.45	1.53
6	d	247	LEU	C-N	5.75	1.41	1.33
3	l	392	GLU	CA-C	-5.74	1.45	1.52
3	l	720	PHE	CA-CB	5.74	1.61	1.53
3	l	834	ARG	CZ-NH2	5.74	1.41	1.33
5	c	134	ASN	CA-CB	5.74	1.62	1.53
1	X	264	LEU	CA-C	-5.74	1.45	1.52
1	X	280	ALA	CA-CB	5.74	1.63	1.53
6	d	32	THR	CA-C	-5.74	1.45	1.52
9	g	221	LEU	C-N	5.74	1.41	1.33
3	l	975	ARG	NE-CZ	5.74	1.39	1.33
4	m	575	LEU	C-N	5.74	1.42	1.33
1	X	1280	LEU	C-N	5.74	1.41	1.33
1	X	1313	ARG	CZ-NH2	5.74	1.41	1.33
6	d	57	TRP	C-N	5.74	1.42	1.33
8	f	624	SER	CA-C	-5.74	1.44	1.52
6	o	268	VAL	CA-C	-5.74	1.45	1.52
1	X	1336	LEU	C-N	5.74	1.41	1.34
3	a	565	THR	C-N	5.74	1.41	1.34
1	X	1435	ASP	N-CA	5.73	1.53	1.46
3	a	211	PHE	N-CA	5.73	1.53	1.46
6	d	144	HIS	CG-ND1	5.73	1.44	1.38
4	b	403	HIS	ND1-CE1	5.73	1.38	1.32
8	q	724	LEU	N-CA	5.73	1.53	1.46
9	g	288	ASN	N-CA	-5.73	1.38	1.46
3	l	565	THR	N-CA	-5.73	1.39	1.46
8	q	516	TRP	NE1-CE2	5.73	1.43	1.37
1	X	1026	THR	CA-CB	5.73	1.60	1.53
4	m	144	VAL	C-O	-5.73	1.18	1.24
3	a	251	PHE	CA-C	-5.72	1.44	1.52
3	a	24	VAL	C-N	5.72	1.41	1.33
1	X	208	ILE	C-N	5.72	1.40	1.34
1	X	291	ASP	N-CA	-5.72	1.39	1.45
1	X	645	SER	N-CA	-5.72	1.39	1.46
4	b	211	TRP	CA-CB	5.72	1.63	1.53
4	b	304	ARG	NE-CZ	5.72	1.39	1.33
5	c	190	LEU	CA-C	5.72	1.60	1.52
8	f	676	LYS	N-CA	-5.72	1.39	1.46
4	m	593	ALA	CA-C	-5.72	1.45	1.52
1	X	1048	LYS	C-N	5.71	1.40	1.33
4	b	516	ASN	N-CA	-5.71	1.38	1.46
9	g	755	GLN	CA-C	-5.71	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	240	LEU	CA-C	-5.71	1.47	1.53
6	o	58	ARG	NE-CZ	5.71	1.39	1.33
3	a	864	PHE	CA-C	-5.71	1.44	1.52
8	f	265	SER	N-CA	-5.71	1.39	1.46
7	e	3	PRO	CA-CB	5.71	1.61	1.53
3	l	588	ASN	C-N	5.71	1.41	1.33
9	r	504	PHE	CA-C	5.71	1.60	1.52
1	X	1404	PHE	N-CA	-5.71	1.39	1.46
5	n	472	GLU	CA-CB	5.71	1.62	1.53
9	r	257	TRP	C-N	5.71	1.41	1.33
3	a	548	GLU	N-CA	-5.71	1.39	1.46
3	a	878	HIS	CG-ND1	5.70	1.44	1.38
8	q	275	GLU	CA-CB	5.70	1.63	1.53
8	q	401	PRO	N-CA	-5.70	1.43	1.47
7	e	26	THR	CA-CB	-5.70	1.46	1.52
4	m	637	ARG	NE-CZ	5.70	1.39	1.33
4	m	690	THR	CA-C	5.70	1.60	1.52
4	m	310	VAL	CA-C	5.70	1.60	1.52
8	q	68	TRP	CA-C	-5.70	1.44	1.52
5	n	452	TYR	CZ-OH	5.70	1.50	1.38
4	b	532	PRO	CA-CB	-5.70	1.47	1.53
4	b	53	VAL	CA-C	-5.70	1.45	1.52
7	e	156	VAL	CA-CB	-5.70	1.47	1.54
9	g	657	LEU	C-N	5.70	1.42	1.34
3	l	583	LEU	N-CA	-5.70	1.39	1.46
3	l	622	LEU	CA-C	5.70	1.60	1.52
9	r	590	LYS	C-O	-5.70	1.17	1.24
9	g	779	ASN	CA-CB	5.69	1.63	1.53
1	X	706	THR	C-N	5.69	1.41	1.33
1	X	837	ASP	CA-CB	5.69	1.61	1.53
7	p	61	ILE	C-O	-5.69	1.18	1.23
1	X	978	SER	CA-CB	5.69	1.63	1.53
3	a	1003	VAL	CA-CB	-5.69	1.47	1.54
3	l	802	TYR	CA-C	-5.68	1.45	1.52
7	p	64	ALA	N-CA	-5.68	1.39	1.45
4	b	214	ARG	CZ-NH2	5.68	1.40	1.33
8	f	202	LEU	C-N	5.68	1.41	1.33
9	r	904	LYS	CA-CB	5.68	1.62	1.53
7	p	27	CYS	N-CA	-5.68	1.39	1.45
3	l	620	HIS	N-CA	-5.68	1.39	1.46
3	l	1002	MET	CA-C	-5.68	1.45	1.52
6	o	278	VAL	N-CA	-5.68	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	206	VAL	C-N	5.68	1.41	1.33
1	X	1171	ARG	CD-NE	5.68	1.54	1.46
5	n	317	HIS	CA-C	-5.68	1.45	1.52
8	q	719	ALA	CA-C	-5.68	1.44	1.52
1	X	773	LEU	C-N	5.67	1.41	1.33
5	n	519	ARG	CA-CB	5.67	1.60	1.53
4	b	524	SER	CA-CB	5.67	1.63	1.53
3	l	364	GLN	CA-C	-5.67	1.45	1.52
6	o	17	LEU	CA-CB	5.67	1.62	1.53
3	a	974	GLU	CA-C	-5.67	1.45	1.52
6	d	120	SER	CA-C	-5.67	1.45	1.52
7	e	183	LEU	N-CA	-5.67	1.39	1.46
9	g	356	CYS	C-N	5.67	1.40	1.33
6	d	142	ASP	CB-CG	5.67	1.66	1.52
3	l	304	LEU	CA-C	-5.67	1.45	1.52
1	X	1043	LEU	CA-C	5.67	1.60	1.52
5	c	567	LEU	CA-CB	5.67	1.61	1.53
8	f	243	TRP	CA-CB	5.67	1.62	1.53
9	g	575	PHE	N-CA	5.67	1.53	1.46
3	l	875	LEU	C-N	5.67	1.41	1.33
8	f	645	ASP	C-N	5.67	1.42	1.33
4	m	341	GLY	C-N	5.67	1.40	1.33
1	X	1507	LEU	N-CA	-5.67	1.39	1.46
3	a	351	LEU	C-N	5.67	1.38	1.33
3	a	488	THR	C-N	5.67	1.41	1.34
7	e	43	SER	CA-CB	5.67	1.59	1.52
6	o	101	SER	CA-CB	5.67	1.62	1.53
6	d	284	ASN	CA-C	-5.66	1.45	1.53
9	g	962	ASN	CA-C	-5.66	1.44	1.52
4	m	331	TYR	CA-C	-5.66	1.45	1.52
5	n	141	GLU	CA-CB	5.66	1.62	1.53
7	p	23	HIS	CA-C	-5.66	1.45	1.52
4	b	276	ASP	CA-C	-5.66	1.45	1.52
5	n	281	GLU	C-N	5.66	1.41	1.33
8	q	620	LEU	CA-C	-5.66	1.45	1.52
8	f	430	PRO	C-N	5.66	1.41	1.33
9	g	125	ARG	CD-NE	5.66	1.54	1.46
9	g	901	ASN	N-CA	-5.66	1.39	1.46
9	r	663	GLN	N-CA	-5.66	1.39	1.46
8	f	161	PRO	CA-C	-5.66	1.47	1.52
3	l	900	VAL	CA-C	-5.66	1.45	1.52
3	a	432	ILE	N-CA	-5.65	1.38	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	p	228	TYR	C-N	5.65	1.41	1.33
7	e	173	TRP	CA-CB	5.65	1.62	1.53
6	o	189	SER	C-N	5.65	1.41	1.33
8	q	244	ARG	CZ-NH2	5.65	1.40	1.33
3	a	630	THR	C-O	-5.65	1.17	1.24
5	c	579	ARG	CA-C	-5.65	1.48	1.53
9	g	1050	ALA	C-N	5.65	1.41	1.33
1	X	134	ARG	NE-CZ	5.65	1.39	1.33
9	g	533	LEU	N-CA	5.65	1.53	1.45
7	p	299	GLU	N-CA	-5.65	1.39	1.46
3	l	320	PRO	CA-CB	5.64	1.61	1.53
3	l	984	TYR	C-N	5.64	1.40	1.34
1	X	1319	LEU	CA-C	5.64	1.60	1.52
1	X	1600	ALA	N-CA	5.64	1.53	1.46
4	b	328	LEU	C-N	5.64	1.41	1.33
3	l	84	LEU	CA-C	-5.64	1.45	1.52
3	l	97	LEU	CA-CB	5.64	1.61	1.53
9	g	1079	PRO	N-CA	5.64	1.53	1.47
3	l	862	GLN	C-N	5.64	1.42	1.33
8	q	474	ASN	N-CA	-5.64	1.38	1.46
1	X	1450	LEU	N-CA	-5.64	1.39	1.46
4	b	492	SER	CA-C	-5.64	1.45	1.52
7	e	53	ALA	C-O	-5.64	1.16	1.24
9	g	387	MET	CA-C	-5.64	1.45	1.52
3	l	4	LEU	C-N	5.64	1.40	1.33
5	n	360	LEU	C-O	-5.64	1.17	1.24
7	p	189	GLU	C-N	5.64	1.41	1.33
8	q	406	GLU	CA-C	-5.64	1.45	1.52
3	a	820	ARG	CZ-NH1	5.63	1.40	1.32
5	c	176	PRO	N-CA	-5.63	1.40	1.47
1	X	895	HIS	N-CA	-5.63	1.39	1.46
4	b	295	TYR	CA-CB	5.63	1.61	1.53
6	d	184	ILE	CA-C	-5.63	1.45	1.52
8	f	610	GLU	CA-C	5.63	1.60	1.52
5	n	393	GLN	C-N	5.63	1.41	1.33
8	q	328	LEU	CA-CB	-5.63	1.44	1.53
9	r	634	VAL	N-CA	-5.63	1.39	1.46
3	l	174	SER	CA-C	-5.63	1.45	1.52
3	a	180	ASP	CA-C	-5.62	1.48	1.52
6	o	278	VAL	C-N	5.62	1.41	1.33
9	r	994	THR	C-N	5.62	1.41	1.33
3	l	970	LEU	N-CA	-5.62	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	1423	ASN	N-CA	-5.62	1.39	1.46
3	a	880	ARG	NE-CZ	5.62	1.39	1.33
9	g	158	GLN	CA-CB	5.62	1.60	1.53
5	n	610	TRP	CD2-CE3	-5.62	1.31	1.40
6	d	134	GLY	C-N	5.62	1.41	1.33
9	g	552	THR	N-CA	-5.62	1.38	1.46
9	r	963	LYS	CA-CB	5.62	1.62	1.53
1	X	1492	HIS	CB-CG	5.61	1.58	1.50
7	e	343	SER	CA-C	-5.61	1.46	1.52
9	g	475	LEU	CA-C	-5.61	1.46	1.52
3	l	179	GLU	CA-CB	5.61	1.60	1.52
5	n	569	GLU	CA-CB	5.61	1.61	1.53
7	p	50	SER	CA-CB	5.61	1.61	1.53
8	f	535	ARG	CD-NE	5.61	1.54	1.46
4	m	669	LYS	CA-C	-5.61	1.45	1.52
7	p	116	PHE	C-N	5.61	1.41	1.33
1	X	1602	LEU	C-N	5.61	1.41	1.33
9	g	559	VAL	CA-CB	-5.61	1.46	1.54
7	e	303	HIS	CA-C	-5.61	1.45	1.52
7	e	339	PHE	CA-CB	5.61	1.66	1.53
9	g	945	ARG	NE-CZ	5.61	1.39	1.33
3	l	214	ARG	CD-NE	5.61	1.54	1.46
3	l	675	LEU	C-N	5.60	1.41	1.33
5	n	197	VAL	CA-C	-5.60	1.45	1.52
1	X	1436	GLU	C-N	5.60	1.39	1.34
3	a	268	SER	CA-CB	5.60	1.61	1.53
3	a	683	SER	C-N	5.60	1.41	1.33
4	b	144	VAL	C-N	5.60	1.41	1.33
8	f	720	ARG	CZ-NH2	5.60	1.40	1.33
4	m	95	ILE	CA-C	5.60	1.58	1.52
1	X	151	ASN	N-CA	-5.60	1.38	1.46
1	X	663	MET	C-N	5.60	1.41	1.33
4	b	690	THR	CA-C	-5.60	1.45	1.53
1	X	666	PRO	CA-C	-5.60	1.46	1.52
5	c	567	LEU	C-N	5.60	1.41	1.33
8	f	59	GLU	C-N	5.60	1.41	1.33
3	l	90	GLY	CA-C	-5.60	1.44	1.51
4	m	736	ASN	CA-CB	5.60	1.62	1.53
6	o	269	LEU	N-CA	-5.60	1.39	1.46
4	b	122	ARG	CZ-NH2	5.60	1.40	1.33
6	d	271	LEU	CA-C	-5.60	1.45	1.52
7	e	123	LEU	C-N	5.60	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	269	SER	C-N	-5.60	1.25	1.33
4	b	136	PHE	CA-CB	5.60	1.62	1.53
3	a	917	ASP	CA-C	5.59	1.60	1.52
8	f	555	ILE	CA-C	-5.59	1.45	1.52
9	g	303	HIS	C-N	5.59	1.40	1.33
9	r	890	GLN	CA-CB	5.59	1.63	1.53
3	l	107	THR	N-CA	-5.59	1.40	1.46
3	a	210	ARG	CD-NE	5.59	1.54	1.46
5	c	463	ARG	CZ-NH1	5.59	1.40	1.32
4	m	639	ARG	CD-NE	5.59	1.54	1.46
9	g	614	TRP	N-CA	-5.59	1.38	1.46
4	m	430	ILE	CA-C	-5.59	1.45	1.52
3	a	54	SER	C-O	-5.59	1.17	1.24
4	b	661	HIS	ND1-CE1	5.59	1.38	1.32
4	b	675	PHE	CA-CB	-5.59	1.44	1.53
9	g	1040	LEU	CA-CB	5.59	1.62	1.53
3	a	551	THR	N-CA	5.58	1.53	1.46
8	f	578	ASP	C-N	5.58	1.41	1.33
4	m	145	ASN	CA-C	5.58	1.60	1.52
4	m	261	ALA	N-CA	-5.58	1.39	1.46
6	o	185	TRP	CD2-CE2	-5.58	1.31	1.41
1	X	1389	LEU	CA-CB	5.58	1.62	1.53
5	n	270	SER	CA-C	-5.58	1.45	1.52
6	o	9	ASN	CA-C	-5.58	1.45	1.52
3	l	995	ARG	N-CA	-5.58	1.39	1.46
3	l	406	ARG	CA-C	-5.57	1.45	1.52
7	e	90	GLN	CA-C	-5.57	1.45	1.52
3	a	695	TYR	CA-C	-5.57	1.44	1.52
3	a	945	VAL	CA-CB	5.57	1.62	1.54
8	q	509	HIS	CD2-NE2	-5.57	1.31	1.37
1	X	950	ARG	CA-CB	5.57	1.61	1.53
4	b	73	PRO	N-CD	-5.57	1.40	1.47
9	g	499	ASP	CA-C	-5.57	1.44	1.52
4	m	89	LYS	CA-CB	5.57	1.62	1.53
7	e	100	LYS	N-CA	-5.57	1.39	1.46
9	g	139	ILE	N-CA	-5.57	1.37	1.45
5	n	142	ARG	C-N	5.57	1.41	1.33
6	d	262	TRP	CA-C	-5.56	1.45	1.52
9	r	1010	ASP	C-N	5.56	1.40	1.33
8	f	43	ARG	CA-C	-5.56	1.45	1.52
6	o	103	ASN	C-O	-5.56	1.17	1.24
8	q	97	HIS	CA-CB	5.56	1.62	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	l	498	HIS	ND1-CE1	5.56	1.38	1.32
8	q	173	ASP	CA-CB	5.56	1.62	1.53
8	f	57	GLY	CA-C	-5.56	1.44	1.52
7	p	146	ARG	NE-CZ	5.56	1.39	1.33
3	a	902	THR	CA-C	5.56	1.59	1.52
1	X	802	LEU	CA-CB	5.55	1.62	1.53
1	X	1647	LEU	N-CA	-5.55	1.39	1.46
8	q	474	ASN	C-N	5.55	1.40	1.33
8	q	542	ARG	NE-CZ	5.55	1.39	1.33
3	a	129	LEU	N-CA	5.55	1.52	1.45
3	a	927	ASN	CA-CB	5.55	1.59	1.52
3	a	430	ASN	C-N	5.55	1.41	1.33
6	d	141	ILE	CA-C	-5.55	1.46	1.52
5	n	177	THR	CA-C	-5.55	1.46	1.52
8	q	320	HIS	C-N	5.55	1.41	1.33
4	b	325	SER	CA-C	-5.55	1.45	1.52
3	l	639	LEU	CA-C	-5.55	1.45	1.52
5	n	312	GLU	CA-C	-5.55	1.45	1.52
9	r	659	PRO	N-CD	5.55	1.55	1.47
7	p	99	ASN	C-N	5.55	1.41	1.33
8	q	162	LEU	CA-C	-5.55	1.45	1.52
4	b	76	TYR	C-N	5.55	1.41	1.33
7	e	300	HIS	ND1-CE1	5.55	1.38	1.32
9	g	629	LEU	CA-C	5.55	1.60	1.52
6	o	250	GLU	C-N	5.55	1.40	1.33
7	p	216	ARG	NE-CZ	5.55	1.39	1.33
7	p	301	ASP	N-CA	-5.55	1.39	1.46
3	l	547	VAL	CA-C	-5.54	1.45	1.52
4	m	379	LEU	CA-C	-5.54	1.44	1.52
9	r	579	ILE	N-CA	-5.54	1.39	1.46
9	r	863	ARG	CD-NE	5.54	1.54	1.46
8	f	651	ILE	CA-CB	-5.54	1.47	1.54
9	g	282	LEU	N-CA	-5.54	1.40	1.46
9	r	1136	THR	CA-C	-5.54	1.45	1.52
5	c	333	ARG	CD-NE	5.54	1.54	1.46
3	l	81	PHE	CA-CB	5.54	1.62	1.53
9	r	1094	TYR	CA-CB	5.54	1.62	1.53
6	d	151	ALA	CA-C	-5.54	1.45	1.52
1	X	1253	GLU	CA-C	-5.54	1.45	1.52
4	m	627	TYR	CB-CG	-5.54	1.39	1.51
1	X	638	ILE	C-N	5.54	1.40	1.33
5	c	156	GLY	CA-C	-5.54	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	l	698	LEU	CA-CB	5.54	1.62	1.53
5	n	260	LEU	CA-CB	5.54	1.62	1.53
3	a	342	LEU	CB-CG	5.53	1.64	1.53
9	g	86	LEU	CA-C	-5.53	1.45	1.52
3	l	527	SER	CA-CB	5.53	1.62	1.53
3	l	686	PHE	CA-C	-5.53	1.45	1.52
4	b	515	THR	C-N	5.53	1.41	1.33
3	a	245	ILE	C-N	5.53	1.41	1.33
9	g	282	LEU	C-N	5.53	1.39	1.33
4	m	731	LEU	C-N	5.53	1.41	1.33
4	b	190	PHE	C-N	5.53	1.39	1.34
6	d	96	ALA	N-CA	-5.53	1.40	1.46
7	e	96	ARG	CD-NE	5.53	1.53	1.46
8	f	610	GLU	N-CA	-5.53	1.38	1.46
9	r	923	HIS	ND1-CE1	5.53	1.38	1.32
6	o	218	LEU	N-CA	-5.53	1.39	1.46
4	b	235	ALA	CA-C	-5.52	1.41	1.52
1	X	158	SER	CA-CB	5.52	1.64	1.54
6	o	275	ASP	C-N	5.52	1.41	1.33
3	a	751	ARG	NE-CZ	5.52	1.39	1.33
3	a	991	LEU	C-N	5.52	1.40	1.33
9	g	96	TYR	C-N	5.52	1.39	1.33
8	q	544	LYS	CA-CB	5.52	1.62	1.53
7	p	18	ASP	CA-CB	5.52	1.61	1.53
3	a	875	LEU	CA-C	5.51	1.61	1.52
9	g	1020	ARG	NE-CZ	5.51	1.39	1.33
3	a	322	ASN	CA-C	-5.51	1.46	1.52
3	a	492	ASN	C-N	5.51	1.40	1.33
7	e	94	SER	C-N	5.51	1.41	1.33
4	b	559	PHE	C-N	-5.51	1.26	1.33
8	f	600	TRP	C-N	5.51	1.41	1.33
9	r	714	TYR	C-N	5.51	1.41	1.33
1	X	366	SER	C-N	5.51	1.41	1.33
3	l	749	TYR	CA-C	5.50	1.60	1.53
3	l	293	LEU	N-CA	-5.50	1.38	1.46
8	q	672	VAL	N-CA	-5.50	1.41	1.46
5	c	489	HIS	CG-CD2	5.50	1.42	1.35
6	d	147	GLY	CA-C	-5.50	1.43	1.52
9	g	299	ALA	C-N	5.50	1.40	1.33
3	l	263	SER	C-N	5.50	1.41	1.33
4	b	640	GLU	CA-C	5.50	1.59	1.52
9	g	887	TRP	NE1-CE2	-5.50	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	906	TYR	CA-CB	5.50	1.62	1.53
9	g	373	ASN	C-N	5.50	1.41	1.33
4	m	237	LYS	CA-C	-5.50	1.46	1.52
1	X	1515	LEU	CA-C	5.50	1.59	1.52
3	l	479	TYR	CA-CB	5.50	1.61	1.54
3	l	624	SER	CA-CB	5.50	1.62	1.53
1	X	446	ALA	CA-C	-5.50	1.45	1.52
3	a	968	ARG	N-CA	-5.50	1.40	1.46
8	f	156	CYS	CA-CB	5.50	1.61	1.53
9	g	319	SER	C-N	5.50	1.41	1.33
5	n	373	LYS	N-CA	-5.50	1.39	1.46
7	p	130	ASN	CA-CB	5.50	1.62	1.53
5	n	375	LEU	CA-C	-5.49	1.46	1.52
4	b	617	THR	C-N	5.49	1.41	1.33
6	d	257	LEU	CA-C	-5.49	1.46	1.52
7	p	134	LEU	N-CA	-5.49	1.39	1.46
1	X	1564	LEU	C-N	5.49	1.40	1.33
3	a	768	GLY	CA-C	-5.49	1.44	1.51
3	a	890	ARG	NE-CZ	5.49	1.39	1.33
4	b	294	GLN	CA-CB	5.49	1.62	1.53
4	b	533	GLU	CA-CB	5.49	1.62	1.53
6	o	137	SER	C-N	-5.49	1.27	1.33
9	r	1126	ASP	CA-C	-5.49	1.45	1.52
9	g	381	TYR	N-CA	-5.49	1.40	1.46
3	l	653	THR	N-CA	-5.49	1.39	1.46
1	X	950	ARG	CZ-NH1	5.49	1.40	1.32
1	X	1540	LYS	N-CA	-5.49	1.39	1.46
5	n	428	ASN	CA-CB	5.49	1.62	1.53
8	q	394	ILE	CA-CB	-5.49	1.48	1.54
1	X	402	LYS	C-N	5.48	1.40	1.33
3	a	466	TYR	CA-C	-5.48	1.46	1.52
8	q	295	GLN	CA-CB	5.48	1.62	1.53
4	b	702	ALA	C-N	5.48	1.40	1.33
4	m	724	MET	C-N	5.48	1.40	1.33
9	r	619	SER	N-CA	-5.48	1.39	1.45
3	a	793	PHE	CA-C	-5.48	1.45	1.53
9	g	801	CYS	C-N	5.48	1.40	1.34
5	c	582	LEU	N-CA	-5.48	1.39	1.46
8	f	287	HIS	ND1-CE1	5.48	1.38	1.32
3	a	1035	ARG	CD-NE	5.48	1.53	1.46
5	n	271	TRP	NE1-CE2	-5.48	1.31	1.37
9	r	671	ASN	C-N	5.48	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	g	1011	ASP	CA-C	-5.47	1.45	1.52
9	g	1110	ARG	CD-NE	5.47	1.53	1.46
4	m	455	PHE	CA-CB	5.47	1.62	1.53
5	n	578	PRO	CA-C	5.47	1.60	1.52
5	c	356	LYS	N-CA	5.47	1.53	1.46
8	f	712	LYS	CA-CB	5.47	1.62	1.53
3	l	1031	ARG	CD-NE	5.47	1.53	1.46
5	n	149	THR	C-N	5.47	1.40	1.33
1	X	963	LYS	C-N	5.47	1.41	1.33
5	c	202	ARG	NE-CZ	5.47	1.39	1.33
3	l	440	GLU	C-N	5.47	1.39	1.33
5	n	542	GLN	N-CA	-5.47	1.40	1.46
5	c	147	SER	C-N	5.47	1.41	1.33
3	l	281	SER	C-N	5.47	1.40	1.33
4	b	365	ILE	CA-C	-5.47	1.47	1.52
1	X	869	LYS	CA-CB	5.47	1.62	1.54
4	b	293	LYS	CA-CB	5.47	1.62	1.53
3	l	598	LYS	C-N	5.47	1.41	1.33
6	o	134	GLY	CA-C	-5.47	1.44	1.51
7	p	165	LEU	C-N	-5.47	1.25	1.33
3	a	808	TRP	CA-CB	5.46	1.62	1.53
4	b	275	SER	CA-CB	5.46	1.62	1.53
8	q	347	MET	CA-CB	5.46	1.61	1.53
1	X	1403	ASN	C-N	5.46	1.40	1.33
3	a	770	PHE	N-CA	-5.46	1.38	1.45
4	b	275	SER	C-N	5.46	1.41	1.33
3	l	274	GLU	CA-C	5.46	1.60	1.52
3	l	422	ARG	CZ-NH1	5.46	1.40	1.32
3	a	911	GLU	CA-C	-5.46	1.45	1.52
5	c	573	VAL	C-N	5.46	1.41	1.33
3	a	977	ALA	C-N	5.46	1.41	1.33
8	f	695	ALA	CA-C	5.46	1.59	1.52
3	l	996	LYS	C-N	5.46	1.41	1.33
3	l	240	ASN	CA-C	-5.46	1.45	1.52
8	q	15	PHE	CA-C	-5.46	1.45	1.52
9	g	731	GLU	CA-CB	5.46	1.62	1.53
3	l	117	LEU	CA-C	-5.46	1.45	1.52
3	l	764	LEU	CA-C	-5.46	1.44	1.52
3	l	536	ILE	CA-CB	5.45	1.62	1.54
7	p	96	ARG	NE-CZ	5.45	1.39	1.33
9	r	1094	TYR	C-N	5.45	1.40	1.33
4	m	171	ARG	CD-NE	5.45	1.53	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	r	957	GLU	C-N	5.45	1.41	1.33
3	a	806	SER	C-N	5.45	1.39	1.33
9	g	850	TYR	CZ-OH	5.45	1.49	1.38
3	l	137	PHE	C-N	5.45	1.41	1.33
5	n	519	ARG	CA-C	-5.45	1.46	1.53
9	r	918	SER	CA-C	5.45	1.59	1.52
3	a	951	GLN	C-O	-5.44	1.17	1.24
4	b	311	LEU	C-N	5.44	1.41	1.33
3	l	677	GLU	N-CA	-5.44	1.39	1.46
3	a	851	TYR	CA-CB	5.44	1.60	1.53
4	b	175	LEU	CA-C	-5.44	1.45	1.52
4	b	334	ASP	CA-C	-5.44	1.45	1.52
5	c	504	GLU	CA-CB	5.44	1.62	1.54
5	c	512	MET	N-CA	5.44	1.53	1.46
3	l	120	ASN	CA-C	5.44	1.59	1.52
3	l	214	ARG	NE-CZ	5.44	1.39	1.33
4	b	156	GLU	CA-CB	5.44	1.61	1.53
8	q	149	THR	C-N	5.44	1.41	1.34
8	q	163	ARG	NE-CZ	5.44	1.39	1.33
9	r	872	ILE	CA-CB	-5.44	1.48	1.54
3	a	750	LEU	C-N	5.43	1.41	1.33
3	a	1011	ASP	CA-CB	5.43	1.62	1.53
6	d	53	GLU	N-CA	-5.43	1.39	1.46
9	r	762	THR	N-CA	-5.43	1.39	1.46
5	c	285	ARG	CZ-NH2	5.43	1.40	1.33
5	c	185	PHE	N-CA	5.43	1.52	1.46
5	n	451	TRP	N-CA	-5.43	1.39	1.46
5	n	495	CYS	C-N	5.43	1.41	1.33
8	q	261	ARG	CZ-NH2	5.43	1.40	1.33
9	r	1121	GLU	CA-C	-5.43	1.45	1.52
4	b	680	LYS	C-N	5.43	1.40	1.33
6	d	61	TRP	N-CA	-5.43	1.38	1.45
9	g	924	LEU	CA-C	-5.43	1.45	1.52
7	e	219	SER	C-N	5.43	1.40	1.33
1	X	1419	LYS	C-N	5.43	1.40	1.33
1	X	1035	LYS	CA-C	-5.42	1.45	1.53
4	b	110	GLY	C-N	5.42	1.41	1.33
4	b	238	LYS	C-N	5.42	1.40	1.33
5	c	498	ASN	C-N	5.42	1.41	1.33
4	m	502	MET	N-CA	-5.42	1.39	1.46
8	q	36	PHE	CG-CD1	5.42	1.50	1.38
9	r	382	ARG	CA-C	5.42	1.59	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	c	423	GLN	C-N	5.42	1.41	1.33
9	g	1092	PRO	N-CA	5.42	1.54	1.47
4	m	365	ILE	N-CA	-5.42	1.41	1.46
5	c	783	ARG	NE-CZ	5.42	1.39	1.33
8	f	507	ASP	N-CA	-5.42	1.39	1.46
9	g	399	ILE	N-CA	-5.42	1.39	1.46
8	q	523	TYR	C-O	-5.42	1.16	1.24
6	d	225	VAL	CA-C	5.42	1.59	1.52
4	b	527	VAL	N-CA	-5.42	1.39	1.46
3	l	81	PHE	CA-C	-5.42	1.46	1.53
4	b	668	ALA	C-N	5.41	1.40	1.33
4	m	171	ARG	C-N	5.41	1.42	1.33
1	X	1248	THR	C-N	5.41	1.40	1.33
3	a	149	TRP	C-N	5.41	1.40	1.33
8	q	292	GLN	CA-C	5.41	1.59	1.52
8	f	629	GLU	N-CA	-5.41	1.38	1.45
3	l	774	TYR	C-O	-5.41	1.17	1.24
8	q	588	GLU	CA-CB	5.41	1.62	1.53
3	a	199	PHE	C-N	5.41	1.40	1.33
6	d	248	LEU	CA-C	-5.41	1.46	1.52
3	l	784	GLU	CB-CG	5.41	1.68	1.52
5	n	191	ASP	N-CA	-5.41	1.39	1.46
6	o	263	SER	CA-C	-5.41	1.46	1.52
7	p	63	TRP	N-CA	5.41	1.52	1.46
8	q	535	ARG	CD-NE	5.41	1.53	1.46
5	c	265	HIS	CA-CB	5.40	1.61	1.53
1	X	916	TYR	CA-C	-5.40	1.46	1.52
4	b	79	MET	N-CA	-5.40	1.39	1.46
8	f	163	ARG	CD-NE	5.40	1.53	1.46
7	e	122	GLY	CA-C	-5.40	1.44	1.51
8	f	178	HIS	N-CA	-5.40	1.39	1.46
9	g	455	ILE	CA-C	-5.40	1.45	1.52
5	n	358	TYR	N-CA	-5.40	1.39	1.46
5	n	775	GLY	N-CA	-5.40	1.39	1.45
9	r	1007	SER	CA-CB	5.40	1.62	1.53
9	r	493	PHE	CA-C	-5.40	1.45	1.52
4	b	474	CYS	C-N	5.40	1.41	1.33
8	f	524	VAL	C-N	5.40	1.41	1.33
4	m	569	LYS	N-CA	-5.40	1.39	1.46
5	c	651	CYS	CA-C	-5.40	1.45	1.52
7	e	227	TRP	NE1-CE2	5.40	1.43	1.37
9	r	927	ALA	CA-C	-5.40	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	457	PHE	CA-CB	-5.39	1.45	1.53
6	d	265	SER	CA-CB	5.39	1.62	1.53
3	l	463	ILE	N-CA	-5.39	1.39	1.46
1	X	156	THR	N-CA	5.39	1.53	1.45
3	a	57	SER	CA-C	-5.39	1.46	1.52
3	a	867	LYS	N-CA	-5.39	1.39	1.46
4	b	165	GLN	CA-CB	5.39	1.62	1.53
9	g	702	ASP	N-CA	-5.39	1.39	1.46
9	r	1016	PHE	C-N	5.39	1.39	1.33
3	a	393	HIS	CA-C	-5.39	1.45	1.52
5	c	398	SER	CA-C	5.39	1.59	1.52
5	c	464	VAL	CA-CB	-5.39	1.48	1.54
3	l	948	ILE	C-N	5.39	1.40	1.33
5	n	523	ASN	C-N	5.39	1.40	1.33
1	X	404	ILE	C-N	5.39	1.41	1.33
4	b	112	PHE	CA-CB	5.39	1.61	1.53
8	f	274	GLN	CA-CB	5.39	1.61	1.53
9	g	134	VAL	N-CA	-5.39	1.40	1.46
5	n	285	ARG	CA-C	-5.38	1.45	1.52
1	X	1490	ARG	NE-CZ	5.38	1.39	1.33
5	c	295	PHE	N-CA	-5.38	1.39	1.46
9	g	622	ASN	CA-CB	5.38	1.61	1.53
4	m	344	ARG	N-CA	-5.38	1.39	1.46
6	o	221	TYR	N-CA	-5.38	1.39	1.45
3	l	724	PHE	C-N	5.38	1.41	1.33
5	n	438	VAL	C-N	5.38	1.41	1.33
9	r	1001	ASP	CB-CG	5.38	1.65	1.52
1	X	640	GLU	N-CA	-5.38	1.38	1.46
3	a	974	GLU	N-CA	5.38	1.52	1.46
4	b	201	ARG	CZ-NH2	5.38	1.40	1.33
5	c	396	GLU	CA-C	-5.38	1.45	1.52
5	c	492	PHE	N-CA	-5.38	1.39	1.46
9	g	450	ARG	CD-NE	5.38	1.53	1.46
3	l	366	LEU	CA-C	-5.38	1.45	1.52
4	m	425	GLU	N-CA	-5.38	1.39	1.46
4	m	479	LYS	CA-C	-5.38	1.47	1.52
8	f	44	SER	C-N	5.38	1.41	1.33
9	g	621	TYR	C-N	5.38	1.37	1.33
4	m	70	LYS	CA-CB	5.38	1.61	1.53
4	m	664	VAL	CA-CB	-5.38	1.48	1.54
9	g	292	PHE	CA-C	-5.38	1.46	1.52
3	a	908	LEU	CA-C	-5.37	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	f	40	ARG	CD-NE	5.37	1.53	1.46
9	g	1154	THR	C-N	5.37	1.40	1.33
4	m	97	ARG	NE-CZ	5.37	1.39	1.33
4	m	346	ILE	CA-C	-5.37	1.45	1.52
6	o	232	ILE	CA-C	-5.37	1.46	1.52
1	X	693	MET	CA-CB	5.37	1.60	1.53
8	f	423	GLN	C-N	5.37	1.40	1.33
5	n	499	ASP	CA-CB	5.37	1.61	1.53
8	q	362	SER	N-CA	-5.37	1.39	1.46
4	m	369	GLU	CA-CB	5.37	1.62	1.53
3	a	284	ASN	CA-C	-5.37	1.45	1.52
5	c	606	GLU	CA-C	-5.37	1.45	1.52
3	l	157	ASP	CA-C	5.37	1.59	1.52
4	m	578	ALA	N-CA	-5.37	1.38	1.46
6	o	148	VAL	N-CA	-5.37	1.39	1.46
8	q	287	HIS	CA-C	-5.37	1.46	1.52
7	e	52	ARG	N-CA	-5.37	1.39	1.46
4	m	212	ILE	CA-C	5.37	1.60	1.52
4	b	138	LYS	N-CA	-5.37	1.40	1.46
5	c	250	THR	CA-C	-5.37	1.46	1.52
8	f	442	LEU	CA-CB	5.37	1.61	1.53
4	m	307	LYS	C-N	5.37	1.41	1.33
1	X	298	VAL	CA-CB	-5.36	1.48	1.54
3	l	131	LEU	CA-C	-5.36	1.46	1.52
3	l	722	THR	CB-OG1	-5.36	1.35	1.43
9	r	1076	PHE	CA-CB	5.36	1.61	1.53
1	X	375	TYR	N-CA	-5.36	1.39	1.46
1	X	1187	ILE	C-N	5.36	1.41	1.33
1	X	267	ILE	CB-CG1	5.36	1.64	1.53
4	b	345	LYS	C-N	-5.36	1.27	1.33
9	g	256	ILE	N-CA	-5.36	1.40	1.46
3	l	564	ILE	C-N	5.36	1.41	1.34
7	p	203	HIS	CA-C	-5.36	1.46	1.52
1	X	153	ASP	C-N	5.36	1.40	1.33
1	X	731	SER	CA-CB	5.36	1.62	1.53
3	a	340	LEU	CA-C	-5.36	1.46	1.52
4	b	156	GLU	CA-C	-5.36	1.46	1.52
4	b	217	GLY	CA-C	-5.36	1.44	1.51
7	e	311	SER	CA-C	-5.36	1.46	1.52
9	g	1127	ASN	CA-CB	5.36	1.61	1.53
9	r	653	VAL	C-N	5.36	1.40	1.33
9	g	676	CYS	C-N	5.36	1.41	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	637	VAL	C-N	5.35	1.39	1.34
3	l	151	HIS	CG-ND1	5.35	1.44	1.38
3	l	186	LEU	CA-CB	5.35	1.62	1.53
1	X	989	ASP	N-CA	-5.35	1.39	1.46
7	e	222	PRO	C-N	5.35	1.40	1.33
8	f	429	ILE	C-N	5.35	1.40	1.34
9	r	915	GLU	N-CA	-5.35	1.39	1.46
4	m	142	ALA	CA-C	5.35	1.59	1.52
4	m	462	ALA	C-N	5.35	1.41	1.33
5	n	500	ASP	N-CA	5.35	1.52	1.46
6	o	13	HIS	ND1-CE1	5.35	1.37	1.32
3	a	320	PRO	CA-CB	5.35	1.60	1.53
5	c	523	ASN	CA-CB	5.35	1.61	1.53
8	f	243	TRP	NE1-CE2	5.35	1.43	1.37
5	c	170	VAL	CA-C	5.35	1.58	1.52
8	f	633	THR	N-CA	-5.35	1.39	1.46
9	r	912	LYS	CA-C	-5.35	1.45	1.52
5	c	609	LYS	C-N	5.34	1.40	1.33
6	o	139	ILE	CA-CB	5.34	1.60	1.53
9	r	778	ASN	C-N	5.34	1.41	1.33
5	n	631	GLN	CA-CB	5.34	1.62	1.53
1	X	340	SER	N-CA	5.34	1.52	1.46
3	a	271	ARG	C-N	5.34	1.40	1.33
5	c	512	MET	C-N	5.34	1.41	1.33
3	l	384	LYS	CA-C	-5.34	1.46	1.52
4	m	589	PRO	N-CD	-5.34	1.40	1.47
6	o	171	ARG	C-N	5.34	1.40	1.33
5	c	652	ARG	CD-NE	5.34	1.53	1.46
9	g	719	ASN	CA-C	-5.34	1.45	1.52
1	X	427	ILE	CA-CB	-5.34	1.47	1.54
3	a	224	ILE	CA-CB	-5.34	1.48	1.54
9	g	690	ARG	CZ-NH2	5.34	1.40	1.33
9	g	1067	ASP	CA-CB	5.33	1.63	1.53
4	m	582	GLU	CA-CB	5.33	1.62	1.53
3	a	635	LEU	N-CA	-5.33	1.39	1.46
6	o	205	ASP	N-CA	-5.33	1.39	1.45
3	a	20	PRO	CA-C	-5.33	1.44	1.52
3	a	938	ARG	NE-CZ	5.33	1.39	1.33
4	b	694	VAL	N-CA	5.33	1.51	1.46
3	l	278	GLU	CA-C	-5.33	1.47	1.53
9	r	1073	ASN	C-N	5.33	1.40	1.33
8	f	479	THR	C-N	5.33	1.42	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	g	522	LEU	CA-CB	5.33	1.61	1.53
9	r	956	ALA	CA-CB	5.33	1.62	1.53
9	r	1071	PRO	N-CD	-5.33	1.40	1.47
1	X	1263	TYR	C-N	5.33	1.41	1.33
8	q	413	ILE	CA-CB	-5.33	1.47	1.54
8	f	313	LEU	CA-CB	5.33	1.60	1.53
3	l	681	LYS	CA-CB	5.33	1.61	1.53
9	r	942	ASN	CA-CB	5.33	1.61	1.53
1	X	440	ILE	CA-C	-5.33	1.47	1.52
3	a	53	GLY	N-CA	5.33	1.54	1.45
3	a	602	ILE	N-CA	-5.33	1.39	1.46
6	d	95	HIS	C-N	5.33	1.41	1.33
7	e	55	ASP	CA-CB	5.33	1.60	1.53
9	r	894	GLY	C-N	5.33	1.40	1.33
3	a	745	GLU	N-CA	-5.32	1.39	1.46
3	a	1001	LEU	CA-C	-5.32	1.45	1.52
4	b	405	ILE	N-CA	-5.32	1.39	1.46
5	c	202	ARG	CD-NE	5.32	1.53	1.46
5	c	208	PRO	C-N	5.32	1.37	1.33
7	e	48	SER	C-N	5.32	1.40	1.33
7	e	183	LEU	C-N	5.32	1.41	1.33
9	r	592	GLU	CA-CB	5.32	1.62	1.53
8	q	213	CYS	CA-C	-5.32	1.45	1.52
4	b	274	LEU	C-N	5.32	1.41	1.33
5	c	308	LYS	N-CA	-5.32	1.40	1.46
8	f	408	ASP	CA-C	5.32	1.59	1.52
4	m	322	THR	N-CA	-5.32	1.40	1.46
5	n	173	LYS	CA-C	-5.32	1.46	1.52
1	X	990	LYS	C-N	5.32	1.41	1.33
7	e	328	VAL	CA-CB	-5.32	1.47	1.54
9	g	827	THR	CA-CB	5.32	1.60	1.53
7	p	31	GLN	CD-NE2	5.32	1.44	1.33
3	a	801	ASN	CA-C	-5.31	1.45	1.52
8	f	336	PRO	CA-C	5.31	1.59	1.52
8	f	669	LYS	CA-C	-5.31	1.45	1.52
9	r	1086	ASP	CA-C	-5.31	1.46	1.52
9	r	1112	GLU	C-N	5.31	1.40	1.33
3	a	1001	LEU	CA-CB	5.31	1.61	1.53
9	g	258	SER	CA-C	-5.31	1.46	1.52
5	c	563	SER	CA-CB	5.31	1.61	1.53
9	g	435	SER	C-N	5.31	1.41	1.33
7	p	148	TRP	NE1-CE2	-5.31	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	d	110	HIS	CD2-NE2	5.31	1.43	1.37
9	r	1057	LEU	CA-C	5.31	1.59	1.52
4	b	512	PRO	CA-C	-5.31	1.45	1.52
4	b	638	ASP	N-CA	-5.31	1.39	1.46
9	g	632	LYS	CA-CB	5.31	1.62	1.53
3	l	22	ASN	N-CA	-5.31	1.39	1.46
9	r	519	GLU	CA-C	-5.31	1.45	1.52
4	m	492	SER	C-N	5.30	1.40	1.33
3	a	996	LYS	CA-CB	5.30	1.62	1.53
6	d	88	ARG	CD-NE	5.30	1.53	1.46
8	f	175	GLU	C-N	5.30	1.41	1.33
1	X	1187	ILE	CB-CG1	5.30	1.64	1.53
4	b	242	THR	CA-C	-5.30	1.45	1.52
4	b	736	ASN	C-N	5.30	1.41	1.33
7	e	32	HIS	C-O	-5.30	1.16	1.23
8	f	338	GLU	C-N	5.30	1.41	1.34
9	r	646	PHE	CA-C	-5.30	1.46	1.52
1	X	845	SER	C-O	-5.30	1.18	1.24
1	X	1387	LEU	CA-C	5.30	1.59	1.52
3	a	512	THR	CA-C	5.30	1.60	1.52
9	g	669	VAL	N-CA	5.30	1.52	1.46
3	l	428	SER	N-CA	5.30	1.53	1.46
4	m	586	LEU	CA-C	-5.30	1.46	1.52
5	n	603	PRO	C-N	5.30	1.40	1.33
8	f	707	SER	CA-C	-5.29	1.45	1.52
9	r	529	HIS	CA-CB	5.29	1.61	1.53
4	b	737	PHE	N-CA	-5.29	1.40	1.46
4	m	266	GLU	CA-CB	5.29	1.62	1.53
5	n	210	ILE	CA-C	-5.29	1.46	1.52
6	o	68	THR	CA-C	-5.29	1.46	1.52
9	r	526	SER	CA-CB	5.29	1.60	1.52
3	l	808	TRP	NE1-CE2	-5.29	1.31	1.37
4	b	411	SER	N-CA	-5.29	1.39	1.46
9	g	1088	SER	CA-CB	5.29	1.62	1.53
4	m	219	PRO	N-CD	-5.29	1.40	1.47
9	r	1005	LEU	C-N	5.29	1.41	1.33
9	r	1064	ARG	C-N	5.29	1.40	1.33
6	d	51	GLY	CA-C	-5.29	1.44	1.51
6	o	247	LEU	C-N	5.29	1.41	1.33
3	a	286	THR	CA-CB	-5.29	1.46	1.52
3	l	663	LEU	CA-C	-5.29	1.46	1.52
5	n	369	LEU	C-N	5.29	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
6	d	222	LEU	C-N	5.28	1.40	1.33
8	q	697	GLU	CA-CB	5.28	1.60	1.53
1	X	685	TYR	CA-C	-5.28	1.48	1.53
1	X	1063	ASP	C-N	5.28	1.41	1.33
9	g	102	HIS	CA-C	-5.28	1.45	1.52
3	l	743	ASN	C-N	5.28	1.40	1.33
6	o	86	ASN	CG-ND2	5.28	1.44	1.33
9	r	713	ASP	N-CA	-5.28	1.39	1.46
3	a	178	LEU	N-CA	-5.28	1.38	1.45
3	a	780	HIS	CB-CG	-5.28	1.42	1.50
8	f	297	GLU	C-N	5.28	1.40	1.33
3	l	875	LEU	N-CA	-5.28	1.40	1.46
7	p	30	ASP	N-CA	5.28	1.52	1.46
5	n	432	GLU	CA-C	-5.28	1.46	1.52
6	o	9	ASN	N-CA	-5.28	1.39	1.46
1	X	728	ILE	CB-CG1	5.28	1.64	1.53
8	f	169	LEU	N-CA	-5.28	1.40	1.46
9	g	299	ALA	CA-C	-5.28	1.46	1.52
5	n	577	GLY	CA-C	5.28	1.59	1.51
9	r	1147	THR	N-CA	-5.28	1.39	1.46
1	X	176	LEU	N-CA	-5.28	1.40	1.46
1	X	1633	ARG	N-CA	5.28	1.56	1.46
3	a	758	PHE	CA-C	5.28	1.59	1.52
5	c	386	ASN	C-N	5.28	1.41	1.34
8	f	276	VAL	CA-CB	-5.28	1.47	1.54
1	X	1291	GLY	CA-C	-5.27	1.44	1.51
3	a	801	ASN	C-N	5.27	1.41	1.33
9	g	327	ALA	N-CA	5.27	1.52	1.45
3	l	12	LEU	N-CA	-5.27	1.39	1.46
4	m	567	LEU	C-N	5.27	1.39	1.33
5	n	622	LYS	C-N	5.27	1.40	1.33
6	d	285	LEU	CA-C	-5.27	1.45	1.52
5	n	647	GLN	N-CA	-5.27	1.39	1.46
7	p	182	LYS	CA-C	-5.27	1.46	1.52
8	q	462	ILE	N-CA	-5.27	1.40	1.46
9	r	601	ASN	C-N	5.27	1.41	1.33
4	b	286	SER	CA-CB	5.27	1.62	1.53
7	e	238	GLY	C-N	5.27	1.41	1.33
9	g	261	PHE	CA-C	-5.27	1.45	1.52
9	g	492	GLY	C-N	5.27	1.42	1.33
3	l	599	LYS	CA-C	-5.27	1.46	1.52
1	X	1518	THR	C-N	5.27	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	616	LEU	CA-CB	5.27	1.61	1.53
3	a	1008	SER	C-N	5.27	1.40	1.33
9	g	652	HIS	CG-CD2	5.27	1.41	1.35
9	g	977	ASN	CA-C	-5.27	1.46	1.52
4	m	183	ASN	C-N	5.27	1.41	1.33
4	m	403	HIS	CA-CB	5.27	1.62	1.53
8	q	189	LEU	C-N	5.27	1.42	1.33
9	g	101	ASP	CA-C	-5.27	1.46	1.52
9	r	862	PHE	CA-C	-5.27	1.46	1.53
3	a	451	ARG	NE-CZ	5.26	1.38	1.33
4	m	174	GLU	CA-CB	5.26	1.61	1.53
5	n	342	LYS	CA-C	-5.26	1.46	1.52
7	p	312	TRP	N-CA	-5.26	1.39	1.45
1	X	1441	GLN	C-N	5.26	1.39	1.33
9	g	1018	PRO	C-N	5.26	1.41	1.34
4	m	430	ILE	CA-CB	-5.26	1.47	1.54
4	b	647	ARG	CD-NE	5.26	1.53	1.46
4	m	281	SER	CA-CB	5.26	1.60	1.53
3	a	336	LEU	CA-CB	5.25	1.63	1.53
6	d	70	LEU	N-CA	-5.25	1.40	1.46
6	d	199	THR	CA-C	-5.25	1.46	1.52
4	m	572	SER	C-N	5.25	1.41	1.34
9	r	719	ASN	CA-C	-5.25	1.46	1.52
9	g	881	LYS	CA-C	-5.25	1.46	1.52
5	n	617	PHE	CA-CB	5.25	1.62	1.53
5	c	428	ASN	N-CA	-5.25	1.39	1.46
5	n	307	SER	CA-CB	5.25	1.61	1.53
8	q	707	SER	CA-CB	5.25	1.61	1.53
4	b	596	SER	C-N	5.25	1.40	1.33
5	c	341	GLN	C-N	5.25	1.41	1.33
5	c	531	LYS	C-N	5.25	1.39	1.33
7	e	83	LEU	CA-C	-5.25	1.46	1.52
3	l	448	THR	N-CA	-5.25	1.39	1.46
3	a	220	TYR	C-N	5.25	1.41	1.33
4	m	699	TRP	CA-C	-5.25	1.45	1.52
7	p	317	THR	C-O	-5.25	1.18	1.24
9	g	555	GLN	CA-C	5.24	1.59	1.52
9	g	758	ILE	CA-CB	5.24	1.61	1.54
3	l	269	HIS	ND1-CE1	5.24	1.37	1.32
6	o	185	TRP	CA-CB	5.24	1.59	1.52
9	g	701	VAL	N-CA	-5.24	1.40	1.46
3	l	754	GLU	C-O	-5.24	1.18	1.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	l	821	HIS	CA-C	-5.24	1.45	1.52
4	m	712	THR	C-N	5.24	1.39	1.33
8	q	45	ALA	CA-C	-5.24	1.46	1.52
3	a	313	TYR	CA-CB	5.24	1.60	1.53
4	b	250	ASN	CG-ND2	5.24	1.44	1.33
6	d	13	HIS	CA-C	5.24	1.59	1.52
3	l	699	ILE	C-N	5.24	1.40	1.33
5	n	546	ASP	C-N	5.24	1.40	1.33
5	c	603	PRO	N-CD	-5.24	1.40	1.47
4	m	337	LEU	C-N	5.24	1.40	1.33
5	c	522	THR	C-N	5.24	1.40	1.33
3	l	334	LEU	CA-C	-5.24	1.46	1.52
9	g	538	ILE	CA-CB	5.23	1.60	1.54
5	n	664	GLU	C-N	5.23	1.40	1.33
7	e	204	VAL	CA-C	5.23	1.59	1.52
4	m	469	PHE	CA-C	-5.23	1.46	1.52
8	q	245	ARG	CA-C	5.23	1.59	1.52
9	r	533	LEU	N-CA	-5.23	1.40	1.46
4	b	631	SER	N-CA	-5.23	1.39	1.46
5	c	463	ARG	CD-NE	5.23	1.53	1.46
9	g	968	GLU	C-O	5.23	1.30	1.24
9	g	1069	GLU	CA-CB	5.23	1.61	1.53
3	l	820	ARG	CZ-NH1	5.23	1.40	1.32
8	q	279	TYR	C-N	5.23	1.41	1.33
1	X	720	ARG	NE-CZ	5.23	1.38	1.33
4	m	243	GLN	C-O	-5.23	1.18	1.24
3	a	888	VAL	CA-C	-5.22	1.46	1.53
1	X	1186	GLU	C-N	5.22	1.40	1.33
4	b	133	ASN	CA-CB	5.22	1.63	1.53
9	g	531	LEU	C-N	5.22	1.41	1.33
8	q	202	LEU	CA-C	-5.22	1.45	1.52
8	q	218	TYR	N-CA	5.22	1.52	1.46
9	r	823	GLN	C-N	5.22	1.40	1.33
5	n	287	SER	CA-CB	5.22	1.62	1.53
3	a	497	MET	CA-CB	5.22	1.62	1.53
3	a	671	ASP	CA-CB	5.22	1.62	1.53
3	a	698	LEU	CA-C	-5.22	1.45	1.52
3	a	933	GLY	N-CA	-5.22	1.41	1.45
4	b	435	GLU	CA-C	-5.22	1.46	1.52
5	c	275	GLN	CA-C	-5.22	1.45	1.52
5	c	332	ILE	CA-C	-5.22	1.45	1.52
3	l	510	LEU	CA-C	-5.22	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
7	p	111	LEU	C-O	5.22	1.30	1.23
9	r	494	VAL	CA-C	-5.22	1.46	1.52
4	b	565	TYR	C-N	5.22	1.40	1.33
4	b	701	ASP	CA-C	-5.22	1.46	1.52
8	f	313	LEU	C-N	5.22	1.39	1.33
9	g	925	ASN	C-N	5.22	1.40	1.33
9	r	1130	GLU	CA-CB	5.22	1.61	1.53
1	X	403	ILE	CA-CB	5.21	1.61	1.54
1	X	853	LYS	C-N	5.21	1.40	1.34
4	b	52	THR	CA-C	-5.21	1.46	1.52
3	l	905	LEU	CA-C	5.21	1.59	1.52
7	p	93	CYS	CA-C	5.21	1.59	1.52
8	q	75	TRP	NE1-CE2	5.21	1.43	1.37
1	X	738	ILE	CA-C	-5.21	1.45	1.52
9	g	1143	GLU	CA-CB	5.21	1.62	1.53
3	l	737	ILE	CA-CB	-5.21	1.47	1.54
1	X	1036	ASP	CA-C	-5.21	1.47	1.53
8	f	606	LEU	CA-C	-5.21	1.46	1.52
9	r	919	GLU	CA-C	5.21	1.59	1.52
9	r	969	VAL	N-CA	-5.21	1.40	1.46
1	X	354	GLU	CA-CB	5.21	1.62	1.53
8	q	192	ALA	CA-C	-5.21	1.45	1.52
7	e	204	VAL	C-N	5.21	1.41	1.33
7	e	235	CYS	C-N	5.21	1.41	1.33
3	l	181	GLY	N-CA	5.21	1.53	1.45
3	l	691	LYS	CA-CB	5.21	1.60	1.53
5	n	556	VAL	C-N	5.21	1.41	1.34
5	n	587	VAL	C-N	5.21	1.40	1.33
7	p	309	SER	N-CA	-5.21	1.39	1.46
4	b	488	LEU	C-N	5.21	1.40	1.33
4	b	665	LEU	N-CA	-5.21	1.39	1.46
5	c	607	ARG	CA-CB	5.21	1.61	1.53
9	g	292	PHE	CA-CB	5.21	1.60	1.53
9	g	961	SER	CA-C	-5.21	1.46	1.52
7	p	155	LYS	CA-CB	5.21	1.61	1.53
8	q	192	ALA	C-N	5.21	1.38	1.33
3	l	608	ASP	CA-C	-5.21	1.46	1.52
4	m	423	ILE	N-CA	-5.21	1.40	1.46
5	n	321	LEU	CA-CB	5.21	1.61	1.53
9	r	820	THR	N-CA	-5.20	1.39	1.46
9	r	982	GLU	CA-C	-5.20	1.46	1.52
3	l	1010	PHE	CA-C	-5.20	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	m	261	ALA	C-N	5.20	1.40	1.33
4	b	344	ARG	CA-C	-5.20	1.45	1.52
6	d	232	ILE	CA-CB	5.20	1.60	1.53
7	p	304	ASN	C-N	5.20	1.39	1.32
8	q	109	LEU	CA-C	-5.20	1.46	1.52
9	g	953	THR	CA-C	-5.20	1.45	1.52
3	l	958	TRP	CA-CB	5.20	1.62	1.53
4	m	301	SER	CA-C	-5.20	1.46	1.52
5	c	283	LYS	CA-CB	5.20	1.62	1.53
8	f	53	LEU	N-CA	-5.20	1.39	1.46
9	g	996	VAL	CA-CB	-5.20	1.48	1.54
9	g	1142	LYS	N-CA	-5.20	1.40	1.46
5	n	192	LYS	C-N	5.20	1.41	1.34
1	X	1495	TRP	CD2-CE2	5.19	1.50	1.41
3	a	169	VAL	CA-C	-5.19	1.46	1.52
3	l	415	TYR	N-CA	5.19	1.57	1.46
1	X	931	PHE	CA-C	-5.19	1.46	1.53
1	X	996	THR	CA-C	-5.19	1.45	1.52
1	X	1461	ILE	CA-C	-5.19	1.46	1.52
4	b	639	ARG	NE-CZ	5.19	1.38	1.33
9	g	1009	LEU	CA-CB	5.19	1.61	1.53
6	d	38	VAL	N-CA	-5.19	1.40	1.46
9	g	714	TYR	N-CA	-5.19	1.39	1.46
3	l	197	LEU	CA-C	-5.19	1.46	1.53
5	n	649	LYS	N-CA	-5.19	1.39	1.46
8	f	104	LEU	CA-C	-5.19	1.46	1.52
4	b	209	LEU	CA-C	-5.19	1.45	1.52
9	g	937	ASP	N-CA	-5.19	1.39	1.46
5	n	422	PHE	C-N	5.19	1.41	1.34
1	X	1352	LEU	C-N	5.19	1.41	1.33
8	f	649	TYR	CA-CB	5.19	1.61	1.53
3	a	232	ARG	CD-NE	5.18	1.53	1.46
3	a	794	LEU	C-N	5.18	1.41	1.33
4	b	125	ASN	CA-C	-5.18	1.46	1.52
5	c	205	ASN	C-N	-5.18	1.26	1.34
5	n	209	GLN	C-O	5.18	1.29	1.24
1	X	142	ILE	CA-CB	-5.18	1.48	1.54
1	X	1008	THR	CA-C	-5.18	1.46	1.52
1	X	1259	PHE	N-CA	-5.18	1.40	1.46
3	a	81	PHE	N-CA	-5.18	1.40	1.46
3	a	230	HIS	CG-CD2	5.18	1.41	1.35
9	r	611	ASN	CA-CB	5.18	1.62	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	998	LEU	N-CA	-5.18	1.39	1.46
3	l	328	ILE	CA-C	-5.18	1.46	1.52
3	a	324	SER	CA-CB	5.18	1.61	1.53
9	g	706	LEU	CA-C	5.18	1.59	1.52
5	n	255	VAL	C-N	5.18	1.40	1.33
3	l	438	GLU	CA-C	-5.18	1.46	1.52
3	l	350	ASN	CG-ND2	5.18	1.44	1.33
3	l	414	ARG	CA-C	-5.18	1.46	1.52
5	n	318	LEU	CA-C	-5.18	1.46	1.52
3	l	976	ALA	N-CA	5.17	1.52	1.46
4	m	104	PHE	CA-C	-5.17	1.46	1.52
9	r	897	ALA	C-N	5.17	1.40	1.33
1	X	1414	GLU	N-CA	5.17	1.52	1.46
1	X	1623	GLU	CA-C	-5.17	1.46	1.52
3	a	408	PHE	CA-C	-5.17	1.45	1.52
5	c	257	MET	N-CA	-5.17	1.39	1.46
8	f	363	VAL	N-CA	-5.17	1.39	1.46
9	g	1066	PHE	C-N	5.17	1.41	1.33
7	p	80	THR	C-N	5.17	1.40	1.33
8	q	109	LEU	CA-CB	5.17	1.61	1.53
3	a	863	ASP	CA-CB	5.17	1.61	1.54
3	a	964	LEU	N-CA	-5.17	1.39	1.46
5	c	162	LYS	C-N	5.17	1.40	1.33
3	l	674	LEU	C-N	5.17	1.41	1.34
3	l	953	LEU	N-CA	-5.17	1.39	1.46
4	m	293	LYS	C-N	5.17	1.40	1.33
5	n	465	PHE	N-CA	-5.17	1.39	1.46
1	X	1622	GLU	C-N	5.17	1.40	1.33
4	b	741	GLN	N-CA	-5.17	1.39	1.46
3	l	377	GLU	N-CA	-5.17	1.39	1.46
9	g	411	ASN	CA-C	-5.17	1.47	1.53
9	g	677	PHE	CA-CB	5.17	1.61	1.53
9	g	1122	THR	C-N	5.17	1.40	1.33
3	l	796	ASP	C-N	5.17	1.41	1.33
1	X	1432	ARG	NE-CZ	5.16	1.38	1.33
3	l	788	ASP	C-N	5.16	1.41	1.33
9	r	1110	ARG	CD-NE	5.16	1.53	1.46
9	g	212	LEU	CA-CB	5.16	1.62	1.54
3	a	144	THR	CA-C	5.16	1.58	1.52
4	b	686	ASP	CA-C	5.16	1.59	1.53
7	e	63	TRP	C-N	5.16	1.41	1.33
9	g	160	GLU	CA-C	-5.16	1.45	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	g	516	LEU	CA-CB	5.16	1.60	1.53
4	m	140	HIS	CE1-NE2	5.16	1.37	1.32
4	b	121	ASP	CA-CB	5.16	1.57	1.53
6	d	99	SER	N-CA	-5.16	1.40	1.46
4	m	653	ILE	N-CA	-5.16	1.40	1.46
9	g	66	ARG	CD-NE	5.16	1.53	1.46
4	m	350	SER	CA-C	5.16	1.59	1.52
4	m	394	CYS	CA-C	5.16	1.59	1.52
5	n	529	ARG	CD-NE	5.16	1.53	1.46
8	f	79	GLU	C-N	5.15	1.40	1.33
6	o	120	SER	CA-C	-5.15	1.46	1.52
7	e	98	TRP	CA-CB	5.15	1.59	1.52
8	f	390	THR	N-CA	-5.15	1.40	1.46
3	l	102	MET	N-CA	-5.15	1.40	1.46
1	X	820	LEU	CA-C	-5.15	1.47	1.53
7	e	136	LEU	C-N	5.15	1.40	1.33
9	g	273	GLY	N-CA	5.15	1.51	1.44
4	m	133	ASN	CA-CB	5.15	1.62	1.53
1	X	389	PHE	CA-C	5.15	1.58	1.52
1	X	1188	THR	C-N	5.15	1.40	1.33
1	X	1401	SER	CA-C	-5.15	1.46	1.52
3	a	230	HIS	ND1-CE1	5.15	1.37	1.32
5	c	321	LEU	CA-C	-5.15	1.45	1.52
1	X	185	LEU	C-N	5.15	1.40	1.33
4	b	706	SER	C-N	5.14	1.40	1.33
6	d	81	ILE	N-CA	-5.14	1.40	1.46
7	p	242	ILE	C-N	5.14	1.40	1.33
4	b	578	ALA	N-CA	-5.14	1.40	1.46
9	g	377	ILE	C-N	5.14	1.40	1.33
3	l	868	GLN	CA-C	-5.14	1.45	1.52
5	n	430	ASN	C-N	5.14	1.40	1.33
8	q	445	CYS	CA-C	-5.14	1.45	1.52
9	g	365	THR	N-CA	-5.14	1.40	1.46
9	g	548	PRO	C-N	5.14	1.40	1.33
9	r	807	PHE	CA-C	-5.14	1.46	1.52
1	X	980	LYS	C-N	5.14	1.40	1.33
9	g	156	ASN	CA-CB	5.14	1.62	1.53
3	l	198	LEU	CB-CG	5.14	1.63	1.53
5	n	532	ILE	CA-CB	-5.14	1.47	1.54
8	q	325	GLN	CA-C	5.14	1.59	1.52
5	c	240	LEU	N-CA	-5.14	1.39	1.46
8	f	167	ASN	CA-C	-5.14	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	f	581	LEU	N-CA	-5.14	1.40	1.46
9	g	1088	SER	C-N	5.14	1.41	1.33
6	o	141	ILE	CA-CB	-5.14	1.46	1.54
9	r	560	ARG	CD-NE	5.14	1.53	1.46
5	c	468	GLU	CA-C	-5.13	1.45	1.52
8	f	304	GLU	CA-C	-5.13	1.46	1.52
9	g	177	ASP	CA-C	-5.13	1.46	1.52
9	g	202	SER	CA-C	-5.13	1.46	1.52
5	n	252	ASN	CG-ND2	5.13	1.44	1.33
5	n	307	SER	CA-C	-5.13	1.46	1.52
9	g	120	ILE	CA-CB	5.13	1.59	1.53
9	g	404	MET	CA-C	-5.13	1.45	1.52
3	a	918	PHE	CA-C	-5.13	1.45	1.52
5	c	564	SER	CA-CB	5.13	1.62	1.53
6	d	293	GLY	CA-C	5.13	1.61	1.52
4	m	623	THR	N-CA	-5.13	1.39	1.46
7	p	24	VAL	N-CA	-5.13	1.40	1.46
8	q	244	ARG	CD-NE	5.13	1.53	1.46
1	X	403	ILE	C-N	5.13	1.40	1.33
1	X	1443	THR	C-N	5.13	1.40	1.33
9	g	811	LEU	CA-CB	5.13	1.62	1.53
5	n	344	SER	CA-C	-5.13	1.46	1.52
1	X	1527	LYS	CA-C	5.13	1.59	1.52
3	a	880	ARG	C-N	5.13	1.40	1.33
4	b	386	ILE	CB-CG1	5.13	1.63	1.53
3	a	197	LEU	N-CA	-5.13	1.39	1.46
3	a	803	HIS	CE1-NE2	-5.13	1.27	1.32
3	l	326	SER	C-O	5.13	1.30	1.23
6	o	199	THR	N-CA	-5.13	1.39	1.46
1	X	1388	LEU	CA-C	5.12	1.59	1.52
5	c	570	MET	CA-C	-5.12	1.46	1.52
9	g	492	GLY	CA-C	-5.12	1.44	1.51
9	g	666	LYS	CA-CB	5.12	1.61	1.53
9	r	552	THR	C-N	5.12	1.40	1.33
5	c	554	SER	CA-CB	5.12	1.61	1.53
7	e	120	HIS	ND1-CE1	5.12	1.37	1.32
4	m	74	LEU	CA-C	-5.12	1.46	1.52
4	m	407	PRO	C-O	-5.12	1.17	1.24
5	n	519	ARG	C-N	5.12	1.41	1.33
8	q	297	GLU	C-N	5.12	1.40	1.33
1	X	1481	GLY	CA-C	5.12	1.57	1.52
9	g	446	ILE	N-CA	-5.12	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	n	579	ARG	CA-CB	5.12	1.60	1.53
4	b	237	LYS	CA-C	-5.12	1.46	1.52
5	c	236	LEU	C-N	5.12	1.40	1.34
4	b	290	GLU	C-N	5.12	1.40	1.33
7	e	157	LEU	CA-C	-5.12	1.46	1.52
6	o	129	GLU	CA-CB	5.12	1.61	1.53
8	q	662	PHE	CA-CB	5.12	1.61	1.53
9	r	561	LYS	C-O	5.12	1.30	1.24
1	X	1229	LEU	C-N	5.12	1.40	1.33
1	X	1521	PHE	C-N	5.12	1.40	1.33
5	c	223	TYR	C-N	5.12	1.40	1.33
5	c	599	LEU	CB-CG	5.12	1.63	1.53
9	g	355	SER	N-CA	-5.12	1.39	1.46
9	g	939	LEU	CB-CG	5.12	1.63	1.53
4	m	347	LEU	CA-CB	5.12	1.61	1.53
5	n	240	LEU	CA-C	-5.12	1.46	1.52
9	r	790	HIS	CG-CD2	5.12	1.41	1.35
8	f	73	ARG	C-O	-5.11	1.17	1.24
9	g	449	LEU	C-N	5.11	1.41	1.34
9	g	778	ASN	CA-C	-5.11	1.46	1.52
4	m	166	ASP	C-N	5.11	1.41	1.33
6	o	53	GLU	C-N	5.11	1.41	1.33
4	b	58	ILE	N-CA	-5.11	1.40	1.46
5	c	246	TYR	CA-CB	5.11	1.59	1.53
3	a	259	MET	CA-CB	5.11	1.59	1.52
3	a	322	ASN	N-CA	5.11	1.52	1.46
9	g	762	THR	CA-C	-5.11	1.46	1.52
9	g	922	LEU	N-CA	-5.11	1.40	1.46
3	l	987	MET	CA-C	-5.11	1.46	1.52
4	m	590	VAL	CA-C	-5.11	1.46	1.52
8	q	101	SER	N-CA	-5.11	1.39	1.46
8	q	235	GLN	CA-CB	5.11	1.63	1.54
5	c	510	LEU	CA-C	-5.11	1.46	1.52
5	c	603	PRO	C-O	5.11	1.29	1.23
7	p	54	HIS	ND1-CE1	5.11	1.37	1.32
8	q	341	HIS	ND1-CE1	5.11	1.37	1.32
6	d	283	GLU	N-CA	-5.11	1.39	1.46
3	l	266	ASP	N-CA	-5.11	1.37	1.45
4	m	420	THR	CA-C	-5.11	1.46	1.52
4	m	658	LEU	CA-CB	5.11	1.61	1.52
8	q	595	ARG	CA-C	-5.11	1.46	1.52
1	X	887	VAL	C-N	5.11	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	X	939	LEU	CA-CB	5.11	1.59	1.53
5	c	303	VAL	CA-CB	-5.11	1.48	1.54
7	e	135	ARG	CA-C	-5.11	1.46	1.52
8	q	333	SER	N-CA	5.11	1.52	1.46
3	a	808	TRP	C-O	-5.10	1.17	1.24
1	X	153	ASP	CA-C	-5.10	1.46	1.52
1	X	1563	LEU	CA-CB	5.10	1.61	1.53
4	b	384	VAL	CA-C	-5.10	1.46	1.52
7	e	4	PHE	N-CA	-5.10	1.39	1.46
7	e	296	LEU	N-CA	-5.10	1.39	1.46
9	g	833	GLU	N-CA	-5.10	1.39	1.46
4	m	66	PRO	CA-C	-5.10	1.47	1.53
6	o	137	SER	CA-C	5.10	1.58	1.52
5	c	581	LEU	CA-CB	5.10	1.61	1.53
6	d	219	ARG	CA-C	-5.10	1.46	1.52
7	e	2	GLN	CA-C	5.10	1.56	1.52
8	f	522	LEU	CA-CB	5.10	1.62	1.53
8	f	580	PHE	CA-CB	5.10	1.62	1.53
9	g	979	SER	C-N	5.10	1.39	1.34
3	l	800	GLU	N-CA	5.10	1.52	1.46
4	m	58	ILE	CA-C	5.10	1.58	1.52
5	n	525	HIS	ND1-CE1	5.10	1.37	1.32
9	r	1024	VAL	CA-C	-5.10	1.46	1.52
1	X	864	SER	C-N	5.10	1.40	1.33
5	c	655	ALA	CA-CB	5.10	1.61	1.53
4	m	614	CYS	CA-C	-5.10	1.46	1.52
9	g	794	LYS	C-N	5.10	1.39	1.33
3	l	978	ALA	CA-CB	5.09	1.61	1.53
7	p	150	LEU	N-CA	5.09	1.52	1.46
9	r	313	TYR	N-CA	-5.09	1.40	1.46
3	a	990	ASP	CA-CB	5.09	1.61	1.53
8	f	39	ILE	CA-C	-5.09	1.45	1.52
8	f	695	ALA	N-CA	-5.09	1.40	1.46
3	l	180	ASP	C-N	5.09	1.40	1.33
3	l	404	VAL	C-N	5.09	1.40	1.33
8	q	453	GLU	N-CA	-5.09	1.41	1.46
9	r	1013	GLU	CA-C	-5.09	1.46	1.52
1	X	996	THR	N-CA	5.09	1.52	1.46
1	X	1280	LEU	CA-CB	5.09	1.61	1.53
4	b	591	LEU	CA-C	-5.09	1.46	1.52
5	c	406	HIS	ND1-CE1	5.09	1.37	1.32
9	g	663	GLN	N-CA	-5.09	1.39	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
9	g	980	ILE	CA-C	-5.09	1.45	1.52
5	n	616	VAL	N-CA	-5.09	1.40	1.46
9	r	559	VAL	CA-CB	5.09	1.61	1.54
3	a	986	LEU	C-N	5.09	1.41	1.33
4	b	645	ALA	CA-CB	5.09	1.62	1.53
9	r	1101	ARG	CZ-NH1	5.09	1.39	1.32
6	o	52	HIS	CG-CD2	-5.09	1.30	1.35
5	c	356	LYS	C-N	5.09	1.40	1.33
3	l	71	HIS	CB-CG	5.09	1.57	1.50
5	n	546	ASP	CA-CB	5.09	1.62	1.53
8	f	170	ASP	CA-C	-5.08	1.46	1.53
3	l	258	ASP	C-N	5.08	1.40	1.33
1	X	181	LYS	N-CA	-5.08	1.39	1.46
3	a	511	ARG	NE-CZ	5.08	1.38	1.33
9	g	278	LYS	C-N	5.08	1.39	1.33
9	g	303	HIS	ND1-CE1	5.08	1.37	1.32
4	m	526	CYS	CA-C	-5.08	1.46	1.52
7	p	333	ALA	N-CA	-5.08	1.39	1.46
9	g	687	LYS	CA-C	5.08	1.59	1.52
3	l	131	LEU	CA-CB	5.08	1.61	1.53
3	l	929	HIS	N-CA	-5.08	1.39	1.46
4	b	250	ASN	N-CA	-5.08	1.40	1.46
4	b	471	PHE	CG-CD2	5.08	1.49	1.38
8	f	265	SER	CA-CB	5.08	1.61	1.53
3	a	890	ARG	CD-NE	5.08	1.53	1.46
3	l	251	PHE	CA-CB	5.08	1.61	1.53
4	m	544	ASN	C-N	5.08	1.40	1.33
7	p	149	THR	C-N	5.08	1.40	1.33
7	p	236	LYS	N-CA	-5.08	1.39	1.46
9	r	835	PHE	N-CA	-5.08	1.39	1.46
3	a	609	GLY	CA-C	-5.08	1.45	1.52
4	m	317	PHE	CA-CB	5.08	1.61	1.54
3	a	703	ASP	N-CA	5.08	1.52	1.46
4	b	214	ARG	CZ-NH1	5.08	1.39	1.32
6	d	277	LYS	N-CA	-5.08	1.40	1.46
3	l	730	GLU	CA-C	-5.08	1.46	1.52
4	m	284	ALA	N-CA	-5.08	1.40	1.46
9	r	731	GLU	CA-CB	5.08	1.60	1.53
1	X	839	ILE	CA-C	5.07	1.59	1.52
1	X	1492	HIS	ND1-CE1	5.07	1.37	1.32
5	c	194	ILE	N-CA	-5.07	1.40	1.46
4	m	280	VAL	CA-CB	-5.07	1.47	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	m	685	GLU	CA-C	-5.07	1.46	1.52
8	q	457	VAL	CA-CB	-5.07	1.47	1.54
9	r	601	ASN	CA-C	-5.07	1.45	1.52
1	X	960	LEU	CA-C	5.07	1.59	1.52
8	f	382	LYS	N-CA	-5.07	1.38	1.46
8	f	536	ARG	C-N	5.07	1.41	1.33
8	f	627	THR	CA-C	-5.07	1.46	1.52
7	p	165	LEU	CA-C	-5.07	1.45	1.52
9	g	334	TRP	NE1-CE2	-5.07	1.31	1.37
3	l	880	ARG	CD-NE	5.07	1.53	1.46
6	o	109	PRO	C-N	5.07	1.40	1.33
6	o	199	THR	CA-C	5.07	1.58	1.52
1	X	704	ASP	C-N	5.07	1.40	1.33
4	m	211	TRP	CA-C	-5.07	1.45	1.52
6	o	206	TRP	CG-CD2	5.07	1.52	1.43
6	d	95	HIS	CG-ND1	-5.07	1.32	1.38
6	d	252	LYS	CA-C	-5.07	1.46	1.52
8	f	138	ASN	CA-C	-5.07	1.46	1.52
3	l	464	THR	C-O	-5.07	1.19	1.24
4	b	497	ARG	CA-C	-5.07	1.45	1.52
5	c	234	TRP	C-O	-5.07	1.18	1.24
5	n	355	SER	N-CA	-5.07	1.39	1.46
6	o	291	PRO	CA-C	5.07	1.58	1.52
9	r	1140	VAL	CA-C	5.07	1.59	1.52
3	a	555	LYS	CA-C	-5.06	1.46	1.52
1	X	366	SER	CA-CB	5.06	1.61	1.53
1	X	1544	SER	C-N	5.06	1.40	1.34
3	a	797	LEU	CB-CG	5.06	1.63	1.53
4	b	535	ALA	C-N	5.06	1.40	1.33
3	a	917	ASP	C-N	5.06	1.40	1.33
4	b	65	MET	CA-C	-5.06	1.46	1.52
1	X	663	MET	CA-CB	5.06	1.61	1.53
3	a	970	LEU	C-N	5.06	1.40	1.33
9	g	888	ILE	CA-C	-5.06	1.45	1.52
8	q	549	PHE	C-N	5.06	1.40	1.33
3	a	214	ARG	CZ-NH2	5.06	1.40	1.33
9	g	625	GLN	C-N	5.06	1.40	1.33
1	X	766	GLU	C-N	5.06	1.40	1.33
6	o	245	LYS	N-CA	5.06	1.52	1.46
3	a	1031	ARG	NE-CZ	5.05	1.38	1.33
5	c	204	SER	CA-CB	-5.05	1.45	1.53
9	g	554	GLY	CA-C	-5.05	1.44	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
5	n	230	ASP	CA-CB	5.05	1.61	1.53
1	X	1286	THR	CA-C	5.05	1.59	1.52
1	X	880	ASN	CA-CB	5.05	1.62	1.53
7	e	155	LYS	C-N	5.05	1.40	1.33
1	X	835	LEU	C-O	-5.05	1.17	1.24
3	a	350	ASN	CA-CB	5.05	1.59	1.53
9	g	593	ILE	C-N	5.05	1.41	1.33
9	g	993	SER	CA-C	-5.05	1.46	1.52
4	m	418	ALA	CA-C	-5.05	1.45	1.52
9	r	307	LEU	N-CA	-5.05	1.39	1.46
9	r	314	GLU	C-O	-5.05	1.18	1.24
3	a	640	PHE	CA-CB	5.05	1.64	1.54
4	b	332	ILE	C-N	5.05	1.40	1.33
5	n	382	LEU	N-CA	-5.05	1.39	1.46
6	o	269	LEU	CB-CG	5.05	1.63	1.53
7	p	242	ILE	CA-C	-5.05	1.47	1.52
8	q	363	VAL	N-CA	5.05	1.51	1.46
9	r	972	CYS	CA-C	5.05	1.59	1.52
5	c	404	GLN	CA-C	-5.04	1.46	1.52
5	n	631	GLN	C-N	5.04	1.40	1.33
3	a	243	LEU	CA-C	-5.04	1.46	1.52
4	b	414	SER	CA-CB	5.04	1.61	1.53
3	l	718	SER	N-CA	-5.04	1.39	1.46
6	o	236	GLN	N-CA	-5.04	1.39	1.46
8	q	419	LEU	C-N	5.04	1.41	1.33
1	X	961	GLU	N-CA	-5.04	1.40	1.46
3	a	556	ASN	C-N	5.04	1.40	1.33
9	r	536	GLU	N-CA	-5.04	1.39	1.46
9	r	874	PHE	CA-CB	5.04	1.62	1.53
5	c	305	ARG	CZ-NH1	5.04	1.39	1.32
5	n	239	ILE	C-O	-5.04	1.17	1.24
9	r	929	LEU	CA-C	-5.04	1.46	1.52
3	l	814	THR	C-N	5.04	1.40	1.33
7	e	217	SER	C-N	5.04	1.40	1.33
9	g	571	VAL	CA-CB	-5.04	1.49	1.54
3	l	701	TYR	CA-C	-5.04	1.46	1.52
4	m	155	LEU	C-N	5.04	1.41	1.33
1	X	1210	LEU	CA-C	-5.03	1.46	1.52
1	X	1236	LEU	C-N	5.03	1.41	1.34
1	X	1541	LEU	CA-CB	5.03	1.61	1.53
3	a	473	VAL	CA-C	-5.03	1.48	1.53
3	a	585	ASP	CA-C	-5.03	1.46	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	a	670	GLN	CA-C	-5.03	1.46	1.52
3	a	700	ALA	N-CA	-5.03	1.40	1.46
4	b	261	ALA	CA-CB	5.03	1.61	1.53
4	b	420	THR	CA-CB	5.03	1.61	1.53
5	c	143	ARG	CZ-NH2	5.03	1.40	1.33
8	f	704	LEU	N-CA	-5.03	1.39	1.46
3	l	408	PHE	CA-CB	5.03	1.61	1.53
3	l	837	SER	C-N	5.03	1.41	1.34
4	m	280	VAL	CA-C	5.03	1.59	1.52
5	n	199	ILE	C-N	5.03	1.41	1.33
1	X	1398	VAL	CA-C	-5.03	1.47	1.52
7	p	34	LYS	C-N	5.03	1.39	1.33
1	X	1051	LYS	C-N	5.03	1.40	1.33
4	b	426	ALA	C-N	5.03	1.40	1.33
5	c	265	HIS	ND1-CE1	5.03	1.37	1.32
5	c	435	TYR	CA-C	-5.03	1.46	1.52
9	g	977	ASN	C-N	5.03	1.40	1.33
3	l	565	THR	CA-CB	-5.03	1.45	1.53
8	q	237	ILE	C-N	5.03	1.40	1.33
8	q	408	ASP	C-N	5.03	1.40	1.33
1	X	1309	ARG	CA-CB	5.03	1.60	1.53
4	b	477	GLY	C-N	5.03	1.40	1.33
8	f	177	ASP	C-N	5.03	1.40	1.33
3	a	662	PHE	C-O	-5.03	1.17	1.24
5	c	264	ARG	CD-NE	5.03	1.53	1.46
8	f	169	LEU	CA-C	-5.03	1.46	1.52
6	o	152	SER	CA-C	-5.03	1.46	1.52
7	p	320	SER	CA-CB	5.03	1.59	1.52
5	c	656	ALA	C-N	5.03	1.40	1.34
6	d	58	ARG	NE-CZ	5.03	1.38	1.33
7	e	70	ARG	CD-NE	5.03	1.53	1.46
3	l	96	HIS	CA-C	5.03	1.58	1.52
7	p	138	ASP	C-N	5.03	1.40	1.33
9	r	1148	ILE	CA-CB	5.03	1.62	1.54
1	X	809	PRO	C-O	5.02	1.30	1.24
3	a	498	HIS	ND1-CE1	5.02	1.37	1.32
8	f	210	MET	C-O	-5.02	1.18	1.24
7	p	121	LEU	C-N	5.02	1.40	1.33
5	c	324	TYR	CA-CB	5.02	1.60	1.52
7	e	220	TRP	N-CA	-5.02	1.39	1.46
8	f	535	ARG	CZ-NH1	5.02	1.39	1.32
9	g	1146	TYR	CA-CB	5.02	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	m	590	VAL	C-N	5.02	1.40	1.33
7	p	133	ILE	N-CA	-5.02	1.40	1.46
4	b	168	ARG	CA-C	-5.02	1.46	1.52
5	n	626	ASP	C-N	5.02	1.40	1.33
3	a	413	SER	C-N	5.02	1.40	1.34
3	a	743	ASN	CG-ND2	5.02	1.43	1.33
6	d	213	SER	CA-C	5.02	1.58	1.53
7	e	8	HIS	ND1-CE1	5.02	1.37	1.32
8	f	349	SER	CA-CB	5.02	1.61	1.53
8	f	703	LEU	CA-CB	5.02	1.61	1.53
5	n	147	SER	CA-C	-5.02	1.46	1.52
5	n	489	HIS	CB-CG	5.02	1.57	1.50
7	p	53	ALA	C-N	5.02	1.40	1.33
9	r	623	LEU	C-N	5.02	1.40	1.33
1	X	382	PHE	CA-C	-5.02	1.46	1.52
1	X	1427	SER	N-CA	-5.02	1.39	1.46
5	c	466	SER	CA-C	-5.02	1.46	1.52
7	e	13	HIS	ND1-CE1	5.02	1.37	1.32
7	e	146	ARG	CD-NE	5.02	1.53	1.46
5	n	369	LEU	C-O	5.02	1.30	1.24
7	e	304	ASN	CA-C	-5.02	1.47	1.53
3	l	573	GLU	CA-C	5.02	1.59	1.52
5	c	509	ARG	N-CA	-5.01	1.40	1.46
5	c	643	ILE	CA-CB	-5.01	1.47	1.54
5	c	773	PRO	C-N	5.01	1.40	1.33
8	f	19	LEU	C-N	5.01	1.40	1.33
8	f	43	ARG	CZ-NH1	5.01	1.39	1.32
3	l	874	ASN	CA-C	-5.01	1.46	1.52
4	m	71	LEU	CA-CB	5.01	1.59	1.53
7	p	8	HIS	ND1-CE1	5.01	1.37	1.32
4	b	724	MET	CG-SD	5.01	1.93	1.80
6	d	144	HIS	ND1-CE1	5.01	1.37	1.32
3	l	157	ASP	CA-CB	5.01	1.61	1.53
4	b	149	GLU	CA-C	5.01	1.59	1.52
7	e	184	ALA	N-CA	-5.01	1.39	1.46
8	f	355	LEU	CA-C	5.01	1.59	1.52
6	o	289	TRP	NE1-CE2	-5.01	1.31	1.37
9	r	868	HIS	CG-ND1	5.01	1.43	1.38
9	r	553	LEU	N-CA	-5.01	1.40	1.46
6	d	34	LYS	CA-CB	5.01	1.59	1.52
3	l	161	ARG	NE-CZ	5.01	1.38	1.33
3	l	349	LEU	CA-CB	5.01	1.61	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	b	142	ALA	CA-CB	5.00	1.61	1.53
5	c	439	ARG	NE-CZ	5.00	1.38	1.33
8	f	478	ARG	CD-NE	5.00	1.53	1.46
6	o	261	SER	CA-C	-5.00	1.46	1.52
8	q	124	VAL	CA-C	5.00	1.59	1.52
7	e	305	GLY	N-CA	5.00	1.50	1.45
9	g	790	HIS	CA-C	-5.00	1.46	1.52
3	l	442	TYR	C-N	5.00	1.40	1.33
3	l	452	ASP	CA-C	-5.00	1.48	1.53
8	q	469	ARG	CD-NE	5.00	1.53	1.46

All (5348) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	72	LEU	O-C-N	-85.55	23.37	121.76
9	r	325	PRO	N-CA-CB	65.10	148.57	102.35
9	r	431	SER	O-C-N	-59.46	43.50	122.59
9	r	155	PRO	N-CA-CB	44.27	148.65	102.17
9	r	274	PRO	N-CA-CB	43.52	148.95	103.25
9	r	304	PRO	N-CA-CB	43.32	148.74	103.25
9	r	150	PRO	N-CA-CB	42.57	148.78	103.23
9	r	251	PRO	N-CA-CB	41.67	148.57	103.15
9	r	155	PRO	CA-N-CD	-33.49	65.11	112.00
9	r	325	PRO	CA-N-CD	-33.38	65.27	112.00
9	r	150	PRO	CA-N-CD	-33.37	65.29	112.00
9	r	251	PRO	CA-N-CD	-33.30	65.37	112.00
9	r	304	PRO	CA-N-CD	-32.86	66.00	112.00
9	r	274	PRO	CA-N-CD	-32.83	66.04	112.00
1	X	794	ILE	N-CA-CB	31.60	163.36	111.23
9	r	74	THR	N-CA-CB	31.17	155.86	110.04
9	r	300	THR	N-CA-CB	31.07	155.79	110.12
9	r	155	PRO	CB-CA-C	-30.79	75.52	110.00
9	r	391	THR	N-CA-CB	29.93	156.10	110.60
9	r	286	THR	N-CA-CB	29.31	156.38	110.65
9	r	287	THR	N-CA-CB	29.07	155.52	110.46
9	r	263	THR	N-CA-CB	29.05	155.41	109.51
9	r	393	THR	N-CA-CB	29.02	155.83	110.56
9	r	325	PRO	CB-CA-C	-28.04	74.95	113.09
9	r	414	THR	N-CA-CB	27.98	156.04	110.43
9	r	268	VAL	N-CA-CB	27.97	142.25	110.65
9	r	280	THR	N-CA-CB	27.11	156.35	110.81
9	r	413	VAL	N-CA-CB	26.57	142.30	111.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	410	THR	N-CA-CB	26.15	156.04	110.80
9	r	145	THR	N-CA-CB	25.16	156.15	110.87
9	r	215	GLU	C-N-CD	-24.43	24.84	125.00
9	r	263	THR	CB-CA-C	-23.77	75.93	110.16
9	r	150	PRO	CB-CA-C	-23.02	76.47	113.06
1	X	1304	LYS	N-CA-CB	22.61	148.70	110.49
9	r	251	PRO	CB-CA-C	-22.23	75.64	113.20
1	X	794	ILE	N-CA-C	-21.90	63.79	109.34
9	r	304	PRO	CB-CA-C	-21.47	76.14	111.56
9	r	268	VAL	CB-CA-C	-21.01	84.77	111.87
9	r	267	VAL	N-CA-CB	20.97	142.03	110.58
1	X	1059	ASN	N-CA-C	20.91	142.89	109.85
9	r	274	PRO	CB-CA-C	-20.66	77.47	111.56
9	r	267	VAL	CB-CA-C	-20.64	83.73	112.22
9	r	300	THR	CB-CA-C	-20.37	76.97	110.79
9	r	287	THR	CB-CA-C	-19.64	76.47	110.45
9	r	393	THR	CB-CA-C	-19.62	77.43	109.80
9	r	125	ARG	NH1-CZ-NH2	19.45	144.58	119.30
9	r	271	ARG	NH1-CZ-NH2	19.45	144.58	119.30
9	r	281	ARG	NH1-CZ-NH2	19.44	144.57	119.30
9	r	450	ARG	NH1-CZ-NH2	19.43	144.56	119.30
9	r	234	ARG	NH1-CZ-NH2	19.41	144.53	119.30
9	r	227	ARG	NH1-CZ-NH2	19.39	144.51	119.30
9	r	382	ARG	NH1-CZ-NH2	19.38	144.50	119.30
9	r	137	ARG	NH1-CZ-NH2	19.38	144.50	119.30
9	r	441	ARG	NH1-CZ-NH2	19.37	144.48	119.30
9	r	166	ILE	N-CA-CB	19.37	131.83	110.72
9	r	440	ARG	NH1-CZ-NH2	19.36	144.47	119.30
9	r	413	VAL	CB-CA-C	-19.34	84.48	110.98
9	r	414	THR	CB-CA-C	-19.25	77.98	109.75
9	r	416	ILE	N-CA-CB	18.55	131.82	110.49
9	r	286	THR	CB-CA-C	-18.54	79.38	110.16
9	r	74	THR	CB-CA-C	-18.09	77.24	109.62
3	l	416	GLY	N-CA-C	18.05	155.97	113.18
9	r	367	ILE	N-CA-CB	17.71	131.93	111.39
9	r	391	THR	CB-CA-C	-17.41	78.22	111.48
9	r	410	THR	CB-CA-C	-17.35	78.30	109.70
9	r	280	THR	CB-CA-C	-17.26	79.45	109.65
1	X	1304	LYS	N-CA-C	-17.22	74.13	110.80
8	q	482	ARG	N-CA-CB	17.15	139.65	110.50
9	r	291	ILE	N-CA-CB	17.07	131.30	110.31
9	r	94	ILE	CB-CA-C	-16.91	90.37	111.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	367	ILE	CB-CA-C	-16.79	93.10	111.23
9	r	260	ILE	N-CA-CB	16.64	130.77	110.31
9	r	80	PHE	O-C-N	-16.57	100.56	122.59
4	b	253	VAL	N-CA-C	-16.55	97.20	112.43
9	r	233	ILE	N-CA-CB	15.98	130.97	111.31
9	r	366	ILE	N-CA-CB	15.59	131.91	111.64
3	l	415	TYR	N-CA-CB	15.47	139.04	111.96
9	r	167	ILE	CB-CA-C	-15.46	90.88	112.22
1	X	1059	ASN	CB-CA-C	-15.45	79.70	109.66
9	r	233	ILE	CB-CA-C	-15.44	91.64	111.25
9	r	256	ILE	CB-CA-C	-15.40	92.10	111.20
3	l	415	TYR	CB-CA-C	15.04	136.97	111.86
9	r	256	ILE	N-CA-CB	14.70	131.22	112.26
9	r	145	THR	CB-CA-C	-14.69	78.37	113.19
9	r	166	ILE	CB-CA-C	-14.32	93.15	110.91
9	g	852	ILE	N-CA-C	-14.31	100.31	111.62
4	m	402	ILE	N-CA-C	-14.31	99.26	112.43
1	X	1277	ILE	CB-CA-C	14.10	134.42	111.29
9	r	125	ARG	NE-CZ-NH1	-13.83	107.67	121.50
9	r	450	ARG	NE-CZ-NH1	-13.82	107.68	121.50
9	r	281	ARG	NE-CZ-NH1	-13.80	107.70	121.50
9	r	137	ARG	NE-CZ-NH1	-13.78	107.72	121.50
9	r	227	ARG	NE-CZ-NH1	-13.78	107.72	121.50
9	r	234	ARG	NE-CZ-NH1	-13.77	107.73	121.50
9	r	271	ARG	NE-CZ-NH1	-13.74	107.75	121.50
9	r	440	ARG	NE-CZ-NH1	-13.72	107.78	121.50
9	r	441	ARG	NE-CZ-NH1	-13.72	107.78	121.50
9	r	382	ARG	NE-CZ-NH1	-13.68	107.82	121.50
9	r	94	ILE	N-CA-CB	13.56	130.32	112.28
9	r	260	ILE	CB-CA-C	-13.54	91.15	111.33
9	r	390	ILE	CB-CA-C	-13.52	90.26	110.81
9	r	396	LYS	C-N-CD	-13.44	69.90	125.00
9	r	167	ILE	N-CA-CB	13.30	130.53	110.58
8	f	576	ASN	CA-C-O	-13.26	101.54	120.51
9	r	165	ILE	CB-CA-C	-13.22	90.92	110.62
1	X	265	PHE	CA-CB-CG	13.11	126.91	113.80
9	g	405	GLU	N-CA-C	-13.04	96.77	113.72
9	g	1011	ASP	CA-CB-CG	12.93	125.53	112.60
9	r	291	ILE	CB-CA-C	-12.92	92.07	111.33
4	b	76	TYR	N-CA-C	-12.89	98.19	114.56
9	r	340	GLN	O-C-N	-12.86	107.93	123.36
1	X	794	ILE	CB-CA-C	12.85	132.36	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	271	ARG	NE-CZ-NH2	-12.82	107.66	119.20
9	r	382	ARG	NE-CZ-NH2	-12.80	107.68	119.20
1	X	793	LEU	N-CA-CB	12.77	132.21	110.50
9	g	845	PHE	CA-CB-CG	-12.77	101.03	113.80
9	r	281	ARG	NE-CZ-NH2	-12.75	107.72	119.20
9	r	234	ARG	NE-CZ-NH2	-12.74	107.73	119.20
9	r	441	ARG	NE-CZ-NH2	-12.74	107.74	119.20
9	r	440	ARG	NE-CZ-NH2	-12.72	107.75	119.20
9	r	125	ARG	NE-CZ-NH2	-12.72	107.75	119.20
9	r	450	ARG	NE-CZ-NH2	-12.71	107.76	119.20
9	r	227	ARG	NE-CZ-NH2	-12.71	107.76	119.20
1	X	1060	LEU	CB-CA-C	12.69	135.68	110.42
9	r	137	ARG	NE-CZ-NH2	-12.69	107.78	119.20
3	l	397	ILE	N-CA-C	-12.68	100.66	113.47
1	X	1277	ILE	CA-C-O	12.57	136.49	120.78
9	r	275	ILE	N-CA-CB	12.52	131.88	111.23
8	f	575	GLU	CB-CA-C	-12.46	86.42	110.10
9	r	372	SER	CB-CA-C	-12.42	94.09	111.73
8	q	575	GLU	N-CA-C	-12.42	76.22	111.00
9	r	366	ILE	CB-CA-C	-12.35	93.23	110.77
9	r	81	SER	N-CA-CB	12.34	127.03	110.25
3	l	415	TYR	N-CA-C	-12.26	83.55	108.18
1	X	1303	LEU	N-CA-CB	12.25	131.33	110.50
9	r	90	ILE	N-CA-CB	12.17	131.40	111.44
1	X	1304	LYS	CB-CA-C	12.13	134.56	110.42
1	X	1165	ILE	N-CA-C	-12.13	102.08	111.90
1	X	134	ARG	N-CA-C	-12.09	99.52	114.75
9	r	416	ILE	CB-CA-C	-11.94	93.06	111.69
9	r	90	ILE	CB-CA-C	-11.93	92.13	110.50
1	X	793	LEU	CB-CA-C	-11.93	87.44	110.10
9	r	885	VAL	N-CA-C	-11.86	101.81	113.20
9	r	265	SER	CB-CA-C	-11.83	92.51	110.26
9	r	302	SER	CB-CA-C	-11.81	94.87	112.11
9	r	343	SER	CB-CA-C	-11.79	93.15	111.66
4	b	695	ILE	N-CA-C	-11.74	101.63	112.90
8	f	37	ASN	CA-CB-CG	11.69	124.29	112.60
4	b	121	ASP	CA-CB-CG	11.66	124.26	112.60
4	m	606	ILE	CA-C-N	11.55	127.52	120.24
4	m	606	ILE	C-N-CA	11.55	127.52	120.24
8	q	561	ASN	N-CA-C	-11.53	99.35	113.41
8	q	576	ASN	CA-CB-CG	-11.50	101.10	112.60
9	r	144	ALA	O-C-N	-11.45	107.36	122.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	146	SER	N-CA-C	11.44	123.83	111.36
3	a	931	ASP	CA-CB-CG	11.42	124.02	112.60
3	a	22	ASN	CA-CB-CG	11.36	123.95	112.60
5	n	633	THR	N-CA-C	-11.34	98.97	113.72
8	f	637	ASP	CA-CB-CG	11.34	123.94	112.60
9	r	415	SER	N-CA-CB	11.33	127.30	110.65
1	X	1276	LYS	N-CA-CB	11.25	129.63	110.50
3	a	1032	ASP	CA-CB-CG	11.13	123.73	112.60
8	q	423	GLN	N-CA-C	-11.12	99.13	111.14
3	l	293	LEU	N-CA-C	-11.12	94.16	110.06
5	c	659	ASN	CA-CB-CG	11.10	123.70	112.60
8	q	575	GLU	CB-CA-C	-11.10	89.01	110.10
9	r	165	ILE	N-CA-CB	11.07	130.66	111.39
9	r	436	SER	N-CA-CB	11.06	126.74	109.71
1	X	262	SER	CA-C-N	11.06	136.52	120.38
1	X	262	SER	C-N-CA	11.06	136.52	120.38
7	p	69	GLY	CA-C-O	-11.00	114.64	122.23
9	r	275	ILE	CB-CA-C	-10.97	93.30	111.29
9	g	409	ASP	N-CA-C	10.96	124.49	110.24
9	r	236	SER	N-CA-CB	10.86	126.08	110.12
3	a	569	ILE	N-CA-C	10.84	121.67	110.62
9	r	154	ASN	C-N-CD	10.83	169.40	125.00
4	m	102	LYS	N-CA-C	-10.75	100.70	114.04
9	g	229	PHE	CA-CB-CG	-10.75	103.05	113.80
9	r	251	PRO	N-CD-CG	-10.73	87.11	103.20
9	r	344	SER	CB-CA-C	-10.72	94.57	111.51
9	r	713	ASP	CA-CB-CG	10.72	123.32	112.60
9	r	77	SER	N-CA-CB	10.68	126.08	110.06
3	l	963	LYS	N-CA-C	-10.65	100.34	113.97
3	a	343	ASN	CA-CB-CG	10.61	123.21	112.60
9	r	78	SER	N-CA-CB	10.60	126.71	110.28
9	r	298	SER	N-CA-CB	10.56	127.81	110.39
3	a	927	ASN	CA-CB-CG	-10.54	102.06	112.60
1	X	1223	ASN	N-CA-C	-10.52	99.76	112.59
8	f	435	PHE	CA-CB-CG	-10.51	103.29	113.80
1	X	793	LEU	N-CA-C	10.48	140.34	111.00
6	o	146	ILE	N-CA-C	-10.47	102.85	112.90
6	d	130	PHE	CA-CB-CG	-10.46	103.34	113.80
9	r	370	SER	CB-CA-C	-10.46	93.79	111.26
9	g	1078	LEU	CA-C-O	-10.43	111.43	120.19
9	r	150	PRO	N-CD-CG	-10.41	87.58	103.20
9	g	860	LEU	N-CA-C	-10.40	100.60	113.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	236	SER	CB-CA-C	-10.37	93.57	110.79
3	a	199	PHE	CA-CB-CG	-10.36	103.44	113.80
9	r	266	SER	CB-CA-C	-10.35	93.57	110.74
4	b	692	ILE	N-CA-C	-10.34	102.16	113.43
8	f	663	LEU	CA-C-N	10.32	134.48	120.54
8	f	663	LEU	C-N-CA	10.32	134.48	120.54
9	r	436	SER	CB-CA-C	-10.32	94.78	110.26
1	X	694	ILE	N-CA-C	-10.32	102.94	112.43
8	f	576	ASN	CB-CA-C	10.31	130.94	110.42
9	r	96	TYR	N-CA-CB	10.31	125.39	109.83
9	r	390	ILE	N-CA-CB	10.30	130.26	111.21
3	l	840	PHE	CA-CB-CG	-10.28	103.52	113.80
7	e	342	MET	N-CA-C	-10.26	102.92	114.62
9	r	354	SER	N-CA-CB	10.26	126.35	110.14
1	X	1060	LEU	N-CA-CB	10.26	127.82	110.49
9	g	682	LEU	N-CA-C	-10.25	100.85	113.97
8	q	281	ASP	CA-CB-CG	10.20	122.80	112.60
9	r	269	SER	N-CA-CB	10.17	127.68	110.49
4	m	352	THR	CA-C-N	10.16	133.65	120.44
4	m	352	THR	C-N-CA	10.16	133.65	120.44
3	l	735	LYS	N-CA-C	-10.16	100.97	113.97
3	a	575	ASN	CA-CB-CG	10.15	122.75	112.60
9	g	702	ASP	CA-CB-CG	10.14	122.74	112.60
4	b	606	ILE	CA-C-N	10.13	126.62	120.24
4	b	606	ILE	C-N-CA	10.13	126.62	120.24
9	r	265	SER	N-CA-CB	10.09	125.24	109.71
7	e	18	ASP	CA-CB-CG	10.08	122.68	112.60
4	b	603	ASP	N-CA-CB	10.08	127.53	110.49
9	r	435	SER	N-CA-CB	10.07	127.28	110.87
4	m	686	ASP	CA-CB-CG	10.04	122.64	112.60
1	X	1059	ASN	CA-CB-CG	-10.03	102.57	112.60
8	f	575	GLU	N-CA-C	-10.03	82.93	111.00
4	b	552	ILE	N-CA-C	-10.02	103.19	111.81
9	r	149	SER	C-N-CD	10.02	166.09	125.00
9	r	273	GLY	C-N-CD	10.02	166.09	125.00
8	f	323	THR	N-CA-C	-10.01	95.71	110.52
9	r	77	SER	CB-CA-C	-10.00	93.68	110.68
9	r	324	TYR	C-N-CD	9.99	165.97	125.00
3	a	807	ILE	N-CA-C	-9.93	103.80	113.53
7	p	41	ASP	CA-CB-CG	9.93	122.53	112.60
4	m	366	PRO	N-CA-CB	9.92	109.97	102.73
9	r	266	SER	N-CA-CB	9.92	125.94	109.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	453	VAL	N-CA-C	-9.91	103.87	111.90
9	r	199	PRO	CA-N-CD	-9.89	98.15	112.00
9	r	435	SER	CB-CA-C	-9.89	95.94	111.17
1	X	766	GLU	N-CA-C	-9.88	99.01	112.94
7	e	239	ARG	NE-CZ-NH2	9.87	128.09	119.20
1	X	1616	ILE	N-CA-CB	9.85	121.46	110.72
3	l	549	LYS	CA-C-O	-9.84	110.49	120.82
3	l	944	ILE	N-CA-C	-9.83	103.94	111.90
9	g	82	ASN	OD1-CG-ND2	-9.82	112.78	122.60
3	l	416	GLY	CA-C-O	9.81	137.64	120.57
3	a	893	HIS	N-CA-C	-9.80	100.82	113.17
9	r	355	SER	N-CA-CB	9.80	126.29	110.42
8	f	37	ASN	CA-C-N	9.80	134.33	120.42
8	f	37	ASN	C-N-CA	9.80	134.33	120.42
9	r	437	TYR	CB-CA-C	-9.77	98.77	111.86
9	g	266	SER	N-CA-C	-9.76	100.87	113.17
9	r	356	CYS	N-CA-CB	9.76	125.89	110.57
3	l	878	HIS	CA-CB-CG	-9.75	104.05	113.80
8	f	662	PHE	CA-CB-CG	9.73	123.53	113.80
9	r	155	PRO	N-CD-CG	-9.73	88.60	103.20
9	r	158	GLN	N-CA-CB	9.72	124.33	109.85
9	r	208	CYS	CB-CA-C	-9.71	94.36	110.29
1	X	1235	LYS	N-CA-C	-9.71	101.44	113.38
1	X	182	PHE	CA-CB-CG	-9.70	104.10	113.80
1	X	704	ASP	N-CA-C	-9.70	99.13	112.12
9	r	208	CYS	N-CA-CB	9.68	125.64	109.87
9	g	656	VAL	N-CA-C	-9.67	95.02	108.27
9	r	92	MET	N-CA-CB	9.67	124.33	110.12
6	d	53	GLU	CA-C-O	9.62	130.75	120.36
4	b	530	ARG	NE-CZ-NH2	9.62	127.85	119.20
9	r	437	TYR	N-CA-CB	9.61	126.52	111.91
1	X	801	LYS	CA-C-N	9.61	133.52	120.54
1	X	801	LYS	C-N-CA	9.61	133.52	120.54
9	r	371	SER	N-CA-CB	9.61	126.33	110.39
5	c	277	GLY	CA-C-N	9.60	129.32	118.85
5	c	277	GLY	C-N-CA	9.60	129.32	118.85
1	X	1465	LEU	N-CA-C	-9.59	100.45	112.72
9	g	923	HIS	CA-CB-CG	9.55	123.36	113.80
4	m	604	ASP	N-CA-C	-9.55	100.48	113.18
3	l	523	ASP	CA-CB-CG	9.54	122.14	112.60
9	g	128	ASP	N-CA-C	-9.54	101.19	112.92
8	q	42	PHE	CA-CB-CG	9.53	123.33	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	143	ASN	CA-CB-CG	-9.52	103.08	112.60
8	f	17	ASP	CA-CB-CG	9.52	122.12	112.60
4	b	226	GLN	N-CA-C	-9.52	99.52	112.94
9	r	302	SER	N-CA-CB	9.50	126.75	111.74
3	l	559	GLU	CA-C-O	-9.50	111.21	121.56
3	a	1010	PHE	CA-CB-CG	-9.50	104.30	113.80
4	m	196	ASP	CA-C-N	9.49	132.84	120.60
4	m	196	ASP	C-N-CA	9.49	132.84	120.60
9	r	438	SER	N-CA-CB	9.49	126.14	110.39
9	r	76	TYR	N-CA-CB	9.49	125.10	109.92
1	X	1250	ILE	N-CA-C	-9.48	104.10	113.20
9	g	298	SER	CA-C-N	9.46	132.74	120.44
9	g	298	SER	C-N-CA	9.46	132.74	120.44
9	r	344	SER	N-CA-CB	9.46	126.67	112.30
9	r	717	CYS	N-CA-C	-9.44	102.14	114.31
8	f	629	GLU	N-CA-C	-9.43	98.99	113.89
9	r	92	MET	CB-CA-C	-9.43	95.13	110.79
9	r	149	SER	N-CA-CB	9.43	127.15	110.37
5	c	204	SER	CA-C-O	-9.43	110.92	120.82
9	r	325	PRO	N-CD-CG	-9.42	89.08	103.20
5	n	221	LEU	N-CA-CB	9.39	121.15	110.35
5	c	624	VAL	N-CA-C	-9.36	104.36	113.53
9	g	826	SER	N-CA-C	-9.35	101.57	113.72
5	c	147	SER	N-CA-CB	9.34	126.28	110.49
9	r	372	SER	N-CA-CB	9.34	126.23	112.13
8	q	482	ARG	CB-CA-C	-9.32	92.39	110.10
6	d	175	THR	CA-C-N	9.31	129.13	122.33
6	d	175	THR	C-N-CA	9.31	129.13	122.33
4	b	166	ASP	CA-CB-CG	9.31	121.91	112.60
9	g	354	SER	CA-C-O	-9.30	110.78	121.66
3	a	979	GLU	N-CA-C	9.28	121.39	111.28
3	l	81	PHE	CA-CB-CG	-9.28	104.52	113.80
9	r	304	PRO	N-CD-CG	-9.26	89.31	103.20
4	m	486	ILE	CA-C-N	9.26	131.98	120.22
4	m	486	ILE	C-N-CA	9.26	131.98	120.22
5	c	650	HIS	CA-CB-CG	9.25	123.05	113.80
1	X	1545	SER	CA-C-N	9.24	133.01	120.54
1	X	1545	SER	C-N-CA	9.24	133.01	120.54
4	m	387	THR	N-CA-C	-9.24	102.52	113.88
8	q	222	VAL	N-CA-C	-9.22	104.95	113.71
9	g	1067	ASP	CA-CB-CG	9.21	121.81	112.60
8	q	179	ILE	N-CA-C	9.21	119.19	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1130	PHE	N-CA-C	-9.19	99.39	111.71
3	l	124	LYS	N-CA-C	9.19	121.38	111.36
9	r	274	PRO	N-CD-CG	-9.19	89.42	103.20
9	r	450	ARG	N-CA-C	9.19	124.37	109.76
3	l	835	ASN	N-CA-C	-9.18	102.59	113.88
9	r	817	THR	N-CA-C	-9.18	102.91	114.56
5	n	289	ASN	CA-CB-CG	9.17	121.77	112.60
1	X	1059	ASN	N-CA-CB	9.15	126.03	111.20
8	f	73	ARG	CA-C-N	9.14	132.87	120.44
8	f	73	ARG	C-N-CA	9.14	132.87	120.44
9	r	836	PHE	CA-C-N	9.14	132.87	120.44
9	r	836	PHE	C-N-CA	9.14	132.87	120.44
3	a	10	ASN	CA-CB-CG	-9.14	103.46	112.60
9	r	199	PRO	N-CA-CB	9.13	112.83	103.25
4	m	433	ILE	N-CA-C	-9.12	104.26	113.10
3	l	705	LEU	CA-C-N	9.11	132.49	120.28
3	l	705	LEU	C-N-CA	9.11	132.49	120.28
3	a	7	ILE	CA-C-O	9.10	129.46	120.27
6	d	38	VAL	CB-CA-C	-9.09	101.42	111.23
7	p	131	ASP	CA-CB-CG	9.08	121.68	112.60
9	r	118	PRO	CA-N-CD	-9.07	99.30	112.00
8	f	597	TYR	N-CA-C	-9.06	101.12	112.72
8	q	17	ASP	CA-C-N	9.05	132.76	120.54
8	q	17	ASP	C-N-CA	9.05	132.76	120.54
9	r	237	MET	CB-CA-C	-9.05	94.25	109.99
9	g	493	PHE	N-CA-C	-9.04	99.12	111.87
9	r	404	MET	N-CA-CB	9.03	124.53	110.44
3	a	335	VAL	N-CA-C	-9.03	97.80	108.82
5	n	524	ASP	CA-C-O	-9.03	111.24	120.90
3	l	14	TYR	N-CA-C	-9.01	91.61	110.80
5	n	366	PHE	N-CA-C	-9.01	103.40	114.75
8	q	181	PHE	CA-CB-CG	-9.01	104.79	113.80
8	q	679	LYS	N-CA-C	-9.01	102.45	112.72
9	r	343	SER	N-CA-CB	9.01	125.68	112.08
1	X	1277	ILE	N-CA-CB	9.00	126.09	111.23
3	l	685	GLU	N-CA-C	-9.00	102.43	113.41
7	p	57	SER	O-C-N	9.00	134.98	123.01
1	X	923	LEU	CA-C-N	8.98	132.74	121.06
1	X	923	LEU	C-N-CA	8.98	132.74	121.06
9	g	498	VAL	CA-C-O	8.97	130.16	120.47
5	c	242	ASP	N-CA-C	-8.96	95.06	109.40
3	l	109	THR	CA-C-N	8.96	131.47	122.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	109	THR	C-N-CA	8.96	131.47	122.96
4	b	694	VAL	O-C-N	-8.96	112.56	121.78
9	r	250	LYS	C-N-CD	8.95	161.70	125.00
3	l	752	HIS	CG-CD2-NE2	8.95	116.15	107.20
5	c	267	ARG	CA-C-N	8.95	135.42	121.19
5	c	267	ARG	C-N-CA	8.95	135.42	121.19
6	d	99	SER	N-CA-C	-8.95	100.13	112.12
1	X	1172	SER	CA-C-O	-8.94	107.73	120.51
1	X	949	LEU	CA-C-N	8.94	132.06	120.44
1	X	949	LEU	C-N-CA	8.94	132.06	120.44
4	b	532	PRO	N-CA-C	-8.94	103.24	114.68
8	q	580	PHE	CA-CB-CG	-8.93	104.87	113.80
3	a	103	ASN	CA-CB-CG	8.93	121.53	112.60
6	d	91	GLN	OE1-CD-NE2	8.90	131.50	122.60
5	n	412	LEU	N-CA-C	-8.90	96.87	109.24
3	a	940	VAL	CA-C-O	-8.86	114.72	120.66
1	X	1193	ASN	CA-CB-CG	8.85	121.45	112.60
8	q	561	ASN	CA-C-N	8.85	137.63	121.70
8	q	561	ASN	C-N-CA	8.85	137.63	121.70
6	d	149	ASN	CA-CB-CG	-8.84	103.76	112.60
1	X	1276	LYS	N-CA-C	8.84	135.75	111.00
3	a	1017	TRP	N-CA-CB	8.84	125.42	110.49
7	e	313	ASN	CA-CB-CG	8.82	121.42	112.60
3	l	640	PHE	CA-CB-CG	-8.82	104.98	113.80
3	l	781	ASP	CA-CB-CG	8.82	121.42	112.60
3	l	180	ASP	CA-CB-CG	8.81	121.41	112.60
9	g	1124	ASN	N-CA-C	-8.81	102.27	113.72
9	r	237	MET	N-CA-CB	8.80	123.92	110.80
9	g	130	ASP	CA-CB-CG	8.80	121.40	112.60
6	d	176	GLY	CA-C-N	8.80	129.48	120.60
6	d	176	GLY	C-N-CA	8.80	129.48	120.60
3	l	158	PHE	CA-CB-CG	8.78	122.58	113.80
4	b	190	PHE	N-CA-CB	8.77	123.33	110.26
1	X	205	PRO	CB-CA-C	8.77	122.45	111.23
9	r	517	PRO	N-CA-C	8.76	121.38	110.70
1	X	881	SER	CA-C-N	8.75	134.71	120.63
1	X	881	SER	C-N-CA	8.75	134.71	120.63
5	n	272	ILE	CA-C-N	8.75	131.58	120.56
5	n	272	ILE	C-N-CA	8.75	131.58	120.56
3	l	542	ASP	CA-CB-CG	8.74	121.34	112.60
9	r	89	TYR	O-C-N	-8.73	112.16	123.16
4	b	213	ASN	CA-CB-CG	-8.73	103.87	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	m	525	ILE	N-CA-C	-8.73	104.09	112.29
9	r	546	ILE	N-CA-CB	8.73	123.43	111.21
5	c	505	ASP	CA-CB-CG	8.72	121.32	112.60
9	r	952	ASP	CA-CB-CG	-8.72	103.88	112.60
8	f	78	VAL	CA-C-N	8.72	131.78	120.44
8	f	78	VAL	C-N-CA	8.72	131.78	120.44
6	o	12	ILE	CA-C-O	-8.71	112.87	121.58
8	f	698	ASN	CA-CB-CG	-8.70	103.90	112.60
3	l	643	ASP	CA-CB-CG	-8.69	103.92	112.60
9	r	298	SER	CB-CA-C	-8.68	96.72	111.31
9	r	356	CYS	CB-CA-C	-8.68	94.71	109.72
9	r	352	TYR	O-C-N	-8.67	111.46	123.34
9	r	93	GLN	N-CA-CB	8.66	122.56	109.91
9	g	556	HIS	CG-CD2-NE2	8.66	115.86	107.20
9	g	794	LYS	N-CA-C	-8.65	103.85	114.75
4	m	49	VAL	CA-C-O	-8.65	115.44	119.94
1	X	1236	LEU	N-CA-C	-8.64	100.75	112.94
4	b	655	PHE	CA-CB-CG	-8.64	105.16	113.80
8	q	36	PHE	CA-CB-CG	-8.64	105.16	113.80
3	a	8	ASP	CA-CB-CG	8.64	121.24	112.60
4	b	321	ALA	N-CA-CB	8.63	122.66	109.97
3	l	992	ASP	CA-CB-CG	8.62	121.22	112.60
9	r	240	PRO	N-CA-CB	8.61	112.29	103.25
9	r	985	ASN	CA-CB-CG	-8.60	104.00	112.60
3	l	70	TYR	N-CA-CB	8.60	122.67	110.46
5	c	445	LEU	CA-C-N	8.59	133.45	120.82
5	c	445	LEU	C-N-CA	8.59	133.45	120.82
9	r	136	PRO	N-CD-CG	-8.59	90.31	103.20
6	d	43	HIS	CA-CB-CG	-8.59	105.21	113.80
4	m	674	ILE	CB-CA-C	-8.58	102.00	111.35
9	r	727	PHE	N-CA-C	8.58	121.77	111.82
8	q	648	ASP	N-CA-C	-8.57	102.58	113.72
6	o	181	LEU	CA-C-N	8.57	131.10	122.96
6	o	181	LEU	C-N-CA	8.57	131.10	122.96
9	r	78	SER	CA-C-N	8.56	129.41	120.00
9	r	78	SER	C-N-CA	8.56	129.41	120.00
5	c	242	ASP	O-C-N	-8.56	113.77	121.39
1	X	663	MET	O-C-N	8.55	132.53	122.19
9	g	605	ARG	NE-CZ-NH2	-8.55	111.51	119.20
3	l	796	ASP	N-CA-C	-8.55	101.46	112.23
9	r	324	TYR	N-CA-CB	8.54	126.16	110.10
1	X	1092	SER	N-CA-CB	8.54	124.92	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	387	LEU	CA-C-N	8.53	132.05	120.54
1	X	387	LEU	C-N-CA	8.53	132.05	120.54
9	g	693	LEU	N-CA-C	-8.52	104.91	114.62
9	g	1033	VAL	CA-C-N	8.52	131.69	120.28
9	g	1033	VAL	C-N-CA	8.52	131.69	120.28
5	c	325	LEU	N-CA-C	-8.50	103.35	114.31
9	r	234	ARG	N-CA-CB	8.50	123.53	109.94
8	q	454	ASP	CA-C-N	8.49	128.48	119.05
8	q	454	ASP	C-N-CA	8.49	128.48	119.05
6	o	213	SER	O-C-N	-8.49	113.29	121.18
3	l	451	ARG	CA-C-N	8.48	133.50	121.71
3	l	451	ARG	C-N-CA	8.48	133.50	121.71
8	q	335	HIS	CE1-NE2-CD2	-8.48	100.52	109.00
5	c	424	LEU	N-CA-C	-8.48	102.85	113.02
3	l	614	ILE	N-CA-C	-8.47	100.94	113.39
9	r	958	LYS	CA-C-N	8.47	132.31	120.29
9	r	958	LYS	C-N-CA	8.47	132.31	120.29
7	e	178	PHE	N-CA-C	-8.46	101.41	112.41
4	m	679	ASP	N-CA-C	-8.46	100.92	113.61
9	r	146	MET	N-CA-CB	8.46	124.78	110.49
1	X	1347	GLY	CA-C-N	8.46	134.68	120.64
1	X	1347	GLY	C-N-CA	8.46	134.68	120.64
9	r	355	SER	CB-CA-C	-8.46	94.05	110.11
8	q	576	ASN	CB-CA-C	8.44	127.22	110.42
9	r	240	PRO	CA-N-CD	-8.44	100.18	112.00
1	X	1390	SER	N-CA-C	8.44	120.48	111.28
9	g	1052	ASN	CA-C-O	8.44	129.81	120.70
9	r	1041	VAL	N-CA-CB	8.43	120.18	110.65
5	c	320	VAL	N-CA-C	-8.43	96.72	108.27
8	q	639	THR	N-CA-C	8.43	120.64	110.19
1	X	1072	TYR	N-CA-C	-8.42	103.01	113.28
7	p	163	ASN	CA-CB-CG	8.42	121.02	112.60
9	r	1027	ASN	CA-CB-CG	-8.42	104.18	112.60
3	l	549	LYS	O-C-N	8.41	130.74	122.07
4	m	198	GLU	CA-C-N	8.41	131.55	120.28
4	m	198	GLU	C-N-CA	8.41	131.55	120.28
4	m	146	LEU	N-CA-C	-8.40	101.89	112.90
8	q	315	LEU	CA-C-O	-8.40	113.03	119.59
4	b	674	ILE	N-CA-C	-8.40	104.52	112.83
9	r	246	LYS	N-CA-CB	8.39	122.58	110.16
9	r	136	PRO	N-CA-CB	8.37	111.85	103.48
8	f	713	GLU	CA-C-N	8.36	131.31	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	713	GLU	C-N-CA	8.36	131.31	120.44
9	g	115	LYS	N-CA-C	-8.36	97.91	109.95
1	X	659	GLU	N-CA-C	-8.36	102.50	114.12
1	X	366	SER	O-C-N	8.36	130.98	122.12
9	r	354	SER	CB-CA-C	-8.36	94.25	110.46
9	g	925	ASN	N-CA-CB	8.35	123.22	110.28
9	r	370	SER	N-CA-CB	8.35	126.08	112.63
9	r	78	SER	CB-CA-C	-8.34	94.67	110.67
4	m	691	VAL	N-CA-C	-8.33	96.45	108.11
5	n	246	TYR	N-CA-C	-8.31	98.84	110.31
6	d	255	ASP	CA-CB-CG	8.31	120.91	112.60
1	X	1022	TYR	CA-C-N	8.31	134.24	120.62
1	X	1022	TYR	C-N-CA	8.31	134.24	120.62
3	a	338	ARG	NE-CZ-NH2	8.30	126.67	119.20
3	l	540	LEU	CA-C-N	8.30	128.33	119.78
3	l	540	LEU	C-N-CA	8.30	128.33	119.78
6	o	225	VAL	N-CA-C	-8.30	97.92	109.21
3	a	396	ASP	N-CA-C	-8.30	103.19	112.57
9	g	1063	LYS	CA-C-O	-8.30	111.76	120.55
9	g	362	ILE	N-CA-C	-8.29	96.19	108.12
9	r	93	GLN	CB-CA-C	-8.29	98.20	110.96
9	g	796	ASN	OD1-CG-ND2	8.28	130.88	122.60
3	a	430	ASN	CA-CB-CG	8.28	120.88	112.60
4	m	409	MET	CA-C-N	8.27	132.19	120.28
1	X	685	TYR	N-CA-CB	8.27	123.09	110.11
1	X	1633	ARG	NE-CZ-NH2	-8.27	111.76	119.20
3	a	242	HIS	CE1-NE2-CD2	-8.27	100.73	109.00
9	g	601	ASN	N-CA-C	8.27	120.29	111.28
4	m	409	MET	C-N-CA	8.27	132.19	120.28
3	a	264	ASP	N-CA-C	-8.26	102.52	112.59
5	n	379	PHE	CA-CB-CG	-8.26	105.54	113.80
9	r	415	SER	CB-CA-C	-8.26	95.68	109.55
8	f	680	ILE	N-CA-C	-8.25	99.69	109.01
4	m	285	VAL	N-CA-C	-8.25	101.03	112.50
1	X	1594	ASP	N-CA-C	-8.25	101.67	113.21
8	f	17	ASP	CA-C-N	8.24	131.99	120.29
8	f	17	ASP	C-N-CA	8.24	131.99	120.29
8	f	677	LEU	N-CA-C	-8.24	103.01	113.72
3	l	1019	LEU	N-CA-CB	8.23	124.41	110.49
8	f	236	GLY	N-CA-C	-8.23	103.77	112.08
9	g	1057	LEU	CA-C-N	8.23	131.30	120.28
9	g	1057	LEU	C-N-CA	8.23	131.30	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	972	LYS	N-CA-C	-8.22	102.47	114.39
5	n	430	ASN	CA-CB-CG	8.21	120.81	112.60
3	a	566	ASN	N-CA-CB	8.21	123.00	110.28
4	b	548	SER	N-CA-C	-8.21	101.37	114.09
4	b	638	ASP	CA-CB-CG	8.21	120.81	112.60
9	r	901	ASN	CA-CB-CG	8.21	120.81	112.60
9	r	421	PRO	CA-N-CD	-8.20	100.52	112.00
9	r	635	VAL	N-CA-C	8.20	118.29	110.42
4	m	363	TYR	N-CA-CB	8.20	122.62	110.49
1	X	1276	LYS	CB-CA-C	-8.19	94.53	110.10
8	q	67	ASP	N-CA-CB	8.19	122.16	110.12
5	c	460	ASN	CA-CB-CG	8.19	120.79	112.60
4	b	156	GLU	N-CA-CB	8.19	121.85	109.98
5	c	459	PHE	CA-CB-CG	-8.18	105.62	113.80
6	d	285	LEU	CA-C-N	8.18	134.38	120.72
6	d	285	LEU	C-N-CA	8.18	134.38	120.72
1	X	1126	LEU	N-CA-C	-8.18	103.09	113.72
3	l	162	VAL	CB-CA-C	8.18	118.06	110.13
6	d	41	GLU	N-CA-C	-8.16	102.89	113.17
8	f	288	ILE	O-C-N	8.16	130.23	121.83
5	n	607	ARG	NE-CZ-NH2	-8.15	111.87	119.20
3	l	101	SER	CA-C-N	8.14	131.19	120.28
3	l	101	SER	C-N-CA	8.14	131.19	120.28
4	b	69	PHE	CA-CB-CG	8.13	121.93	113.80
9	g	420	PHE	CA-CB-CG	8.13	121.93	113.80
9	r	328	HIS	CB-CA-C	-8.13	97.81	110.81
1	X	939	LEU	CA-C-O	8.12	128.99	120.54
3	l	457	PHE	CA-CB-CG	8.13	121.93	113.80
3	a	298	PHE	CA-CB-CG	-8.12	105.68	113.80
8	f	428	ASN	CA-C-O	8.12	128.60	120.32
3	a	578	ASP	CA-C-N	8.12	126.82	120.33
3	a	578	ASP	C-N-CA	8.12	126.82	120.33
3	a	680	LEU	CA-C-N	8.12	131.97	120.28
3	a	680	LEU	C-N-CA	8.12	131.97	120.28
8	q	64	SER	N-CA-CB	8.11	121.78	110.01
4	b	247	LYS	N-CA-C	-8.11	102.40	113.18
7	e	74	SER	N-CA-C	8.11	120.70	107.32
3	l	161	ARG	N-CA-C	-8.10	94.19	108.13
3	l	415	TYR	CA-CB-CG	8.10	128.49	113.90
3	l	820	ARG	NE-CZ-NH2	8.10	126.49	119.20
1	X	821	THR	N-CA-C	-8.10	101.52	112.94
9	r	643	PRO	CA-C-N	8.10	130.93	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	643	PRO	C-N-CA	8.10	130.93	120.56
1	X	1193	ASN	CA-C-O	-8.09	111.89	120.63
9	g	111	HIS	ND1-CE1-NE2	8.09	116.49	108.40
1	X	344	SER	N-CA-C	8.09	120.81	111.11
3	l	170	SER	CA-C-N	8.09	129.95	119.84
3	l	170	SER	C-N-CA	8.09	129.95	119.84
7	e	166	GLN	N-CA-C	-8.09	93.58	110.80
1	X	769	PHE	N-CA-C	-8.08	103.21	113.72
3	a	630	THR	CA-C-N	8.08	132.03	120.79
3	a	630	THR	C-N-CA	8.08	132.03	120.79
4	b	396	ASP	CA-CB-CG	8.08	120.68	112.60
4	b	267	ARG	N-CA-C	-8.08	102.73	112.59
5	n	377	SER	N-CA-C	-8.07	102.90	114.12
4	m	466	LEU	CB-CA-C	-8.06	97.25	110.79
8	q	715	LEU	CA-C-N	8.06	131.08	120.28
8	q	715	LEU	C-N-CA	8.06	131.08	120.28
5	n	592	LEU	N-CA-C	-8.06	101.29	112.25
3	l	709	VAL	O-C-N	8.06	130.13	121.83
7	p	22	ARG	NE-CZ-NH1	-8.05	113.45	121.50
9	r	397	PRO	N-CD-CG	-8.05	91.12	103.20
1	X	918	PHE	CA-CB-CG	-8.05	105.75	113.80
6	o	250	GLU	N-CA-C	-8.05	101.94	112.41
9	r	1066	PHE	CA-CB-CG	-8.05	105.75	113.80
1	X	419	ASP	CA-CB-CG	8.04	120.64	112.60
5	n	524	ASP	O-C-N	8.04	130.45	122.09
3	a	351	LEU	CA-C-N	8.04	129.20	121.65
3	a	351	LEU	C-N-CA	8.04	129.20	121.65
4	m	528	GLU	N-CA-C	-8.03	102.11	112.23
3	l	995	ARG	N-CA-C	-8.03	103.61	113.41
3	l	883	GLU	N-CA-C	-8.03	100.60	110.88
8	f	335	HIS	ND1-CE1-NE2	8.03	116.43	108.40
3	l	430	ASN	CA-CB-CG	-8.03	104.58	112.60
5	c	456	THR	N-CA-C	-8.02	102.12	111.03
9	r	928	LYS	CA-C-N	8.02	130.87	120.44
9	r	928	LYS	C-N-CA	8.02	130.87	120.44
9	g	712	PHE	O-C-N	8.02	130.11	121.85
1	X	1514	VAL	N-CA-C	-8.02	104.76	112.29
3	l	954	ARG	NE-CZ-NH2	-8.01	111.99	119.20
5	n	361	LEU	N-CA-C	8.01	122.31	112.54
1	X	1036	ASP	CA-C-O	-8.00	112.07	120.23
1	X	212	TRP	N-CA-C	-8.00	100.97	110.41
8	f	70	LEU	CA-C-N	8.00	134.26	120.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	70	LEU	C-N-CA	8.00	134.26	120.58
7	p	69	GLY	N-CA-C	-8.00	103.33	112.29
9	g	595	ASN	N-CA-C	-8.00	104.04	113.88
9	r	248	LEU	N-CA-CB	7.99	121.86	110.12
4	m	99	ASP	N-CA-C	-7.99	95.39	108.41
5	c	353	ASN	N-CA-C	-7.98	103.49	113.55
3	l	75	ARG	CA-C-N	7.98	136.77	121.54
3	l	75	ARG	C-N-CA	7.98	136.77	121.54
8	q	313	LEU	CA-C-O	-7.98	112.92	121.45
9	r	801	CYS	CA-C-O	-7.98	112.09	120.55
7	e	245	ILE	CA-C-N	7.97	132.03	120.71
7	e	245	ILE	C-N-CA	7.97	132.03	120.71
1	X	1198	ASN	OD1-CG-ND2	7.97	130.57	122.60
9	g	334	TRP	CA-CB-CG	7.96	128.73	113.60
9	r	715	LEU	CA-C-N	7.96	136.75	121.54
9	r	715	LEU	C-N-CA	7.96	136.75	121.54
9	r	1077	PRO	CA-C-N	7.96	131.48	120.65
9	r	1077	PRO	C-N-CA	7.96	131.48	120.65
9	r	170	SER	CB-CA-C	-7.96	95.15	110.35
3	l	661	GLN	OE1-CD-NE2	-7.96	114.64	122.60
9	r	438	SER	CB-CA-C	-7.96	93.68	110.31
9	g	330	THR	N-CA-C	-7.95	102.48	112.90
1	X	644	ILE	N-CA-CB	7.95	119.85	110.55
5	c	447	VAL	N-CA-C	7.94	120.98	111.05
9	r	153	LEU	N-CA-CB	7.94	121.53	110.01
9	g	704	SER	N-CA-C	-7.94	104.48	114.56
9	g	959	ASN	CA-CB-CG	7.94	120.54	112.60
7	p	173	TRP	CB-CG-CD2	-7.94	115.69	126.80
8	f	618	GLU	N-CA-C	7.93	119.92	111.28
5	n	544	LEU	CA-C-N	7.93	131.25	120.38
5	n	544	LEU	C-N-CA	7.93	131.25	120.38
1	X	1595	LYS	N-CA-C	7.93	122.05	112.38
3	l	491	GLU	N-CA-C	-7.93	101.73	111.40
3	a	82	TYR	CA-C-N	7.92	127.98	119.90
3	a	82	TYR	C-N-CA	7.92	127.98	119.90
4	b	406	LEU	CA-C-N	7.92	128.35	119.32
4	b	406	LEU	C-N-CA	7.92	128.35	119.32
9	g	854	HIS	N-CA-C	-7.92	102.44	114.16
3	a	929	HIS	N-CA-C	-7.92	101.78	112.94
7	e	114	VAL	N-CA-CB	7.92	121.11	110.26
5	n	371	SER	CA-C-O	-7.92	112.15	120.70
5	c	236	LEU	CA-C-N	7.92	131.68	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	236	LEU	C-N-CA	7.92	131.68	120.28
9	g	1044	ARG	NE-CZ-NH1	-7.91	113.59	121.50
9	r	216	PRO	N-CD-CG	-7.91	91.34	103.20
5	n	506	THR	N-CA-C	7.91	119.90	111.28
9	g	80	PHE	N-CA-C	-7.91	103.21	113.17
9	g	1066	PHE	CA-CB-CG	7.90	121.70	113.80
3	l	732	THR	N-CA-C	-7.90	102.95	112.59
1	X	1467	SER	CA-C-N	7.90	131.28	120.46
1	X	1467	SER	C-N-CA	7.90	131.28	120.46
7	e	226	ARG	N-CA-C	-7.90	97.02	109.50
1	X	885	VAL	N-CA-C	7.90	118.00	110.42
9	g	759	TRP	CB-CG-CD2	-7.90	115.74	126.80
9	r	835	PHE	N-CA-CB	7.90	123.84	110.49
3	a	574	LEU	N-CA-C	7.89	120.65	111.02
9	g	655	PHE	CA-CB-CG	-7.89	105.91	113.80
9	g	525	GLU	N-CA-CB	7.89	121.56	109.97
1	X	156	THR	N-CA-C	-7.88	103.16	114.12
1	X	1050	SER	N-CA-CB	7.88	123.81	110.49
8	q	111	GLN	N-CA-CB	7.88	121.88	110.06
3	a	552	ASP	CA-CB-CG	7.87	120.47	112.60
5	c	254	GLN	N-CA-C	-7.86	103.91	113.97
3	a	495	TYR	CA-C-O	7.86	129.06	119.31
6	o	120	SER	N-CA-C	-7.86	97.25	108.96
9	r	819	GLN	N-CA-C	-7.86	102.20	112.41
1	X	199	ILE	N-CA-C	-7.85	105.06	112.83
5	c	222	ASP	CA-CB-CG	-7.85	104.75	112.60
8	f	576	ASN	N-CA-CB	7.85	123.76	110.49
9	g	1036	PHE	CA-CB-CG	7.85	121.65	113.80
9	r	143	PRO	N-CD-CG	-7.85	91.42	103.20
5	n	270	SER	CA-C-N	7.85	130.64	120.44
5	n	270	SER	C-N-CA	7.85	130.64	120.44
3	l	940	VAL	CA-C-N	7.85	133.00	121.31
3	l	940	VAL	C-N-CA	7.85	133.00	121.31
7	p	44	ASN	CA-CB-CG	-7.84	104.75	112.60
5	n	583	SER	N-CA-CB	7.84	123.75	110.49
4	b	729	LYS	N-CA-C	-7.83	103.70	113.18
8	f	223	ILE	N-CA-C	-7.83	105.56	111.90
9	r	151	LEU	N-CA-CB	7.83	121.64	110.12
5	c	136	LYS	O-C-N	7.83	130.23	122.09
1	X	1538	ASP	CA-CB-CG	7.83	120.43	112.60
8	q	724	LEU	N-CA-C	-7.83	103.75	113.38
9	r	968	GLU	N-CA-C	-7.83	103.75	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	1010	ASP	CA-CB-CG	7.83	120.42	112.60
3	a	871	HIS	ND1-CE1-NE2	7.82	116.22	108.40
8	q	555	ILE	N-CA-C	-7.82	102.47	111.00
1	X	1041	ASN	CA-CB-CG	7.82	120.42	112.60
8	q	621	GLN	CA-C-N	7.82	128.60	120.00
8	q	621	GLN	C-N-CA	7.82	128.60	120.00
9	r	820	THR	N-CA-C	-7.81	102.80	112.88
5	n	199	ILE	CA-C-O	-7.81	111.95	120.85
6	o	14	ASP	CA-CB-CG	7.81	120.41	112.60
9	r	884	HIS	CE1-NE2-CD2	-7.81	101.19	109.00
8	f	335	HIS	CE1-NE2-CD2	-7.81	101.19	109.00
9	g	736	ASP	CA-C-N	7.81	132.17	120.31
9	g	736	ASP	C-N-CA	7.81	132.17	120.31
5	c	242	ASP	CA-C-N	7.80	129.16	120.66
5	c	242	ASP	C-N-CA	7.80	129.16	120.66
6	o	255	ASP	CA-C-N	7.80	132.16	120.77
6	o	255	ASP	C-N-CA	7.80	132.16	120.77
8	q	341	HIS	CA-C-O	-7.80	112.81	119.36
9	r	171	LYS	N-CA-CB	7.80	121.61	109.83
1	X	934	GLU	N-CA-C	-7.80	103.83	112.72
1	X	1622	GLU	CA-C-N	7.80	130.73	120.28
1	X	1622	GLU	C-N-CA	7.80	130.73	120.28
3	l	1022	SER	CA-C-N	7.80	131.63	120.79
3	l	1022	SER	C-N-CA	7.80	131.63	120.79
3	a	803	HIS	ND1-CE1-NE2	7.80	116.20	108.40
3	a	437	ASN	CA-CB-CG	7.80	120.40	112.60
4	b	636	LEU	CA-C-O	7.80	128.75	120.33
6	d	125	VAL	N-CA-C	-7.79	96.85	108.85
4	m	380	GLU	N-CA-C	-7.79	103.77	112.57
4	m	596	SER	CA-C-N	7.79	130.71	120.28
4	m	596	SER	C-N-CA	7.79	130.71	120.28
6	o	237	ASP	CA-CB-CG	7.78	120.38	112.60
5	c	229	SER	CA-C-N	7.78	130.56	120.44
5	c	229	SER	C-N-CA	7.78	130.56	120.44
5	n	191	ASP	N-CA-C	7.78	120.65	111.71
3	l	170	SER	CA-C-O	-7.77	113.19	121.27
3	l	537	THR	CA-CB-OG1	7.77	121.25	109.60
9	r	170	SER	N-CA-CB	7.76	127.00	114.27
5	c	294	ILE	CA-C-N	7.75	130.67	120.28
5	c	294	ILE	C-N-CA	7.75	130.67	120.28
1	X	178	GLN	CA-C-N	7.75	130.51	120.44
1	X	178	GLN	C-N-CA	7.75	130.51	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	e	49	ASP	CB-CA-C	-7.75	99.50	110.34
3	a	738	ARG	N-CA-C	-7.74	101.34	111.71
3	a	727	TYR	N-CA-CB	7.74	121.29	110.07
9	r	250	LYS	N-CA-CB	7.74	121.83	110.30
8	f	561	ASN	N-CA-C	-7.73	103.67	113.72
9	g	837	ASN	N-CA-C	-7.73	100.98	111.87
6	d	132	GLU	N-CA-C	-7.72	102.92	112.88
3	l	398	VAL	N-CA-CB	7.72	119.58	110.55
6	d	144	HIS	CG-CD2-NE2	7.72	114.92	107.20
9	g	279	GLY	CA-C-O	-7.72	112.91	121.71
5	n	459	PHE	CA-CB-CG	-7.71	106.09	113.80
3	a	414	ARG	NE-CZ-NH2	-7.71	112.26	119.20
3	a	219	ASP	N-CA-CB	7.71	123.52	110.49
4	b	145	ASN	CA-CB-CG	-7.71	104.89	112.60
8	f	312	GLU	N-CA-C	-7.71	103.44	112.92
9	r	371	SER	CB-CA-C	-7.70	94.21	110.31
8	f	439	SER	N-CA-C	-7.70	103.20	112.59
3	a	665	LEU	N-CA-C	-7.70	103.42	114.12
8	q	540	ASN	OD1-CG-ND2	7.70	130.30	122.60
5	c	188	VAL	CA-C-N	7.70	130.59	120.28
5	c	188	VAL	C-N-CA	7.70	130.59	120.28
3	l	435	ALA	N-CA-C	-7.70	103.69	113.23
1	X	725	LEU	N-CA-CB	7.69	121.25	110.17
1	X	281	GLN	N-CA-C	-7.69	105.06	114.75
9	g	264	ASN	OD1-CG-ND2	7.69	130.29	122.60
1	X	1306	ASN	N-CA-C	-7.69	103.95	112.72
8	f	51	LEU	N-CA-C	-7.69	104.42	113.88
1	X	1339	PHE	CA-C-N	7.69	130.58	120.28
1	X	1339	PHE	C-N-CA	7.69	130.58	120.28
1	X	433	PRO	N-CA-CB	7.69	110.01	103.17
1	X	1461	ILE	N-CA-CB	7.68	119.04	110.51
9	g	331	LEU	CA-C-O	7.68	128.86	119.79
8	q	439	SER	N-CA-C	7.68	119.44	111.14
3	l	903	ASN	N-CA-C	-7.68	102.97	112.88
1	X	676	LEU	CA-C-O	-7.68	112.34	120.63
3	a	1006	VAL	N-CA-C	-7.68	105.68	111.90
8	q	314	ILE	N-CA-C	-7.68	105.72	113.47
9	r	1073	ASN	CA-CB-CG	-7.67	104.93	112.60
3	a	365	ILE	N-CA-CB	7.67	121.34	111.67
4	b	611	ILE	N-CA-CB	7.67	120.06	110.47
8	f	529	SER	CA-C-N	7.67	130.08	120.72
8	f	529	SER	C-N-CA	7.67	130.08	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	345	GLN	CB-CA-C	-7.67	97.71	109.29
8	f	115	GLN	N-CA-C	-7.67	104.06	113.41
8	q	717	LEU	N-CA-C	7.67	119.72	111.36
9	r	566	ASN	CA-CB-CG	-7.66	104.94	112.60
9	r	997	VAL	N-CA-C	-7.66	97.05	108.46
3	l	658	HIS	CE1-NE2-CD2	-7.66	101.34	109.00
3	a	953	LEU	N-CA-C	7.65	119.62	111.28
4	m	220	ASP	CA-CB-CG	7.65	120.25	112.60
9	r	73	GLN	N-CA-CB	7.65	122.90	110.43
9	r	96	TYR	CB-CA-C	-7.65	97.02	109.72
7	e	16	VAL	N-CA-C	-7.64	97.80	108.27
5	n	136	LYS	N-CA-C	7.64	119.24	111.07
8	q	105	PHE	CA-CB-CG	-7.64	106.16	113.80
8	q	172	LYS	N-CA-C	-7.64	103.03	112.88
1	X	343	ASP	CA-CB-CG	7.63	120.23	112.60
9	r	123	PRO	CA-N-CD	-7.63	101.31	112.00
9	r	143	PRO	CA-N-CD	-7.63	101.32	112.00
1	X	673	SER	CA-C-N	7.63	130.84	120.54
1	X	673	SER	C-N-CA	7.63	130.84	120.54
1	X	1064	GLU	CA-C-N	7.63	131.26	120.28
1	X	1064	GLU	C-N-CA	7.63	131.26	120.28
3	a	929	HIS	CA-CB-CG	-7.62	106.18	113.80
6	o	122	ASP	N-CA-C	-7.62	103.99	113.28
3	a	94	ASN	O-C-N	-7.62	114.67	123.27
3	a	994	ILE	CA-C-N	7.61	130.81	120.38
3	a	994	ILE	C-N-CA	7.61	130.81	120.38
8	f	111	GLN	CA-C-O	7.61	128.79	120.80
8	q	273	ASN	N-CA-C	-7.61	103.10	113.30
9	r	368	PHE	CB-CA-C	-7.61	97.86	110.72
5	c	305	ARG	CA-C-N	7.61	131.09	120.29
5	c	305	ARG	C-N-CA	7.61	131.09	120.29
5	c	307	SER	CA-C-N	7.61	130.47	120.28
5	c	307	SER	C-N-CA	7.61	130.47	120.28
4	m	140	HIS	CE1-NE2-CD2	-7.61	101.39	109.00
1	X	1439	LEU	CA-C-N	7.60	128.36	120.00
1	X	1439	LEU	C-N-CA	7.60	128.36	120.00
1	X	1493	ASN	CA-CB-CG	-7.60	105.00	112.60
8	q	542	ARG	N-CA-CB	7.60	123.33	110.49
8	q	696	ASN	CA-CB-CG	7.60	120.20	112.60
1	X	1615	ARG	NE-CZ-NH1	-7.60	113.90	121.50
8	f	518	ILE	N-CA-C	-7.59	106.50	113.71
5	n	428	ASN	CA-C-N	7.59	130.31	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	428	ASN	C-N-CA	7.59	130.31	120.44
8	f	122	VAL	O-C-N	7.59	129.23	121.87
8	f	231	PHE	N-CA-CB	7.59	123.15	111.46
7	e	154	MET	CA-C-O	7.58	128.36	120.40
3	l	770	PHE	CA-CB-CG	-7.58	106.22	113.80
4	b	307	LYS	N-CA-C	-7.58	99.96	111.56
9	g	443	TRP	CB-CG-CD2	-7.58	116.19	126.80
8	q	687	ALA	N-CA-C	-7.58	104.00	112.57
3	a	833	ASP	CA-CB-CG	-7.58	105.03	112.60
3	l	14	TYR	CA-CB-CG	-7.58	100.27	113.90
3	l	15	TYR	N-CA-C	-7.58	101.22	113.19
9	r	86	LEU	N-CA-CB	7.58	121.81	110.29
9	r	421	PRO	N-CA-CB	7.58	111.20	103.25
3	l	1020	ASN	CA-CB-CG	-7.57	105.03	112.60
9	r	885	VAL	CA-CB-CG2	7.57	123.27	110.40
9	g	240	PRO	CA-C-N	7.57	134.39	122.74
9	g	240	PRO	C-N-CA	7.57	134.39	122.74
3	l	22	ASN	CA-CB-CG	7.57	120.17	112.60
7	e	189	GLU	N-CA-CB	7.56	123.58	110.65
8	q	391	HIS	CA-CB-CG	-7.56	106.24	113.80
9	g	372	SER	N-CA-CB	7.56	122.49	110.85
3	l	436	HIS	CE1-NE2-CD2	-7.56	101.44	109.00
9	r	405	GLU	N-CA-C	7.56	124.63	114.12
9	r	701	VAL	CA-C-O	-7.56	113.19	121.05
5	n	564	SER	N-CA-C	-7.56	104.56	114.31
1	X	1124	ASP	CA-CB-CG	7.55	120.15	112.60
9	r	247	LEU	N-CA-CB	7.54	121.32	110.16
9	g	278	LYS	CA-C-N	7.54	127.26	120.10
9	g	278	LYS	C-N-CA	7.54	127.26	120.10
9	g	636	ILE	CB-CA-C	7.54	122.56	111.33
3	l	283	TYR	N-CA-C	-7.54	106.03	114.62
5	n	657	CYS	CA-C-N	7.54	131.14	120.28
5	n	657	CYS	C-N-CA	7.54	131.14	120.28
7	p	51	TRP	CA-CB-CG	7.53	127.92	113.60
3	a	105	ARG	NE-CZ-NH1	7.53	129.03	121.50
4	m	53	VAL	N-CA-C	-7.52	105.23	113.43
6	o	85	GLU	CA-C-N	7.52	133.57	122.74
6	o	85	GLU	C-N-CA	7.52	133.57	122.74
9	r	240	PRO	N-CD-CG	-7.52	91.92	103.20
3	a	94	ASN	OD1-CG-ND2	-7.52	115.08	122.60
9	g	198	LEU	CA-C-N	7.52	127.56	119.89
9	g	198	LEU	C-N-CA	7.52	127.56	119.89

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	m	164	ASP	CA-CB-CG	7.51	120.11	112.60
3	a	547	VAL	O-C-N	7.51	129.15	121.87
3	l	901	ARG	NE-CZ-NH2	-7.50	112.45	119.20
5	n	265	HIS	CA-C-O	-7.50	112.60	120.55
7	e	15	VAL	O-C-N	7.50	131.15	123.20
4	b	375	LEU	N-CA-C	-7.49	104.02	113.01
3	l	303	LEU	O-C-N	7.49	131.33	122.94
4	b	625	ALA	O-C-N	-7.49	112.71	121.32
8	f	215	ILE	N-CA-C	-7.49	105.71	112.90
3	l	17	LYS	N-CA-C	-7.49	96.38	109.48
6	o	63	HIS	CA-CB-CG	7.49	121.29	113.80
3	a	583	LEU	CA-C-O	7.48	128.62	119.79
3	l	386	LEU	CA-C-N	7.48	131.43	120.74
3	l	386	LEU	C-N-CA	7.48	131.43	120.74
3	l	408	PHE	N-CA-C	7.48	119.07	111.07
3	l	1017	TRP	N-CA-C	-7.48	98.04	109.41
8	q	303	LEU	N-CA-C	-7.48	103.11	112.90
7	e	163	ASN	CA-CB-CG	-7.47	105.13	112.60
6	o	63	HIS	CA-C-O	-7.47	112.40	120.17
4	b	348	GLN	N-CA-C	7.47	120.37	111.33
8	f	289	HIS	ND1-CE1-NE2	7.47	115.87	108.40
1	X	649	LYS	CA-C-N	7.46	133.38	122.63
1	X	649	LYS	C-N-CA	7.46	133.38	122.63
5	n	546	ASP	CA-CB-CG	-7.46	105.14	112.60
9	r	118	PRO	N-CD-CG	-7.46	92.00	103.20
5	n	310	ALA	CA-C-N	7.46	130.68	120.46
5	n	310	ALA	C-N-CA	7.46	130.68	120.46
1	X	1564	LEU	N-CA-C	-7.46	104.03	113.72
8	q	604	VAL	N-CA-CB	7.45	117.75	111.64
3	l	904	PHE	CA-CB-CG	-7.45	106.35	113.80
3	l	863	ASP	N-CA-C	-7.45	102.53	111.69
3	a	403	ASP	CA-C-O	-7.45	113.62	117.94
6	d	139	ILE	N-CA-C	-7.45	97.75	108.17
5	n	265	HIS	CE1-NE2-CD2	-7.44	101.56	109.00
9	r	912	LYS	N-CA-CB	7.44	123.07	110.49
9	r	982	GLU	O-C-N	7.44	130.63	122.15
9	g	674	ASN	N-CA-CB	7.44	122.53	110.40
1	X	1637	VAL	CA-C-N	7.43	130.10	120.44
1	X	1637	VAL	C-N-CA	7.43	130.10	120.44
3	l	602	ILE	N-CA-C	-7.43	97.76	108.17
5	c	144	PHE	CA-CB-CG	7.43	121.23	113.80
9	g	223	THR	N-CA-C	-7.43	97.83	109.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	149	SER	CB-CA-C	-7.43	95.53	110.17
9	r	504	PHE	N-CA-C	-7.43	103.18	111.28
1	X	895	HIS	ND1-CE1-NE2	7.43	115.83	108.40
4	b	320	SER	CA-C-N	7.43	131.42	120.87
4	b	320	SER	C-N-CA	7.43	131.42	120.87
5	c	318	LEU	N-CA-C	-7.42	103.62	114.39
3	l	984	TYR	CA-C-O	7.42	128.35	119.59
3	a	489	THR	N-CA-C	-7.42	103.21	111.82
5	c	297	TYR	CB-CG-CD2	-7.42	109.67	120.80
9	g	556	HIS	CE1-NE2-CD2	-7.42	101.58	109.00
8	f	528	HIS	CA-CB-CG	7.42	121.22	113.80
6	d	259	ARG	N-CA-CB	7.42	121.49	109.69
9	r	1010	ASP	N-CA-C	-7.42	97.17	108.96
5	n	341	GLN	N-CA-C	7.42	120.42	111.82
8	q	726	ASN	CA-CB-CG	-7.42	105.18	112.60
4	b	561	ARG	NE-CZ-NH2	7.42	125.87	119.20
8	f	524	VAL	N-CA-C	-7.42	105.49	112.83
3	l	556	ASN	OD1-CG-ND2	7.42	130.01	122.60
3	l	746	CYS	CB-CA-C	-7.41	98.48	109.97
4	m	552	ILE	CA-C-N	7.41	135.31	121.97
4	m	552	ILE	C-N-CA	7.41	135.31	121.97
9	r	76	TYR	CB-CA-C	-7.41	96.52	109.64
8	f	384	TYR	N-CA-C	-7.41	102.81	111.03
3	l	694	ASN	N-CA-C	-7.41	98.52	108.74
9	r	118	PRO	N-CA-CB	7.41	111.06	102.76
1	X	1565	ASN	N-CA-C	-7.41	99.56	111.04
8	f	576	ASN	CA-CB-CG	7.41	120.00	112.60
3	l	902	THR	N-CA-C	-7.40	103.84	113.17
5	c	551	ASN	N-CA-C	-7.40	101.56	110.44
7	e	89	ASP	CA-C-N	7.40	131.22	120.71
7	e	89	ASP	C-N-CA	7.40	131.22	120.71
9	r	146	MET	CB-CA-C	-7.40	95.69	110.42
9	g	377	ILE	N-CA-C	-7.40	104.12	113.22
5	c	569	GLU	N-CA-C	-7.39	104.28	113.38
3	l	350	ASN	CA-CB-CG	-7.39	105.21	112.60
4	m	64	LYS	CB-CA-C	-7.39	99.86	111.17
1	X	899	GLN	CA-C-N	7.39	129.87	120.56
1	X	899	GLN	C-N-CA	7.39	129.87	120.56
4	m	61	ASN	N-CA-C	-7.39	103.57	112.59
3	a	10	ASN	N-CA-C	-7.39	96.50	109.06
9	g	893	ASP	CA-CB-CG	7.39	119.99	112.60
1	X	770	HIS	CA-CB-CG	-7.38	106.42	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	o	86	ASN	N-CA-C	-7.38	103.57	112.58
5	n	555	GLU	N-CA-C	-7.37	105.20	114.56
3	l	929	HIS	CE1-NE2-CD2	-7.37	101.63	109.00
8	q	589	HIS	ND1-CE1-NE2	7.37	115.77	108.40
5	c	762	LYS	N-CA-C	-7.37	104.80	114.31
1	X	1206	ALA	CA-C-N	7.37	130.15	120.28
1	X	1206	ALA	C-N-CA	7.37	130.15	120.28
5	c	408	ASP	O-C-N	-7.36	114.48	122.07
3	l	904	PHE	N-CA-C	-7.36	103.43	113.30
4	m	658	LEU	CA-C-N	7.36	129.04	119.84
4	m	658	LEU	C-N-CA	7.36	129.04	119.84
9	r	278	LYS	N-CA-CB	7.36	121.14	110.47
4	b	642	TRP	CA-C-N	7.35	129.33	120.14
4	b	642	TRP	C-N-CA	7.35	129.33	120.14
3	l	284	ASN	CA-C-N	7.35	131.27	120.90
3	l	284	ASN	C-N-CA	7.35	131.27	120.90
1	X	713	LYS	N-CA-CB	7.35	120.93	110.12
1	X	758	TYR	CA-C-O	-7.35	112.20	120.43
3	l	744	VAL	CA-C-O	-7.34	113.39	121.17
3	a	715	THR	N-CA-C	-7.34	95.16	110.80
8	q	706	GLN	N-CA-CB	7.34	120.74	110.17
9	r	960	ILE	O-C-N	7.34	129.10	121.91
5	c	302	ASP	CA-C-N	7.34	130.51	120.46
5	c	302	ASP	C-N-CA	7.34	130.51	120.46
6	d	196	LEU	CA-C-N	7.34	130.61	120.63
6	d	196	LEU	C-N-CA	7.34	130.61	120.63
9	g	544	LYS	CA-C-O	-7.34	110.59	119.32
4	m	672	TYR	CA-C-O	-7.34	111.75	118.79
8	q	122	VAL	N-CA-C	7.34	117.46	110.42
8	q	604	VAL	CB-CA-C	-7.34	104.52	111.05
5	n	345	THR	N-CA-C	-7.33	104.22	113.02
5	c	464	VAL	N-CA-C	7.33	119.03	109.58
9	g	1104	ILE	CA-C-N	7.33	131.28	120.87
9	g	1104	ILE	C-N-CA	7.33	131.28	120.87
4	m	238	LYS	CA-C-O	7.33	127.07	118.79
8	q	71	GLU	CA-C-N	7.33	129.97	120.44
8	q	71	GLU	C-N-CA	7.33	129.97	120.44
9	r	276	LEU	N-CA-CB	7.33	122.33	110.90
7	e	11	LEU	N-CA-CB	7.32	121.08	109.51
9	r	753	PHE	CA-C-O	-7.32	112.12	120.24
1	X	143	SER	N-CA-CB	7.31	120.93	109.82
6	d	287	GLY	N-CA-C	-7.31	104.68	115.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1468	VAL	CA-C-N	7.31	129.94	120.44
1	X	1468	VAL	C-N-CA	7.31	129.94	120.44
9	r	257	TRP	N-CA-CB	7.31	122.96	110.68
5	c	173	LYS	CA-C-O	-7.31	112.48	120.30
7	e	188	LEU	N-CA-CB	7.31	122.84	110.49
9	r	523	ASP	N-CA-CB	7.30	119.65	110.45
7	p	173	TRP	CB-CG-CD1	7.30	137.85	126.90
1	X	723	LEU	N-CA-C	-7.29	103.04	112.23
9	g	230	PHE	CA-CB-CG	-7.29	106.50	113.80
3	l	753	ASN	OD1-CG-ND2	7.29	129.89	122.60
5	n	642	LYS	N-CA-CB	7.29	120.95	110.16
3	a	933	GLY	N-CA-C	-7.29	99.18	110.77
5	c	558	ASN	N-CA-C	-7.29	104.27	113.02
4	b	658	LEU	N-CA-CB	7.29	123.34	110.37
3	a	7	ILE	O-C-N	-7.29	115.60	123.18
4	b	527	VAL	N-CA-C	-7.29	105.91	112.90
8	q	355	LEU	O-C-N	-7.29	112.94	121.32
1	X	162	HIS	CE1-NE2-CD2	-7.28	101.72	109.00
8	f	607	LEU	CA-C-O	-7.28	113.83	121.55
8	q	622	GLY	CA-C-O	-7.28	112.94	120.66
6	d	215	THR	CA-C-O	-7.28	113.10	121.47
7	e	148	TRP	N-CA-C	-7.28	98.00	109.50
9	r	199	PRO	N-CD-CG	-7.28	92.28	103.20
9	g	239	LYS	CA-C-N	7.28	127.24	120.03
9	g	239	LYS	C-N-CA	7.28	127.24	120.03
5	c	639	SER	O-C-N	7.28	129.66	122.09
3	l	880	ARG	CA-C-N	7.27	135.43	121.54
3	l	880	ARG	C-N-CA	7.27	135.43	121.54
9	r	982	GLU	N-CA-C	7.27	119.29	111.36
7	p	234	GLY	N-CA-C	-7.27	100.85	111.03
9	r	261	PHE	N-CA-CB	7.27	122.48	110.85
8	q	242	LEU	N-CA-C	-7.27	103.07	112.23
9	r	1080	SER	N-CA-C	-7.27	97.99	108.60
1	X	146	SER	CB-CA-C	-7.27	98.50	110.85
3	a	507	PHE	CA-C-N	7.26	131.35	120.31
3	a	507	PHE	C-N-CA	7.26	131.35	120.31
9	r	421	PRO	N-CD-CG	-7.26	92.30	103.20
4	m	420	THR	N-CA-CB	7.26	120.54	110.01
7	p	199	ASP	CA-CB-CG	7.26	119.86	112.60
6	d	139	ILE	CA-C-O	7.26	128.17	120.48
3	a	845	ILE	N-CA-C	-7.26	106.42	113.53
6	d	182	VAL	CA-C-O	7.26	128.13	120.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	537	PHE	CA-CB-CG	-7.25	106.55	113.80
5	c	174	ARG	O-C-N	7.25	131.47	123.13
7	e	337	ASN	OD1-CG-ND2	7.25	129.85	122.60
3	a	970	LEU	N-CA-C	-7.24	102.73	112.94
3	l	286	THR	CA-C-N	7.24	131.16	120.87
3	l	286	THR	C-N-CA	7.24	131.16	120.87
1	X	950	ARG	O-C-N	7.24	129.53	122.07
6	o	38	VAL	O-C-N	-7.24	114.72	122.83
5	n	254	GLN	N-CA-CB	7.24	120.76	110.12
8	q	79	GLU	N-CA-C	-7.24	104.58	113.41
9	r	960	ILE	CA-C-O	-7.24	113.50	121.17
9	g	1046	VAL	CA-C-O	-7.23	113.43	120.95
9	r	292	PHE	N-CA-CB	7.23	122.63	110.69
1	X	850	ASN	CA-CB-CG	-7.23	105.37	112.60
3	a	332	VAL	N-CA-C	-7.23	106.84	113.71
8	f	633	THR	N-CA-CB	7.23	122.71	110.49
7	e	211	HIS	CB-CG-CD2	-7.23	121.80	131.20
3	l	658	HIS	ND1-CE1-NE2	7.23	115.63	108.40
4	m	388	ASN	CA-CB-CG	-7.23	105.37	112.60
9	r	790	HIS	ND1-CE1-NE2	7.23	115.63	108.40
7	e	324	ASP	CA-CB-CG	7.23	119.83	112.60
5	n	207	TYR	CA-C-N	7.23	127.22	119.78
5	n	207	TYR	C-N-CA	7.23	127.22	119.78
9	r	1078	LEU	N-CA-C	7.23	119.89	109.48
1	X	674	SER	O-C-N	7.23	129.60	122.09
3	l	583	LEU	N-CA-C	7.23	120.58	111.69
7	e	42	THR	CA-CB-OG1	7.22	120.44	109.60
9	g	239	LYS	O-C-N	-7.22	113.01	121.32
9	g	865	PRO	CA-C-O	-7.22	113.50	121.23
7	e	30	ASP	CA-CB-CG	7.22	119.82	112.60
1	X	289	TYR	N-CA-CB	7.21	122.68	110.49
1	X	1018	GLU	N-CA-C	-7.21	102.42	112.45
8	f	142	SER	N-CA-CB	7.21	122.68	110.49
8	q	676	LYS	N-CA-C	-7.21	96.76	108.52
3	l	715	THR	N-CA-C	-7.21	104.61	113.41
6	o	116	LEU	CA-C-O	-7.21	112.39	120.54
6	d	198	SER	CA-C-N	7.21	134.43	121.89
6	d	198	SER	C-N-CA	7.21	134.43	121.89
9	g	67	TYR	N-CA-CB	7.21	120.56	109.97
5	n	294	ILE	O-C-N	7.21	129.15	121.94
9	r	136	PRO	CA-N-CD	-7.21	101.91	112.00
9	g	539	PHE	N-CA-C	-7.21	104.37	113.02

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	598	ILE	CA-C-N	7.21	129.94	120.28
5	n	598	ILE	C-N-CA	7.21	129.94	120.28
3	a	955	SER	N-CA-CB	7.21	120.71	109.69
4	b	592	ASN	CA-CB-CG	7.21	119.81	112.60
1	X	429	LYS	CA-C-O	7.20	128.16	120.46
8	f	55	ASN	CA-CB-CG	7.20	119.80	112.60
1	X	913	ASN	CA-C-O	-7.20	111.22	119.78
3	l	538	GLY	CA-C-N	7.19	129.92	120.28
3	l	538	GLY	C-N-CA	7.19	129.92	120.28
9	r	403	GLN	O-C-N	-7.19	115.02	122.64
3	l	529	SER	CA-C-N	7.19	129.91	120.28
3	l	529	SER	C-N-CA	7.19	129.91	120.28
8	f	122	VAL	CA-C-O	-7.19	113.48	120.95
5	c	285	ARG	NE-CZ-NH2	-7.18	112.73	119.20
3	l	21	ASN	CA-CB-CG	-7.18	105.42	112.60
6	o	52	HIS	CE1-NE2-CD2	-7.18	101.82	109.00
9	g	478	PHE	CA-CB-CG	7.18	120.98	113.80
8	q	332	ALA	O-C-N	7.18	130.34	122.15
3	a	727	TYR	CB-CA-C	-7.18	99.56	110.90
3	a	814	THR	CA-C-N	7.18	133.43	122.37
3	a	814	THR	C-N-CA	7.18	133.43	122.37
4	b	635	GLU	CA-C-O	-7.18	112.87	120.55
4	m	587	ASP	CA-CB-CG	7.17	119.77	112.60
9	g	792	LEU	N-CA-C	-7.17	104.56	113.38
3	l	752	HIS	CA-CB-CG	7.17	120.97	113.80
5	n	294	ILE	CA-C-O	-7.17	113.81	121.27
5	n	585	ASN	CA-C-O	-7.17	113.74	120.34
8	q	576	ASN	CA-C-O	-7.17	110.26	120.51
9	r	81	SER	CB-CA-C	-7.17	95.31	111.30
3	a	142	ALA	CA-C-O	7.17	130.76	120.51
3	a	997	ARG	N-CA-CB	-7.17	99.47	110.44
9	g	309	ASP	CA-CB-CG	7.17	119.77	112.60
3	a	925	LEU	N-CA-C	-7.17	97.25	108.14
3	a	272	LYS	N-CA-C	-7.16	100.61	110.35
3	l	424	GLN	CA-C-O	7.16	126.96	119.51
3	a	254	ILE	CA-C-O	-7.16	111.83	120.78
1	X	1614	SER	N-CA-C	7.16	118.73	111.07
3	l	419	ILE	N-CA-C	-7.16	105.37	112.17
7	p	301	ASP	CA-CB-CG	7.16	119.76	112.60
9	r	326	PHE	N-CA-CB	7.16	121.88	110.85
3	a	85	SER	N-CA-C	-7.16	97.23	108.90
8	f	382	LYS	CA-C-O	-7.16	112.93	120.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	680	LYS	N-CA-C	-7.16	98.14	109.23
5	c	483	PHE	CA-CB-CG	-7.16	106.64	113.80
7	p	159	ILE	CA-C-N	7.15	127.75	120.38
7	p	159	ILE	C-N-CA	7.15	127.75	120.38
1	X	1220	VAL	N-CA-C	-7.15	100.93	109.01
8	f	168	VAL	N-CA-C	-7.15	104.33	111.77
8	f	261	ARG	N-CA-C	-7.15	104.59	113.38
8	q	62	VAL	CA-CB-CG1	7.15	122.55	110.40
9	g	265	SER	N-CA-CB	7.14	122.56	110.49
9	g	634	VAL	CB-CA-C	-7.14	102.67	112.24
9	g	241	GLN	OE1-CD-NE2	7.14	129.74	122.60
8	q	46	ALA	CA-C-O	-7.14	112.85	120.42
3	a	841	ALA	CA-C-N	7.14	129.72	120.44
3	a	841	ALA	C-N-CA	7.14	129.72	120.44
5	c	412	LEU	CA-C-N	7.14	128.76	119.84
5	c	412	LEU	C-N-CA	7.14	128.76	119.84
9	g	793	CYS	N-CA-C	-7.14	104.50	112.57
4	b	345	LYS	N-CA-C	-7.14	104.04	114.39
4	m	641	ASP	N-CA-CB	7.14	122.55	110.49
8	q	102	ARG	NE-CZ-NH2	-7.14	112.78	119.20
9	r	404	MET	CB-CA-C	-7.14	95.06	109.55
6	d	209	ASP	CA-CB-CG	7.13	119.73	112.60
8	f	507	ASP	N-CA-C	-7.13	103.20	112.68
1	X	1462	ASN	N-CA-C	7.13	119.05	111.28
6	o	106	GLN	CA-C-N	7.12	131.61	121.42
6	o	106	GLN	C-N-CA	7.12	131.61	121.42
3	l	650	HIS	N-CA-C	-7.12	104.62	113.38
6	o	122	ASP	CA-CB-CG	7.12	119.72	112.60
8	f	324	VAL	CA-C-N	7.12	129.69	120.44
8	f	324	VAL	C-N-CA	7.12	129.69	120.44
5	n	393	GLN	N-CA-CB	7.12	122.52	110.49
8	q	539	LEU	CA-C-N	7.12	129.69	120.44
8	q	539	LEU	C-N-CA	7.12	129.69	120.44
9	g	139	ILE	N-CA-CB	-7.11	104.48	112.45
9	g	279	GLY	O-C-N	7.11	131.66	122.91
4	m	185	LEU	CA-C-N	7.11	130.39	120.29
4	m	185	LEU	C-N-CA	7.11	130.39	120.29
5	c	302	ASP	N-CA-C	-7.10	95.67	110.80
7	p	308	TRP	CA-C-O	-7.10	110.36	120.51
8	f	553	ASN	CA-CB-CG	-7.10	105.50	112.60
9	r	257	TRP	CA-C-N	-7.10	111.42	121.99
9	r	257	TRP	C-N-CA	-7.10	111.42	121.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1091	ASP	CA-C-O	-7.09	113.44	120.89
7	p	50	SER	CB-CA-C	-7.09	101.57	112.07
8	q	144	TRP	CB-CG-CD1	-7.09	116.27	126.90
9	r	338	PRO	N-CD-CG	-7.09	92.56	103.20
3	l	972	LYS	N-CA-C	-7.09	103.74	112.88
9	g	108	TRP	CB-CG-CD1	7.09	137.53	126.90
5	n	350	ILE	N-CA-C	-7.08	97.14	108.90
9	g	529	HIS	ND1-CE1-NE2	7.08	115.48	108.40
4	b	63	ASP	N-CA-CB	7.08	122.46	110.49
5	n	256	LYS	CA-C-O	7.08	128.25	120.82
6	d	8	HIS	ND1-CE1-NE2	7.08	115.47	108.40
1	X	323	TYR	CA-C-N	7.07	135.05	121.54
1	X	323	TYR	C-N-CA	7.07	135.05	121.54
5	c	506	THR	CA-C-N	7.07	129.61	120.56
5	c	506	THR	C-N-CA	7.07	129.61	120.56
8	f	655	ILE	N-CA-C	-7.07	104.09	111.58
4	m	395	VAL	O-C-N	7.07	128.73	121.87
5	n	431	THR	N-CA-C	7.07	119.89	111.33
1	X	1465	LEU	O-C-N	7.07	130.78	122.09
8	f	270	ALA	N-CA-C	7.07	121.28	107.57
1	X	187	PHE	CA-C-N	7.06	130.13	120.46
1	X	187	PHE	C-N-CA	7.06	130.13	120.46
4	b	99	ASP	CA-CB-CG	-7.06	105.54	112.60
3	l	827	GLN	CA-C-N	7.06	131.04	120.31
3	l	827	GLN	C-N-CA	7.06	131.04	120.31
9	r	778	ASN	N-CA-C	-7.06	104.54	113.72
9	r	153	LEU	CB-CA-C	-7.06	99.80	110.88
6	d	47	ASP	CA-CB-CG	7.05	119.65	112.60
7	e	88	PRO	N-CA-C	-7.05	105.53	114.35
4	m	712	THR	CA-CB-OG1	7.05	120.18	109.60
9	r	918	SER	N-CA-C	7.05	119.05	111.36
8	q	229	ASN	CA-CB-CG	-7.05	105.55	112.60
3	a	802	TYR	CA-C-N	7.05	133.09	121.39
3	a	802	TYR	C-N-CA	7.05	133.09	121.39
3	a	764	LEU	N-CA-C	-7.05	104.56	113.72
7	e	207	LYS	N-CA-C	-7.04	96.86	108.76
5	n	511	VAL	N-CA-C	7.04	117.15	110.53
9	r	345	GLN	N-CA-CB	7.04	122.26	111.06
9	r	269	SER	CB-CA-C	-7.04	96.42	110.42
1	X	1492	HIS	N-CA-C	7.03	118.59	111.07
5	c	331	ARG	CA-C-N	7.03	132.17	120.64
5	c	331	ARG	C-N-CA	7.03	132.17	120.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1287	ILE	CA-C-N	7.03	130.01	120.38
1	X	1287	ILE	C-N-CA	7.03	130.01	120.38
7	e	8	HIS	CE1-NE2-CD2	-7.03	101.97	109.00
3	l	453	VAL	N-CA-C	-7.03	98.05	108.45
5	n	451	TRP	CA-C-O	-7.03	113.46	120.70
3	l	189	VAL	N-CA-C	-7.03	107.04	113.71
8	q	146	ASN	CA-CB-CG	-7.03	105.57	112.60
6	o	33	ILE	CA-CB-CG1	7.02	122.34	110.40
9	g	177	ASP	CA-C-N	7.02	129.41	120.56
9	g	177	ASP	C-N-CA	7.02	129.41	120.56
1	X	1638	LYS	O-C-N	7.02	129.30	122.07
8	f	642	ASN	OD1-CG-ND2	-7.02	115.58	122.60
5	n	561	LEU	O-C-N	7.02	129.56	122.12
8	f	384	TYR	CB-CG-CD2	-7.02	110.27	120.80
9	r	324	TYR	CB-CA-C	-7.02	98.17	108.91
5	c	393	GLN	CA-C-N	7.02	129.40	120.56
5	c	393	GLN	C-N-CA	7.02	129.40	120.56
3	l	396	ASP	N-CA-CB	7.02	120.81	110.35
6	o	188	ASN	CA-CB-CG	7.02	119.62	112.60
9	r	550	LEU	CB-CA-C	-7.02	99.56	110.37
3	l	746	CYS	CA-C-N	7.02	127.06	119.90
3	l	746	CYS	C-N-CA	7.02	127.06	119.90
4	b	610	ASP	CA-CB-CG	7.01	119.61	112.60
8	q	279	TYR	CA-C-N	7.01	134.93	121.54
8	q	279	TYR	C-N-CA	7.01	134.93	121.54
3	l	782	TYR	CA-C-N	7.01	127.16	119.87
3	l	782	TYR	C-N-CA	7.01	127.16	119.87
8	f	507	ASP	O-C-N	7.00	131.37	122.19
4	b	659	PRO	CA-C-O	-7.00	113.44	122.12
3	l	929	HIS	ND1-CE1-NE2	7.00	115.40	108.40
1	X	177	VAL	CB-CA-C	-7.00	102.69	112.14
4	b	56	GLN	CA-C-N	7.00	126.52	119.24
4	b	56	GLN	C-N-CA	7.00	126.52	119.24
4	b	214	ARG	O-C-N	-7.00	113.16	122.19
8	f	273	ASN	CA-CB-CG	-7.00	105.60	112.60
3	l	809	LYS	CA-CB-CG	7.00	128.10	114.10
5	n	585	ASN	CA-C-N	7.00	126.70	119.56
5	n	585	ASN	C-N-CA	7.00	126.70	119.56
8	q	666	GLU	CA-C-N	7.00	130.95	120.31
8	q	666	GLU	C-N-CA	7.00	130.95	120.31
5	n	465	PHE	N-CA-C	-7.00	97.21	108.55
3	l	715	THR	N-CA-CB	7.00	120.69	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	752	HIS	CE1-NE2-CD2	-7.00	102.00	109.00
4	m	372	ALA	N-CA-C	-7.00	100.92	111.34
9	g	761	ASN	OD1-CG-ND2	7.00	129.59	122.60
3	l	842	LEU	O-C-N	-6.99	114.71	122.12
8	q	341	HIS	CA-C-N	6.99	126.62	119.56
8	q	341	HIS	C-N-CA	6.99	126.62	119.56
3	a	705	LEU	CA-C-N	6.99	129.53	120.44
3	a	705	LEU	C-N-CA	6.99	129.53	120.44
5	n	282	GLU	O-C-N	-6.99	114.71	122.12
8	q	115	GLN	OE1-CD-NE2	6.99	129.59	122.60
1	X	1386	LEU	N-CA-C	6.99	118.59	110.97
9	g	232	THR	CA-CB-OG1	6.99	120.08	109.60
1	X	190	GLN	CA-C-N	6.98	130.03	120.46
1	X	190	GLN	C-N-CA	6.98	130.03	120.46
3	a	553	ILE	CA-CB-CG1	-6.98	98.53	110.40
9	r	1046	VAL	CB-CA-C	6.98	121.57	112.14
1	X	1503	VAL	CA-C-N	6.98	129.52	120.44
1	X	1503	VAL	C-N-CA	6.98	129.52	120.44
7	e	134	LEU	CA-C-O	6.98	128.18	120.92
9	g	100	ASN	CA-CB-CG	6.98	119.58	112.60
4	m	225	GLU	CA-C-O	6.98	126.72	118.69
5	n	217	PHE	CA-C-O	6.98	127.73	119.56
4	b	146	LEU	N-CA-C	6.98	119.92	111.82
7	p	300	HIS	ND1-CE1-NE2	6.98	115.38	108.40
3	a	481	HIS	CA-CB-CG	-6.98	106.82	113.80
3	a	1010	PHE	N-CA-C	-6.98	104.40	113.12
3	l	520	LEU	O-C-N	6.98	131.45	122.87
6	o	98	HIS	N-CA-CB	6.97	122.27	110.49
9	r	945	ARG	CA-C-N	6.97	129.50	120.44
9	r	945	ARG	C-N-CA	6.97	129.50	120.44
9	g	608	ASP	CB-CA-C	-6.97	98.78	110.56
3	l	753	ASN	N-CA-C	6.97	118.96	111.36
4	b	61	ASN	N-CA-C	-6.97	103.12	111.69
8	f	282	TRP	O-C-N	-6.97	113.70	122.27
5	n	168	SER	N-CA-C	-6.97	104.66	113.72
8	q	619	LYS	CA-C-N	6.96	130.18	120.29
8	q	619	LYS	C-N-CA	6.96	130.18	120.29
7	e	105	ASN	N-CA-C	-6.96	96.30	108.20
9	g	327	ALA	O-C-N	-6.96	113.57	122.20
1	X	1410	SER	N-CA-CB	6.95	120.15	110.07
3	l	454	LYS	CB-CA-C	6.95	124.25	110.42
5	n	131	GLU	CA-C-N	6.95	129.20	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	131	GLU	C-N-CA	6.95	129.20	120.72
6	o	211	ALA	CA-C-O	6.95	128.62	120.70
7	e	310	VAL	N-CA-C	-6.95	98.58	108.58
6	o	88	ARG	NE-CZ-NH1	-6.95	114.56	121.50
8	q	672	VAL	N-CA-C	-6.95	107.11	113.71
9	r	207	LYS	CB-CA-C	-6.94	98.44	110.17
3	a	151	HIS	CA-C-O	-6.94	112.62	120.32
9	r	1101	ARG	NE-CZ-NH1	6.94	128.44	121.50
8	q	576	ASN	N-CA-CB	6.94	122.22	110.49
9	g	912	LYS	N-CA-C	6.93	120.73	111.30
1	X	1303	LEU	N-CA-C	6.93	130.40	111.00
5	c	617	PHE	CA-CB-CG	-6.93	106.87	113.80
4	b	177	GLU	CA-C-O	6.92	127.66	119.28
3	l	355	TRP	N-CA-C	6.92	120.69	110.30
9	r	96	TYR	CA-C-N	-6.92	116.28	121.61
9	r	96	TYR	C-N-CA	-6.92	116.28	121.61
7	e	17	TYR	N-CA-C	-6.92	99.72	110.17
3	l	201	ASP	CA-CB-CG	-6.92	105.68	112.60
3	a	451	ARG	NE-CZ-NH2	-6.92	112.97	119.20
4	b	227	VAL	CA-C-O	6.92	127.84	119.54
7	e	89	ASP	CA-C-O	6.92	127.76	120.42
8	f	178	HIS	CE1-NE2-CD2	-6.92	102.08	109.00
5	n	577	GLY	CA-C-N	6.92	128.49	119.84
5	n	577	GLY	C-N-CA	6.92	128.49	119.84
9	g	795	VAL	N-CA-C	-6.92	104.57	111.77
4	b	743	PHE	N-CA-C	-6.92	98.21	108.79
3	l	820	ARG	NE-CZ-NH1	-6.91	114.59	121.50
9	g	169	GLY	CA-C-N	6.91	133.29	122.78
9	g	169	GLY	C-N-CA	6.91	133.29	122.78
5	n	376	GLU	N-CA-C	-6.91	103.24	113.61
7	p	30	ASP	CA-C-N	6.91	137.19	125.02
7	p	30	ASP	C-N-CA	6.91	137.19	125.02
9	r	785	HIS	CA-CB-CG	-6.91	106.89	113.80
3	a	746	CYS	CA-C-N	6.91	126.52	119.19
3	a	746	CYS	C-N-CA	6.91	126.52	119.19
9	r	606	GLN	N-CA-C	-6.91	105.78	114.56
5	c	542	GLN	CB-CG-CD	-6.90	100.87	112.60
8	q	287	HIS	CA-C-N	6.90	132.16	120.29
8	q	287	HIS	C-N-CA	6.90	132.16	120.29
9	g	337	HIS	CB-CG-CD2	-6.90	122.23	131.20
4	m	91	TYR	CA-C-O	6.90	125.15	119.36
8	q	535	ARG	NE-CZ-NH2	-6.89	113.00	119.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	705	LYS	N-CA-C	6.89	118.44	111.07
6	d	42	THR	N-CA-CB	6.89	121.86	110.63
9	r	143	PRO	N-CA-CB	6.89	110.18	102.67
3	a	131	LEU	N-CA-C	-6.89	98.97	109.85
5	c	334	ASP	CA-CB-CG	6.89	119.49	112.60
9	g	756	PHE	N-CA-C	-6.88	104.00	112.88
4	b	597	LYS	CA-C-N	6.88	130.19	120.28
4	b	597	LYS	C-N-CA	6.88	130.19	120.28
1	X	1465	LEU	CA-C-O	-6.88	111.76	119.81
8	q	97	HIS	CB-CG-CD2	-6.88	122.25	131.20
3	l	963	LYS	CA-C-O	6.88	126.33	118.97
4	b	685	GLU	CA-C-N	6.88	132.79	122.68
4	b	685	GLU	C-N-CA	6.88	132.79	122.68
9	g	165	ILE	CA-C-N	6.88	130.79	120.75
9	g	165	ILE	C-N-CA	6.88	130.79	120.75
3	l	457	PHE	N-CA-C	-6.88	98.98	109.85
8	f	184	ILE	O-C-N	6.88	128.54	121.87
9	g	529	HIS	CE1-NE2-CD2	-6.88	102.12	109.00
7	p	65	SER	O-C-N	-6.88	115.33	121.31
3	l	735	LYS	N-CA-CB	6.88	120.23	110.67
1	X	1060	LEU	N-CA-C	-6.87	96.16	110.80
9	g	183	ASN	CA-CB-CG	6.87	119.47	112.60
9	g	540	HIS	CA-C-O	6.87	127.59	119.48
3	l	868	GLN	CA-C-N	6.87	130.75	120.31
3	l	868	GLN	C-N-CA	6.87	130.75	120.31
6	d	8	HIS	CE1-NE2-CD2	-6.87	102.13	109.00
3	a	929	HIS	CG-CD2-NE2	6.87	114.07	107.20
3	a	1029	ASP	CA-CB-CG	6.87	119.47	112.60
8	f	694	VAL	CA-C-O	-6.87	113.81	120.95
5	n	347	GLY	CA-C-O	-6.87	114.25	121.67
8	q	575	GLU	CA-CB-CG	-6.87	100.36	114.10
3	a	835	ASN	CA-CB-CG	6.87	119.47	112.60
4	b	618	ASN	N-CA-C	-6.87	104.52	113.17
8	f	276	VAL	N-CA-C	-6.86	106.03	112.83
9	g	819	GLN	N-CA-CB	6.86	122.09	110.49
3	l	1016	GLN	OE1-CD-NE2	6.86	129.46	122.60
5	c	202	ARG	NE-CZ-NH1	6.86	128.36	121.50
5	c	486	LEU	CA-C-N	6.86	129.47	120.28
5	c	486	LEU	C-N-CA	6.86	129.47	120.28
7	e	233	THR	CA-C-N	6.86	128.81	120.92
7	e	233	THR	C-N-CA	6.86	128.81	120.92
4	m	328	LEU	CA-C-N	6.86	129.47	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	m	328	LEU	C-N-CA	6.86	129.47	120.28
3	l	219	ASP	N-CA-CB	6.86	123.22	112.25
4	b	288	SER	N-CA-CB	6.86	120.31	110.16
4	b	432	ASN	OD1-CG-ND2	-6.86	115.75	122.60
5	c	415	ASP	CA-CB-CG	-6.86	105.74	112.60
8	f	516	TRP	CD2-CE2-CZ2	-6.86	115.55	122.40
9	g	217	ALA	N-CA-CB	6.86	122.07	110.49
9	g	566	ASN	CA-CB-CG	6.85	119.45	112.60
5	c	538	ILE	CA-C-N	6.85	130.01	120.29
5	c	538	ILE	C-N-CA	6.85	130.01	120.29
9	r	503	TYR	CB-CG-CD2	-6.85	110.53	120.80
1	X	207	ASP	CA-CB-CG	6.85	119.45	112.60
1	X	614	ILE	CA-C-O	6.85	127.64	120.25
9	r	826	SER	N-CA-C	-6.85	97.81	109.24
1	X	204	VAL	O-C-N	-6.84	116.12	121.46
5	c	276	ILE	N-CA-C	-6.84	105.42	113.42
9	r	254	LEU	N-CA-CB	6.84	121.23	110.56
3	l	566	ASN	CA-CB-CG	-6.84	105.76	112.60
9	r	999	LEU	N-CA-C	-6.83	105.22	113.97
8	f	388	ILE	N-CA-C	-6.83	103.55	111.00
9	r	823	GLN	CB-CG-CD	-6.83	100.98	112.60
3	a	867	LYS	N-CA-C	-6.83	103.91	111.36
6	d	33	ILE	N-CA-CB	6.83	120.42	112.15
8	f	699	ASP	N-CA-C	-6.83	104.62	114.12
3	l	274	GLU	N-CA-C	-6.83	105.50	114.31
8	f	291	ASN	CA-C-N	6.83	129.99	120.29
8	f	291	ASN	C-N-CA	6.83	129.99	120.29
9	g	101	ASP	N-CA-C	-6.83	99.03	109.41
3	l	449	ILE	CA-C-N	6.83	133.68	121.66
3	l	449	ILE	C-N-CA	6.83	133.68	121.66
1	X	665	THR	CA-C-N	6.83	127.90	119.98
1	X	665	THR	C-N-CA	6.83	127.90	119.98
9	r	646	PHE	CA-CB-CG	6.83	120.63	113.80
5	c	261	LYS	N-CA-C	6.83	118.37	111.07
9	r	368	PHE	N-CA-CB	6.83	121.31	110.73
9	r	405	GLU	CB-CA-C	-6.82	97.92	109.38
3	a	294	GLU	N-CA-CB	6.82	122.02	110.49
3	a	637	PHE	CA-C-N	6.82	129.15	120.56
3	a	637	PHE	C-N-CA	6.82	129.15	120.56
9	g	648	GLN	N-CA-CB	6.82	120.72	110.22
9	g	930	SER	N-CA-CB	6.82	119.96	110.07
3	l	487	ASN	CA-C-N	6.82	130.56	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	487	ASN	C-N-CA	6.82	130.56	120.87
9	r	1120	VAL	CA-C-N	6.82	130.68	120.31
9	r	1120	VAL	C-N-CA	6.82	130.68	120.31
3	a	889	LEU	N-CA-C	-6.82	104.28	114.64
5	c	346	GLY	CA-C-O	-6.82	116.77	122.29
3	l	261	SER	CA-C-O	-6.82	111.37	119.35
3	a	777	PHE	CA-CB-CG	6.82	120.62	113.80
9	r	713	ASP	N-CA-C	-6.82	103.64	112.23
1	X	1224	ASP	N-CA-C	-6.81	105.52	114.31
3	a	449	ILE	CA-C-O	-6.81	113.11	120.47
8	q	113	ASN	OD1-CG-ND2	6.81	129.41	122.60
1	X	822	ASN	CA-CB-CG	6.81	119.41	112.60
3	a	183	LEU	N-CA-C	-6.81	99.13	109.95
9	r	922	LEU	CA-C-N	6.81	132.09	120.72
9	r	922	LEU	C-N-CA	6.81	132.09	120.72
5	c	489	HIS	CE1-NE2-CD2	-6.81	102.19	109.00
9	g	167	ILE	N-CA-CB	6.81	119.80	110.54
1	X	1535	ASN	CA-CB-CG	6.80	119.40	112.60
3	a	649	GLN	OE1-CD-NE2	-6.80	115.80	122.60
8	f	710	LYS	N-CA-C	-6.80	105.60	114.04
3	l	429	GLU	CA-C-O	6.80	126.22	118.47
5	n	265	HIS	CG-CD2-NE2	6.80	114.00	107.20
3	a	116	GLN	N-CA-CB	6.80	121.98	110.49
4	b	168	ARG	N-CA-C	-6.80	97.33	108.41
5	c	438	VAL	CA-C-N	6.80	132.07	120.72
5	c	438	VAL	C-N-CA	6.80	132.07	120.72
5	n	191	ASP	CA-CB-CG	6.79	119.39	112.60
8	f	643	PHE	N-CA-C	-6.79	98.55	109.96
4	m	372	ALA	O-C-N	6.79	128.45	121.79
8	q	160	PHE	O-C-N	6.79	126.53	120.48
6	o	276	ASN	N-CA-CB	6.79	123.11	112.25
5	c	489	HIS	CA-C-N	6.79	129.37	120.28
5	c	489	HIS	C-N-CA	6.79	129.37	120.28
9	g	964	LEU	CA-C-N	6.78	130.62	120.31
9	g	964	LEU	C-N-CA	6.78	130.62	120.31
5	n	505	ASP	CA-CB-CG	6.78	119.38	112.60
8	q	613	ILE	O-C-N	-6.78	113.37	121.10
3	a	616	LEU	N-CA-C	6.78	121.60	113.12
9	g	820	THR	N-CA-C	-6.78	99.48	109.11
1	X	654	ILE	O-C-N	-6.78	113.17	122.05
1	X	823	ILE	N-CA-C	-6.78	104.40	111.58
8	q	295	GLN	N-CA-C	6.78	120.77	112.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	622	GLY	O-C-N	6.78	128.76	122.19
3	a	993	VAL	N-CA-C	6.77	123.43	109.34
9	g	730	GLU	N-CA-C	-6.77	102.64	111.71
1	X	1427	SER	N-CA-C	-6.77	96.38	110.80
9	g	680	GLY	N-CA-C	-6.77	105.54	115.63
3	a	684	SER	N-CA-C	-6.77	104.77	113.16
8	f	438	GLU	CB-CG-CD	-6.77	101.09	112.60
9	r	688	THR	CA-CB-OG1	6.77	119.75	109.60
4	b	663	LEU	N-CA-C	-6.77	102.28	111.55
4	b	550	HIS	CE1-NE2-CD2	-6.77	102.23	109.00
4	m	728	LEU	CA-C-O	6.77	127.27	119.35
3	l	511	ARG	NE-CZ-NH1	6.76	128.26	121.50
1	X	938	ASP	CA-C-O	6.76	130.18	120.51
5	c	271	TRP	CA-C-N	6.76	129.72	120.46
5	c	271	TRP	C-N-CA	6.76	129.72	120.46
3	l	979	GLU	CA-C-N	-6.76	114.64	122.14
3	l	979	GLU	C-N-CA	-6.76	114.64	122.14
9	g	229	PHE	N-CA-C	-6.76	98.23	109.24
5	n	580	LEU	CA-C-O	6.75	127.45	119.28
3	a	929	HIS	CE1-NE2-CD2	-6.75	102.25	109.00
4	b	54	ASN	CA-CB-CG	6.75	119.35	112.60
4	b	728	LEU	N-CA-C	-6.75	104.35	112.59
4	b	116	ARG	NE-CZ-NH1	6.75	128.25	121.50
9	g	781	TYR	CA-C-N	6.75	129.21	120.44
9	g	781	TYR	C-N-CA	6.75	129.21	120.44
9	g	833	GLU	N-CA-CB	6.75	121.90	110.49
1	X	1122	PHE	CA-CB-CG	-6.75	107.06	113.80
3	l	520	LEU	N-CA-C	6.75	120.01	110.23
3	a	91	LYS	CA-C-N	6.74	132.50	123.00
3	a	91	LYS	C-N-CA	6.74	132.50	123.00
8	q	617	ILE	N-CA-C	-6.74	106.22	112.96
1	X	1179	SER	CA-C-O	-6.74	113.14	121.02
9	g	742	LEU	O-C-N	6.74	131.46	122.43
8	q	578	ASP	O-C-N	-6.74	113.63	122.59
9	r	73	GLN	CB-CA-C	-6.74	98.63	109.75
1	X	1450	LEU	N-CA-CB	6.74	119.75	109.98
4	b	369	GLU	O-C-N	6.74	129.13	122.19
9	g	392	ASP	CA-CB-CG	-6.74	105.86	112.60
5	n	612	VAL	N-CA-C	-6.74	106.46	112.12
5	c	583	SER	N-CA-C	-6.73	102.39	113.50
1	X	1008	THR	CA-C-O	-6.73	111.81	118.34
4	b	419	PHE	O-C-N	-6.73	112.43	122.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	594	LEU	N-CA-C	-6.73	105.83	112.97
6	d	225	VAL	CA-C-O	-6.73	113.32	121.13
3	l	89	HIS	CE1-NE2-CD2	-6.73	102.27	109.00
3	l	536	ILE	CA-C-O	-6.73	112.85	119.92
8	q	237	ILE	CA-C-O	-6.73	113.35	120.48
9	g	628	HIS	CA-C-O	6.72	126.14	119.08
4	m	381	ALA	N-CA-CB	6.72	121.85	110.49
3	a	636	THR	CA-CB-OG1	6.72	119.68	109.60
4	b	92	PRO	CA-C-O	-6.72	114.04	121.23
8	f	360	HIS	CB-CG-CD2	-6.72	122.46	131.20
5	c	267	ARG	N-CA-C	6.72	118.26	111.07
9	g	738	TYR	N-CA-CB	-6.72	100.19	110.20
3	l	449	ILE	N-CA-C	-6.72	103.93	113.07
3	a	719	PHE	O-C-N	-6.72	114.50	123.23
1	X	1217	ARG	NE-CZ-NH2	6.72	125.25	119.20
1	X	1289	LYS	CA-C-N	6.71	134.37	121.54
1	X	1289	LYS	C-N-CA	6.71	134.37	121.54
3	l	699	ILE	CA-C-N	6.71	129.76	120.63
3	l	699	ILE	C-N-CA	6.71	129.76	120.63
8	f	44	SER	N-CA-CB	6.71	120.10	110.16
9	r	168	LYS	N-CA-CB	6.71	120.40	110.33
4	b	468	SER	N-CA-C	6.71	120.73	112.54
4	b	625	ALA	CA-C-N	6.71	128.23	119.84
4	b	625	ALA	C-N-CA	6.71	128.23	119.84
4	m	251	GLN	OE1-CD-NE2	6.71	129.31	122.60
3	a	573	GLU	N-CA-CB	6.71	120.20	110.20
4	b	473	LEU	N-CA-CB	6.71	120.39	110.53
9	g	605	ARG	NE-CZ-NH1	6.71	128.21	121.50
9	g	1074	ASN	CA-C-N	6.71	130.28	120.82
9	g	1074	ASN	C-N-CA	6.71	130.28	120.82
8	q	474	ASN	CA-CB-CG	-6.71	105.89	112.60
8	q	423	GLN	OE1-CD-NE2	6.71	129.31	122.60
4	b	310	VAL	N-CA-C	-6.71	102.90	112.35
4	b	532	PRO	N-CA-CB	6.71	107.46	101.83
3	l	386	LEU	N-CA-C	6.70	119.44	111.33
5	n	303	VAL	O-C-N	-6.70	116.82	121.98
9	r	292	PHE	CB-CA-C	-6.70	99.97	111.23
4	b	154	GLU	CB-CG-CD	-6.70	101.21	112.60
5	n	339	GLN	N-CA-C	6.70	118.66	111.36
9	r	123	PRO	N-CD-CG	-6.70	93.15	103.20
7	p	146	ARG	NE-CZ-NH1	6.70	128.20	121.50
9	r	151	LEU	CB-CA-C	-6.70	99.67	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	615	THR	CA-CB-CG2	-6.70	99.12	110.50
7	e	9	ASP	N-CA-C	-6.69	102.74	111.71
3	l	540	LEU	CA-C-O	-6.69	113.43	119.59
5	n	528	ASN	OD1-CG-ND2	6.69	129.29	122.60
6	d	52	HIS	CE1-NE2-CD2	-6.69	102.31	109.00
7	p	208	LEU	O-C-N	-6.69	113.62	121.32
8	q	611	SER	CA-C-N	6.69	134.32	121.54
8	q	611	SER	C-N-CA	6.69	134.32	121.54
4	m	227	VAL	N-CA-CB	6.69	122.27	111.23
4	b	546	MET	N-CA-C	-6.69	105.10	112.72
9	g	713	ASP	CA-C-N	6.69	134.31	121.54
9	g	713	ASP	C-N-CA	6.69	134.31	121.54
8	f	223	ILE	CA-C-O	-6.69	114.02	120.30
9	r	247	LEU	CB-CA-C	-6.69	99.48	110.85
3	l	128	PHE	N-CA-C	-6.68	96.56	110.80
3	l	285	ASN	N-CA-C	6.68	119.66	110.24
9	g	219	ILE	CA-C-O	6.68	127.71	120.43
9	r	433	LEU	N-CA-CB	6.68	121.48	110.39
4	m	397	ILE	CA-C-N	6.68	129.61	120.46
4	m	397	ILE	C-N-CA	6.68	129.61	120.46
3	a	180	ASP	N-CA-C	-6.68	102.98	112.13
5	n	559	LEU	N-CA-C	-6.68	104.77	113.12
8	f	525	ASP	N-CA-C	-6.67	104.36	113.30
9	g	759	TRP	CB-CG-CD1	6.67	136.91	126.90
4	b	280	VAL	CA-CB-CG1	-6.67	99.06	110.40
9	g	428	GLN	OE1-CD-NE2	6.67	129.27	122.60
3	l	250	SER	CA-C-N	6.67	132.29	122.82
3	l	250	SER	C-N-CA	6.67	132.29	122.82
4	m	171	ARG	N-CA-C	-6.67	104.09	111.36
1	X	1415	VAL	CA-C-O	-6.67	114.09	121.23
3	a	137	PHE	N-CA-C	-6.67	103.35	113.89
4	b	696	GLU	CA-C-N	6.67	129.11	120.44
4	b	696	GLU	C-N-CA	6.67	129.11	120.44
9	g	1046	VAL	O-C-N	6.67	128.34	121.87
3	a	945	VAL	CA-C-O	-6.67	112.45	120.78
8	q	301	TYR	CA-C-O	6.67	127.48	120.42
1	X	763	GLN	CA-C-N	6.66	134.27	121.54
1	X	763	GLN	C-N-CA	6.66	134.27	121.54
8	q	42	PHE	N-CA-CB	6.66	120.61	110.28
8	f	240	HIS	CE1-NE2-CD2	-6.66	102.34	109.00
6	d	88	ARG	CA-C-O	-6.66	114.10	121.23
3	l	587	ILE	N-CA-CB	6.66	117.88	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	256	LEU	N-CA-CB	6.66	120.60	109.94
1	X	1029	ASN	CA-C-O	6.66	127.84	120.92
5	n	584	ASN	N-CA-C	-6.66	97.56	108.41
3	l	407	GLY	CA-C-N	6.66	129.09	120.44
3	l	407	GLY	C-N-CA	6.66	129.09	120.44
9	g	353	ASP	CA-CB-CG	6.66	119.26	112.60
1	X	1099	PHE	CA-CB-CG	-6.65	107.15	113.80
9	g	984	PHE	N-CA-C	-6.65	102.46	112.04
9	r	807	PHE	CA-CB-CG	6.65	120.45	113.80
1	X	195	LEU	N-CA-C	-6.65	105.13	113.18
4	b	303	PHE	N-CA-C	-6.65	105.32	113.50
5	c	329	ASP	N-CA-C	-6.65	95.11	109.81
1	X	634	ILE	CA-C-N	6.65	129.01	120.70
1	X	634	ILE	C-N-CA	6.65	129.01	120.70
4	b	679	ASP	CA-CB-CG	-6.65	105.95	112.60
8	f	340	GLU	N-CA-C	-6.65	103.49	112.26
3	l	6	ARG	NE-CZ-NH1	-6.65	114.85	121.50
1	X	1534	TYR	CA-C-N	6.64	134.23	121.54
1	X	1534	TYR	C-N-CA	6.64	134.23	121.54
5	c	575	SER	N-CA-C	-6.64	102.59	111.96
7	p	78	ASP	N-CA-C	-6.64	104.92	113.16
9	r	884	HIS	CG-CD2-NE2	6.64	113.84	107.20
3	a	378	TRP	CB-CG-CD2	-6.64	117.50	126.80
4	b	623	THR	O-C-N	6.64	129.98	122.27
8	f	723	THR	N-CA-C	-6.64	105.05	113.02
7	e	302	ASP	N-CA-C	-6.64	103.80	114.09
9	g	662	ASN	N-CA-C	-6.64	104.80	113.17
4	m	300	SER	CA-C-O	-6.64	111.76	119.59
1	X	134	ARG	NE-CZ-NH2	-6.64	113.23	119.20
1	X	1539	ASN	N-CA-C	-6.64	96.94	108.69
3	a	457	PHE	N-CA-C	-6.64	104.41	113.30
3	a	724	PHE	CA-CB-CG	6.64	120.44	113.80
1	X	618	LEU	O-C-N	6.63	128.93	122.03
3	l	410	ASN	CA-C-N	6.63	129.07	120.44
3	l	410	ASN	C-N-CA	6.63	129.07	120.44
4	b	162	VAL	CA-C-O	6.63	128.07	119.85
9	r	1111	GLU	N-CA-C	6.63	118.16	111.07
1	X	682	LEU	N-CA-CB	6.63	121.57	110.77
8	q	260	GLU	CA-C-N	6.62	131.78	120.72
8	q	260	GLU	C-N-CA	6.62	131.78	120.72
9	r	629	LEU	N-CA-C	-6.62	104.94	113.16
3	a	1003	VAL	N-CA-C	-6.62	105.07	113.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	113	ASN	CA-CB-CG	6.62	119.22	112.60
3	a	419	ILE	CA-C-N	6.62	129.69	120.29
3	a	419	ILE	C-N-CA	6.62	129.69	120.29
4	b	619	SER	N-CA-C	-6.62	103.15	113.02
8	f	178	HIS	ND1-CE1-NE2	6.62	115.02	108.40
3	a	345	GLU	N-CA-C	-6.62	103.68	113.61
3	l	567	LEU	N-CA-CB	6.62	119.85	110.12
1	X	1031	LYS	N-CA-C	-6.62	103.68	113.61
3	a	829	SER	CA-C-N	6.62	129.04	120.44
3	a	829	SER	C-N-CA	6.62	129.04	120.44
4	b	70	LYS	O-C-N	6.62	131.18	123.30
4	b	240	PHE	CA-CB-CG	-6.62	107.18	113.80
5	n	504	GLU	CA-C-O	-6.62	113.85	120.80
6	o	286	GLU	N-CA-CB	6.62	121.68	110.49
4	m	315	GLN	CB-CG-CD	-6.62	101.35	112.60
8	q	382	LYS	N-CA-C	-6.62	98.80	109.58
4	b	98	LEU	N-CA-C	-6.62	96.71	110.80
3	l	821	HIS	CG-CD2-NE2	6.62	113.81	107.20
4	m	106	ALA	O-C-N	6.61	129.69	122.15
5	c	130	ASP	N-CA-C	-6.61	105.03	113.23
4	b	675	PHE	CA-CB-CG	-6.61	107.19	113.80
8	q	67	ASP	CA-CB-CG	-6.61	105.99	112.60
4	m	78	ASN	CA-CB-CG	-6.61	105.99	112.60
9	r	253	LYS	N-CA-CB	6.61	120.55	110.44
1	X	1311	LEU	N-CA-C	-6.61	104.00	111.07
3	a	781	ASP	CA-CB-CG	6.61	119.20	112.60
6	d	225	VAL	N-CA-CB	6.61	118.98	110.13
8	f	417	ILE	N-CA-C	6.60	117.39	110.72
8	f	209	CYS	CA-C-N	6.60	129.66	120.29
8	f	209	CYS	C-N-CA	6.60	129.66	120.29
5	n	436	LYS	CA-C-O	6.60	127.55	120.55
4	m	609	GLN	OE1-CD-NE2	6.60	129.20	122.60
9	r	1103	PRO	N-CD-CG	6.60	113.10	103.20
4	b	713	ILE	N-CA-C	-6.60	106.81	113.47
4	m	644	GLN	N-CA-CB	6.60	119.77	109.94
9	g	702	ASP	CA-C-O	-6.60	113.09	120.54
6	o	43	HIS	ND1-CE1-NE2	6.60	115.00	108.40
7	p	210	GLY	CA-C-O	6.60	127.18	119.13
3	a	615	SER	N-CA-C	-6.59	105.05	113.23
3	l	821	HIS	CE1-NE2-CD2	-6.59	102.41	109.00
5	n	287	SER	O-C-N	-6.59	114.76	122.87
5	c	441	ARG	N-CA-CB	6.59	117.07	108.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	e	205	ALA	N-CA-C	-6.59	104.86	113.17
7	p	24	VAL	N-CA-CB	6.59	121.14	111.52
8	q	654	GLU	CA-C-O	6.59	127.57	119.79
4	b	92	PRO	CB-CA-C	-6.59	103.34	111.64
4	b	708	ASN	O-C-N	6.59	129.66	122.15
9	g	868	HIS	CE1-NE2-CD2	-6.59	102.41	109.00
3	a	980	VAL	CA-C-O	-6.59	113.05	118.98
4	b	63	ASP	CA-C-N	6.59	130.17	120.95
4	b	63	ASP	C-N-CA	6.59	130.17	120.95
3	l	586	LEU	CA-C-N	6.58	128.93	120.70
3	l	586	LEU	C-N-CA	6.58	128.93	120.70
8	f	291	ASN	OD1-CG-ND2	6.58	129.18	122.60
3	l	89	HIS	CG-CD2-NE2	6.58	113.78	107.20
3	a	458	ASN	CA-CB-CG	-6.58	106.02	112.60
3	a	803	HIS	CA-CB-CG	6.58	120.38	113.80
9	r	689	ILE	N-CA-CB	6.58	119.49	110.54
9	r	1054	GLY	CA-C-N	6.58	134.11	121.54
9	r	1054	GLY	C-N-CA	6.58	134.11	121.54
5	c	423	GLN	OE1-CD-NE2	6.58	129.18	122.60
7	e	199	ASP	N-CA-C	-6.58	98.99	108.60
9	r	1042	TRP	N-CA-C	6.58	120.40	112.38
9	r	753	PHE	CA-C-N	6.57	130.30	120.31
9	r	753	PHE	C-N-CA	6.57	130.30	120.31
9	g	947	ILE	O-C-N	-6.57	115.45	121.89
4	b	295	TYR	O-C-N	6.57	127.49	120.85
3	l	154	ASN	CA-C-O	-6.57	112.72	119.49
3	l	749	TYR	CA-CB-CG	-6.57	102.08	113.90
4	b	516	ASN	CA-CB-CG	6.57	119.17	112.60
9	g	274	PRO	N-CA-CB	6.57	110.15	103.25
9	g	751	TYR	N-CA-C	-6.57	105.23	112.72
1	X	422	GLU	N-CA-C	-6.57	103.76	113.61
9	r	276	LEU	CB-CA-C	-6.57	101.03	110.62
4	b	576	PHE	N-CA-C	-6.56	105.19	113.72
7	e	8	HIS	ND1-CE1-NE2	6.56	114.96	108.40
9	r	515	ASN	OD1-CG-ND2	-6.56	116.04	122.60
1	X	1208	GLY	O-C-N	6.56	128.49	122.19
4	m	282	PHE	N-CA-C	-6.56	104.67	114.64
5	n	540	ASN	N-CA-CB	6.56	120.33	110.22
9	r	826	SER	CA-C-O	6.56	128.21	120.66
3	a	693	PHE	N-CA-C	-6.56	105.57	113.97
4	b	339	ILE	N-CA-C	-6.56	104.25	110.42
8	q	550	MET	CA-C-N	6.56	132.53	122.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	550	MET	C-N-CA	6.56	132.53	122.23
9	r	515	ASN	CA-CB-CG	6.56	119.16	112.60
4	b	55	ASP	N-CA-CB	6.56	121.25	110.69
3	a	66	GLU	N-CA-C	-6.56	97.68	108.76
8	f	430	PRO	CA-C-O	-6.56	110.14	118.86
9	g	1149	ASN	CA-CB-CG	-6.56	106.04	112.60
9	r	289	LYS	N-CA-CB	6.56	121.04	110.42
1	X	1020	ILE	CA-CB-CG1	6.56	121.54	110.40
5	n	646	ASP	N-CA-CB	6.56	119.76	110.12
5	c	585	ASN	CA-CB-CG	6.55	119.16	112.60
3	a	723	PHE	CA-C-N	6.55	129.95	120.38
3	a	723	PHE	C-N-CA	6.55	129.95	120.38
7	p	177	ARG	NE-CZ-NH2	6.55	125.10	119.20
1	X	814	ASP	CA-CB-CG	6.55	119.15	112.60
4	b	639	ARG	CB-CG-CD	6.55	126.37	111.30
5	c	581	LEU	N-CA-C	6.55	119.98	110.42
4	m	398	ILE	O-C-N	-6.55	115.51	121.87
5	c	362	SER	CA-C-O	6.55	127.43	119.31
4	m	268	SER	CA-C-N	6.55	131.14	122.30
4	m	268	SER	C-N-CA	6.55	131.14	122.30
3	l	689	GLY	CA-C-O	-6.54	115.82	122.56
5	n	214	SER	N-CA-C	-6.54	103.90	112.41
9	r	148	GLU	N-CA-CB	6.54	119.84	110.16
1	X	699	GLU	O-C-N	-6.54	116.42	123.42
1	X	1004	LEU	N-CA-C	-6.54	103.80	113.61
7	e	231	ILE	O-C-N	6.54	129.38	123.03
9	g	151	LEU	CA-C-N	6.54	134.04	121.54
9	g	151	LEU	C-N-CA	6.54	134.04	121.54
9	r	790	HIS	CE1-NE2-CD2	-6.54	102.46	109.00
4	b	389	ASP	N-CA-C	-6.54	103.72	112.94
9	r	976	LYS	N-CA-C	-6.54	104.49	114.16
1	X	220	PHE	CA-CB-CG	6.53	120.33	113.80
5	c	159	LEU	CB-CA-C	-6.53	99.02	109.80
4	b	534	ILE	N-CA-C	-6.53	103.88	111.00
9	g	859	ASP	CA-CB-CG	6.53	119.13	112.60
3	a	719	PHE	CA-C-O	6.53	127.75	120.70
9	g	311	ASN	N-CA-CB	6.53	120.93	110.16
4	m	281	SER	N-CA-C	-6.53	104.62	112.59
1	X	1025	ASN	CA-CB-CG	6.53	119.13	112.60
3	a	1023	LYS	N-CA-C	-6.53	104.89	112.92
3	a	636	THR	N-CA-C	-6.52	104.47	112.88
3	a	706	ASN	CA-CB-CG	-6.52	106.08	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	260	VAL	CA-CB-CG1	6.52	121.49	110.40
9	r	1126	ASP	N-CA-CB	6.52	121.52	110.49
1	X	1626	GLN	N-CA-CB	6.52	121.81	110.39
7	e	159	ILE	N-CA-C	-6.52	99.85	107.61
3	l	130	THR	N-CA-C	-6.52	96.75	108.48
9	r	1142	LYS	N-CA-C	-6.52	105.20	113.02
3	a	385	SER	CA-C-O	6.52	129.25	121.88
3	a	512	THR	CA-CB-CG2	-6.52	99.42	110.50
3	a	819	TYR	CA-CB-CG	-6.52	102.17	113.90
9	g	290	GLY	CA-C-O	6.52	126.00	118.96
9	g	565	GLN	CA-C-O	-6.52	113.01	120.24
3	a	216	SER	CA-C-N	6.51	129.01	120.28
3	a	216	SER	C-N-CA	6.51	129.01	120.28
9	g	599	LYS	CA-C-O	6.51	127.33	120.42
7	p	2	GLN	O-C-N	-6.51	115.59	121.39
7	p	14	ASP	CA-CB-CG	6.51	119.11	112.60
7	e	63	TRP	CA-C-O	-6.51	112.87	120.62
5	n	402	LEU	CA-C-N	6.51	130.98	120.30
5	n	402	LEU	C-N-CA	6.51	130.98	120.30
7	p	55	ASP	CA-C-O	6.51	127.63	119.95
9	g	1036	PHE	N-CA-C	-6.51	104.82	112.89
3	l	564	ILE	N-CA-C	6.51	117.29	110.72
9	r	597	CYS	CA-C-N	6.51	129.66	120.42
9	r	597	CYS	C-N-CA	6.51	129.66	120.42
1	X	262	SER	N-CA-C	-6.50	102.67	112.04
4	m	228	PHE	N-CA-C	-6.50	104.54	114.16
7	e	154	MET	O-C-N	-6.50	114.54	123.12
9	g	332	LYS	N-CA-C	-6.50	104.28	111.82
6	o	223	ALA	CA-C-N	6.50	132.66	122.26
6	o	223	ALA	C-N-CA	6.50	132.66	122.26
8	q	351	ILE	CA-C-N	6.50	128.99	120.28
8	q	351	ILE	C-N-CA	6.50	128.99	120.28
9	r	614	TRP	CA-C-N	6.50	131.00	120.60
9	r	614	TRP	C-N-CA	6.50	131.00	120.60
1	X	1558	GLN	OE1-CD-NE2	6.50	129.10	122.60
3	a	658	HIS	N-CA-C	6.50	118.36	111.28
6	d	153	TRP	CB-CG-CD2	-6.50	117.70	126.80
9	r	977	ASN	N-CA-C	-6.50	99.46	109.14
1	X	650	ASP	CA-CB-CG	6.50	119.09	112.60
4	b	86	ASP	CA-CB-CG	6.50	119.09	112.60
8	f	597	TYR	CA-C-N	6.50	130.18	120.31
8	f	597	TYR	C-N-CA	6.50	130.18	120.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	m	629	VAL	N-CA-C	-6.50	95.83	109.34
9	g	445	ASP	N-CA-CB	6.49	119.62	109.69
7	p	300	HIS	CE1-NE2-CD2	-6.49	102.51	109.00
8	q	287	HIS	N-CA-CB	6.49	119.42	110.01
9	g	351	ILE	N-CA-C	-6.49	98.30	108.23
3	a	418	GLN	OE1-CD-NE2	-6.49	116.11	122.60
3	a	442	TYR	O-C-N	6.49	129.10	122.09
9	r	123	PRO	N-CA-CB	6.49	110.06	103.25
1	X	1084	LEU	N-CA-C	-6.49	104.29	111.36
5	n	497	LEU	N-CA-CB	6.49	120.32	109.94
7	p	75	ALA	N-CA-CB	6.49	121.14	110.69
6	d	218	LEU	N-CA-CB	6.49	120.24	109.60
4	m	550	HIS	CE1-NE2-CD2	-6.49	102.51	109.00
1	X	915	ASP	CA-CB-CG	6.49	119.09	112.60
5	c	593	LYS	CA-C-N	6.49	129.62	120.28
5	c	593	LYS	C-N-CA	6.49	129.62	120.28
3	l	1006	VAL	O-C-N	6.48	129.32	123.03
1	X	1305	ASN	N-CA-C	-6.48	102.58	110.88
5	n	641	MET	CA-C-N	6.48	129.50	120.29
5	n	641	MET	C-N-CA	6.48	129.50	120.29
7	p	203	HIS	ND1-CE1-NE2	6.48	114.88	108.40
8	q	347	MET	CA-C-N	6.48	128.87	120.44
8	q	347	MET	C-N-CA	6.48	128.87	120.44
8	q	554	ASN	CA-CB-CG	6.48	119.08	112.60
9	r	839	PHE	CA-CB-CG	6.48	120.28	113.80
9	r	652	HIS	CE1-NE2-CD2	-6.48	102.52	109.00
9	r	1148	ILE	N-CA-C	-6.48	98.86	108.45
9	g	419	MET	N-CA-CB	6.48	120.97	110.41
3	l	622	LEU	CA-C-O	6.48	127.35	119.38
5	n	450	CYS	CA-C-N	6.48	129.25	120.44
5	n	450	CYS	C-N-CA	6.48	129.25	120.44
8	q	157	ASP	CA-CB-CG	6.48	119.08	112.60
9	r	979	SER	N-CA-C	-6.48	105.13	113.16
8	f	192	ALA	CA-C-O	6.48	129.77	120.51
3	l	799	SER	N-CA-CB	6.48	119.83	110.37
1	X	931	PHE	N-CA-C	-6.47	103.72	112.26
1	X	939	LEU	O-C-N	-6.47	115.35	123.05
5	c	648	TYR	CB-CG-CD1	6.47	130.51	120.80
4	m	161	ARG	NE-CZ-NH2	-6.47	113.37	119.20
9	r	252	PHE	N-CA-CB	6.47	121.33	110.32
1	X	1345	SER	CA-C-N	6.47	133.46	122.26
1	X	1345	SER	C-N-CA	6.47	133.46	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	588	ASN	N-CA-C	-6.47	105.31	113.72
8	f	622	GLY	O-C-N	6.47	129.33	122.28
5	c	650	HIS	CE1-NE2-CD2	-6.47	102.53	109.00
4	m	727	LEU	N-CA-C	-6.47	98.83	108.99
7	p	8	HIS	CA-CB-CG	6.47	120.27	113.80
9	g	905	ASN	N-CA-C	6.47	119.15	111.71
5	c	210	ILE	O-C-N	6.46	129.90	123.18
3	a	847	LYS	N-CA-CB	6.46	121.41	110.49
4	b	503	VAL	N-CA-C	-6.46	105.27	113.22
3	l	1015	ASP	N-CA-CB	6.46	119.47	110.17
7	p	244	LYS	CA-C-N	6.46	129.70	122.59
7	p	244	LYS	C-N-CA	6.46	129.70	122.59
5	c	217	PHE	N-CA-C	-6.46	104.97	112.92
5	c	218	LYS	CA-C-N	6.46	132.44	121.14
5	c	218	LYS	C-N-CA	6.46	132.44	121.14
7	e	304	ASN	CA-C-O	-6.46	114.13	122.14
1	X	1565	ASN	N-CA-CB	6.46	119.27	110.10
3	l	682	ASP	N-CA-C	-6.46	105.16	113.16
9	r	250	LYS	CB-CA-C	-6.45	100.76	112.76
1	X	1001	ASN	CA-CB-CG	6.45	119.05	112.60
7	p	57	SER	N-CA-CB	6.45	119.70	109.51
9	g	855	LYS	CA-C-O	-6.45	113.79	121.66
6	o	54	GLY	O-C-N	-6.45	115.32	121.77
7	e	225	GLY	CA-C-O	-6.45	111.06	119.44
1	X	675	TYR	CA-C-N	6.45	129.21	120.38
1	X	675	TYR	C-N-CA	6.45	129.21	120.38
1	X	1431	ILE	CB-CA-C	-6.45	103.67	111.85
5	n	150	PHE	CA-CB-CG	-6.45	107.35	113.80
9	g	244	LEU	CA-C-O	6.44	127.17	120.40
5	n	489	HIS	ND1-CE1-NE2	6.44	114.84	108.40
1	X	1410	SER	CA-C-N	6.44	128.91	120.28
1	X	1410	SER	C-N-CA	6.44	128.91	120.28
1	X	1491	LEU	CA-C-N	6.44	128.81	120.44
1	X	1491	LEU	C-N-CA	6.44	128.81	120.44
9	g	864	PHE	CB-CA-C	-6.44	99.58	108.86
7	p	211	HIS	CE1-NE2-CD2	-6.44	102.56	109.00
3	a	180	ASP	CA-CB-CG	-6.44	106.16	112.60
1	X	1605	PHE	CA-CB-CG	-6.44	107.36	113.80
9	g	635	VAL	CA-C-N	6.44	129.74	120.98
9	g	635	VAL	C-N-CA	6.44	129.74	120.98
5	n	407	LEU	N-CA-C	6.44	118.30	111.28
8	f	300	ASN	OD1-CG-ND2	-6.43	116.17	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	105	PHE	N-CA-CB	6.43	119.34	110.01
8	f	463	GLU	N-CA-C	6.43	118.29	111.28
8	q	147	SER	N-CA-CB	6.43	119.40	110.07
5	c	286	ASN	N-CA-C	-6.43	105.31	113.02
3	l	494	PHE	CA-CB-CG	-6.43	107.37	113.80
9	r	207	LYS	N-CA-CB	6.43	120.32	110.61
9	r	559	VAL	CB-CA-C	-6.43	101.84	112.26
9	r	1091	THR	N-CA-C	-6.43	94.19	107.95
4	b	519	ILE	N-CA-C	-6.43	107.23	113.53
3	l	763	THR	N-CA-CB	6.43	119.59	109.82
8	q	174	LYS	CA-C-N	6.43	128.89	120.28
8	q	174	LYS	C-N-CA	6.43	128.89	120.28
9	r	248	LEU	CB-CA-C	-6.43	100.12	110.79
1	X	136	ASN	OD1-CG-ND2	-6.42	116.17	122.60
1	X	698	VAL	CA-C-O	6.42	125.06	118.96
1	X	1123	HIS	CE1-NE2-CD2	-6.42	102.58	109.00
4	m	75	SER	N-CA-CB	6.42	121.34	110.49
3	l	513	LEU	O-C-N	6.42	129.47	122.15
3	l	570	LEU	N-CA-C	6.42	117.97	110.97
1	X	1460	LEU	CA-C-N	6.42	128.88	120.60
1	X	1460	LEU	C-N-CA	6.42	128.88	120.60
3	l	874	ASN	N-CA-CB	6.42	119.55	110.12
8	f	14	LYS	N-CA-C	6.41	119.08	111.71
6	o	108	ALA	N-CA-C	-6.41	102.05	110.39
3	a	87	ALA	N-CA-C	6.41	117.93	111.07
4	m	388	ASN	OD1-CG-ND2	6.41	129.01	122.60
6	o	292	ALA	N-CA-C	-6.41	104.23	113.21
3	a	80	THR	O-C-N	6.41	130.54	123.04
3	a	903	ASN	CA-C-O	6.41	127.04	119.28
9	g	782	ASP	CA-C-O	-6.41	114.09	120.82
9	g	818	LEU	CA-C-O	6.41	127.22	119.78
3	l	923	LEU	N-CA-C	6.41	118.80	111.11
3	a	447	GLU	O-C-N	6.41	129.46	122.15
8	f	335	HIS	CB-CG-CD2	-6.41	122.87	131.20
4	b	160	GLY	CA-C-N	6.40	129.34	120.63
4	b	160	GLY	C-N-CA	6.40	129.34	120.63
5	c	479	ALA	N-CA-C	6.40	118.26	111.28
7	p	6	SER	N-CA-C	-6.40	105.77	113.97
3	l	195	GLU	CA-C-N	6.40	126.16	119.76
3	l	195	GLU	C-N-CA	6.40	126.16	119.76
3	l	1027	LEU	N-CA-C	-6.40	103.81	112.26
4	b	306	TRP	CE2-CD2-CE3	6.40	125.20	118.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	e	294	VAL	N-CA-CB	6.40	118.70	111.21
4	m	376	GLN	N-CA-CB	6.40	120.08	110.22
9	r	254	LEU	CB-CA-C	-6.40	99.24	109.80
1	X	1203	THR	CA-C-N	6.40	129.33	120.63
1	X	1203	THR	C-N-CA	6.40	129.33	120.63
4	b	456	SER	N-CA-CB	6.40	121.31	110.49
1	X	734	SER	CA-C-O	-6.40	113.14	120.24
4	b	283	ASP	CA-CB-CG	6.40	119.00	112.60
3	a	105	ARG	NE-CZ-NH2	-6.39	113.44	119.20
3	a	607	PHE	CA-C-O	-6.39	113.35	120.70
3	l	528	ILE	CB-CA-C	-6.39	103.78	111.97
3	a	11	LEU	N-CA-C	-6.39	104.63	112.88
9	r	713	ASP	CA-C-N	6.39	133.75	121.54
9	r	713	ASP	C-N-CA	6.39	133.75	121.54
5	c	313	SER	N-CA-C	-6.39	105.42	113.72
5	c	378	GLU	N-CA-C	-6.39	104.03	113.61
8	f	345	VAL	CA-C-N	6.39	129.36	120.29
8	f	345	VAL	C-N-CA	6.39	129.36	120.29
3	l	824	PHE	N-CA-CB	6.39	119.51	110.12
5	n	615	ASN	N-CA-C	-6.39	104.74	113.30
7	p	17	TYR	O-C-N	6.39	130.25	123.03
1	X	899	GLN	CA-C-O	6.38	126.07	119.05
1	X	1413	ASN	CA-C-O	-6.38	113.78	120.55
4	b	388	ASN	OD1-CG-ND2	6.38	128.99	122.60
8	f	687	ALA	N-CA-C	-6.38	107.34	114.62
4	m	140	HIS	CG-CD2-NE2	6.38	113.58	107.20
5	n	259	LEU	CA-C-O	-6.38	111.39	119.31
9	r	432	LYS	CB-CA-C	-6.38	98.08	110.46
9	r	854	HIS	CG-CD2-NE2	6.38	113.58	107.20
1	X	1634	LEU	CA-C-N	6.38	133.73	121.54
1	X	1634	LEU	C-N-CA	6.38	133.73	121.54
6	o	110	HIS	CE1-NE2-CD2	-6.38	102.62	109.00
8	f	654	GLU	N-CA-CB	6.38	120.80	110.40
8	f	69	GLU	N-CA-CB	6.38	119.26	110.01
4	m	106	ALA	CA-C-O	-6.38	113.66	120.42
9	r	395	PHE	CA-CB-CG	-6.38	107.42	113.80
1	X	775	PHE	CA-CB-CG	6.38	120.18	113.80
3	a	826	TYR	CB-CG-CD2	-6.38	111.23	120.80
8	f	589	HIS	CE1-NE2-CD2	-6.38	102.62	109.00
3	l	384	LYS	CA-C-O	6.38	128.98	121.58
9	g	1051	SER	N-CA-C	-6.38	105.25	113.16
6	o	194	TYR	CA-C-O	-6.38	113.84	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	p	76	SER	N-CA-C	-6.38	99.99	108.34
9	r	573	LYS	N-CA-CB	6.38	120.12	110.30
9	g	631	THR	CB-CA-C	6.37	123.10	110.42
9	g	1071	PRO	N-CA-C	-6.37	106.38	114.35
3	l	596	PHE	CA-CB-CG	-6.37	107.43	113.80
8	q	480	THR	N-CA-C	-6.37	105.44	113.72
3	a	588	ASN	CB-CG-ND2	-6.37	106.84	116.40
7	e	23	HIS	CE1-NE2-CD2	-6.37	102.63	109.00
9	g	252	PHE	CB-CG-CD1	6.37	131.53	120.70
4	m	215	SER	N-CA-C	-6.37	101.33	111.02
5	n	151	ALA	N-CA-C	-6.37	97.86	108.75
1	X	796	SER	N-CA-C	-6.37	97.23	110.80
3	l	922	LEU	N-CA-C	-6.37	105.47	113.18
8	q	323	THR	N-CA-C	-6.37	99.44	109.50
9	g	228	ILE	N-CA-C	-6.37	98.29	107.78
9	g	452	ASP	CB-CA-C	6.37	121.89	112.09
5	c	134	ASN	CA-CB-CG	6.37	118.97	112.60
9	r	252	PHE	CA-CB-CG	-6.37	107.44	113.80
8	f	380	ILE	CA-C-N	6.36	128.81	120.28
8	f	380	ILE	C-N-CA	6.36	128.81	120.28
9	g	959	ASN	O-C-N	6.36	129.40	122.15
1	X	1239	ASP	N-CA-C	-6.36	97.25	110.80
8	f	144	TRP	CB-CG-CD2	6.36	135.70	126.80
3	l	1005	ASN	N-CA-C	-6.36	106.11	114.31
9	r	515	ASN	N-CA-CB	6.36	121.24	110.49
8	f	315	LEU	CA-C-N	6.36	127.79	119.84
8	f	315	LEU	C-N-CA	6.36	127.79	119.84
9	r	478	PHE	CA-CB-CG	-6.36	107.44	113.80
9	r	642	PHE	O-C-N	-6.36	115.36	120.38
3	a	647	PHE	CA-C-N	6.36	128.09	120.14
3	a	647	PHE	C-N-CA	6.36	128.09	120.14
8	f	686	GLU	N-CA-CB	6.36	121.23	110.49
7	p	164	HIS	CE1-NE2-CD2	-6.36	102.64	109.00
3	a	393	HIS	CA-CB-CG	6.35	120.15	113.80
3	a	959	GLU	N-CA-C	-6.35	99.01	108.99
7	e	42	THR	CA-C-O	6.35	128.11	120.99
3	a	582	VAL	O-C-N	-6.35	113.35	122.12
6	o	102	VAL	CB-CA-C	-6.35	102.82	111.33
1	X	1420	VAL	N-CA-C	-6.35	106.61	112.96
8	q	10	GLU	N-CA-C	-6.35	104.58	112.90
7	p	39	ASP	N-CA-C	-6.35	98.89	109.24
5	c	478	ALA	N-CA-C	-6.35	104.46	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	709	PHE	CA-C-O	6.35	126.98	119.56
4	b	245	PHE	CA-C-O	6.34	126.73	119.18
7	p	189	GLU	N-CA-CB	6.34	121.21	110.49
4	m	641	ASP	CA-CB-CG	-6.34	106.26	112.60
8	q	257	ASP	CA-CB-CG	6.34	118.94	112.60
3	a	210	ARG	NE-CZ-NH2	-6.34	113.50	119.20
8	f	37	ASN	O-C-N	-6.34	114.92	122.15
9	r	696	LEU	CA-C-N	6.34	128.75	120.26
9	r	696	LEU	C-N-CA	6.34	128.75	120.26
4	b	454	LEU	N-CA-C	6.34	119.17	111.82
6	d	178	ALA	N-CA-C	-6.34	105.48	113.72
6	o	83	LYS	CA-C-N	6.34	129.71	120.71
6	o	83	LYS	C-N-CA	6.34	129.71	120.71
9	g	339	LEU	CB-CA-C	-6.34	99.85	110.56
9	g	628	HIS	N-CA-C	-6.34	102.79	112.99
1	X	749	ILE	CA-C-O	6.33	127.09	120.25
9	g	832	TYR	N-CA-C	-6.33	98.89	108.96
9	r	292	PHE	CA-CB-CG	-6.33	107.47	113.80
5	c	663	GLN	N-CA-C	6.33	120.11	112.38
9	g	597	CYS	CB-CA-C	-6.33	100.89	110.90
4	m	249	LEU	N-CA-C	6.33	118.26	111.36
9	r	613	ILE	N-CA-C	-6.33	103.18	111.09
3	a	211	PHE	CA-CB-CG	6.33	120.13	113.80
5	c	172	ILE	CA-C-N	6.33	131.92	123.00
5	c	172	ILE	C-N-CA	6.33	131.92	123.00
9	g	259	LYS	N-CA-C	-6.33	104.12	113.61
7	p	167	SER	N-CA-CB	6.33	120.51	110.57
9	r	1124	ASN	CA-C-O	-6.33	113.78	120.80
4	b	323	ASP	CA-C-N	6.33	129.71	120.91
4	b	323	ASP	C-N-CA	6.33	129.71	120.91
9	g	325	PRO	CA-C-O	-6.33	113.57	120.97
5	n	241	PHE	CB-CG-CD1	6.33	131.45	120.70
6	o	66	PHE	CA-CB-CG	6.33	120.13	113.80
9	r	368	PHE	CA-CB-CG	-6.33	107.47	113.80
1	X	1122	PHE	N-CA-CB	6.32	119.95	110.65
7	e	37	LYS	N-CA-CB	6.32	120.59	110.16
8	q	108	LYS	CA-C-O	6.32	127.24	119.97
9	r	230	PHE	CA-CB-CG	-6.32	107.48	113.80
8	f	645	ASP	CA-CB-CG	6.32	118.92	112.60
9	r	400	PHE	CA-CB-CG	-6.32	107.48	113.80
9	r	142	PHE	CA-CB-CG	-6.32	107.48	113.80
3	a	810	ASP	N-CA-CB	6.32	120.12	110.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	632	GLU	CA-C-O	6.32	129.54	120.51
1	X	1436	GLU	N-CA-C	-6.32	100.60	110.14
1	X	1210	LEU	N-CA-CB	6.31	119.40	110.12
5	n	540	ASN	CA-C-O	-6.31	112.97	120.10
1	X	365	LEU	N-CA-C	6.31	118.97	111.71
3	a	496	ASN	OD1-CG-ND2	6.31	128.91	122.60
9	g	179	ASN	CA-CB-CG	-6.31	106.29	112.60
6	o	193	THR	N-CA-C	-6.31	99.71	109.24
8	q	612	ASN	N-CA-CB	6.31	121.16	110.49
4	b	602	GLU	CA-C-O	6.31	127.11	120.42
4	b	652	LEU	N-CA-C	-6.31	104.74	112.88
3	l	481	HIS	CB-CG-CD2	-6.31	123.00	131.20
5	n	479	ALA	CB-CA-C	-6.31	98.56	110.67
9	r	420	PHE	CA-CB-CG	-6.31	107.49	113.80
5	c	333	ARG	NE-CZ-NH2	-6.31	113.52	119.20
8	f	188	ILE	CA-C-N	6.31	128.73	120.28
8	f	188	ILE	C-N-CA	6.31	128.73	120.28
9	r	124	PHE	CA-CB-CG	-6.31	107.49	113.80
4	b	349	TYR	CA-C-O	6.31	127.03	119.59
1	X	636	GLN	CA-C-N	6.30	128.41	120.72
1	X	636	GLN	C-N-CA	6.30	128.41	120.72
1	X	843	LEU	CA-C-N	6.30	128.64	120.44
1	X	843	LEU	C-N-CA	6.30	128.64	120.44
3	a	338	ARG	CA-C-N	6.30	127.72	119.84
3	a	338	ARG	C-N-CA	6.30	127.72	119.84
9	r	80	PHE	CA-CB-CG	-6.30	107.50	113.80
9	r	229	PHE	CA-CB-CG	-6.30	107.50	113.80
9	r	477	PHE	CA-CB-CG	-6.30	107.50	113.80
8	q	17	ASP	CA-CB-CG	6.30	118.90	112.60
1	X	1621	LEU	CB-CA-C	-6.30	100.33	110.79
6	d	149	ASN	N-CA-C	-6.30	105.63	113.38
4	m	661	HIS	CE1-NE2-CD2	-6.30	102.70	109.00
7	e	58	ILE	N-CA-C	-6.30	99.40	108.53
3	l	480	ASN	CA-CB-CG	-6.30	106.30	112.60
7	p	207	LYS	N-CA-C	-6.30	97.98	108.75
8	q	611	SER	N-CA-C	-6.30	104.40	113.21
9	g	538	ILE	N-CA-C	-6.29	104.51	113.07
9	r	386	PHE	CA-CB-CG	-6.29	107.51	113.80
3	a	995	ARG	NE-CZ-NH2	-6.29	113.54	119.20
9	g	212	LEU	CA-C-O	-6.29	114.28	121.58
9	g	852	ILE	N-CA-CB	6.29	116.80	111.64
3	l	541	PRO	CA-C-O	-6.29	114.26	121.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	315	ALA	N-CA-C	6.29	117.80	111.07
9	r	326	PHE	CA-CB-CG	-6.29	107.51	113.80
9	r	1052	ASN	N-CA-C	-6.29	97.40	110.80
9	r	253	LYS	CB-CA-C	-6.29	98.69	110.01
3	a	697	GLN	N-CA-C	6.29	121.75	111.37
9	g	736	ASP	CA-C-O	6.29	127.20	120.10
9	r	347	PHE	CA-CB-CG	-6.29	107.51	113.80
1	X	153	ASP	CA-CB-CG	6.29	118.89	112.60
1	X	1303	LEU	CB-CA-C	-6.29	98.16	110.10
9	r	786	LEU	O-C-N	6.29	129.78	122.17
1	X	834	ILE	CB-CA-C	6.29	120.39	110.52
3	l	230	HIS	CA-CB-CG	6.29	120.09	113.80
8	q	51	LEU	CA-C-O	6.29	126.90	119.67
9	r	378	PHE	CA-CB-CG	-6.29	107.52	113.80
4	b	297	LYS	N-CA-C	-6.28	102.94	111.55
4	b	507	LEU	CA-C-N	6.28	130.27	120.97
4	b	507	LEU	C-N-CA	6.28	130.27	120.97
3	a	529	SER	N-CA-CB	6.28	119.46	110.16
1	X	857	LEU	N-CA-CB	6.28	119.48	110.06
6	d	43	HIS	N-CA-C	-6.28	99.79	109.14
9	g	369	ASP	N-CA-C	-6.28	99.48	109.59
9	r	261	PHE	CA-CB-CG	-6.28	107.52	113.80
5	c	426	ALA	N-CA-C	-6.27	104.44	111.28
8	q	717	LEU	O-C-N	-6.27	115.00	122.15
8	f	650	GLU	CA-C-N	6.27	130.04	122.26
8	f	650	GLU	C-N-CA	6.27	130.04	122.26
3	l	998	LYS	N-CA-C	6.27	118.12	111.28
1	X	1195	GLN	CA-C-N	6.27	129.00	120.54
1	X	1195	GLN	C-N-CA	6.27	129.00	120.54
1	X	1566	TYR	N-CA-CB	6.27	121.09	110.49
3	a	406	ARG	N-CA-C	-6.27	104.94	112.59
9	g	878	SER	N-CA-CB	6.27	119.69	110.35
9	r	628	HIS	CA-CB-CG	6.27	120.07	113.80
9	r	747	LYS	CA-C-N	6.27	129.05	120.46
9	r	747	LYS	C-N-CA	6.27	129.05	120.46
1	X	838	LYS	N-CA-C	-6.27	104.26	112.41
1	X	914	ASP	N-CA-C	-6.27	106.85	114.75
3	a	672	LYS	N-CA-C	-6.27	105.30	114.39
3	l	259	MET	N-CA-C	-6.27	104.94	112.59
5	n	193	GLU	CB-CG-CD	-6.27	101.95	112.60
1	X	1088	ASN	CA-CB-CG	-6.26	106.33	112.60
8	f	665	MET	N-CA-C	6.26	119.08	111.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	375	PHE	CA-CB-CG	-6.26	107.54	113.80
6	o	183	LYS	CA-C-N	6.26	130.90	122.01
6	o	183	LYS	C-N-CA	6.26	130.90	122.01
3	l	667	LEU	N-CA-CB	6.26	119.09	110.01
3	l	771	ASP	N-CA-C	-6.26	104.81	112.88
1	X	297	THR	N-CA-CB	6.26	119.08	110.01
1	X	186	LYS	CA-C-N	6.26	128.66	120.28
1	X	186	LYS	C-N-CA	6.26	128.66	120.28
6	d	213	SER	O-C-N	-6.26	115.73	121.30
9	g	200	ILE	N-CA-C	-6.25	99.22	108.85
6	o	249	LYS	CA-C-O	6.25	127.25	120.43
4	b	553	ILE	O-C-N	-6.25	115.49	122.05
5	c	294	ILE	CA-C-O	-6.25	114.54	121.17
8	f	250	LEU	N-CA-CB	6.25	119.52	110.20
9	g	982	GLU	CA-C-O	6.25	126.62	119.18
9	r	513	ASP	O-C-N	6.25	130.41	123.16
1	X	693	MET	N-CA-C	-6.24	104.29	112.41
1	X	216	TYR	CB-CG-CD1	-6.24	111.44	120.80
7	e	325	ASP	CA-CB-CG	6.24	118.84	112.60
8	f	342	PRO	N-CA-C	6.24	121.74	113.57
8	f	706	GLN	N-CA-CB	6.24	119.85	109.56
4	m	193	ASP	N-CA-CB	6.24	121.03	110.49
1	X	1596	LYS	CA-C-N	6.24	128.55	120.44
1	X	1596	LYS	C-N-CA	6.24	128.55	120.44
5	c	232	ASN	CA-C-N	6.24	128.55	120.44
5	c	232	ASN	C-N-CA	6.24	128.55	120.44
3	l	285	ASN	CB-CG-ND2	6.24	125.75	116.40
4	m	368	LEU	CA-C-O	6.24	127.03	120.54
1	X	366	SER	CA-C-N	6.23	129.14	120.29
1	X	366	SER	C-N-CA	6.23	129.14	120.29
1	X	687	LYS	CA-C-N	6.23	130.41	121.50
1	X	687	LYS	C-N-CA	6.23	130.41	121.50
7	e	190	GLN	N-CA-CB	6.23	120.92	110.77
8	f	352	LEU	N-CA-CB	6.23	119.89	110.30
9	r	497	HIS	ND1-CE1-NE2	6.23	114.63	108.40
3	a	208	LEU	N-CA-C	-6.23	97.67	108.69
4	m	184	CYS	CA-C-N	6.23	128.62	120.28
4	m	184	CYS	C-N-CA	6.23	128.62	120.28
1	X	970	LEU	N-CA-C	-6.23	105.70	113.55
8	q	545	ALA	N-CA-CB	6.23	120.15	110.44
1	X	854	LEU	N-CA-C	6.22	119.72	111.75
8	f	358	VAL	O-C-N	6.22	128.24	121.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	606	GLN	CB-CG-CD	-6.22	102.02	112.60
6	o	207	VAL	CA-C-N	6.22	129.13	120.29
6	o	207	VAL	C-N-CA	6.22	129.13	120.29
9	r	432	LYS	N-CA-CB	6.22	119.97	110.14
9	g	536	GLU	O-C-N	6.22	130.44	122.10
4	m	728	LEU	N-CA-C	-6.22	105.33	113.17
4	b	239	VAL	CA-C-O	-6.22	114.78	121.19
4	b	355	GLU	N-CA-C	6.22	120.13	112.54
4	b	736	ASN	CA-CB-CG	-6.22	106.38	112.60
8	q	682	LYS	N-CA-C	-6.22	101.00	110.14
8	f	578	ASP	CA-CB-CG	6.22	118.82	112.60
3	l	139	PHE	N-CA-C	-6.22	105.64	113.72
5	n	432	GLU	CB-CG-CD	-6.22	102.03	112.60
4	b	269	ASP	N-CA-C	-6.22	100.64	109.96
3	l	247	ASP	CA-CB-CG	6.22	118.82	112.60
3	l	1014	TYR	N-CA-C	-6.22	98.49	109.06
6	o	76	ASP	N-CA-CB	6.22	119.08	110.07
8	q	637	ASP	N-CA-CB	6.22	121.09	110.77
4	b	581	MET	CA-C-N	6.21	131.56	121.74
4	b	581	MET	C-N-CA	6.21	131.56	121.74
1	X	710	GLN	N-CA-CB	6.21	119.25	110.12
5	n	278	PRO	N-CA-CB	6.21	110.40	103.44
5	c	427	ALA	N-CA-CB	6.21	120.41	110.16
4	m	54	ASN	CA-C-N	6.21	133.40	121.54
4	m	54	ASN	C-N-CA	6.21	133.40	121.54
9	g	542	ASN	CA-CB-CG	6.21	118.81	112.60
3	l	217	LYS	N-CA-C	-6.21	105.71	113.28
4	b	224	ILE	N-CA-C	-6.21	106.46	112.29
9	r	1067	ASP	N-CA-CB	6.21	119.53	110.47
5	c	380	SER	CA-C-N	6.20	129.44	120.38
5	c	380	SER	C-N-CA	6.20	129.44	120.38
6	d	103	ASN	CA-CB-CG	6.20	118.80	112.60
9	r	949	TYR	CA-C-N	6.20	129.74	120.31
9	r	949	TYR	C-N-CA	6.20	129.74	120.31
8	f	136	PRO	O-C-N	-6.20	113.08	123.00
9	g	752	GLN	N-CA-CB	6.20	119.44	110.88
4	m	610	ASP	CB-CA-C	6.20	121.07	111.02
3	a	4	LEU	N-CA-CB	6.20	119.42	110.06
6	o	82	TRP	CB-CG-CD2	6.20	135.48	126.80
9	r	840	PRO	N-CA-CB	6.20	109.22	103.39
9	g	256	ILE	CA-CB-CG2	-6.20	99.96	110.50
9	r	825	ASP	CA-C-O	6.20	128.81	120.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1263	TYR	CB-CG-CD2	6.20	130.09	120.80
9	g	108	TRP	CB-CG-CD2	-6.20	118.13	126.80
5	n	602	PHE	CA-C-O	-6.20	114.43	120.19
8	q	578	ASP	CA-CB-CG	6.20	118.80	112.60
9	r	328	HIS	N-CA-C	6.19	118.54	111.11
8	f	723	THR	CB-CA-C	6.19	121.39	110.37
4	m	699	TRP	N-CA-CB	6.19	119.75	110.53
5	n	349	SER	CA-C-N	6.19	131.48	122.69
5	n	349	SER	C-N-CA	6.19	131.48	122.69
9	r	839	PHE	CA-C-N	6.19	126.54	119.92
9	r	839	PHE	C-N-CA	6.19	126.54	119.92
6	d	42	THR	N-CA-C	-6.19	100.21	110.17
4	m	588	ASP	CA-CB-CG	6.19	118.79	112.60
7	p	297	LEU	O-C-N	-6.19	114.36	122.59
8	f	544	LYS	N-CA-C	-6.19	105.73	113.28
9	g	618	LEU	N-CA-C	-6.19	104.45	112.68
5	c	767	ASN	OD1-CG-ND2	6.18	128.78	122.60
9	r	786	LEU	CA-C-O	-6.18	113.94	120.55
1	X	139	GLY	CA-C-N	6.18	129.18	120.28
1	X	139	GLY	C-N-CA	6.18	129.18	120.28
3	a	25	ASP	CA-CB-CG	-6.18	106.42	112.60
4	b	295	TYR	CA-C-O	-6.18	114.70	119.71
1	X	865	ASN	OD1-CG-ND2	6.18	128.78	122.60
3	l	953	LEU	N-CA-CB	6.18	120.93	110.49
6	o	142	ASP	N-CA-CB	6.18	120.73	110.47
7	p	36	PHE	CA-CB-CG	-6.18	107.62	113.80
1	X	760	ASN	N-CA-C	-6.18	99.58	109.96
8	q	536	ARG	N-CA-C	6.18	118.81	111.71
3	a	166	LEU	O-C-N	-6.17	115.97	123.19
7	p	26	THR	CA-C-N	6.17	133.13	122.64
7	p	26	THR	C-N-CA	6.17	133.13	122.64
3	a	708	ASN	N-CA-C	6.17	118.09	111.36
7	e	66	PRO	N-CA-CB	6.17	108.82	103.27
8	q	591	ILE	N-CA-CB	-6.17	102.15	110.54
8	q	656	ARG	NE-CZ-NH2	-6.17	113.64	119.20
5	c	765	GLU	N-CA-CB	6.17	120.91	110.49
7	p	81	VAL	O-C-N	-6.17	116.73	122.71
6	o	63	HIS	CE1-NE2-CD2	-6.17	102.83	109.00
1	X	865	ASN	CA-CB-CG	-6.17	106.44	112.60
1	X	1615	ARG	NE-CZ-NH2	6.16	124.75	119.20
4	m	597	LYS	O-C-N	6.16	128.65	122.12
6	o	235	THR	CA-C-O	6.16	127.10	120.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	379	SER	CB-CA-C	-6.16	99.93	110.16
9	r	854	HIS	CE1-NE2-CD2	-6.16	102.84	109.00
3	a	947	SER	CA-C-N	6.16	128.45	120.56
3	a	947	SER	C-N-CA	6.16	128.45	120.56
6	d	251	GLU	CB-CG-CD	-6.16	102.13	112.60
4	m	151	ILE	N-CA-C	6.16	116.33	110.42
4	m	388	ASN	N-CA-C	-6.16	99.77	109.50
5	n	439	ARG	N-CA-C	-6.16	105.03	112.54
8	f	578	ASP	CA-C-N	6.16	128.81	120.44
8	f	578	ASP	C-N-CA	6.16	128.81	120.44
5	n	634	ILE	O-C-N	6.16	128.17	121.83
9	r	662	ASN	N-CA-CB	6.16	118.94	110.01
1	X	334	ALA	N-CA-CB	6.16	119.86	110.14
5	c	150	PHE	CA-CB-CG	-6.15	107.65	113.80
5	n	202	ARG	NE-CZ-NH1	6.15	127.65	121.50
5	n	375	LEU	N-CA-C	-6.15	103.93	112.30
7	p	26	THR	N-CA-C	-6.15	99.97	109.76
3	a	273	VAL	N-CA-C	-6.15	100.84	109.21
9	g	950	ASN	CA-C-N	6.15	129.66	120.31
9	g	950	ASN	C-N-CA	6.15	129.66	120.31
4	m	120	ASP	N-CA-C	-6.15	105.35	112.92
8	q	201	LYS	N-CA-C	6.15	119.89	112.38
1	X	1263	TYR	CB-CG-CD1	-6.15	111.58	120.80
3	a	971	ASN	CA-C-O	6.15	127.71	120.58
4	b	216	ASP	N-CA-CB	6.15	120.88	110.49
3	l	425	GLN	N-CA-C	-6.15	105.68	113.43
4	m	461	MET	CA-C-N	6.15	128.77	120.65
4	m	461	MET	C-N-CA	6.15	128.77	120.65
6	o	125	VAL	N-CA-C	-6.15	98.62	107.78
8	q	193	ILE	N-CA-C	-6.15	107.87	113.71
1	X	708	THR	O-C-N	6.15	129.41	122.22
1	X	849	ASN	OD1-CG-ND2	-6.15	116.45	122.60
8	f	147	SER	CB-CA-C	-6.15	101.23	110.88
4	m	63	ASP	CA-CB-CG	6.15	118.75	112.60
7	p	169	PHE	CA-CB-CG	-6.15	107.65	113.80
9	r	265	SER	N-CA-C	6.15	118.63	109.59
1	X	1518	THR	N-CA-C	6.14	118.95	111.82
5	c	244	VAL	O-C-N	6.14	128.06	122.65
6	d	133	ASN	CA-C-N	6.14	130.85	121.51
6	d	133	ASN	C-N-CA	6.14	130.85	121.51
1	X	162	HIS	CG-CD2-NE2	6.14	113.34	107.20
8	f	275	GLU	CA-C-O	6.14	128.20	120.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	198	GLU	N-CA-CB	6.14	119.80	110.28
3	l	533	LEU	N-CA-CB	6.14	119.15	110.12
1	X	323	TYR	CB-CG-CD2	-6.14	111.59	120.80
3	a	320	PRO	O-C-N	-6.14	116.53	123.03
3	a	623	LEU	CB-CA-C	-6.14	99.33	110.56
7	e	225	GLY	O-C-N	6.14	129.93	122.32
3	l	446	LEU	CA-C-N	6.14	131.82	122.37
3	l	446	LEU	C-N-CA	6.14	131.82	122.37
4	b	491	LEU	CA-C-O	-6.13	115.12	121.87
8	f	116	LEU	O-C-N	6.13	128.62	122.12
8	q	403	SER	N-CA-CB	6.13	119.55	110.53
6	d	55	PRO	CA-C-N	6.13	131.01	123.10
6	d	55	PRO	C-N-CA	6.13	131.01	123.10
5	n	183	PHE	N-CA-C	-6.13	103.89	113.02
5	n	569	GLU	N-CA-C	6.13	119.80	112.93
6	o	186	LYS	CA-C-N	6.13	133.25	121.54
6	o	186	LYS	C-N-CA	6.13	133.25	121.54
3	a	851	TYR	N-CA-C	-6.13	104.17	112.26
4	m	634	TYR	CA-CB-CG	6.13	124.93	113.90
8	q	640	SER	CA-C-O	6.13	126.52	119.35
3	a	808	TRP	N-CA-CB	6.13	119.33	110.20
1	X	1163	LEU	N-CA-C	-6.13	104.30	112.94
9	r	235	ASN	N-CA-C	6.13	118.74	111.33
9	r	640	ASP	O-C-N	6.13	128.38	122.07
4	b	429	LEU	N-CA-CB	6.12	119.73	110.42
7	e	118	PRO	CA-C-N	6.12	132.56	121.97
7	e	118	PRO	C-N-CA	6.12	132.56	121.97
9	g	652	HIS	CG-CD2-NE2	6.12	113.32	107.20
6	o	63	HIS	CB-CG-ND1	6.12	131.88	122.70
5	c	202	ARG	NH1-CZ-NH2	-6.12	111.34	119.30
6	d	109	PRO	CB-CA-C	6.12	119.23	111.39
3	l	195	GLU	O-C-N	-6.12	113.57	121.10
1	X	1000	LYS	N-CA-CB	6.12	119.51	110.33
5	c	138	ILE	N-CA-CB	6.12	118.40	110.57
1	X	1060	LEU	CA-C-O	-6.12	111.76	120.51
3	a	399	THR	N-CA-CB	6.12	119.05	109.69
4	m	686	ASP	N-CA-CB	6.12	120.37	111.62
8	q	416	TYR	CA-C-O	-6.12	114.06	120.55
3	a	976	ALA	CA-C-N	6.12	132.58	122.73
3	a	976	ALA	C-N-CA	6.12	132.58	122.73
8	f	216	GLN	N-CA-C	-6.12	100.32	110.17
8	f	227	ILE	CA-C-N	6.12	133.22	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	227	ILE	C-N-CA	6.12	133.22	121.54
8	q	668	HIS	CA-C-O	-6.12	113.94	120.42
6	o	63	HIS	CG-CD2-NE2	6.12	113.31	107.20
5	c	289	ASN	N-CA-C	-6.11	100.60	110.32
3	l	872	TYR	CA-CB-CG	6.11	124.90	113.90
1	X	1194	LEU	CA-C-N	6.11	128.72	120.65
1	X	1194	LEU	C-N-CA	6.11	128.72	120.65
8	f	239	LYS	N-CA-C	-6.11	106.49	112.97
3	a	168	TYR	CA-C-N	6.11	132.97	121.97
3	a	168	TYR	C-N-CA	6.11	132.97	121.97
4	b	208	LEU	N-CA-C	6.11	117.94	111.28
8	f	68	TRP	CA-C-N	6.11	128.38	120.44
8	f	68	TRP	C-N-CA	6.11	128.38	120.44
8	f	230	GLU	N-CA-CB	6.11	120.82	110.49
8	q	380	ILE	N-CA-C	-6.11	106.77	113.43
5	n	592	LEU	N-CA-CB	6.11	119.83	110.79
7	p	59	VAL	CA-C-O	6.11	125.06	119.20
8	q	214	GLY	CA-C-N	6.11	130.78	120.64
8	q	214	GLY	C-N-CA	6.11	130.78	120.64
9	r	328	HIS	N-CA-CB	6.11	119.04	109.94
1	X	942	PRO	CA-C-N	-6.11	114.94	121.84
1	X	942	PRO	C-N-CA	-6.11	114.94	121.84
3	a	397	ILE	CA-CB-CG1	6.11	120.78	110.40
3	l	724	PHE	CA-CB-CG	6.11	119.91	113.80
8	q	590	LEU	CA-C-N	6.11	128.82	120.46
8	q	590	LEU	C-N-CA	6.11	128.82	120.46
4	m	360	PHE	CB-CG-CD1	-6.10	110.32	120.70
5	n	541	ALA	CA-C-N	6.10	129.28	120.79
5	n	541	ALA	C-N-CA	6.10	129.28	120.79
5	c	542	GLN	N-CA-C	6.10	118.43	111.11
8	f	315	LEU	N-CA-CB	6.10	121.23	110.37
9	g	385	THR	N-CA-C	-6.10	105.64	114.12
4	m	549	ALA	CA-C-N	6.10	131.26	122.35
4	m	549	ALA	C-N-CA	6.10	131.26	122.35
8	q	592	LYS	N-CA-CB	6.10	119.74	110.28
9	r	551	ASN	OD1-CG-ND2	6.10	128.70	122.60
6	d	206	TRP	CA-C-N	6.10	129.39	120.91
6	d	206	TRP	C-N-CA	6.10	129.39	120.91
7	e	211	HIS	CB-CG-ND1	6.10	131.85	122.70
3	l	609	GLY	N-CA-C	6.10	119.58	112.50
9	r	914	GLY	CA-C-N	6.10	129.37	120.71
9	r	914	GLY	C-N-CA	6.10	129.37	120.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	330	ARG	CA-C-O	6.10	126.89	120.42
9	g	529	HIS	CG-CD2-NE2	6.10	113.30	107.20
8	q	630	LEU	CA-C-N	6.10	129.13	120.53
8	q	630	LEU	C-N-CA	6.10	129.13	120.53
1	X	924	GLY	O-C-N	6.10	129.49	122.60
4	b	357	PHE	CA-C-N	6.10	128.45	120.28
4	b	357	PHE	C-N-CA	6.10	128.45	120.28
8	q	233	THR	CA-CB-OG1	6.10	118.75	109.60
6	d	173	PHE	CA-C-N	6.10	131.82	122.25
6	d	173	PHE	C-N-CA	6.10	131.82	122.25
3	l	961	PHE	N-CA-CB	6.10	120.34	110.77
3	l	972	LYS	O-C-N	-6.10	115.00	122.25
1	X	835	LEU	N-CA-C	-6.09	105.13	113.30
3	a	717	ASN	N-CA-C	-6.09	106.82	114.56
8	q	31	ASN	N-CA-C	-6.09	101.18	108.25
8	f	212	LEU	CA-C-O	-6.09	112.60	119.79
3	a	541	PRO	N-CA-CB	6.09	109.06	103.15
3	a	974	GLU	CA-C-O	-6.09	113.98	120.92
9	g	462	SER	CB-CA-C	-6.09	102.91	111.80
3	l	410	ASN	OD1-CG-ND2	-6.09	116.51	122.60
5	n	182	LYS	N-CA-C	-6.09	105.61	113.16
9	r	278	LYS	CB-CA-C	-6.09	99.53	110.37
8	q	403	SER	CA-C-O	6.09	125.84	119.14
3	l	96	HIS	CB-CG-ND1	6.08	131.83	122.70
3	l	808	TRP	CD2-CE2-CZ2	-6.08	116.31	122.40
1	X	1182	ASN	CB-CA-C	-6.08	100.34	110.68
1	X	1214	PHE	CA-C-N	6.08	129.06	120.42
1	X	1214	PHE	C-N-CA	6.08	129.06	120.42
4	b	214	ARG	NE-CZ-NH1	6.08	127.58	121.50
9	g	102	HIS	CA-CB-CG	-6.08	107.72	113.80
9	g	1134	HIS	CG-CD2-NE2	6.08	113.28	107.20
4	m	413	ASP	CA-C-N	6.08	129.56	120.31
4	m	413	ASP	C-N-CA	6.08	129.56	120.31
6	d	98	HIS	CE1-NE2-CD2	-6.08	102.92	109.00
8	f	240	HIS	N-CA-C	6.08	118.70	111.71
8	f	243	TRP	N-CA-C	6.08	118.69	111.33
9	g	407	ALA	N-CA-C	-6.08	104.49	113.61
9	g	510	ASN	N-CA-C	6.08	123.25	109.81
1	X	1523	SER	N-CA-C	6.08	117.91	111.28
4	m	77	GLN	N-CA-CB	6.08	120.08	110.84
1	X	1608	HIS	CA-C-N	6.08	125.63	119.19
1	X	1608	HIS	C-N-CA	6.08	125.63	119.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	341	HIS	CA-C-O	-6.08	114.38	120.64
3	l	890	ARG	CA-C-O	6.08	127.91	120.92
3	a	583	LEU	CA-C-N	6.08	128.34	120.44
3	a	583	LEU	C-N-CA	6.08	128.34	120.44
4	m	391	GLU	N-CA-C	-6.08	106.50	114.04
1	X	1636	PHE	CA-CB-CG	6.08	119.88	113.80
4	m	406	LEU	O-C-N	6.08	126.42	120.71
1	X	1130	PHE	CA-CB-CG	-6.07	107.73	113.80
1	X	1442	ILE	N-CA-C	-6.07	106.98	111.90
1	X	1604	LYS	N-CA-CB	6.07	118.82	110.01
8	q	37	ASN	OD1-CG-ND2	6.07	128.67	122.60
3	l	319	ILE	CA-C-N	6.07	127.43	119.84
3	l	319	ILE	C-N-CA	6.07	127.43	119.84
4	m	51	MET	N-CA-CB	6.07	119.04	110.12
4	m	473	LEU	N-CA-CB	6.07	119.04	110.12
8	q	519	GLU	CA-C-N	6.07	133.31	121.41
8	q	519	GLU	C-N-CA	6.07	133.31	121.41
9	g	1075	ASP	CA-CB-CG	6.07	118.67	112.60
1	X	866	ARG	CA-C-O	6.07	129.19	120.51
9	g	825	ASP	CA-CB-CG	6.07	118.67	112.60
5	n	567	LEU	N-CA-C	-6.07	97.88	110.80
1	X	1286	THR	N-CA-CB	6.07	118.99	110.07
5	c	650	HIS	ND1-CE1-NE2	6.07	114.47	108.40
9	g	858	ASN	CA-C-N	6.07	132.24	121.75
9	g	858	ASN	C-N-CA	6.07	132.24	121.75
9	r	397	PRO	CA-N-CD	-6.07	103.51	112.00
9	r	563	PHE	CA-CB-CG	-6.07	107.73	113.80
3	l	968	ARG	N-CA-C	-6.06	104.72	113.21
1	X	899	GLN	N-CA-C	-6.06	105.84	113.72
9	g	775	ILE	N-CA-C	6.06	116.72	110.36
6	o	43	HIS	N-CA-CB	6.06	120.73	110.49
7	e	70	ARG	O-C-N	6.06	130.32	122.87
8	f	535	ARG	CA-C-N	6.06	128.72	120.54
8	f	535	ARG	C-N-CA	6.06	128.72	120.54
9	g	633	THR	N-CA-C	-6.06	105.15	112.54
3	l	404	VAL	N-CA-CB	6.06	117.74	110.95
5	c	135	ALA	CA-C-N	6.06	128.72	120.54
5	c	135	ALA	C-N-CA	6.06	128.72	120.54
5	n	297	TYR	CA-C-N	6.06	129.00	120.28
5	n	297	TYR	C-N-CA	6.06	129.00	120.28
4	b	723	SER	CB-CA-C	-6.05	100.87	110.86
5	c	515	ILE	N-CA-C	-6.05	104.45	110.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	548	GLN	CA-C-N	-6.05	112.85	122.29
8	q	548	GLN	C-N-CA	-6.05	112.85	122.29
8	q	301	TYR	O-C-N	-6.05	115.25	122.15
9	r	547	PRO	N-CA-C	6.05	118.08	110.70
1	X	198	MET	N-CA-C	-6.05	105.08	112.88
8	f	61	ASN	CA-CB-CG	6.05	118.65	112.60
3	l	765	PHE	CA-C-N	6.05	128.88	120.29
3	l	765	PHE	C-N-CA	6.05	128.88	120.29
8	q	516	TRP	N-CA-C	-6.05	105.94	113.38
9	g	376	THR	CA-C-N	6.05	130.48	121.77
9	g	376	THR	C-N-CA	6.05	130.48	121.77
9	g	125	ARG	O-C-N	-6.05	115.59	122.97
4	m	644	GLN	OE1-CD-NE2	-6.05	116.55	122.60
8	q	404	VAL	N-CA-C	-6.05	99.03	107.80
1	X	1638	LYS	N-CA-CB	6.04	118.78	110.01
7	e	221	ALA	CB-CA-C	-6.04	104.19	110.17
9	g	512	ILE	N-CA-C	-6.04	99.34	108.17
1	X	901	ILE	CA-C-N	6.04	129.19	120.79
1	X	901	ILE	C-N-CA	6.04	129.19	120.79
3	a	530	LYS	N-CA-CB	6.04	119.00	110.12
9	g	704	SER	CA-C-N	6.04	133.08	121.54
9	g	704	SER	C-N-CA	6.04	133.08	121.54
8	q	482	ARG	N-CA-C	6.04	127.92	111.00
9	r	829	VAL	CA-C-N	6.04	133.09	121.54
9	r	829	VAL	C-N-CA	6.04	133.09	121.54
9	r	1006	TYR	N-CA-C	6.04	117.95	111.36
4	b	271	LEU	O-C-N	-6.04	115.61	120.38
5	c	364	SER	CA-C-N	6.04	127.39	119.84
5	c	364	SER	C-N-CA	6.04	127.39	119.84
6	d	181	LEU	N-CA-CB	6.04	119.98	110.56
3	a	666	ASN	CB-CG-ND2	-6.04	107.34	116.40
9	g	411	ASN	CA-CB-CG	6.04	118.64	112.60
4	m	691	VAL	N-CA-CB	-6.04	103.08	111.41
6	o	276	ASN	N-CA-C	-6.04	102.92	111.56
3	a	557	CYS	O-C-N	6.04	129.58	122.34
8	f	543	VAL	CA-C-N	6.04	133.29	122.06
8	f	543	VAL	C-N-CA	6.04	133.29	122.06
3	a	754	GLU	CB-CA-C	-6.03	100.47	110.37
8	f	640	SER	CA-C-O	6.03	125.78	119.51
9	g	1067	ASP	N-CA-C	-6.03	105.92	113.28
6	o	139	ILE	CA-C-N	6.03	129.99	121.66
6	o	139	ILE	C-N-CA	6.03	129.99	121.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	757	LYS	CA-C-N	6.03	128.08	120.72
9	r	757	LYS	C-N-CA	6.03	128.08	120.72
4	b	329	ARG	NH1-CZ-NH2	6.03	127.14	119.30
4	b	343	GLN	CB-CA-C	-6.03	102.62	112.03
9	g	1044	ARG	NH1-CZ-NH2	6.03	127.14	119.30
9	r	239	LYS	CA-C-N	-6.03	112.30	119.84
9	r	239	LYS	C-N-CA	-6.03	112.30	119.84
1	X	839	ILE	CA-C-N	6.03	130.79	120.72
1	X	839	ILE	C-N-CA	6.03	130.79	120.72
3	a	95	ILE	N-CA-CB	6.03	118.88	110.56
3	a	262	GLN	N-CA-C	-6.03	105.23	112.59
4	b	537	GLU	CA-C-N	6.03	130.53	120.64
4	b	537	GLU	C-N-CA	6.03	130.53	120.64
9	g	1026	GLY	CA-C-N	6.03	128.85	120.29
9	g	1026	GLY	C-N-CA	6.03	128.85	120.29
3	l	1005	ASN	OD1-CG-ND2	6.03	128.63	122.60
8	q	558	ILE	CA-C-O	-6.03	113.24	120.78
8	q	609	SER	CA-C-O	-6.03	114.82	121.33
3	a	1020	ASN	CA-CB-CG	6.03	118.63	112.60
8	f	358	VAL	CA-C-O	-6.03	114.46	120.85
6	o	94	VAL	CA-C-O	6.03	126.75	120.36
3	l	651	ILE	CA-C-N	6.02	130.92	120.68
3	l	651	ILE	C-N-CA	6.02	130.92	120.68
3	l	586	LEU	O-C-N	6.02	129.30	122.19
4	b	708	ASN	CA-C-O	-6.02	114.04	120.42
3	l	240	ASN	OD1-CG-ND2	6.02	128.62	122.60
6	o	259	ARG	NH1-CZ-NH2	-6.02	111.47	119.30
1	X	813	ILE	N-CA-C	6.02	121.86	109.34
4	b	94	ARG	N-CA-C	6.02	118.68	110.55
5	n	404	GLN	N-CA-C	6.02	117.92	111.36
7	p	224	ILE	O-C-N	6.02	129.58	122.66
7	e	163	ASN	N-CA-C	-6.02	106.07	113.41
4	m	267	ARG	NE-CZ-NH1	-6.02	115.48	121.50
5	n	250	THR	N-CA-CB	6.02	120.44	110.63
5	n	628	VAL	CA-CB-CG1	6.02	120.63	110.40
8	f	633	THR	N-CA-C	-6.01	97.99	110.80
3	l	769	ASN	N-CA-C	-6.01	97.99	110.80
5	n	152	LYS	N-CA-C	-6.01	100.18	109.14
8	q	343	ILE	CA-C-N	6.01	128.94	120.28
8	q	343	ILE	C-N-CA	6.01	128.94	120.28
8	q	468	LEU	CA-C-N	6.01	131.92	122.78
8	q	468	LEU	C-N-CA	6.01	131.92	122.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	470	SER	O-C-N	6.01	128.26	122.07
7	p	219	SER	N-CA-C	-6.01	98.61	108.76
4	b	287	ASP	N-CA-C	-6.01	105.19	113.18
5	c	205	ASN	CA-CB-CG	6.01	118.61	112.60
5	c	355	SER	CA-C-N	6.01	129.44	120.31
5	c	355	SER	C-N-CA	6.01	129.44	120.31
9	g	285	ILE	N-CA-CB	6.01	121.14	111.23
4	m	57	PRO	N-CD-CG	6.01	112.21	103.20
9	r	326	PHE	CB-CA-C	-6.01	98.90	109.71
3	l	451	ARG	N-CA-C	-6.00	105.25	113.30
3	l	875	LEU	CA-C-N	6.00	128.33	120.28
3	l	875	LEU	C-N-CA	6.00	128.33	120.28
3	l	930	SER	O-C-N	-6.00	116.49	123.27
4	m	253	VAL	CA-C-N	6.00	128.92	120.28
4	m	253	VAL	C-N-CA	6.00	128.92	120.28
6	o	23	ARG	NE-CZ-NH1	6.00	127.50	121.50
9	r	657	LEU	N-CA-C	-6.00	105.14	112.88
3	a	383	ASN	CB-CG-ND2	-6.00	107.40	116.40
5	c	464	VAL	CA-C-N	6.00	132.69	122.37
5	c	464	VAL	C-N-CA	6.00	132.69	122.37
6	d	17	LEU	CA-C-O	-6.00	114.87	121.89
7	e	205	ALA	O-C-N	-6.00	114.84	122.34
8	f	382	LYS	CA-C-N	6.00	125.62	119.56
8	f	382	LYS	C-N-CA	6.00	125.62	119.56
3	l	210	ARG	NE-CZ-NH1	-6.00	115.50	121.50
3	a	620	HIS	ND1-CE1-NE2	6.00	114.40	108.40
3	l	744	VAL	N-CA-C	-6.00	104.66	110.42
4	m	321	ALA	N-CA-C	6.00	118.51	110.35
5	n	272	ILE	CB-CA-C	6.00	119.65	111.97
5	n	523	ASN	OD1-CG-ND2	-6.00	116.60	122.60
5	n	205	ASN	O-C-N	-6.00	115.64	121.94
8	q	12	PHE	CA-C-N	6.00	128.32	120.28
8	q	12	PHE	C-N-CA	6.00	128.32	120.28
9	r	896	TYR	N-CA-C	-6.00	105.83	113.02
3	a	502	ASP	CA-CB-CG	6.00	118.59	112.60
1	X	1334	ASP	CA-C-O	5.99	126.86	119.79
6	d	98	HIS	CG-CD2-NE2	5.99	113.19	107.20
3	l	957	ASP	CB-CG-OD1	5.99	132.19	118.40
5	n	477	PHE	CA-CB-CG	5.99	119.79	113.80
9	r	642	PHE	N-CA-CB	5.99	117.49	110.42
3	a	386	LEU	CA-C-N	5.99	130.15	121.52
3	a	386	LEU	C-N-CA	5.99	130.15	121.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	869	HIS	CE1-NE2-CD2	-5.99	103.01	109.00
4	m	204	PHE	CA-C-N	5.99	128.67	120.46
4	m	204	PHE	C-N-CA	5.99	128.67	120.46
4	b	363	TYR	O-C-N	-5.99	114.57	122.42
9	g	995	THR	CA-C-O	5.99	128.30	120.21
3	a	856	ILE	N-CA-C	-5.99	104.87	113.07
3	l	458	ASN	N-CA-C	-5.99	105.27	112.58
1	X	1202	SER	N-CA-C	5.99	118.59	111.71
5	c	325	LEU	O-C-N	-5.99	115.75	122.34
5	c	487	HIS	CA-CB-CG	-5.99	107.81	113.80
5	c	568	ALA	N-CA-C	-5.99	104.63	112.41
9	g	786	LEU	N-CA-CB	5.99	119.58	110.42
3	a	242	HIS	CG-CD2-NE2	5.99	113.19	107.20
8	f	199	GLU	CA-C-O	-5.99	114.08	120.42
9	g	721	CYS	CA-C-N	5.99	128.58	120.38
9	g	721	CYS	C-N-CA	5.99	128.58	120.38
3	l	249	THR	N-CA-C	-5.98	106.02	113.38
3	l	272	LYS	O-C-N	5.98	130.42	123.30
5	n	485	GLN	OE1-CD-NE2	5.98	128.58	122.60
1	X	193	GLN	CA-C-N	5.98	130.11	120.30
1	X	193	GLN	C-N-CA	5.98	130.11	120.30
1	X	1188	THR	N-CA-CB	5.98	118.91	110.12
5	n	465	PHE	O-C-N	-5.98	116.66	123.48
8	q	231	PHE	CA-CB-CG	-5.98	107.82	113.80
5	c	525	HIS	CG-CD2-NE2	5.98	113.18	107.20
6	d	153	TRP	CB-CG-CD1	5.98	135.87	126.90
8	f	251	SER	CA-C-O	-5.98	114.21	120.55
9	g	111	HIS	CE1-NE2-CD2	-5.98	103.02	109.00
8	f	235	GLN	N-CA-C	5.98	118.90	110.23
5	n	605	SER	N-CA-C	-5.98	98.07	110.80
8	q	66	LYS	CA-C-N	5.98	128.29	120.28
8	q	66	LYS	C-N-CA	5.98	128.29	120.28
4	b	91	TYR	CA-C-O	-5.98	114.79	119.99
3	l	165	PHE	CA-C-N	5.98	132.43	121.85
3	l	165	PHE	C-N-CA	5.98	132.43	121.85
5	n	209	GLN	N-CA-C	-5.98	99.82	108.07
4	b	612	LEU	N-CA-C	-5.97	105.56	114.64
9	g	934	VAL	N-CA-CB	5.97	117.81	111.00
8	q	704	LEU	N-CA-C	-5.97	106.03	113.38
3	l	803	HIS	CG-CD2-NE2	5.97	113.17	107.20
4	m	197	VAL	CB-CA-C	-5.97	104.24	111.88
4	m	699	TRP	CA-CB-CG	5.97	124.95	113.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	678	LEU	N-CA-C	-5.97	98.08	110.80
8	f	153	LEU	CA-C-O	-5.97	111.60	119.06
1	X	1179	SER	O-C-N	5.97	129.42	122.20
9	g	1037	LEU	CA-C-N	5.97	128.28	120.28
9	g	1037	LEU	C-N-CA	5.97	128.28	120.28
5	c	181	ARG	N-CA-CB	5.97	121.81	111.13
5	n	439	ARG	NE-CZ-NH2	-5.96	113.83	119.20
9	r	830	SER	N-CA-CB	5.96	120.57	110.49
3	a	422	ARG	CA-C-O	-5.96	114.67	121.58
4	b	389	ASP	CA-C-O	-5.96	112.44	119.48
8	f	703	LEU	N-CA-C	5.96	120.28	112.89
9	g	697	ASP	CA-C-N	5.96	126.39	119.47
9	g	697	ASP	C-N-CA	5.96	126.39	119.47
4	m	413	ASP	CA-CB-CG	5.96	118.56	112.60
3	a	264	ASP	CA-CB-CG	5.96	118.56	112.60
4	m	223	TYR	N-CA-C	-5.96	104.14	113.02
5	n	406	HIS	CG-CD2-NE2	5.96	113.16	107.20
5	n	565	TYR	CB-CG-CD2	-5.96	111.86	120.80
6	o	17	LEU	N-CA-CB	5.96	119.86	110.56
1	X	1611	TYR	N-CA-CB	5.95	119.39	110.22
7	e	162	ALA	CA-C-N	5.95	132.75	122.09
7	e	162	ALA	C-N-CA	5.95	132.75	122.09
9	g	64	ASN	N-CA-CB	5.95	119.98	110.16
5	n	583	SER	CA-C-N	5.95	131.40	123.00
5	n	583	SER	C-N-CA	5.95	131.40	123.00
3	a	943	LYS	N-CA-CB	-5.95	101.35	110.16
6	d	108	ALA	CA-C-N	5.95	125.96	119.89
6	d	108	ALA	C-N-CA	5.95	125.96	119.89
8	q	645	ASP	CA-CB-CG	5.95	118.55	112.60
1	X	995	LEU	CD1-CG-CD2	5.95	123.89	110.80
3	l	234	LEU	CA-C-N	5.95	132.68	121.97
3	l	234	LEU	C-N-CA	5.95	132.68	121.97
3	l	627	TYR	CB-CA-C	5.95	120.67	110.79
3	l	753	ASN	CB-CG-ND2	-5.95	107.47	116.40
9	r	716	ASN	N-CA-CB	5.95	120.54	110.49
3	a	880	ARG	CA-C-N	5.95	132.90	121.54
3	a	880	ARG	C-N-CA	5.95	132.90	121.54
3	l	317	ASN	O-C-N	-5.95	116.47	123.25
3	a	731	ASN	CA-C-N	5.95	131.70	122.49
3	a	731	ASN	C-N-CA	5.95	131.70	122.49
5	n	652	ARG	O-C-N	5.95	128.19	122.07
8	q	158	LEU	N-CA-C	-5.95	105.94	112.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	3	CYS	N-CA-C	-5.94	107.26	114.75
3	a	403	ASP	CA-CB-CG	5.94	118.54	112.60
8	q	265	SER	O-C-N	5.94	128.21	122.03
1	X	718	PHE	N-CA-C	5.94	117.44	110.97
3	a	910	GLN	N-CA-C	5.94	117.75	111.28
4	m	203	GLU	CA-C-N	5.94	128.49	120.65
4	m	203	GLU	C-N-CA	5.94	128.49	120.65
3	a	1005	ASN	N-CA-C	-5.94	104.69	112.41
9	g	1026	GLY	N-CA-C	-5.94	107.54	115.32
4	b	170	ASN	CA-C-N	5.94	128.24	120.28
4	b	170	ASN	C-N-CA	5.94	128.24	120.28
6	d	68	THR	CB-CA-C	5.94	119.55	109.75
6	d	122	ASP	CA-CB-CG	5.94	118.54	112.60
8	f	389	VAL	CA-C-O	-5.94	112.40	119.58
4	m	351	ARG	NE-CZ-NH2	-5.94	113.86	119.20
5	n	625	LEU	CA-C-N	5.94	131.19	123.00
5	n	625	LEU	C-N-CA	5.94	131.19	123.00
6	o	8	HIS	CA-CB-CG	-5.94	107.86	113.80
3	a	878	HIS	CE1-NE2-CD2	-5.94	103.06	109.00
4	b	329	ARG	NE-CZ-NH1	-5.94	115.56	121.50
5	c	436	LYS	CB-CA-C	-5.94	97.58	109.99
9	r	239	LYS	CB-CA-C	-5.94	99.95	109.69
6	d	54	GLY	CA-C-N	5.93	127.26	119.84
6	d	54	GLY	C-N-CA	5.93	127.26	119.84
1	X	901	ILE	O-C-N	5.93	127.86	121.87
4	b	49	VAL	CA-C-N	5.93	126.28	119.93
4	b	49	VAL	C-N-CA	5.93	126.28	119.93
7	e	65	SER	CA-C-N	5.93	126.24	119.83
7	e	65	SER	C-N-CA	5.93	126.24	119.83
8	q	224	ASP	CA-CB-CG	-5.93	106.67	112.60
4	b	186	ARG	O-C-N	5.93	128.41	122.12
4	b	420	THR	N-CA-C	-5.93	106.18	113.41
8	f	116	LEU	CA-C-O	-5.93	114.27	120.55
9	g	174	TYR	N-CA-C	-5.93	98.75	108.41
4	m	397	ILE	N-CA-C	-5.93	104.96	110.53
1	X	866	ARG	O-C-N	-5.93	114.71	122.59
5	c	515	ILE	CA-C-N	5.93	130.08	120.60
5	c	515	ILE	C-N-CA	5.93	130.08	120.60
5	c	572	ILE	CA-C-N	5.93	130.36	120.64
5	c	572	ILE	C-N-CA	5.93	130.36	120.64
9	r	518	PRO	CA-C-O	-5.93	112.17	118.92
5	c	298	LEU	N-CA-C	5.92	117.74	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	565	TYR	N-CA-C	-5.92	101.43	110.14
9	g	357	ASN	CA-C-O	5.92	127.18	121.67
3	l	825	TYR	N-CA-C	-5.92	105.54	112.89
7	e	240	ILE	CA-CB-CG2	5.92	120.56	110.50
9	g	540	HIS	CE1-NE2-CD2	-5.92	103.08	109.00
3	l	19	GLU	CA-C-O	-5.92	114.14	119.59
4	m	385	ASP	CA-CB-CG	5.92	118.52	112.60
1	X	322	HIS	CA-CB-CG	5.92	119.72	113.80
5	c	656	ALA	N-CA-C	-5.92	105.89	113.23
6	o	63	HIS	CA-C-N	5.92	125.94	119.90
6	o	63	HIS	C-N-CA	5.92	125.94	119.90
7	p	41	ASP	N-CA-C	-5.92	106.03	113.72
1	X	1388	LEU	CA-C-N	5.92	129.30	120.31
1	X	1388	LEU	C-N-CA	5.92	129.30	120.31
3	a	640	PHE	CA-CB-CG	-5.92	107.88	113.80
5	c	371	SER	O-C-N	-5.92	116.85	123.48
3	l	379	ILE	N-CA-CB	5.92	118.59	111.31
4	b	141	ASN	N-CA-C	-5.92	106.10	113.38
7	p	151	THR	O-C-N	-5.92	113.99	122.03
3	a	650	HIS	CG-CD2-NE2	5.91	113.11	107.20
9	g	940	ASP	CA-C-N	5.91	129.61	122.16
9	g	940	ASP	C-N-CA	5.91	129.61	122.16
9	r	636	ILE	CA-C-O	-5.91	114.11	120.85
8	q	98	PRO	N-CA-CB	5.91	109.46	103.25
9	g	471	GLN	CB-CG-CD	5.91	122.65	112.60
4	m	265	ILE	CA-C-O	-5.91	114.48	120.69
1	X	446	ALA	N-CA-C	-5.91	100.09	109.07
3	a	841	ALA	N-CA-C	5.91	117.39	111.07
4	b	694	VAL	N-CA-C	-5.91	107.53	113.20
7	p	176	SER	CA-C-N	5.91	132.29	122.54
7	p	176	SER	C-N-CA	5.91	132.29	122.54
9	r	563	PHE	CA-C-O	5.91	126.81	120.55
1	X	1069	ILE	CA-C-O	-5.91	114.25	120.57
5	c	442	THR	CA-C-O	5.91	127.78	121.05
3	l	261	SER	N-CA-C	-5.91	105.73	113.17
1	X	267	ILE	N-CA-C	5.91	116.03	110.30
3	a	157	ASP	N-CA-CB	5.91	118.81	109.71
5	c	173	LYS	O-C-N	5.91	130.12	123.27
3	l	743	ASN	CA-C-N	5.91	128.00	120.56
3	l	743	ASN	C-N-CA	5.91	128.00	120.56
6	o	61	TRP	CB-CG-CD2	-5.91	118.53	126.80
6	o	267	ASN	CA-CB-CG	-5.91	106.69	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	337	LEU	CA-C-O	-5.90	114.29	120.55
3	a	632	GLN	N-CA-C	5.90	117.71	111.28
4	b	54	ASN	N-CA-C	-5.90	104.56	113.89
9	g	597	CYS	CA-C-N	5.90	128.55	120.46
9	g	597	CYS	C-N-CA	5.90	128.55	120.46
8	q	112	ASP	N-CA-C	-5.90	105.39	112.59
3	l	751	ARG	NE-CZ-NH2	5.90	124.51	119.20
4	m	429	LEU	N-CA-C	-5.90	106.24	113.50
9	r	788	TRP	N-CA-C	-5.90	104.93	111.36
6	d	144	HIS	CE1-NE2-CD2	-5.90	103.10	109.00
5	c	140	LYS	N-CA-C	-5.90	106.22	113.41
9	g	864	PHE	CA-CB-CG	-5.90	107.90	113.80
1	X	1634	LEU	N-CA-C	-5.89	103.37	110.44
4	b	479	LYS	CG-CD-CE	5.89	124.86	111.30
6	d	250	GLU	CB-CG-CD	-5.89	102.58	112.60
3	a	590	GLN	N-CA-CB	5.89	120.45	110.49
1	X	752	SER	N-CA-C	5.89	117.70	111.28
7	e	99	ASN	CB-CG-OD1	-5.89	109.02	120.80
1	X	1412	LEU	N-CA-C	5.89	117.78	111.36
3	a	214	ARG	N-CA-C	-5.89	105.28	112.88
4	b	370	LEU	N-CA-C	-5.89	105.28	112.88
5	c	178	GLU	CA-C-O	5.89	126.79	120.55
4	b	560	SER	O-C-N	-5.89	114.74	122.39
6	d	94	VAL	N-CA-C	-5.89	99.69	108.46
8	f	97	HIS	CA-CB-CG	5.89	119.69	113.80
5	n	769	PRO	CA-C-N	5.89	132.30	121.70
5	n	769	PRO	C-N-CA	5.89	132.30	121.70
7	p	330	LEU	N-CA-CB	5.89	119.08	109.95
9	r	654	VAL	O-C-N	5.89	129.61	121.84
6	o	280	LEU	CA-C-O	-5.88	113.75	120.58
3	a	805	ASP	CA-CB-CG	5.88	118.48	112.60
9	g	96	TYR	N-CA-C	-5.88	100.11	109.23
1	X	1022	TYR	N-CA-C	5.88	118.17	111.11
8	f	396	LEU	CA-C-N	5.88	128.16	120.28
8	f	396	LEU	C-N-CA	5.88	128.16	120.28
4	m	553	ILE	CA-CB-CG2	-5.88	100.50	110.50
1	X	157	ALA	N-CA-C	-5.88	101.31	110.42
9	r	873	GLN	CA-C-N	5.88	130.54	120.72
9	r	873	GLN	C-N-CA	5.88	130.54	120.72
1	X	753	TYR	CA-CB-CG	5.88	124.48	113.90
1	X	950	ARG	CB-CG-CD	5.88	124.82	111.30
4	b	611	ILE	CA-C-O	-5.88	114.94	121.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	827	PRO	CA-C-N	5.88	128.16	120.28
1	X	827	PRO	C-N-CA	5.88	128.16	120.28
3	a	477	GLN	CA-C-N	5.88	127.19	119.84
3	a	477	GLN	C-N-CA	5.88	127.19	119.84
3	a	780	HIS	CA-C-O	5.88	127.78	121.55
5	n	415	ASP	N-CA-C	-5.88	107.10	114.56
8	q	706	GLN	CA-C-N	5.88	128.43	120.38
8	q	706	GLN	C-N-CA	5.88	128.43	120.38
1	X	1540	LYS	N-CA-C	-5.88	98.29	110.80
4	m	138	LYS	CB-CA-C	-5.87	99.89	110.23
4	m	317	PHE	CA-C-N	5.87	127.48	120.14
4	m	317	PHE	C-N-CA	5.87	127.48	120.14
6	o	128	VAL	CA-C-N	5.87	129.82	121.42
6	o	128	VAL	C-N-CA	5.87	129.82	121.42
1	X	1596	LYS	CB-CA-C	-5.87	99.07	110.46
5	c	476	ALA	O-C-N	5.87	128.34	122.12
9	g	792	LEU	O-C-N	-5.87	114.73	122.42
9	r	595	ASN	CA-CB-CG	5.87	118.47	112.60
3	a	971	ASN	CA-C-N	5.87	130.96	121.98
3	a	971	ASN	C-N-CA	5.87	130.96	121.98
4	b	614	CYS	CA-C-O	-5.87	113.46	120.56
9	g	1147	THR	CA-C-O	-5.87	114.99	121.33
9	r	504	PHE	N-CA-CB	5.87	118.75	110.12
7	e	211	HIS	CE1-NE2-CD2	-5.87	103.13	109.00
9	g	134	VAL	N-CA-C	-5.87	99.17	108.90
4	m	111	LEU	CA-C-O	5.87	126.77	120.55
5	n	588	GLN	CA-C-N	5.87	128.46	120.54
5	n	588	GLN	C-N-CA	5.87	128.46	120.54
7	p	121	LEU	O-C-N	-5.87	115.14	122.35
9	r	761	ASN	OD1-CG-ND2	5.87	128.47	122.60
8	q	382	LYS	CA-C-N	5.86	127.17	119.84
8	q	382	LYS	C-N-CA	5.86	127.17	119.84
9	g	516	LEU	O-C-N	-5.86	115.26	120.48
3	a	972	LYS	N-CA-CB	5.86	118.72	110.98
9	r	963	LYS	N-CA-CB	5.86	118.83	110.16
4	b	690	THR	O-C-N	5.86	130.12	122.15
5	c	330	PRO	N-CA-CB	-5.86	97.10	103.25
3	l	14	TYR	N-CA-CB	5.86	120.39	110.49
3	l	251	PHE	CA-CB-CG	-5.86	107.94	113.80
1	X	869	LYS	CA-C-N	5.86	125.40	119.19
1	X	869	LYS	C-N-CA	5.86	125.40	119.19
4	b	489	ILE	N-CA-C	-5.86	107.20	112.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	695	TYR	CA-CB-CG	-5.86	103.36	113.90
5	n	180	GLN	CA-C-N	5.86	129.43	121.05
5	n	180	GLN	C-N-CA	5.86	129.43	121.05
6	d	111	GLU	N-CA-C	-5.85	105.97	113.23
8	q	144	TRP	CB-CG-CD2	5.85	135.00	126.80
9	r	669	VAL	O-C-N	-5.85	115.19	121.80
1	X	213	PHE	CA-CB-CG	5.85	119.65	113.80
1	X	864	SER	CA-C-N	5.85	129.14	120.95
1	X	864	SER	C-N-CA	5.85	129.14	120.95
4	m	611	ILE	N-CA-C	-5.85	107.56	113.47
8	f	252	GLN	N-CA-C	-5.85	103.54	111.55
3	a	101	SER	CA-C-N	5.85	128.12	120.28
3	a	101	SER	C-N-CA	5.85	128.12	120.28
5	c	631	GLN	CA-C-N	5.85	132.71	121.54
5	c	631	GLN	C-N-CA	5.85	132.71	121.54
8	q	720	ARG	N-CA-CB	5.85	118.81	110.16
3	a	524	VAL	CA-C-N	5.85	130.48	120.72
3	a	524	VAL	C-N-CA	5.85	130.48	120.72
7	e	117	ALA	O-C-N	-5.85	114.46	121.12
1	X	342	ASP	CB-CG-OD2	-5.84	104.96	118.40
9	g	468	LEU	CB-CA-C	-5.84	101.17	111.05
9	g	512	ILE	N-CA-CB	5.84	121.05	111.58
3	l	248	LEU	N-CA-C	-5.84	104.81	112.41
3	l	510	LEU	O-C-N	-5.84	115.49	122.15
1	X	799	ALA	CA-C-N	5.84	128.38	120.38
1	X	799	ALA	C-N-CA	5.84	128.38	120.38
3	a	760	PHE	CA-CB-CG	5.84	119.64	113.80
8	f	281	ASP	CA-CB-CG	5.84	118.44	112.60
9	g	659	PRO	N-CA-CB	-5.84	98.22	103.36
3	l	304	LEU	N-CA-C	-5.84	100.17	109.23
9	r	891	ILE	CA-C-O	-5.84	115.04	121.29
5	c	612	VAL	N-CA-C	-5.84	106.80	112.29
1	X	1424	LEU	CA-C-N	5.84	128.58	120.29
1	X	1424	LEU	C-N-CA	5.84	128.58	120.29
7	e	300	HIS	CG-CD2-NE2	5.84	113.04	107.20
6	o	71	ALA	N-CA-CB	5.84	119.76	110.65
9	r	810	ASP	N-CA-C	-5.84	106.20	113.38
7	p	120	HIS	ND1-CE1-NE2	5.84	114.24	108.40
1	X	1179	SER	N-CA-CB	5.84	119.64	109.72
4	b	212	ILE	N-CA-C	-5.84	106.13	111.67
6	d	197	GLU	CA-C-O	-5.84	114.89	120.90
4	m	684	ASP	CA-CB-CG	5.84	118.44	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	447	PHE	N-CA-C	5.84	120.24	113.18
6	d	135	THR	CA-C-N	5.83	129.05	120.82
6	d	135	THR	C-N-CA	5.83	129.05	120.82
1	X	411	PHE	N-CA-CB	5.83	119.22	110.53
9	g	461	ASP	CA-CB-CG	5.83	118.43	112.60
9	g	547	PRO	CA-C-O	-5.83	112.11	120.56
3	l	951	GLN	OE1-CD-NE2	5.83	128.43	122.60
8	q	320	HIS	CA-C-O	5.83	126.79	120.43
1	X	1008	THR	O-C-N	5.83	126.19	120.71
4	b	573	TRP	CA-C-O	-5.83	113.27	119.97
3	a	242	HIS	ND1-CE1-NE2	5.83	114.23	108.40
5	c	328	ASN	N-CA-CB	5.83	121.56	111.13
9	g	946	LYS	CA-C-N	5.83	128.75	120.53
9	g	946	LYS	C-N-CA	5.83	128.75	120.53
5	n	303	VAL	N-CA-C	-5.83	107.02	111.62
6	o	43	HIS	CE1-NE2-CD2	-5.83	103.17	109.00
4	b	606	ILE	O-C-N	-5.83	115.29	122.57
8	f	522	LEU	N-CA-C	-5.83	98.39	110.80
7	p	211	HIS	CG-CD2-NE2	5.83	113.03	107.20
3	l	726	SER	N-CA-C	5.82	119.49	112.38
5	n	241	PHE	CB-CG-CD2	-5.82	110.80	120.70
7	p	23	HIS	CB-CG-CD2	-5.82	123.63	131.20
9	g	1138	GLY	N-CA-C	5.82	122.53	115.31
7	p	163	ASN	N-CA-CB	5.82	120.33	110.49
5	c	414	TYR	N-CA-C	-5.82	104.88	113.61
9	g	295	TRP	N-CA-CB	5.82	119.37	110.70
8	q	507	ASP	O-C-N	5.82	129.18	122.25
8	f	410	SER	N-CA-C	5.82	117.62	111.28
5	n	460	ASN	CA-CB-CG	-5.82	106.78	112.60
9	r	252	PHE	CB-CA-C	-5.82	98.04	110.32
3	l	350	ASN	CA-C-O	-5.82	115.37	122.41
6	o	91	GLN	CA-C-N	5.82	128.01	120.56
6	o	91	GLN	C-N-CA	5.82	128.01	120.56
1	X	204	VAL	CA-C-N	5.82	125.77	119.78
1	X	204	VAL	C-N-CA	5.82	125.77	119.78
8	f	267	LEU	N-CA-CB	5.82	119.20	110.19
7	p	12	VAL	CB-CA-C	5.82	117.69	111.35
4	b	505	ALA	N-CA-CB	5.81	119.39	110.61
7	e	23	HIS	CB-CG-ND1	5.81	131.42	122.70
3	l	315	PHE	CA-CB-CG	5.81	119.61	113.80
3	l	728	ILE	CA-C-O	5.81	128.05	120.78
1	X	1063	ASP	CA-C-N	5.81	128.34	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1063	ASP	C-N-CA	5.81	128.34	120.44
8	f	146	ASN	OD1-CG-ND2	5.81	128.41	122.60
1	X	1427	SER	N-CA-CB	5.81	120.31	110.49
3	l	679	LEU	N-CA-C	5.81	119.63	112.54
4	m	344	ARG	NE-CZ-NH2	-5.81	113.97	119.20
5	n	382	LEU	CA-C-N	5.81	129.14	120.31
5	n	382	LEU	C-N-CA	5.81	129.14	120.31
6	o	291	PRO	N-CA-C	5.81	120.34	111.34
3	a	242	HIS	N-CA-C	-5.81	98.94	108.76
5	c	544	LEU	N-CA-C	-5.81	106.11	113.43
5	c	571	ALA	N-CA-C	-5.81	106.74	113.88
3	a	206	LYS	CA-C-N	5.80	132.63	121.54
3	a	206	LYS	C-N-CA	5.80	132.63	121.54
9	g	540	HIS	ND1-CE1-NE2	5.80	114.20	108.40
8	q	391	HIS	ND1-CE1-NE2	5.80	114.20	108.40
9	r	658	PHE	CA-C-O	-5.80	112.21	120.16
7	e	305	GLY	O-C-N	5.80	130.51	123.37
4	m	52	THR	CA-C-N	5.80	129.47	122.16
4	m	52	THR	C-N-CA	5.80	129.47	122.16
8	q	415	THR	N-CA-CB	5.80	118.65	110.12
3	a	941	ASP	N-CA-C	-5.80	103.05	110.53
3	l	1008	SER	N-CA-C	-5.80	106.24	113.38
4	m	504	ILE	N-CA-CB	5.80	119.75	112.26
3	a	459	GLU	N-CA-CB	5.80	118.99	110.35
8	f	610	GLU	O-C-N	5.80	129.85	123.01
9	g	64	ASN	O-C-N	-5.80	116.61	123.22
6	d	176	GLY	CA-C-O	5.80	126.08	120.57
7	p	331	TRP	CA-C-O	-5.80	114.61	121.16
3	l	975	ARG	N-CA-C	-5.79	103.27	111.56
1	X	867	ASP	CA-C-N	5.79	128.99	120.82
1	X	867	ASP	C-N-CA	5.79	128.99	120.82
3	a	883	GLU	N-CA-C	-5.79	101.35	109.69
5	c	425	TYR	CA-C-N	5.79	128.04	120.28
5	c	425	TYR	C-N-CA	5.79	128.04	120.28
9	g	406	ASN	OD1-CG-ND2	5.79	128.39	122.60
6	o	63	HIS	ND1-CE1-NE2	5.79	114.19	108.40
3	a	422	ARG	N-CA-C	-5.79	100.61	109.41
9	g	552	THR	N-CA-C	-5.79	105.88	113.17
6	o	49	LEU	N-CA-CB	5.79	119.00	110.49
8	q	115	GLN	N-CA-C	-5.79	105.88	113.12
3	a	183	LEU	N-CA-CB	5.79	120.11	110.85
4	b	66	PRO	N-CA-CB	5.79	106.30	102.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	584	ASN	CA-C-N	5.79	128.61	120.28
3	l	584	ASN	C-N-CA	5.79	128.61	120.28
8	q	157	ASP	N-CA-CB	5.79	120.27	110.49
9	r	1087	LYS	N-CA-C	-5.79	105.80	112.92
1	X	990	LYS	CA-C-N	5.79	132.59	121.54
1	X	990	LYS	C-N-CA	5.79	132.59	121.54
6	d	108	ALA	CB-CA-C	-5.79	100.12	109.67
7	e	37	LYS	N-CA-C	-5.79	99.86	109.46
8	f	614	PRO	N-CA-CB	5.79	109.32	103.25
3	a	314	THR	N-CA-CB	5.78	119.71	110.46
7	e	15	VAL	CA-CB-CG2	-5.78	100.57	110.40
7	e	190	GLN	CB-CA-C	-5.78	101.23	110.14
8	f	355	LEU	CA-C-O	-5.78	113.01	118.33
9	g	867	GLN	CA-C-N	5.78	132.58	121.54
9	g	867	GLN	C-N-CA	5.78	132.58	121.54
9	r	136	PRO	CB-CA-C	-5.78	103.64	111.85
4	b	737	PHE	N-CA-C	-5.78	106.84	112.97
3	l	493	TRP	N-CA-CB	5.78	118.39	110.01
4	m	550	HIS	CG-CD2-NE2	5.78	112.98	107.20
3	l	436	HIS	CA-CB-CG	5.78	119.58	113.80
8	q	316	PRO	CA-C-N	5.78	128.70	120.49
8	q	316	PRO	C-N-CA	5.78	128.70	120.49
1	X	335	LEU	CB-CA-C	-5.78	100.08	110.37
1	X	1130	PHE	CA-C-O	5.78	126.21	120.32
9	g	99	VAL	N-CA-C	-5.78	99.80	108.12
3	l	387	VAL	N-CA-C	-5.78	105.22	110.82
4	m	265	ILE	N-CA-CB	5.78	118.83	110.68
1	X	1337	LEU	CA-C-O	5.78	126.61	119.97
9	g	1035	LYS	N-CA-C	5.78	117.58	111.28
3	l	1032	ASP	CA-C-O	5.78	126.30	119.48
1	X	652	THR	N-CA-C	5.77	120.90	111.37
9	g	359	THR	N-CA-C	-5.77	99.11	108.41
7	p	336	SER	N-CA-CB	5.77	120.25	110.49
3	a	134	PRO	N-CA-C	5.77	120.39	111.21
3	a	956	GLY	CA-C-N	5.77	128.96	120.82
3	a	956	GLY	C-N-CA	5.77	128.96	120.82
4	b	178	SER	CA-C-N	5.77	128.01	120.28
4	b	178	SER	C-N-CA	5.77	128.01	120.28
5	c	540	ASN	CA-CB-CG	5.77	118.37	112.60
8	f	509	HIS	CA-C-N	5.77	127.94	120.44
8	f	509	HIS	C-N-CA	5.77	127.94	120.44
4	m	676	LEU	O-C-N	-5.77	117.20	123.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1552	ASN	CB-CG-ND2	5.77	125.05	116.40
7	e	303	HIS	CA-C-N	5.77	131.16	122.68
7	e	303	HIS	C-N-CA	5.77	131.16	122.68
1	X	830	THR	N-CA-C	-5.76	98.89	108.34
8	f	274	GLN	OE1-CD-NE2	5.76	128.37	122.60
5	n	466	SER	N-CA-C	-5.76	103.09	110.53
5	n	538	ILE	N-CA-C	-5.76	104.22	112.35
3	a	71	HIS	N-CA-C	5.76	117.45	109.15
3	a	596	PHE	CA-CB-CG	-5.76	108.04	113.80
5	c	622	LYS	CA-CB-CG	-5.76	102.58	114.10
9	g	999	LEU	CB-CA-C	-5.76	99.70	109.03
4	m	371	SER	CA-C-O	5.76	125.01	119.08
9	r	158	GLN	CB-CA-C	-5.76	100.67	109.89
1	X	1001	ASN	CA-C-N	5.76	128.00	120.28
1	X	1001	ASN	C-N-CA	5.76	128.00	120.28
3	a	279	TYR	CB-CA-C	-5.76	100.59	109.29
4	b	525	ILE	N-CA-CB	5.76	119.36	111.41
5	c	487	HIS	N-CA-CB	5.76	118.59	110.12
9	r	639	PRO	CA-C-N	5.76	127.93	120.44
9	r	639	PRO	C-N-CA	5.76	127.93	120.44
4	b	103	GLU	CA-C-N	5.76	128.31	120.54
4	b	103	GLU	C-N-CA	5.76	128.31	120.54
4	b	717	ASP	N-CA-C	-5.76	105.27	112.93
5	c	265	HIS	CB-CG-CD2	-5.76	123.71	131.20
9	g	787	ASP	CA-C-N	5.76	127.99	120.28
9	g	787	ASP	C-N-CA	5.76	127.99	120.28
3	l	982	TYR	CB-CG-CD1	-5.76	112.17	120.80
3	a	447	GLU	CA-C-O	-5.75	114.32	120.42
7	p	164	HIS	ND1-CE1-NE2	5.75	114.16	108.40
1	X	176	LEU	CA-C-N	5.75	128.34	120.46
1	X	176	LEU	C-N-CA	5.75	128.34	120.46
3	a	84	LEU	CA-C-N	5.75	131.10	122.99
3	a	84	LEU	C-N-CA	5.75	131.10	122.99
7	e	220	TRP	CE2-CD2-CE3	5.75	124.55	118.80
8	f	43	ARG	O-C-N	5.75	128.71	122.15
4	m	581	MET	N-CA-CB	5.75	120.21	110.49
6	o	27	CYS	CA-C-O	5.75	126.65	120.32
3	a	293	LEU	CA-C-N	5.75	132.53	121.54
3	a	293	LEU	C-N-CA	5.75	132.53	121.54
8	f	459	LYS	CA-C-O	5.75	126.62	120.24
5	n	285	ARG	NE-CZ-NH2	5.75	124.38	119.20
3	l	510	LEU	N-CA-CB	5.75	118.67	110.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	631	LEU	N-CA-C	-5.75	104.01	111.02
3	a	816	THR	CA-C-N	5.75	132.77	122.13
3	a	816	THR	C-N-CA	5.75	132.77	122.13
3	a	954	ARG	CA-C-N	5.75	128.93	120.82
3	a	954	ARG	C-N-CA	5.75	128.93	120.82
9	g	935	GLU	N-CA-C	-5.75	103.73	112.99
8	q	445	CYS	CA-C-N	5.75	127.91	120.44
8	q	445	CYS	C-N-CA	5.75	127.91	120.44
8	q	454	ASP	O-C-N	-5.75	115.21	121.53
4	b	266	GLU	N-CA-C	-5.75	106.27	113.28
8	f	207	SER	N-CA-C	-5.75	106.19	113.43
9	g	64	ASN	CA-C-N	5.75	128.54	121.64
9	g	64	ASN	C-N-CA	5.75	128.54	121.64
9	g	141	THR	CA-C-O	5.75	127.03	120.54
9	g	791	VAL	N-CA-CB	5.75	119.83	112.36
5	c	434	LEU	CA-C-N	5.75	127.98	120.28
5	c	434	LEU	C-N-CA	5.75	127.98	120.28
8	q	641	SER	N-CA-C	-5.75	105.85	112.92
1	X	385	PHE	N-CA-C	5.74	117.54	111.28
3	a	995	ARG	NH1-CZ-NH2	5.74	126.77	119.30
4	b	100	THR	N-CA-C	-5.74	106.17	112.72
4	b	737	PHE	CB-CG-CD2	-5.74	110.94	120.70
4	m	317	PHE	N-CA-C	-5.74	106.62	113.97
8	q	479	THR	CA-C-N	-5.74	113.13	122.26
8	q	479	THR	C-N-CA	-5.74	113.13	122.26
1	X	1277	ILE	CA-CB-CG2	5.74	120.26	110.50
9	g	321	GLN	CA-C-O	-5.74	112.19	119.31
9	r	972	CYS	CA-C-O	-5.74	115.30	121.56
9	g	1151	GLU	CA-C-O	-5.74	112.19	119.31
3	l	390	GLN	N-CA-C	5.74	117.54	111.28
5	n	633	THR	CA-C-N	5.74	128.57	120.42
5	n	633	THR	C-N-CA	5.74	128.57	120.42
1	X	1203	THR	O-C-N	-5.74	115.34	122.11
4	b	109	SER	O-C-N	-5.74	115.50	122.22
5	c	528	ASN	CA-C-O	5.74	126.22	119.28
9	g	739	LYS	O-C-N	5.74	127.98	122.07
3	l	860	GLU	CB-CG-CD	-5.74	102.84	112.60
3	a	152	LEU	CA-C-O	-5.74	114.13	120.38
4	b	186	ARG	N-CA-C	5.74	117.53	111.28
5	n	619	VAL	N-CA-C	-5.74	107.18	113.43
4	b	61	ASN	CA-C-O	-5.73	113.88	120.24
7	e	322	ALA	CA-C-N	5.73	129.74	121.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	e	322	ALA	C-N-CA	5.73	129.74	121.54
1	X	880	ASN	N-CA-C	-5.73	98.59	110.80
9	g	1067	ASP	CA-C-O	-5.73	112.36	119.18
3	l	434	MET	N-CA-C	-5.73	100.58	109.24
3	l	683	SER	N-CA-C	-5.73	100.42	108.96
6	o	14	ASP	N-CA-C	-5.73	99.70	108.76
7	p	121	LEU	N-CA-C	-5.73	106.19	112.72
1	X	1184	LYS	CA-C-N	5.73	129.02	120.31
1	X	1184	LYS	C-N-CA	5.73	129.02	120.31
5	n	284	ILE	CA-C-N	5.73	127.96	120.28
5	n	284	ILE	C-N-CA	5.73	127.96	120.28
6	o	214	PRO	N-CD-CG	5.73	111.80	103.20
7	p	50	SER	N-CA-CB	5.73	116.77	110.35
3	a	864	PHE	CA-CB-CG	5.73	119.53	113.80
9	g	176	GLU	N-CA-C	-5.73	106.13	113.23
4	m	54	ASN	OD1-CG-ND2	5.73	128.33	122.60
3	l	322	ASN	O-C-N	5.73	129.97	123.27
3	a	433	ILE	O-C-N	5.72	128.01	122.69
5	c	487	HIS	CE1-NE2-CD2	-5.72	103.28	109.00
3	l	16	GLU	O-C-N	5.72	130.20	122.59
3	l	328	ILE	O-C-N	-5.72	115.41	122.57
3	l	675	LEU	CA-C-N	5.72	127.95	120.28
3	l	675	LEU	C-N-CA	5.72	127.95	120.28
6	o	66	PHE	CD1-CG-CD2	-5.72	110.01	118.60
9	r	630	THR	N-CA-CB	5.72	120.17	110.49
1	X	1232	HIS	CE1-NE2-CD2	-5.72	103.28	109.00
3	a	140	SER	CA-C-O	-5.72	115.15	121.33
3	a	848	SER	N-CA-C	5.72	119.99	112.89
8	q	43	ARG	CA-C-N	5.72	127.95	120.28
8	q	43	ARG	C-N-CA	5.72	127.95	120.28
9	g	121	THR	N-CA-CB	5.72	120.13	110.69
9	g	567	PHE	N-CA-CB	5.72	118.63	110.16
9	g	780	LEU	CA-C-N	5.72	127.95	120.28
9	g	780	LEU	C-N-CA	5.72	127.95	120.28
5	c	660	VAL	CA-CB-CG2	-5.72	100.68	110.40
3	l	210	ARG	CA-C-N	5.72	129.00	120.31
3	l	210	ARG	C-N-CA	5.72	129.00	120.31
3	l	803	HIS	N-CA-C	-5.72	101.91	108.49
3	l	891	LEU	N-CA-CB	5.72	120.16	110.49
3	a	608	ASP	CA-CB-CG	5.72	118.32	112.60
4	m	172	PHE	CA-C-O	-5.72	112.22	119.31
4	b	223	TYR	CA-C-O	5.72	126.40	119.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	341	ASP	CA-CB-CG	5.72	118.32	112.60
3	l	8	ASP	CA-CB-CG	-5.72	106.88	112.60
8	q	475	ILE	N-CA-C	-5.72	105.28	110.82
4	b	411	SER	CA-C-O	5.71	126.41	119.38
9	g	451	ASN	OD1-CG-ND2	5.71	128.31	122.60
1	X	330	TYR	N-CA-C	5.71	117.50	111.28
6	d	221	TYR	N-CA-C	-5.71	101.29	110.14
3	l	541	PRO	N-CA-CB	5.71	108.32	103.35
1	X	1036	ASP	N-CA-C	5.71	117.01	109.93
5	c	565	TYR	N-CA-CB	5.71	119.21	110.70
8	f	292	GLN	OE1-CD-NE2	-5.71	116.89	122.60
4	m	735	LEU	N-CA-C	5.71	120.24	113.16
8	q	335	HIS	CG-CD2-NE2	5.71	112.91	107.20
1	X	713	LYS	CA-C-N	5.71	128.20	120.38
1	X	713	LYS	C-N-CA	5.71	128.20	120.38
1	X	1519	CYS	O-C-N	5.71	127.95	122.07
8	f	162	LEU	CA-C-N	5.71	127.86	120.44
8	f	162	LEU	C-N-CA	5.71	127.86	120.44
1	X	1404	PHE	CA-CB-CG	-5.71	108.09	113.80
8	f	705	PHE	CA-C-N	5.71	129.81	121.31
8	f	705	PHE	C-N-CA	5.71	129.81	121.31
9	g	445	ASP	O-C-N	5.71	130.03	122.95
3	l	89	HIS	ND1-CE1-NE2	5.71	114.11	108.40
3	l	600	ASP	CA-CB-CG	5.71	118.31	112.60
9	r	388	GLU	N-CA-CB	-5.71	101.78	110.45
9	r	389	SER	N-CA-CB	-5.71	102.56	110.38
1	X	1421	ILE	CA-C-N	5.71	127.92	120.28
1	X	1421	ILE	C-N-CA	5.71	127.92	120.28
9	r	239	LYS	N-CA-CB	5.71	121.26	109.45
9	r	975	PHE	CA-CB-CG	-5.71	108.09	113.80
1	X	827	PRO	N-CA-C	-5.70	100.72	112.47
4	b	397	ILE	CA-C-O	-5.70	114.09	120.25
9	g	840	PRO	CA-C-O	-5.70	114.90	121.86
5	c	246	TYR	CA-C-O	-5.70	114.26	119.62
9	r	649	PHE	CA-C-N	5.70	127.92	120.28
9	r	649	PHE	C-N-CA	5.70	127.92	120.28
1	X	1451	CYS	CA-C-N	5.70	128.18	120.65
1	X	1451	CYS	C-N-CA	5.70	128.18	120.65
3	a	746	CYS	O-C-N	-5.70	118.06	121.71
3	a	973	SER	CA-C-N	5.70	128.86	120.82
3	a	973	SER	C-N-CA	5.70	128.86	120.82
5	c	370	PHE	CA-CB-CG	5.70	119.50	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	324	TYR	N-CA-C	-5.70	101.35	109.62
5	n	256	LYS	O-C-N	-5.70	116.20	122.07
6	o	105	VAL	CB-CA-C	5.70	121.84	111.30
3	a	489	THR	O-C-N	-5.70	115.26	122.27
5	n	490	SER	CB-CA-C	-5.70	100.99	110.68
4	m	179	LEU	N-CA-C	-5.70	105.83	112.89
5	n	528	ASN	CA-CB-CG	-5.70	106.90	112.60
5	c	487	HIS	CG-CD2-NE2	5.70	112.89	107.20
7	e	161	PRO	N-CA-CB	5.70	108.38	103.31
8	f	62	VAL	CA-C-N	5.70	129.65	120.82
8	f	62	VAL	C-N-CA	5.70	129.65	120.82
7	p	78	ASP	N-CA-CB	5.70	119.15	110.44
8	q	391	HIS	CE1-NE2-CD2	-5.70	103.31	109.00
8	f	285	ASP	CA-CB-CG	5.69	118.29	112.60
1	X	690	LEU	CA-C-N	5.69	132.41	121.54
1	X	690	LEU	C-N-CA	5.69	132.41	121.54
4	b	531	LEU	N-CA-C	-5.69	97.23	109.81
9	g	866	GLN	CG-CD-NE2	-5.69	107.86	116.40
3	l	380	GLU	N-CA-C	-5.69	102.03	110.46
3	l	803	HIS	CE1-NE2-CD2	-5.69	103.31	109.00
3	l	1006	VAL	N-CA-CB	5.69	119.39	112.10
3	l	1029	ASP	O-C-N	5.69	128.13	122.10
6	o	185	TRP	CA-C-O	-5.69	115.20	121.58
5	c	633	THR	N-CA-CB	5.69	119.15	110.44
3	a	80	THR	CA-C-O	-5.69	114.20	120.69
3	l	760	PHE	CA-CB-CG	5.69	119.49	113.80
8	q	600	TRP	CB-CG-CD1	-5.69	118.37	126.90
9	r	524	GLN	CA-C-N	5.69	128.91	120.95
9	r	524	GLN	C-N-CA	5.69	128.91	120.95
1	X	877	LEU	N-CA-CB	5.69	120.72	110.83
1	X	895	HIS	CE1-NE2-CD2	-5.69	103.31	109.00
4	b	695	ILE	CA-C-N	5.69	127.83	120.44
4	b	695	ILE	C-N-CA	5.69	127.83	120.44
6	d	38	VAL	CA-CB-CG2	-5.69	100.73	110.40
5	n	303	VAL	CA-C-N	5.69	128.25	120.46
5	n	303	VAL	C-N-CA	5.69	128.25	120.46
9	r	547	PRO	CB-CA-C	5.69	117.86	110.92
5	c	551	ASN	CA-CB-CG	5.69	118.29	112.60
3	a	832	PHE	CB-CG-CD2	-5.68	111.04	120.70
7	e	80	THR	N-CA-C	5.68	118.67	109.40
6	o	212	TRP	CB-CG-CD2	5.68	134.76	126.80
8	q	579	GLN	N-CA-C	-5.68	105.45	112.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	189	LEU	CA-C-N	5.68	128.17	120.38
1	X	189	LEU	C-N-CA	5.68	128.17	120.38
1	X	969	ILE	N-CA-CB	-5.68	104.93	112.26
3	a	871	HIS	CE1-NE2-CD2	-5.68	103.32	109.00
7	e	166	GLN	N-CA-CB	5.68	120.09	110.49
3	l	276	VAL	N-CA-C	-5.68	100.40	108.58
3	l	303	LEU	CA-C-O	-5.68	115.01	121.72
9	r	1122	THR	CA-CB-CG2	-5.68	100.84	110.50
3	a	443	LEU	CA-C-O	5.68	126.78	120.82
4	b	195	GLN	N-CA-C	-5.68	101.51	109.69
3	a	980	VAL	N-CA-C	-5.68	107.73	113.47
9	g	817	THR	CA-C-O	-5.68	114.53	120.32
5	n	565	TYR	CA-C-N	5.68	130.81	122.63
5	n	565	TYR	C-N-CA	5.68	130.81	122.63
8	q	551	GLU	N-CA-C	-5.68	106.22	114.12
9	r	754	ASN	CB-CG-ND2	-5.68	107.88	116.40
1	X	1065	THR	CA-C-N	5.68	127.83	120.56
1	X	1065	THR	C-N-CA	5.68	127.83	120.56
4	b	331	TYR	CB-CA-C	-5.68	99.77	110.67
3	l	6	ARG	NE-CZ-NH2	5.68	124.31	119.20
7	p	203	HIS	CE1-NE2-CD2	-5.68	103.32	109.00
3	l	181	GLY	CA-C-N	5.68	129.07	121.01
3	l	181	GLY	C-N-CA	5.68	129.07	121.01
9	r	549	MET	CG-SD-CE	-5.68	88.41	100.90
3	a	441	GLU	N-CA-C	-5.67	106.40	113.55
8	f	588	GLU	CA-C-N	5.67	128.35	120.29
8	f	588	GLU	C-N-CA	5.67	128.35	120.29
9	g	675	LEU	N-CA-C	-5.67	105.08	112.23
9	g	996	VAL	O-C-N	5.67	128.85	122.67
9	r	579	ILE	CA-C-O	5.67	126.60	120.53
1	X	1522	VAL	CA-C-N	5.67	127.88	120.28
1	X	1522	VAL	C-N-CA	5.67	127.88	120.28
3	a	130	THR	N-CA-CB	5.67	120.34	110.81
3	a	232	ARG	O-C-N	5.67	130.13	122.59
4	m	276	ASP	CA-CB-CG	5.67	118.27	112.60
9	r	649	PHE	CB-CG-CD1	5.67	130.34	120.70
3	a	88	TYR	CA-C-O	-5.67	114.54	120.55
4	m	323	ASP	N-CA-C	-5.67	103.73	111.56
5	n	384	LEU	N-CA-CB	5.67	118.55	110.16
6	d	68	THR	N-CA-C	-5.67	100.00	109.24
9	g	568	LEU	N-CA-CB	-5.67	101.56	110.46
7	p	90	GLN	OE1-CD-NE2	-5.67	116.93	122.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	238	LYS	O-C-N	-5.67	116.23	122.07
9	g	1140	VAL	N-CA-C	-5.67	97.55	109.34
3	l	677	GLU	CA-C-O	-5.67	114.54	120.55
9	r	636	ILE	N-CA-CB	5.67	116.71	110.53
4	b	392	GLN	N-CA-C	5.67	122.33	109.81
8	f	200	ALA	CA-C-N	5.66	130.18	120.72
8	f	200	ALA	C-N-CA	5.66	130.18	120.72
3	l	1025	VAL	N-CA-C	-5.66	107.98	113.53
8	q	481	GLN	CB-CG-CD	-5.66	102.97	112.60
3	a	107	THR	CA-CB-OG1	5.66	118.09	109.60
6	d	219	ARG	NE-CZ-NH2	5.66	124.30	119.20
9	g	671	ASN	OD1-CG-ND2	-5.66	116.94	122.60
4	b	478	ASP	CA-CB-CG	-5.66	106.94	112.60
6	d	228	ASP	N-CA-CB	5.66	119.10	110.44
9	g	346	LEU	CA-C-O	-5.66	113.81	120.60
4	m	298	ASP	CA-CB-CG	5.66	118.26	112.60
9	r	171	LYS	CB-CA-C	-5.66	100.32	109.72
1	X	1626	GLN	N-CA-C	-5.66	106.22	113.01
3	a	106	TYR	CA-CB-CG	-5.66	103.72	113.90
8	f	643	PHE	CA-CB-CG	5.66	119.46	113.80
9	g	81	SER	CA-C-N	5.66	129.51	121.42
9	g	81	SER	C-N-CA	5.66	129.51	121.42
9	g	108	TRP	CA-C-O	-5.66	114.84	121.46
4	m	670	PHE	CA-C-N	5.66	128.14	120.44
4	m	670	PHE	C-N-CA	5.66	128.14	120.44
5	n	224	MET	CA-C-O	-5.66	115.55	121.55
5	c	537	LEU	CA-C-O	-5.66	114.56	120.55
5	n	191	ASP	O-C-N	-5.66	115.60	122.22
5	n	460	ASN	N-CA-C	-5.66	106.51	113.41
5	n	661	MET	N-CA-C	5.66	118.21	111.71
9	r	884	HIS	CA-C-N	5.66	128.92	122.36
9	r	884	HIS	C-N-CA	5.66	128.92	122.36
3	a	714	ILE	CA-CB-CG1	5.65	120.01	110.40
5	c	433	LYS	CA-C-N	5.65	128.90	120.31
5	c	433	LYS	C-N-CA	5.65	128.90	120.31
7	p	226	ARG	N-CA-C	-5.65	99.39	108.55
1	X	656	GLN	OE1-CD-NE2	5.65	128.25	122.60
9	g	667	LEU	O-C-N	5.65	127.89	122.07
9	g	998	ASN	N-CA-C	-5.65	100.68	109.72
8	q	243	TRP	O-C-N	5.65	127.89	122.07
3	a	715	THR	N-CA-CB	5.65	120.04	110.49
4	m	475	SER	CA-C-N	5.65	127.85	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	m	475	SER	C-N-CA	5.65	127.85	120.28
4	b	640	GLU	O-C-N	5.65	130.39	123.44
3	l	803	HIS	ND1-CG-CD2	-5.65	100.45	106.10
1	X	333	ARG	N-CA-C	-5.64	107.04	114.04
3	a	132	GLN	N-CA-C	-5.64	98.70	108.69
3	a	709	VAL	N-CA-CB	5.64	117.16	110.55
5	c	474	THR	N-CA-C	5.64	120.68	111.37
9	g	1014	SER	N-CA-CB	5.64	120.03	110.49
3	l	319	ILE	CA-C-O	-5.64	115.13	119.98
4	m	220	ASP	N-CA-CB	5.64	121.34	111.13
6	d	188	ASN	CA-CB-CG	5.64	118.24	112.60
9	g	433	LEU	N-CA-C	-5.64	104.61	113.02
1	X	178	GLN	N-CA-C	5.64	117.11	111.07
1	X	649	LYS	N-CA-C	-5.64	100.85	109.65
3	a	621	GLN	CA-C-N	5.64	130.14	120.72
3	a	621	GLN	C-N-CA	5.64	130.14	120.72
4	b	278	CYS	N-CA-CB	5.64	118.99	110.42
5	c	318	LEU	N-CA-CB	5.64	118.42	110.98
9	g	136	PRO	CA-C-O	-5.64	111.55	118.99
3	l	352	ILE	CB-CA-C	-5.64	105.82	111.80
3	a	1004	ILE	CA-CB-CG1	5.64	119.98	110.40
8	f	516	TRP	CE2-CD2-CE3	5.64	124.44	118.80
8	q	200	ALA	CA-C-O	5.64	126.53	120.55
3	a	131	LEU	N-CA-CB	5.64	120.33	111.20
4	b	526	CYS	N-CA-CB	5.64	120.02	110.49
6	d	37	GLU	N-CA-C	5.64	117.97	110.53
9	g	884	HIS	CE1-NE2-CD2	-5.64	103.36	109.00
5	n	547	ARG	NH1-CZ-NH2	-5.64	111.97	119.30
1	X	1446	PHE	CA-C-N	5.63	129.37	120.47
1	X	1446	PHE	C-N-CA	5.63	129.37	120.47
9	g	517	PRO	CB-CA-C	5.63	117.79	110.92
3	l	456	ALA	N-CA-CB	5.63	120.01	110.49
7	p	144	ASP	CA-CB-CG	-5.63	106.97	112.60
3	a	667	LEU	O-C-N	-5.63	115.10	122.59
4	b	182	LEU	N-CA-C	-5.63	105.13	112.23
9	g	638	SER	N-CA-CB	5.63	120.39	110.37
4	m	241	GLU	N-CA-C	-5.63	104.64	112.30
9	r	994	THR	CA-CB-OG1	5.63	118.05	109.60
7	e	94	SER	N-CA-C	-5.63	99.12	108.75
4	m	394	CYS	CA-C-N	5.63	128.17	120.46
4	m	394	CYS	C-N-CA	5.63	128.17	120.46
1	X	1505	LEU	N-CA-C	-5.63	105.14	111.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	172	PHE	CB-CG-CD1	-5.63	111.13	120.70
8	f	601	GLN	N-CA-CB	5.63	118.39	110.12
5	n	231	TYR	CA-C-N	5.63	128.87	120.31
5	n	231	TYR	C-N-CA	5.63	128.87	120.31
5	n	418	ILE	N-CA-C	-5.63	104.68	112.50
6	o	213	SER	CB-CA-C	-5.63	100.53	109.82
4	b	550	HIS	ND1-CE1-NE2	5.63	114.03	108.40
5	c	584	ASN	CA-CB-CG	5.63	118.23	112.60
3	l	463	ILE	N-CA-C	-5.63	100.34	108.89
4	m	690	THR	N-CA-C	-5.63	105.76	113.30
8	q	201	LYS	CA-C-N	5.63	132.57	122.38
8	q	201	LYS	C-N-CA	5.63	132.57	122.38
9	r	841	LYS	N-CA-C	-5.63	98.81	110.80
6	o	112	TYR	CA-C-N	5.62	130.70	121.87
6	o	112	TYR	C-N-CA	5.62	130.70	121.87
4	b	655	PHE	CA-C-O	-5.62	115.26	120.94
5	c	142	ARG	NH1-CZ-NH2	-5.62	111.99	119.30
8	f	385	LEU	CA-C-N	5.62	127.82	120.28
8	f	385	LEU	C-N-CA	5.62	127.82	120.28
9	g	712	PHE	N-CA-C	-5.62	105.84	114.16
8	q	711	LEU	CA-C-N	5.62	128.27	120.29
8	q	711	LEU	C-N-CA	5.62	128.27	120.29
1	X	921	SER	N-CA-CB	5.62	119.99	110.49
1	X	935	VAL	CA-C-N	5.62	128.27	120.29
1	X	935	VAL	C-N-CA	5.62	128.27	120.29
4	b	279	ALA	CA-C-N	5.62	129.87	121.77
4	b	279	ALA	C-N-CA	5.62	129.87	121.77
3	l	499	SER	N-CA-C	-5.62	105.84	114.16
7	p	303	HIS	CE1-NE2-CD2	-5.62	103.38	109.00
9	g	250	LYS	O-C-N	5.62	125.48	120.48
3	l	630	THR	N-CA-CB	5.62	118.38	110.12
9	r	289	LYS	CB-CA-C	-5.62	99.43	110.11
4	b	88	TYR	N-CA-C	-5.62	105.01	113.89
4	b	529	TRP	CA-C-N	5.62	130.43	121.66
4	b	529	TRP	C-N-CA	5.62	130.43	121.66
8	f	237	ILE	CA-CB-CG1	5.62	119.95	110.40
8	f	589	HIS	N-CA-CB	5.62	118.47	110.16
3	l	929	HIS	CG-CD2-NE2	5.62	112.82	107.20
9	r	712	PHE	CA-C-N	5.62	130.23	120.68
9	r	712	PHE	C-N-CA	5.62	130.23	120.68
5	c	219	ASP	CA-CB-CG	5.62	118.22	112.60
9	g	553	LEU	N-CA-CB	-5.62	102.13	110.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	m	695	ILE	N-CA-C	-5.62	106.85	113.42
8	q	20	LYS	N-CA-CB	5.62	120.05	110.50
4	b	193	ASP	CA-CB-CG	-5.62	106.98	112.60
7	e	156	VAL	CA-C-O	5.62	127.12	121.17
6	o	61	TRP	CB-CG-CD1	5.62	135.32	126.90
1	X	1517	GLU	N-CA-CB	5.61	118.31	109.94
5	c	443	ASN	CA-C-O	5.61	126.55	120.43
3	l	316	GLN	N-CA-C	-5.61	98.84	110.80
3	l	562	PHE	CB-CG-CD1	5.61	130.24	120.70
3	l	788	ASP	N-CA-C	5.61	122.75	110.80
5	n	492	PHE	CA-C-N	5.61	128.39	120.42
5	n	492	PHE	C-N-CA	5.61	128.39	120.42
3	l	245	ILE	N-CA-C	-5.61	99.42	107.78
9	r	673	ILE	CA-CB-CG2	-5.61	100.96	110.50
1	X	136	ASN	CA-CB-CG	5.61	118.21	112.60
4	b	553	ILE	N-CA-C	-5.61	106.84	112.17
8	f	528	HIS	ND1-CE1-NE2	5.61	114.01	108.40
7	p	210	GLY	O-C-N	-5.61	115.40	122.41
9	r	647	LYS	CG-CD-CE	5.61	124.20	111.30
5	n	234	TRP	N-CA-CB	5.61	119.70	110.39
4	b	287	ASP	O-C-N	-5.61	115.63	122.25
5	n	565	TYR	CB-CG-CD1	5.61	129.21	120.80
6	o	113	GLY	N-CA-C	-5.61	100.91	112.34
7	e	135	ARG	CB-CA-C	-5.60	101.56	110.81
1	X	1309	ARG	CA-C-O	-5.60	112.91	118.34
4	b	389	ASP	O-C-N	5.60	128.97	122.19
8	q	157	ASP	N-CA-C	-5.60	98.87	110.80
3	a	193	HIS	ND1-CE1-NE2	5.60	114.00	108.40
5	c	409	LYS	CG-CD-CE	5.60	124.18	111.30
4	m	286	SER	N-CA-C	-5.60	105.32	111.82
9	r	1074	ASN	N-CA-C	-5.60	100.42	108.60
9	g	421	PRO	N-CA-CB	5.60	108.54	103.33
9	g	621	TYR	CA-C-N	-5.60	114.77	122.16
9	g	621	TYR	C-N-CA	-5.60	114.77	122.16
8	q	478	ARG	NE-CZ-NH2	-5.60	114.16	119.20
4	m	505	ALA	N-CA-CB	5.60	118.87	110.53
4	m	623	THR	CA-C-N	5.60	132.23	121.54
4	m	623	THR	C-N-CA	5.60	132.23	121.54
6	o	137	SER	CA-C-N	5.60	125.78	119.90
6	o	137	SER	C-N-CA	5.60	125.78	119.90
3	a	88	TYR	O-C-N	5.60	128.05	122.12
5	c	638	ILE	N-CA-C	-5.60	105.65	111.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	988	GLN	O-C-N	5.60	129.25	122.20
1	X	845	SER	N-CA-CB	5.59	118.12	110.01
9	g	978	GLY	N-CA-C	-5.59	104.54	111.70
4	m	669	LYS	O-C-N	5.59	130.03	122.59
6	o	238	ASN	CA-C-N	5.59	128.23	120.29
6	o	238	ASN	C-N-CA	5.59	128.23	120.29
7	p	11	LEU	N-CA-C	5.59	122.72	110.80
9	r	397	PRO	N-CA-CB	5.59	109.12	103.25
9	r	940	ASP	CA-CB-CG	5.59	118.19	112.60
4	b	620	MET	N-CA-C	-5.59	103.98	111.87
3	a	874	ASN	CA-CB-CG	-5.59	107.01	112.60
9	g	1076	PHE	CA-C-N	5.59	125.35	119.76
9	g	1076	PHE	C-N-CA	5.59	125.35	119.76
5	n	548	TYR	CB-CG-CD1	5.59	129.19	120.80
6	o	228	ASP	N-CA-CB	5.59	119.05	110.61
9	r	965	LYS	N-CA-C	-5.59	105.22	113.61
3	l	177	PHE	CB-CA-C	-5.59	101.74	110.74
4	m	607	ILE	CA-C-O	-5.59	114.10	118.85
4	m	685	GLU	N-CA-C	5.59	118.12	110.24
1	X	996	THR	N-CA-C	-5.59	106.13	113.17
5	c	353	ASN	CA-CB-CG	5.59	118.19	112.60
8	q	162	LEU	N-CA-C	-5.59	106.82	113.97
6	d	131	LYS	CA-CB-CG	5.59	125.27	114.10
8	f	288	ILE	CA-C-O	-5.59	114.93	120.85
9	g	171	LYS	N-CA-C	-5.59	99.32	108.76
9	r	357	ASN	N-CA-C	-5.59	106.30	113.23
9	g	83	ASP	N-CA-CB	5.58	120.45	110.79
3	l	661	GLN	CG-CD-NE2	5.58	124.77	116.40
5	n	432	GLU	N-CA-C	5.58	117.37	111.28
5	n	463	ARG	CA-C-O	-5.58	114.30	120.38
1	X	143	SER	O-C-N	5.58	128.05	122.08
1	X	700	LEU	N-CA-C	-5.58	105.24	113.61
3	l	893	HIS	CA-CB-CG	-5.58	108.22	113.80
3	a	939	THR	CA-C-N	5.58	127.55	121.97
3	a	939	THR	C-N-CA	5.58	127.55	121.97
8	q	76	HIS	CE1-NE2-CD2	-5.58	103.42	109.00
9	g	810	ASP	CA-C-N	5.58	132.19	121.54
9	g	810	ASP	C-N-CA	5.58	132.19	121.54
4	b	50	PRO	N-CA-CB	5.58	108.21	103.19
8	f	355	LEU	CB-CA-C	-5.58	100.20	111.80
1	X	1384	ASP	CA-C-O	-5.57	115.23	121.81
7	e	161	PRO	CA-C-O	-5.57	114.99	121.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	354	ILE	N-CA-CB	5.57	118.12	110.54
8	q	244	ARG	CA-C-O	-5.57	114.51	120.42
8	f	458	ARG	N-CA-C	5.57	118.12	111.71
3	a	272	LYS	N-CA-CB	5.57	118.23	110.04
3	l	498	HIS	N-CA-C	-5.57	104.02	112.99
4	m	659	PRO	N-CA-C	5.57	123.94	112.47
5	n	488	GLY	CA-C-N	5.57	130.10	120.58
5	n	488	GLY	C-N-CA	5.57	130.10	120.58
6	o	225	VAL	N-CA-CB	-5.57	102.63	110.26
7	p	340	LYS	O-C-N	-5.57	115.91	123.10
9	r	1150	TYR	CB-CG-CD1	5.57	129.16	120.80
7	e	305	GLY	CA-C-O	-5.57	116.75	122.26
8	f	183	TYR	CA-C-N	5.57	128.09	120.46
8	f	183	TYR	C-N-CA	5.57	128.09	120.46
9	g	577	TYR	CB-CG-CD2	-5.57	112.45	120.80
5	n	218	LYS	O-C-N	-5.57	115.38	122.34
1	X	349	PHE	CA-C-N	5.57	127.74	120.28
1	X	349	PHE	C-N-CA	5.57	127.74	120.28
1	X	773	LEU	N-CA-C	-5.57	105.09	112.94
5	c	429	GLU	N-CA-C	-5.57	106.49	113.28
8	f	710	LYS	CG-CD-CE	5.57	124.10	111.30
9	g	131	GLU	CA-C-O	5.57	127.31	121.19
1	X	267	ILE	CB-CA-C	-5.57	104.85	111.81
3	a	734	HIS	CB-CG-CD2	-5.57	123.97	131.20
8	q	643	PHE	CA-C-N	5.57	128.61	120.71
8	q	643	PHE	C-N-CA	5.57	128.61	120.71
9	r	561	LYS	CA-C-N	5.57	128.77	120.31
9	r	561	LYS	C-N-CA	5.57	128.77	120.31
1	X	136	ASN	CA-C-O	-5.56	112.55	120.51
3	l	842	LEU	CA-C-O	5.56	126.45	120.55
1	X	1335	GLN	N-CA-CB	5.56	118.30	110.12
3	a	319	ILE	CA-CB-CG2	-5.56	101.04	110.50
6	d	85	GLU	N-CA-C	-5.56	98.18	107.80
7	e	38	LEU	CA-C-O	-5.56	114.20	120.43
9	g	645	ILE	CA-C-N	5.56	128.05	120.54
9	g	645	ILE	C-N-CA	5.56	128.05	120.54
5	n	284	ILE	N-CA-CB	5.56	117.06	110.55
6	o	290	GLU	CA-C-N	5.56	125.87	119.92
6	o	290	GLU	C-N-CA	5.56	125.87	119.92
7	p	178	PHE	CB-CA-C	-5.56	101.16	110.56
3	a	241	CYS	N-CA-C	-5.56	98.96	110.80
4	b	661	HIS	CE1-NE2-CD2	-5.56	103.44	109.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	d	20	TYR	CB-CA-C	-5.56	101.40	110.85
6	d	228	ASP	N-CA-C	-5.56	106.27	113.16
8	f	233	THR	CA-CB-CG2	5.56	119.95	110.50
5	n	356	LYS	CA-C-N	5.56	128.07	120.46
5	n	356	LYS	C-N-CA	5.56	128.07	120.46
5	n	601	GLU	CA-C-O	-5.56	114.66	120.55
9	r	841	LYS	N-CA-CB	5.56	119.88	110.49
4	b	198	GLU	CB-CG-CD	-5.56	103.16	112.60
4	b	227	VAL	CA-C-N	5.56	131.27	122.94
4	b	227	VAL	C-N-CA	5.56	131.27	122.94
4	b	403	HIS	CG-CD2-NE2	5.56	112.76	107.20
4	m	676	LEU	N-CA-C	-5.55	100.49	108.60
9	r	1134	HIS	CE1-NE2-CD2	-5.55	103.44	109.00
4	b	722	SER	N-CA-CB	5.55	118.85	110.30
9	g	883	GLY	O-C-N	5.55	127.97	122.92
1	X	1522	VAL	N-CA-C	5.55	116.33	110.72
3	a	144	THR	N-CA-C	-5.55	105.94	114.16
3	a	342	LEU	N-CA-C	-5.55	98.97	110.80
8	f	599	GLU	CA-C-O	-5.55	113.59	119.97
9	g	142	PHE	CB-CG-CD1	5.55	130.14	120.70
9	r	584	LYS	CA-C-O	5.55	127.38	121.05
1	X	1543	VAL	N-CA-C	-5.55	100.33	108.99
3	a	348	TYR	N-CA-C	-5.55	98.98	110.80
7	e	23	HIS	CG-CD2-NE2	5.55	112.75	107.20
9	g	739	LYS	N-CA-C	5.55	117.01	111.07
9	g	935	GLU	CB-CG-CD	5.55	122.03	112.60
3	l	801	ASN	CA-CB-CG	-5.55	107.05	112.60
3	l	905	LEU	O-C-N	5.55	128.95	122.24
4	m	690	THR	CB-CA-C	5.55	119.55	110.17
5	c	205	ASN	OD1-CG-ND2	5.55	128.15	122.60
8	f	592	LYS	N-CA-C	-5.55	105.31	111.36
9	g	408	ASN	CA-CB-CG	5.55	118.15	112.60
3	l	24	VAL	CA-CB-CG1	5.55	119.83	110.40
3	l	661	GLN	CA-C-N	5.55	128.48	120.38
3	l	661	GLN	C-N-CA	5.55	128.48	120.38
9	g	523	ASP	CA-CB-CG	-5.54	107.06	112.60
1	X	1616	ILE	N-CA-C	-5.54	100.60	108.58
3	a	837	SER	N-CA-CB	5.54	119.86	110.49
7	e	121	LEU	N-CA-CB	5.54	123.13	111.10
7	e	303	HIS	CA-CB-CG	-5.54	108.26	113.80
9	g	858	ASN	N-CA-C	-5.54	101.95	109.54
6	o	110	HIS	CG-CD2-NE2	5.54	112.74	107.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	268	SER	CA-C-O	5.54	124.58	118.65
9	r	392	ASP	N-CA-CB	5.54	118.22	110.07
1	X	425	LEU	CA-C-N	5.54	132.09	122.56
1	X	425	LEU	C-N-CA	5.54	132.09	122.56
1	X	1607	THR	CA-C-O	5.54	126.20	119.11
5	c	339	GLN	N-CA-CB	5.54	118.27	110.12
7	e	212	LYS	N-CA-C	-5.54	104.76	113.02
8	q	537	PHE	CA-CB-CG	-5.54	108.26	113.80
9	r	1152	THR	CA-C-N	5.54	130.00	122.19
9	r	1152	THR	C-N-CA	5.54	130.00	122.19
7	e	179	SER	N-CA-C	-5.54	101.62	110.10
1	X	707	PHE	CA-CB-CG	5.54	119.34	113.80
1	X	860	ALA	CA-C-O	-5.54	114.00	120.20
1	X	1214	PHE	CA-CB-CG	-5.54	108.26	113.80
4	b	194	GLY	CA-C-O	5.54	126.60	119.68
6	d	141	ILE	N-CA-C	-5.54	99.71	108.90
3	l	224	ILE	CA-C-O	-5.54	113.86	120.78
8	f	54	ALA	N-CA-C	-5.54	105.56	112.93
9	g	328	HIS	CE1-NE2-CD2	-5.54	103.46	109.00
4	m	283	ASP	CA-CB-CG	5.54	118.14	112.60
9	r	502	VAL	CA-C-N	5.54	128.15	120.29
9	r	502	VAL	C-N-CA	5.54	128.15	120.29
6	d	173	PHE	CA-CB-CG	5.54	119.34	113.80
7	e	239	ARG	NH1-CZ-NH2	-5.54	112.10	119.30
8	f	97	HIS	CA-C-O	-5.54	113.54	118.63
4	m	661	HIS	CB-CG-CD2	-5.54	124.00	131.20
5	n	776	GLN	O-C-N	-5.54	114.95	121.32
6	o	197	GLU	N-CA-C	5.54	117.12	111.14
3	a	840	PHE	CA-CB-CG	-5.53	108.27	113.80
5	c	412	LEU	CA-C-O	-5.53	114.94	120.64
9	g	223	THR	CA-C-O	-5.53	114.86	121.11
3	l	789	LYS	N-CA-CB	-5.53	102.09	111.17
8	q	390	THR	N-CA-C	5.53	116.99	111.07
4	b	381	ALA	N-CA-CB	5.53	119.84	110.49
8	f	416	TYR	CA-C-N	5.53	128.28	120.42
8	f	416	TYR	C-N-CA	5.53	128.28	120.42
8	f	714	TYR	CA-C-O	-5.53	115.01	120.82
9	g	941	ILE	N-CA-CB	-5.53	106.12	112.21
9	g	1049	ASN	N-CA-C	-5.53	106.53	113.28
5	n	617	PHE	O-C-N	-5.53	115.70	122.34
3	a	599	LYS	CB-CA-C	-5.53	101.78	110.79
3	a	879	PHE	N-CA-C	-5.53	107.18	114.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	795	GLU	N-CA-CB	5.53	118.77	109.92
3	l	929	HIS	CB-CG-CD2	-5.53	124.01	131.20
4	m	336	LEU	CA-C-O	-5.53	113.26	119.79
8	q	308	VAL	N-CA-C	-5.53	100.43	108.17
8	q	314	ILE	CB-CA-C	5.53	116.59	110.62
1	X	1209	ALA	CA-C-N	5.53	127.69	120.28
1	X	1209	ALA	C-N-CA	5.53	127.69	120.28
5	c	525	HIS	CE1-NE2-CD2	-5.53	103.47	109.00
7	e	81	VAL	O-C-N	-5.53	115.36	122.32
7	e	140	LEU	O-C-N	5.53	129.44	122.37
3	l	65	SER	CA-C-N	5.53	129.32	121.42
3	l	65	SER	C-N-CA	5.53	129.32	121.42
3	l	436	HIS	CG-CD2-NE2	5.53	112.73	107.20
1	X	1402	LYS	N-CA-C	-5.53	105.27	112.23
3	a	72	PHE	N-CA-C	-5.53	100.70	109.76
4	m	581	MET	CA-C-N	5.53	132.09	121.54
4	m	581	MET	C-N-CA	5.53	132.09	121.54
5	n	212	GLU	CA-C-N	-5.53	115.31	123.05
5	n	212	GLU	C-N-CA	-5.53	115.31	123.05
9	g	532	LYS	CA-C-O	-5.52	114.56	120.42
8	q	545	ALA	CA-C-O	5.52	125.73	119.27
6	d	46	ILE	O-C-N	-5.52	115.67	122.57
9	g	873	GLN	CA-C-N	5.52	127.68	120.28
9	g	873	GLN	C-N-CA	5.52	127.68	120.28
3	l	173	PHE	N-CA-C	-5.52	100.40	109.40
3	l	823	ALA	CA-C-N	5.52	127.68	120.28
3	l	823	ALA	C-N-CA	5.52	127.68	120.28
6	o	9	ASN	N-CA-C	-5.52	100.02	109.24
1	X	1238	ILE	N-CA-CB	5.52	117.61	110.99
3	a	17	LYS	N-CA-CB	5.52	117.74	110.29
3	a	331	ILE	CA-C-N	5.52	129.26	121.53
3	a	331	ILE	C-N-CA	5.52	129.26	121.53
3	a	551	THR	CA-CB-OG1	5.52	117.88	109.60
4	b	389	ASP	CA-CB-CG	-5.52	107.08	112.60
8	q	101	SER	CA-C-N	5.52	129.94	120.72
8	q	101	SER	C-N-CA	5.52	129.94	120.72
8	q	521	LYS	O-C-N	5.52	126.80	121.56
9	r	758	ILE	N-CA-C	-5.52	105.23	110.42
4	b	489	ILE	CA-C-O	-5.52	115.32	120.34
7	e	121	LEU	N-CA-C	-5.52	104.11	112.99
7	e	293	GLN	OE1-CD-NE2	5.52	128.12	122.60
4	m	158	PHE	O-C-N	-5.52	114.90	122.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	548	TYR	N-CA-C	-5.52	99.05	110.80
6	o	173	PHE	N-CA-C	-5.52	100.78	109.50
8	q	203	SER	N-CA-C	-5.52	106.22	113.17
9	r	304	PRO	CA-C-N	-5.52	114.25	122.74
9	r	304	PRO	C-N-CA	-5.52	114.25	122.74
9	r	604	ILE	CB-CA-C	5.52	118.54	110.98
9	r	1025	ASP	N-CA-CB	5.52	119.17	110.56
1	X	650	ASP	N-CA-C	-5.51	103.83	111.28
3	a	334	LEU	N-CA-CB	5.51	119.89	110.57
4	b	97	ARG	CA-C-N	5.51	132.07	121.54
4	b	97	ARG	C-N-CA	5.51	132.07	121.54
4	b	524	SER	N-CA-C	-5.51	106.22	113.17
3	l	815	PHE	O-C-N	5.51	128.81	122.25
4	b	558	ASN	CA-C-O	5.51	125.74	119.18
5	c	280	ILE	O-C-N	5.51	127.51	121.83
9	g	725	PHE	CA-CB-CG	-5.51	108.29	113.80
9	g	805	ALA	O-C-N	5.51	127.82	122.09
4	m	661	HIS	CA-CB-CG	-5.51	108.29	113.80
1	X	1197	VAL	N-CA-C	5.51	116.29	110.72
3	a	623	LEU	CA-C-N	5.51	128.69	120.31
3	a	623	LEU	C-N-CA	5.51	128.69	120.31
4	b	522	MET	N-CA-C	-5.51	106.76	112.93
5	c	199	ILE	N-CA-CB	5.51	117.09	110.31
6	d	14	ASP	CA-C-N	5.51	132.07	121.54
6	d	14	ASP	C-N-CA	5.51	132.07	121.54
7	e	69	GLY	CA-C-N	5.51	128.53	120.71
7	e	69	GLY	C-N-CA	5.51	128.53	120.71
8	f	387	ARG	NE-CZ-NH1	-5.51	115.99	121.50
8	f	516	TRP	CA-C-O	-5.51	112.05	119.11
3	a	421	GLU	N-CA-C	-5.51	106.51	113.18
9	r	851	LEU	CA-C-O	-5.51	114.71	120.55
9	g	350	SER	CB-CA-C	5.51	120.66	111.30
3	l	912	ASP	CA-CB-CG	5.51	118.11	112.60
3	l	961	PHE	N-CA-C	-5.51	99.31	108.34
5	n	359	LYS	N-CA-CB	5.51	118.31	110.16
7	p	218	ILE	CA-CB-CG2	-5.51	101.14	110.50
9	r	389	SER	O-C-N	-5.51	115.93	122.65
9	r	1004	GLU	N-CA-C	5.51	117.74	111.02
4	b	507	LEU	N-CA-C	-5.51	105.28	111.28
4	b	657	TYR	CB-CG-CD1	5.51	129.06	120.80
5	c	519	ARG	N-CA-C	-5.51	99.93	108.90
8	f	394	ILE	N-CA-CB	-5.51	104.11	110.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	984	PHE	CA-C-N	5.51	128.68	120.31
9	g	984	PHE	C-N-CA	5.51	128.68	120.31
5	n	779	LYS	N-CA-C	-5.51	104.58	112.13
8	q	162	LEU	N-CA-CB	5.51	118.33	110.67
1	X	149	ILE	CB-CA-C	5.50	120.32	111.29
8	f	407	VAL	N-CA-C	-5.50	104.59	112.35
7	p	211	HIS	ND1-CE1-NE2	5.50	113.91	108.40
1	X	761	PHE	O-C-N	-5.50	115.83	122.71
1	X	1237	ASN	CA-CB-CG	5.50	118.10	112.60
1	X	1386	LEU	CB-CA-C	-5.50	102.48	110.96
8	f	192	ALA	N-CA-CB	5.50	119.79	110.49
9	g	586	ASP	N-CA-C	-5.50	106.44	112.72
9	r	168	LYS	CB-CA-C	-5.50	98.61	109.67
9	r	234	ARG	CB-CA-C	-5.50	101.58	110.77
9	r	589	GLU	CA-C-N	5.50	127.66	120.28
9	r	589	GLU	C-N-CA	5.50	127.66	120.28
9	r	901	ASN	CA-C-N	5.50	127.65	120.28
9	r	901	ASN	C-N-CA	5.50	127.65	120.28
3	l	172	GLN	N-CA-CB	5.50	119.79	110.49
3	l	520	LEU	CA-C-O	-5.50	115.14	121.19
5	n	602	PHE	CA-C-N	5.50	125.45	119.78
5	n	602	PHE	C-N-CA	5.50	125.45	119.78
9	r	582	GLU	CB-CA-C	-5.50	99.00	109.95
9	r	699	MET	CG-SD-CE	-5.50	88.80	100.90
4	m	337	LEU	N-CA-CB	-5.50	101.17	110.41
8	f	213	CYS	CA-C-O	5.50	126.28	119.79
9	g	1001	ASP	CA-CB-CG	5.50	118.10	112.60
9	g	1060	HIS	CB-CG-CD2	-5.50	124.05	131.20
3	l	978	ALA	CA-C-O	5.50	126.77	121.00
8	q	173	ASP	CA-C-N	5.50	128.67	120.31
8	q	173	ASP	C-N-CA	5.50	128.67	120.31
4	b	203	GLU	CA-C-N	5.50	129.93	121.19
4	b	203	GLU	C-N-CA	5.50	129.93	121.19
9	g	1052	ASN	O-C-N	-5.50	116.08	123.23
1	X	340	SER	N-CA-C	5.50	117.70	111.11
5	n	254	GLN	CB-CA-C	-5.50	101.67	110.79
8	q	405	GLU	N-CA-CB	5.50	118.30	110.06
3	a	711	ASN	CB-CG-ND2	-5.49	108.16	116.40
3	a	891	LEU	CB-CA-C	5.49	118.93	110.14
7	e	300	HIS	CE1-NE2-CD2	-5.49	103.51	109.00
8	f	36	PHE	N-CA-C	-5.49	106.08	112.89
5	n	200	GLU	N-CA-CB	5.49	119.59	110.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	553	LEU	CA-C-O	5.49	126.59	120.82
8	q	636	VAL	CA-CB-CG2	5.49	119.74	110.40
9	g	712	PHE	CA-C-N	5.49	132.03	121.54
9	g	712	PHE	C-N-CA	5.49	132.03	121.54
8	q	381	ASP	CA-CB-CG	5.49	118.09	112.60
1	X	177	VAL	CA-C-N	5.49	127.58	120.44
1	X	177	VAL	C-N-CA	5.49	127.58	120.44
1	X	1168	LYS	N-CA-C	5.49	122.50	110.80
4	b	56	GLN	OE1-CD-NE2	5.49	128.09	122.60
8	f	358	VAL	N-CA-C	5.49	116.27	110.72
4	m	199	GLU	CA-C-O	-5.49	114.73	120.55
4	m	314	SER	N-CA-C	-5.49	106.08	112.89
6	o	70	LEU	O-C-N	-5.49	116.61	123.04
1	X	1207	TRP	CA-C-N	5.49	126.07	119.98
1	X	1207	TRP	C-N-CA	5.49	126.07	119.98
1	X	1404	PHE	CA-C-N	5.49	127.63	120.28
1	X	1404	PHE	C-N-CA	5.49	127.63	120.28
4	b	305	GLU	N-CA-C	-5.49	104.83	112.30
9	g	173	ILE	N-CA-C	-5.49	98.56	107.28
3	l	58	ASN	CA-CB-CG	5.49	118.09	112.60
1	X	1427	SER	CA-C-O	5.49	128.36	120.51
4	b	657	TYR	CA-C-O	5.49	126.41	120.43
9	g	149	SER	CA-C-O	-5.49	112.64	120.16
3	l	885	VAL	O-C-N	-5.49	116.45	122.05
9	r	529	HIS	CB-CG-CD2	-5.49	124.07	131.20
8	q	406	GLU	CA-C-N	5.49	129.73	120.29
8	q	406	GLU	C-N-CA	5.49	129.73	120.29
6	d	13	HIS	ND1-CE1-NE2	5.48	113.88	108.40
4	m	521	TRP	CG-CD1-NE1	-5.48	103.07	110.20
5	n	660	VAL	N-CA-CB	5.48	117.59	110.57
9	g	614	TRP	N-CA-C	-5.48	106.43	113.23
4	m	83	THR	N-CA-C	-5.48	98.32	108.24
4	m	360	PHE	CB-CG-CD2	5.48	130.02	120.70
5	n	626	ASP	N-CA-CB	5.48	119.18	110.57
8	q	277	LEU	CA-C-O	5.48	126.62	120.70
1	X	1434	ASN	N-CA-CB	5.48	118.03	109.97
1	X	1622	GLU	CA-C-O	5.48	126.76	120.90
8	f	105	PHE	CA-CB-CG	-5.48	108.32	113.80
8	f	427	GLU	CA-C-N	5.48	132.44	121.81
8	f	427	GLU	C-N-CA	5.48	132.44	121.81
4	m	333	GLU	N-CA-CB	5.48	118.27	110.16
4	m	732	ARG	NE-CZ-NH1	-5.48	116.02	121.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	449	PHE	CA-C-N	5.48	128.07	120.29
5	n	449	PHE	C-N-CA	5.48	128.07	120.29
6	o	278	VAL	CA-C-O	5.48	128.15	120.86
9	g	837	ASN	OD1-CG-ND2	-5.48	117.12	122.60
5	n	561	LEU	CA-C-N	5.48	126.02	119.94
5	n	561	LEU	C-N-CA	5.48	126.02	119.94
5	c	466	SER	N-CA-CB	5.48	118.10	109.83
3	l	285	ASN	CA-CB-CG	5.48	118.08	112.60
4	m	76	TYR	N-CA-C	-5.48	106.96	113.97
6	o	125	VAL	N-CA-CB	5.48	120.10	111.99
8	q	591	ILE	N-CA-C	5.48	116.21	110.62
9	r	246	LYS	CB-CA-C	-5.48	101.54	110.85
9	r	719	ASN	OD1-CG-ND2	5.48	128.08	122.60
9	r	342	GLU	N-CA-CB	5.48	119.56	110.47
8	f	380	ILE	O-C-N	5.47	127.80	122.05
9	g	753	PHE	CA-C-N	5.47	127.56	120.44
9	g	753	PHE	C-N-CA	5.47	127.56	120.44
3	l	264	ASP	N-CA-C	-5.47	100.37	109.46
4	m	468	SER	N-CA-C	-5.47	106.60	113.28
8	q	182	LYS	CB-CA-C	5.47	119.88	110.79
8	f	66	LYS	CB-CG-CD	5.47	123.89	111.30
3	l	927	ASN	OD1-CG-ND2	5.47	128.07	122.60
5	n	275	GLN	OE1-CD-NE2	5.47	128.07	122.60
7	p	94	SER	CA-C-N	5.47	131.34	122.09
7	p	94	SER	C-N-CA	5.47	131.34	122.09
9	r	556	HIS	ND1-CE1-NE2	5.47	113.87	108.40
3	a	752	HIS	CB-CG-CD2	5.47	138.31	131.20
8	f	116	LEU	CB-CA-C	-5.47	101.71	110.79
1	X	279	ILE	CA-C-N	5.47	131.99	121.54
1	X	279	ILE	C-N-CA	5.47	131.99	121.54
1	X	1219	THR	O-C-N	5.47	129.31	122.86
3	a	407	GLY	CA-C-N	5.47	131.99	121.54
3	a	407	GLY	C-N-CA	5.47	131.99	121.54
3	l	693	PHE	N-CA-C	-5.47	106.33	114.64
9	r	926	VAL	CA-C-N	5.47	128.06	120.29
9	r	926	VAL	C-N-CA	5.47	128.06	120.29
1	X	1188	THR	N-CA-C	5.47	117.24	111.28
9	g	843	PHE	CA-CB-CG	5.47	119.27	113.80
1	X	896	PHE	N-CA-C	-5.47	100.82	108.96
3	a	790	LEU	CA-C-N	5.47	126.67	119.84
3	a	790	LEU	C-N-CA	5.47	126.67	119.84
6	d	26	THR	CA-C-O	-5.47	114.42	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	729	ILE	O-C-N	-5.47	115.74	122.57
5	n	418	ILE	CA-C-N	5.47	125.90	119.94
5	n	418	ILE	C-N-CA	5.47	125.90	119.94
3	a	866	GLU	O-C-N	5.46	128.60	122.32
8	f	474	ASN	OD1-CG-ND2	5.46	128.06	122.60
7	p	148	TRP	CA-C-N	5.46	130.13	121.99
7	p	148	TRP	C-N-CA	5.46	130.13	121.99
8	q	187	LEU	N-CA-CB	5.46	118.15	110.12
1	X	1090	THR	CA-C-N	5.46	129.09	120.89
1	X	1090	THR	C-N-CA	5.46	129.09	120.89
7	e	240	ILE	N-CA-C	-5.46	99.29	107.37
4	b	304	ARG	NH1-CZ-NH2	5.46	126.40	119.30
1	X	933	LYS	N-CA-C	-5.46	105.98	113.30
3	a	373	PHE	CA-CB-CG	-5.46	108.34	113.80
3	a	936	TYR	O-C-N	5.46	129.58	123.19
5	c	579	ARG	O-C-N	-5.46	118.48	123.50
5	c	454	ILE	N-CA-C	-5.46	105.40	110.53
6	d	96	ALA	CA-C-O	5.46	127.84	120.47
3	l	188	LYS	O-C-N	5.46	129.47	123.25
3	l	558	LEU	N-CA-C	-5.46	106.54	114.12
4	m	509	PRO	CB-CA-C	-5.46	101.88	111.21
7	p	57	SER	CA-C-O	-5.46	114.42	120.70
8	q	530	ILE	CB-CA-C	5.46	118.86	111.88
3	a	416	GLY	N-CA-C	-5.45	104.87	112.18
3	a	756	GLN	CG-CD-NE2	-5.45	108.22	116.40
7	e	219	SER	CA-C-N	5.45	128.46	120.71
7	e	219	SER	C-N-CA	5.45	128.46	120.71
9	g	868	HIS	CG-CD2-NE2	5.45	112.65	107.20
9	g	1063	LYS	N-CA-CB	5.45	118.14	110.12
4	b	506	GLU	N-CA-C	-5.45	107.28	114.04
6	o	18	ASP	CA-CB-CG	-5.45	107.15	112.60
8	q	335	HIS	ND1-CE1-NE2	5.45	113.85	108.40
1	X	1311	LEU	CA-C-O	-5.45	115.10	120.82
3	a	210	ARG	CA-CB-CG	5.45	125.00	114.10
3	l	556	ASN	N-CA-C	5.45	117.03	111.14
4	m	561	ARG	NE-CZ-NH2	-5.45	114.29	119.20
9	r	652	HIS	CG-CD2-NE2	5.45	112.65	107.20
7	e	59	VAL	CB-CA-C	5.45	115.90	111.05
4	m	250	ASN	CA-C-N	5.45	128.13	120.28
4	m	250	ASN	C-N-CA	5.45	128.13	120.28
6	o	186	LYS	N-CA-CB	5.45	119.29	110.41
8	f	446	SER	N-CA-C	-5.45	106.61	113.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	m	48	LEU	O-C-N	5.45	129.72	123.29
1	X	1410	SER	CB-CA-C	-5.45	102.30	110.90
3	a	675	LEU	CA-C-N	5.45	127.52	120.44
3	a	675	LEU	C-N-CA	5.45	127.52	120.44
5	c	187	ASP	CA-C-O	5.45	126.23	119.97
7	e	230	LEU	N-CA-C	-5.45	101.01	109.72
8	f	199	GLU	O-C-N	5.45	128.36	122.15
4	m	79	MET	N-CA-CB	5.45	119.83	110.68
9	r	613	ILE	CA-CB-CG1	5.45	119.66	110.40
3	l	605	ILE	CA-C-O	5.44	126.35	120.47
1	X	1045	ALA	N-CA-CB	5.44	117.96	109.85
3	a	523	ASP	CA-C-N	5.44	127.42	120.56
3	a	523	ASP	C-N-CA	5.44	127.42	120.56
5	c	271	TRP	CG-CD2-CE3	-5.44	128.46	133.90
8	q	404	VAL	N-CA-CB	5.44	118.32	111.46
1	X	1334	ASP	N-CA-CB	5.44	118.68	110.30
3	a	830	LEU	N-CA-C	-5.44	105.25	111.07
6	d	186	LYS	CA-C-N	5.44	129.28	121.50
6	d	186	LYS	C-N-CA	5.44	129.28	121.50
9	g	328	HIS	ND1-CE1-NE2	5.44	113.84	108.40
4	m	115	TYR	CA-CB-CG	5.44	123.69	113.90
9	r	756	PHE	O-C-N	-5.44	115.29	122.42
1	X	769	PHE	CA-CB-CG	-5.44	108.36	113.80
4	b	136	PHE	O-C-N	5.44	127.89	122.12
6	d	265	SER	N-CA-C	-5.44	99.22	110.80
4	m	270	LEU	N-CA-C	-5.44	99.22	110.80
9	r	358	GLU	CA-C-N	5.44	130.66	122.99
9	r	358	GLU	C-N-CA	5.44	130.66	122.99
1	X	1398	VAL	CA-C-O	-5.44	114.91	121.54
4	b	362	LEU	N-CA-C	-5.44	104.77	111.40
4	m	58	ILE	CA-C-O	-5.44	116.39	120.96
8	q	97	HIS	CA-C-N	5.44	126.64	119.84
8	q	97	HIS	C-N-CA	5.44	126.64	119.84
8	q	285	ASP	O-C-N	5.44	127.67	122.07
1	X	958	THR	CA-CB-OG1	5.43	117.75	109.60
4	b	150	ALA	N-CA-C	5.43	117.20	111.28
4	b	543	GLY	CA-C-N	5.43	129.87	120.58
4	b	543	GLY	C-N-CA	5.43	129.87	120.58
4	b	621	ARG	N-CA-C	-5.43	106.42	113.16
5	c	545	LYS	O-C-N	-5.43	115.36	122.59
8	f	209	CYS	N-CA-CB	5.43	118.20	110.16
8	f	553	ASN	N-CA-C	-5.43	100.84	109.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	258	ASP	CA-CB-CG	5.43	118.03	112.60
3	l	807	ILE	O-C-N	-5.43	115.78	122.57
5	n	487	HIS	CA-C-O	5.43	125.63	119.27
8	q	397	ASP	CA-CB-CG	5.43	118.03	112.60
1	X	145	ILE	CA-C-O	-5.43	114.60	120.47
3	a	439	ASP	N-CA-CB	5.43	118.80	110.70
3	a	794	LEU	N-CA-CB	5.43	118.09	109.51
9	g	494	VAL	CA-C-O	-5.43	113.99	120.78
3	l	612	SER	CA-C-O	5.43	125.55	119.41
5	n	511	VAL	CA-C-O	-5.43	115.02	121.05
8	q	696	ASN	O-C-N	-5.43	116.82	122.96
6	d	20	TYR	N-CA-CB	5.43	118.20	110.16
7	e	243	PHE	CA-CB-CG	-5.43	108.37	113.80
9	g	750	TYR	N-CA-C	-5.43	105.88	112.88
5	n	233	LEU	N-CA-C	-5.43	105.28	111.14
9	r	736	ASP	CA-C-N	5.43	127.56	120.28
9	r	736	ASP	C-N-CA	5.43	127.56	120.28
9	r	888	ILE	CB-CA-C	5.43	119.31	111.65
5	c	224	MET	N-CA-CB	5.43	119.66	110.49
9	g	1019	LEU	CA-C-O	-5.43	113.97	120.10
3	l	597	TRP	CB-CG-CD2	-5.43	119.20	126.80
9	r	577	TYR	CB-CA-C	-5.43	100.69	110.35
3	l	709	VAL	N-CA-C	-5.43	105.24	110.72
4	m	221	GLU	CA-C-O	5.43	126.87	120.58
1	X	826	SER	O-C-N	-5.42	115.08	121.32
4	b	713	ILE	CA-C-O	5.42	123.86	118.98
8	f	444	ALA	N-CA-CB	5.42	118.58	110.22
7	p	318	ILE	N-CA-CB	5.42	117.98	111.31
1	X	917	PRO	N-CA-C	-5.42	103.05	111.13
1	X	722	SER	N-CA-C	-5.42	104.94	113.02
1	X	1255	ILE	N-CA-CB	5.42	120.17	111.23
5	c	574	THR	CA-C-N	5.42	130.82	122.42
5	c	574	THR	C-N-CA	5.42	130.82	122.42
8	f	630	LEU	CB-CA-C	-5.42	102.43	110.67
9	g	1060	HIS	CA-CB-CG	5.42	119.22	113.80
5	n	644	PHE	CA-C-N	5.42	128.55	120.31
5	n	644	PHE	C-N-CA	5.42	128.55	120.31
7	p	107	SER	CA-C-O	-5.42	115.23	121.19
9	r	612	ASP	CA-CB-CG	5.42	118.02	112.60
4	b	52	THR	CA-CB-CG2	5.42	119.71	110.50
4	b	623	THR	CA-CB-OG1	5.42	117.73	109.60
5	c	648	TYR	CB-CG-CD2	-5.42	112.67	120.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	238	GLY	CA-C-O	-5.42	113.49	122.00
1	X	383	LEU	CA-C-N	5.42	128.00	120.63
1	X	383	LEU	C-N-CA	5.42	128.00	120.63
3	a	735	LYS	N-CA-C	-5.42	105.89	112.88
3	l	1031	ARG	NH1-CZ-NH2	5.42	126.34	119.30
9	g	462	SER	CA-C-N	5.42	130.25	122.40
9	g	462	SER	C-N-CA	5.42	130.25	122.40
9	r	739	LYS	N-CA-C	-5.42	105.03	111.69
4	b	376	GLN	OE1-CD-NE2	5.41	128.01	122.60
5	n	192	LYS	CA-C-O	-5.41	114.81	120.55
3	l	749	TYR	CB-CA-C	-5.41	102.42	111.13
9	r	959	ASN	CB-CG-ND2	-5.41	108.28	116.40
1	X	861	ILE	CA-C-N	5.41	131.87	121.54
1	X	861	ILE	C-N-CA	5.41	131.87	121.54
3	a	58	ASN	CA-CB-CG	5.41	118.01	112.60
3	a	765	PHE	CA-C-N	5.41	128.07	120.28
3	a	765	PHE	C-N-CA	5.41	128.07	120.28
3	a	869	HIS	ND1-CE1-NE2	5.41	113.81	108.40
4	b	474	CYS	N-CA-C	-5.41	105.04	111.69
8	f	162	LEU	N-CA-C	-5.41	105.74	112.93
9	g	226	GLY	N-CA-C	-5.41	107.89	114.92
9	g	1059	GLN	N-CA-CB	5.41	118.16	110.16
3	l	413	SER	CA-C-N	5.41	127.84	120.54
3	l	413	SER	C-N-CA	5.41	127.84	120.54
3	l	418	GLN	OE1-CD-NE2	5.41	128.01	122.60
5	n	129	ASN	CA-C-N	5.41	127.53	120.28
5	n	129	ASN	C-N-CA	5.41	127.53	120.28
4	b	672	TYR	CA-C-N	5.41	126.60	119.84
4	b	672	TYR	C-N-CA	5.41	126.60	119.84
3	l	693	PHE	CA-C-O	5.41	125.19	118.43
3	l	862	GLN	CA-C-O	-5.41	113.51	119.78
1	X	327	PHE	N-CA-CB	5.41	119.41	110.33
1	X	1429	HIS	CA-C-N	5.41	127.52	120.28
1	X	1429	HIS	C-N-CA	5.41	127.52	120.28
3	a	333	ASP	CA-C-O	-5.41	115.65	121.38
5	n	563	SER	O-C-N	5.41	130.19	123.32
8	q	180	PHE	N-CA-C	-5.41	105.94	112.54
5	c	183	PHE	CB-CG-CD1	5.40	129.89	120.70
9	g	801	CYS	O-C-N	5.40	130.32	122.43
8	q	617	ILE	O-C-N	-5.40	116.26	122.04
1	X	1193	ASN	N-CA-C	5.40	117.87	111.33
5	c	292	GLU	O-C-N	-5.40	115.90	122.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	103	LYS	O-C-N	5.40	129.27	122.19
9	g	493	PHE	CA-C-N	5.40	131.69	121.97
9	g	493	PHE	C-N-CA	5.40	131.69	121.97
3	l	253	LEU	N-CA-C	-5.40	102.28	110.28
3	l	540	LEU	CB-CA-C	-5.40	104.17	110.17
9	r	697	ASP	CA-C-O	-5.40	113.44	118.73
1	X	164	TYR	N-CA-C	-5.40	99.30	110.80
3	a	734	HIS	CG-CD2-NE2	5.40	112.60	107.20
7	e	99	ASN	OD1-CG-ND2	5.40	128.00	122.60
8	f	652	LEU	CA-C-N	5.40	128.30	120.79
8	f	652	LEU	C-N-CA	5.40	128.30	120.79
9	r	837	ASN	N-CA-C	-5.40	105.31	111.14
1	X	147	SER	N-CA-C	5.40	119.61	113.19
1	X	344	SER	CA-C-N	5.40	127.95	120.29
1	X	344	SER	C-N-CA	5.40	127.95	120.29
5	c	455	GLN	CB-CG-CD	5.40	121.77	112.60
8	f	575	GLU	CA-CB-CG	-5.40	103.31	114.10
9	g	442	LYS	CA-C-N	5.40	131.85	121.54
9	g	442	LYS	C-N-CA	5.40	131.85	121.54
7	p	195	GLN	OE1-CD-NE2	5.40	128.00	122.60
1	X	266	THR	N-CA-CB	5.40	118.02	109.82
1	X	808	THR	CA-C-N	5.40	126.58	119.84
1	X	808	THR	C-N-CA	5.40	126.58	119.84
3	a	1029	ASP	N-CA-C	5.40	117.92	111.71
9	g	677	PHE	N-CA-C	-5.39	106.86	113.50
3	l	562	PHE	CA-CB-CG	5.39	119.19	113.80
7	p	144	ASP	CA-C-O	-5.39	114.69	120.46
9	r	827	THR	N-CA-CB	5.39	119.61	110.49
3	a	667	LEU	CA-C-N	5.39	127.77	120.65
3	a	667	LEU	C-N-CA	5.39	127.77	120.65
3	l	98	PRO	O-C-N	5.39	128.44	122.24
3	l	790	LEU	CA-C-O	-5.39	112.77	120.16
4	m	249	LEU	CA-C-N	5.39	127.77	120.65
4	m	249	LEU	C-N-CA	5.39	127.77	120.65
6	o	260	ALA	CA-C-N	5.39	131.39	121.85
6	o	260	ALA	C-N-CA	5.39	131.39	121.85
8	q	586	GLN	CA-C-N	5.39	127.51	120.28
8	q	586	GLN	C-N-CA	5.39	127.51	120.28
9	r	897	ALA	CA-C-N	5.39	127.51	120.28
9	r	897	ALA	C-N-CA	5.39	127.51	120.28
3	l	915	SER	N-CA-C	-5.39	100.24	108.76
4	m	86	ASP	N-CA-C	-5.39	99.32	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	p	175	PRO	CA-C-O	-5.39	111.80	118.81
4	b	122	ARG	NH1-CZ-NH2	-5.39	112.29	119.30
9	g	841	LYS	N-CA-CB	5.39	121.31	112.63
9	g	938	ASN	N-CA-CB	5.39	119.60	110.49
8	q	686	GLU	CB-CG-CD	-5.39	103.44	112.60
4	b	423	ILE	N-CA-CB	5.39	119.00	112.10
5	c	582	LEU	CA-C-N	5.39	128.47	120.17
5	c	582	LEU	C-N-CA	5.39	128.47	120.17
5	n	247	PRO	N-CA-CB	5.39	109.47	103.44
8	q	509	HIS	CG-CD2-NE2	5.39	112.59	107.20
9	r	246	LYS	N-CA-C	-5.39	105.49	111.36
4	b	136	PHE	CA-C-O	-5.38	114.84	120.55
6	d	224	SER	CA-C-N	5.38	127.79	120.63
6	d	224	SER	C-N-CA	5.38	127.79	120.63
3	l	28	VAL	CA-C-O	-5.38	114.58	120.72
3	l	510	LEU	CA-C-O	5.38	126.13	120.42
8	q	226	GLN	N-CA-C	-5.38	105.35	112.94
9	r	762	THR	O-C-N	-5.38	116.97	123.27
9	r	884	HIS	ND1-CE1-NE2	5.38	113.78	108.40
5	n	132	ILE	CA-C-N	5.38	128.49	120.31
5	n	132	ILE	C-N-CA	5.38	128.49	120.31
8	q	151	GLY	CA-C-N	5.38	128.45	122.15
8	q	151	GLY	C-N-CA	5.38	128.45	122.15
3	a	109	THR	N-CA-CB	5.38	119.54	110.77
9	g	447	VAL	CG1-CB-CG2	5.38	122.64	110.80
3	l	166	LEU	CA-C-N	5.38	131.00	121.80
3	l	166	LEU	C-N-CA	5.38	131.00	121.80
3	l	452	ASP	N-CA-C	-5.38	100.12	110.56
4	m	665	LEU	N-CA-C	-5.38	102.36	110.06
6	o	112	TYR	CB-CA-C	-5.38	98.86	109.67
9	r	900	MET	N-CA-C	5.38	117.22	111.36
3	a	827	GLN	N-CA-C	5.38	117.14	111.28
3	a	1004	ILE	N-CA-C	-5.38	107.50	112.83
6	d	91	GLN	N-CA-CB	5.38	119.58	110.49
1	X	825	ILE	N-CA-C	-5.38	98.73	107.28
8	f	287	HIS	CG-CD2-NE2	5.38	112.58	107.20
9	g	291	ILE	CA-CB-CG2	-5.38	101.36	110.50
9	g	303	HIS	CG-CD2-NE2	5.38	112.58	107.20
9	r	329	GLY	CA-C-N	5.38	131.65	121.81
9	r	329	GLY	C-N-CA	5.38	131.65	121.81
9	r	529	HIS	CA-CB-CG	5.38	119.18	113.80
7	e	180	PRO	CA-C-N	5.38	128.50	120.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	e	180	PRO	C-N-CA	5.38	128.50	120.87
8	f	379	ILE	CA-C-N	5.38	131.20	122.76
8	f	379	ILE	C-N-CA	5.38	131.20	122.76
1	X	296	ASP	CA-CB-CG	-5.37	107.23	112.60
8	f	440	ASP	N-CA-CB	5.37	119.57	110.49
8	f	575	GLU	N-CA-CB	-5.37	101.36	110.50
3	l	92	THR	CA-C-N	-5.37	115.18	122.92
3	l	92	THR	C-N-CA	-5.37	115.18	122.92
6	o	263	SER	CB-CA-C	-5.37	100.00	109.62
8	q	66	LYS	CA-C-O	5.37	126.21	120.24
5	c	487	HIS	CB-CG-ND1	5.37	130.76	122.70
9	g	1020	ARG	NE-CZ-NH1	-5.37	116.13	121.50
5	n	630	THR	N-CA-C	5.37	118.59	110.64
6	o	98	HIS	CE1-NE2-CD2	-5.37	103.63	109.00
1	X	323	TYR	N-CA-CB	5.37	118.75	110.21
9	g	1031	PHE	N-CA-CB	5.37	119.56	110.49
3	a	631	LEU	N-CA-CB	5.37	117.98	109.82
3	a	760	PHE	N-CA-C	-5.37	105.47	112.23
4	b	331	TYR	N-CA-CB	5.37	118.60	110.28
5	c	310	ALA	N-CA-C	-5.37	106.23	112.89
5	n	389	LEU	N-CA-CB	5.37	119.78	110.39
1	X	260	ARG	N-CA-C	5.37	117.13	111.28
1	X	1119	ASN	CA-C-N	5.37	131.79	121.54
1	X	1119	ASN	C-N-CA	5.37	131.79	121.54
3	a	414	ARG	NE-CZ-NH1	5.37	126.87	121.50
3	a	887	ASP	N-CA-C	-5.37	104.30	111.87
4	b	223	TYR	CB-CG-CD2	-5.37	112.75	120.80
8	f	323	THR	N-CA-CB	5.37	119.05	110.46
9	g	511	PRO	N-CA-C	-5.37	101.42	112.47
1	X	983	ASN	CB-CA-C	-5.37	101.13	110.09
1	X	1021	THR	CA-C-N	5.37	127.78	120.54
1	X	1021	THR	C-N-CA	5.37	127.78	120.54
9	g	1038	ASN	CA-C-N	5.37	127.47	120.28
9	g	1038	ASN	C-N-CA	5.37	127.47	120.28
5	n	270	SER	N-CA-CB	5.37	118.01	110.12
5	n	347	GLY	O-C-N	5.37	128.30	122.77
8	f	163	ARG	N-CA-C	5.36	116.81	111.07
9	g	1130	GLU	O-C-N	5.36	127.59	122.07
3	l	957	ASP	CB-CG-OD2	-5.36	106.06	118.40
7	p	79	LYS	CA-CB-CG	5.36	124.83	114.10
3	a	71	HIS	CB-CA-C	-5.36	102.52	110.67
7	p	190	GLN	N-CA-C	-5.36	101.97	109.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	e	190	GLN	OE1-CD-NE2	5.36	127.96	122.60
3	a	599	LYS	CA-C-N	5.36	131.78	121.54
3	a	599	LYS	C-N-CA	5.36	131.78	121.54
9	g	950	ASN	OD1-CG-ND2	-5.36	117.24	122.60
1	X	409	GLU	CA-C-N	5.36	127.77	120.54
1	X	409	GLU	C-N-CA	5.36	127.77	120.54
1	X	1043	LEU	CA-C-N	5.36	128.31	120.71
1	X	1043	LEU	C-N-CA	5.36	128.31	120.71
1	X	1213	THR	CA-C-N	5.36	127.46	120.28
1	X	1213	THR	C-N-CA	5.36	127.46	120.28
3	a	963	LYS	N-CA-C	-5.36	105.43	113.89
8	f	641	SER	CA-C-N	5.36	130.61	121.29
8	f	641	SER	C-N-CA	5.36	130.61	121.29
1	X	1077	ARG	CA-C-O	5.35	125.97	119.38
6	d	121	SER	CB-CA-C	5.35	120.07	110.81
8	f	41	GLU	CA-C-N	5.35	127.40	120.44
8	f	41	GLU	C-N-CA	5.35	127.40	120.44
3	l	110	ILE	CB-CG1-CD1	5.35	125.04	113.80
3	a	657	LEU	CA-C-N	5.35	127.45	120.28
3	a	657	LEU	C-N-CA	5.35	127.45	120.28
4	b	544	ASN	CA-C-O	5.35	126.18	120.24
3	a	529	SER	CB-CA-C	-5.35	101.75	110.85
4	m	199	GLU	N-CA-C	5.35	117.11	111.28
9	r	303	HIS	N-CA-CB	5.35	120.81	111.18
4	b	458	ARG	N-CA-CB	5.35	118.57	110.28
7	e	247	GLU	CA-C-O	-5.35	114.54	121.17
9	g	864	PHE	CA-C-N	5.35	125.61	119.83
9	g	864	PHE	C-N-CA	5.35	125.61	119.83
3	l	397	ILE	CA-C-N	5.35	127.30	120.56
3	l	397	ILE	C-N-CA	5.35	127.30	120.56
3	l	970	LEU	N-CA-C	-5.35	100.46	109.07
4	m	274	LEU	N-CA-C	-5.35	104.34	112.04
5	n	643	ILE	CA-CB-CG1	-5.35	101.31	110.40
1	X	662	THR	CA-C-O	-5.35	112.86	120.51
9	g	73	GLN	O-C-N	-5.35	116.55	122.75
9	g	858	ASN	CA-CB-CG	-5.35	107.25	112.60
9	g	181	ILE	CA-CB-CG2	-5.35	101.41	110.50
4	b	554	GLU	CB-CA-C	-5.34	103.24	111.74
8	f	144	TRP	CB-CG-CD1	-5.34	118.88	126.90
3	l	272	LYS	CA-C-N	5.34	132.10	122.43
3	l	272	LYS	C-N-CA	5.34	132.10	122.43
9	r	1070	LEU	CA-C-O	-5.34	112.84	120.16

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	137	VAL	CA-CB-CG1	-5.34	101.32	110.40
6	d	17	LEU	O-C-N	5.34	128.93	122.68
4	m	589	PRO	O-C-N	5.34	128.38	122.24
7	p	34	LYS	CA-C-N	5.34	128.25	120.98
7	p	34	LYS	C-N-CA	5.34	128.25	120.98
1	X	1064	GLU	CB-CG-CD	5.34	121.68	112.60
8	f	404	VAL	N-CA-C	-5.34	100.72	108.36
9	g	890	GLN	CA-C-O	5.34	125.60	119.35
9	g	1008	MET	CA-C-N	5.34	130.61	122.65
9	g	1008	MET	C-N-CA	5.34	130.61	122.65
5	n	252	ASN	CA-C-O	-5.34	115.12	121.16
9	r	1112	GLU	CA-C-N	5.34	127.78	120.46
9	r	1112	GLU	C-N-CA	5.34	127.78	120.46
1	X	1528	GLN	OE1-CD-NE2	-5.34	117.26	122.60
3	a	679	LEU	N-CA-CB	5.34	118.84	110.46
3	a	774	TYR	CA-C-N	5.34	129.53	120.88
3	a	774	TYR	C-N-CA	5.34	129.53	120.88
3	a	774	TYR	N-CA-C	5.34	117.10	111.28
4	b	344	ARG	N-CA-CB	5.34	119.51	110.49
8	f	422	LEU	N-CA-CB	5.34	118.52	110.30
9	g	207	LYS	CA-C-N	5.34	131.78	122.81
9	g	207	LYS	C-N-CA	5.34	131.78	122.81
8	q	324	VAL	CA-C-N	5.34	127.43	120.28
8	q	324	VAL	C-N-CA	5.34	127.43	120.28
9	r	1134	HIS	ND1-CE1-NE2	5.34	113.74	108.40
3	a	878	HIS	CG-CD2-NE2	5.34	112.54	107.20
3	a	184	LEU	CB-CA-C	-5.34	100.31	109.65
4	b	661	HIS	ND1-CE1-NE2	5.34	113.74	108.40
6	o	216	VAL	CA-C-N	5.34	131.12	122.53
6	o	216	VAL	C-N-CA	5.34	131.12	122.53
4	b	738	LYS	O-C-N	-5.33	115.59	122.21
4	m	722	SER	N-CA-C	-5.33	104.70	113.50
9	g	215	GLU	CB-CG-CD	-5.33	103.53	112.60
9	g	604	ILE	N-CA-C	-5.33	100.65	108.54
9	g	708	TRP	CA-C-O	-5.33	114.46	120.43
4	m	609	GLN	CG-CD-OE1	-5.33	110.13	120.80
6	o	88	ARG	NE-CZ-NH2	5.33	124.00	119.20
8	q	342	PRO	N-CA-C	-5.33	107.19	113.86
9	r	448	SER	N-CA-C	-5.33	104.20	111.56
1	X	1563	LEU	N-CA-C	5.33	118.95	112.23
3	a	651	ILE	CA-C-O	-5.33	115.20	120.85
5	c	237	SER	N-CA-CB	5.33	118.43	110.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	252	ASN	N-CA-C	-5.33	100.62	108.99
9	g	748	ILE	N-CA-C	-5.33	107.55	112.83
3	l	620	HIS	CG-CD2-NE2	5.33	112.53	107.20
3	l	642	LEU	CA-C-N	5.33	131.72	121.54
3	l	642	LEU	C-N-CA	5.33	131.72	121.54
9	r	987	LEU	CA-C-N	5.33	127.77	120.46
9	r	987	LEU	C-N-CA	5.33	127.77	120.46
1	X	1315	VAL	N-CA-CB	-5.33	103.81	110.47
3	l	418	GLN	CA-C-O	5.33	124.82	118.69
5	n	421	ILE	CA-C-N	5.33	127.42	120.28
5	n	421	ILE	C-N-CA	5.33	127.42	120.28
3	a	841	ALA	CA-C-O	-5.33	115.22	120.82
3	a	928	ALA	CB-CA-C	-5.33	99.81	110.42
5	c	317	HIS	N-CA-CB	5.33	119.49	110.49
4	m	637	ARG	NE-CZ-NH2	-5.33	114.41	119.20
9	r	641	VAL	CA-C-N	5.33	126.39	119.78
9	r	641	VAL	C-N-CA	5.33	126.39	119.78
1	X	1523	SER	CA-C-O	5.33	126.20	120.55
3	a	829	SER	O-C-N	5.33	127.77	122.12
4	b	435	GLU	CA-C-N	5.33	131.29	121.70
4	b	435	GLU	C-N-CA	5.33	131.29	121.70
6	o	227	GLN	OE1-CD-NE2	5.33	127.93	122.60
7	p	182	LYS	N-CA-C	-5.33	100.34	109.24
9	r	666	LYS	N-CA-C	5.33	117.09	111.28
9	r	983	VAL	O-C-N	5.33	127.04	121.87
1	X	260	ARG	CA-C-N	5.33	128.88	120.47
1	X	260	ARG	C-N-CA	5.33	128.88	120.47
4	m	731	LEU	N-CA-C	-5.33	105.64	111.82
8	q	39	ILE	CA-CB-CG1	5.33	119.45	110.40
8	q	427	GLU	N-CA-C	-5.33	105.43	112.94
9	r	545	TYR	O-C-N	-5.33	116.35	122.95
1	X	647	GLN	N-CA-C	-5.32	106.28	114.16
4	b	140	HIS	O-C-N	5.32	129.62	122.49
4	b	158	PHE	CA-CB-CG	5.32	119.12	113.80
9	g	160	GLU	N-CA-C	-5.32	99.46	110.80
1	X	884	LEU	O-C-N	5.32	129.97	122.41
4	b	636	LEU	N-CA-C	5.32	117.49	108.02
8	f	478	ARG	CA-C-O	5.32	126.45	120.92
5	n	642	LYS	N-CA-C	5.32	117.16	111.36
1	X	941	SER	CA-C-O	-5.32	112.87	120.16
1	X	990	LYS	CA-CB-CG	-5.32	103.46	114.10
8	f	312	GLU	CA-C-N	5.32	130.67	123.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	312	GLU	C-N-CA	5.32	130.67	123.11
8	f	523	TYR	N-CA-C	-5.32	105.76	113.21
9	r	390	ILE	N-CA-C	5.32	116.25	108.53
5	c	195	GLU	N-CA-CB	-5.32	102.76	110.47
3	a	203	SER	N-CA-CB	5.32	119.47	110.49
3	a	338	ARG	NH1-CZ-NH2	-5.32	112.39	119.30
8	f	141	THR	O-C-N	5.32	129.66	122.59
8	f	447	PHE	CA-CB-CG	-5.32	108.48	113.80
9	g	855	LYS	N-CA-CB	5.32	118.85	110.56
3	l	287	LEU	N-CA-CB	5.32	117.79	109.97
1	X	347	THR	CB-CA-C	5.32	119.61	110.79
5	c	273	VAL	CA-C-O	-5.32	115.22	120.85
6	d	127	VAL	N-CA-CB	5.32	117.98	111.60
9	g	82	ASN	O-C-N	-5.32	116.74	123.01
4	m	77	GLN	OE1-CD-NE2	-5.32	117.28	122.60
9	r	407	ALA	N-CA-C	5.32	118.78	112.72
9	r	497	HIS	CE1-NE2-CD2	-5.32	103.68	109.00
9	g	560	ARG	NE-CZ-NH2	-5.31	114.42	119.20
9	g	678	TYR	CA-C-N	5.31	128.39	120.95
9	g	678	TYR	C-N-CA	5.31	128.39	120.95
3	a	317	ASN	OD1-CG-ND2	-5.31	117.29	122.60
4	b	694	VAL	CA-C-O	5.31	123.60	119.46
5	c	531	LYS	N-CA-C	-5.31	102.26	109.54
6	d	190	ASP	N-CA-CB	5.31	118.63	110.61
7	e	17	TYR	N-CA-CB	5.31	119.06	110.51
3	l	230	HIS	CA-C-N	5.31	130.10	122.40
3	l	230	HIS	C-N-CA	5.31	130.10	122.40
8	q	542	ARG	CA-CB-CG	5.31	124.73	114.10
9	r	864	PHE	CB-CG-CD1	-5.31	111.67	120.70
1	X	1292	GLU	CB-CG-CD	-5.31	103.57	112.60
9	g	1038	ASN	OD1-CG-ND2	5.31	127.91	122.60
4	m	216	ASP	O-C-N	-5.31	116.40	122.93
3	a	686	PHE	CA-C-N	5.31	131.68	121.54
3	a	686	PHE	C-N-CA	5.31	131.68	121.54
8	f	117	TYR	CA-C-O	5.31	126.18	120.55
3	l	814	THR	CA-C-N	-5.31	114.32	122.60
3	l	814	THR	C-N-CA	-5.31	114.32	122.60
3	a	544	MET	O-C-N	5.31	129.95	123.10
9	g	461	ASP	N-CA-C	-5.31	99.30	108.69
4	m	434	PHE	N-CA-C	-5.31	99.61	108.32
9	r	540	HIS	CB-CG-ND1	-5.31	114.74	122.70
9	r	848	PHE	CA-C-N	5.31	129.58	120.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	848	PHE	C-N-CA	5.31	129.58	120.72
8	q	213	CYS	CA-C-O	5.31	125.20	119.15
1	X	180	LYS	N-CA-C	5.30	118.85	112.38
3	a	885	VAL	N-CA-C	-5.30	98.31	109.34
4	b	457	TYR	CG-CD1-CE1	5.30	129.16	121.20
5	c	378	GLU	CA-C-N	5.30	131.24	121.85
5	c	378	GLU	C-N-CA	5.30	131.24	121.85
3	l	375	ASN	N-CA-C	-5.30	99.68	108.75
4	m	640	GLU	CA-CB-CG	5.30	124.71	114.10
9	g	874	PHE	CB-CG-CD2	-5.30	111.69	120.70
4	m	109	SER	CA-C-O	5.30	126.13	120.24
8	q	64	SER	N-CA-C	-5.30	105.39	111.07
1	X	319	PRO	N-CA-CB	-5.30	97.69	103.25
3	a	408	PHE	O-C-N	-5.30	115.54	122.59
8	f	538	LEU	CA-C-O	5.30	125.73	120.32
8	f	632	LYS	CA-C-N	5.30	131.66	121.54
8	f	632	LYS	C-N-CA	5.30	131.66	121.54
9	g	339	LEU	N-CA-CB	5.30	118.30	110.56
9	g	948	GLN	CB-CA-C	-5.30	101.84	110.85
7	p	236	LYS	CA-CB-CG	5.30	124.70	114.10
4	m	678	ASP	CA-CB-CG	5.30	117.90	112.60
8	q	140	PRO	CA-C-O	-5.30	115.56	121.23
9	r	261	PHE	CB-CA-C	-5.30	99.67	109.37
9	r	491	VAL	CA-C-N	5.30	131.64	122.05
9	r	491	VAL	C-N-CA	5.30	131.64	122.05
1	X	216	TYR	CB-CG-CD2	5.30	128.74	120.80
4	b	149	GLU	CA-C-N	5.30	127.38	120.28
4	b	149	GLU	C-N-CA	5.30	127.38	120.28
4	b	565	TYR	N-CA-C	-5.30	105.67	113.61
8	f	289	HIS	CE1-NE2-CD2	-5.30	103.70	109.00
8	f	346	LEU	CA-C-N	5.30	127.38	120.28
8	f	346	LEU	C-N-CA	5.30	127.38	120.28
3	l	337	THR	CA-C-N	5.30	128.73	120.68
3	l	337	THR	C-N-CA	5.30	128.73	120.68
3	a	751	ARG	NH1-CZ-NH2	5.29	126.18	119.30
5	c	142	ARG	NE-CZ-NH2	5.29	123.97	119.20
5	c	498	ASN	CA-CB-CG	-5.29	107.31	112.60
8	f	443	GLU	N-CA-CB	5.29	118.32	110.49
3	l	766	SER	CA-C-O	-5.29	114.81	120.42
4	m	583	GLY	N-CA-C	-5.29	105.92	113.86
5	n	381	TRP	CA-C-N	5.29	129.68	120.68
5	n	381	TRP	C-N-CA	5.29	129.68	120.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	l	505	GLU	CB-CG-CD	-5.29	103.60	112.60
4	m	300	SER	CA-C-N	5.29	132.55	122.60
4	m	300	SER	C-N-CA	5.29	132.55	122.60
7	p	172	SER	CA-C-O	-5.29	115.61	121.33
4	b	686	ASP	CB-CA-C	5.29	120.24	112.09
9	g	80	PHE	CA-CB-CG	5.29	119.09	113.80
9	g	1086	ASP	N-CA-CB	5.29	119.31	110.85
8	q	510	LEU	CA-C-N	5.29	127.22	120.56
8	q	510	LEU	C-N-CA	5.29	127.22	120.56
9	r	1084	LEU	N-CA-C	5.29	117.04	111.28
5	c	279	GLU	O-C-N	5.29	129.41	122.33
9	g	643	PRO	O-C-N	5.29	129.04	122.22
1	X	322	HIS	CB-CG-CD2	-5.29	124.33	131.20
3	a	800	GLU	O-C-N	5.29	129.34	123.05
4	b	190	PHE	N-CA-C	-5.29	105.10	112.45
8	f	48	GLN	N-CA-C	5.29	118.89	112.23
9	g	696	LEU	N-CA-CB	5.29	117.64	109.98
9	g	1006	TYR	CB-CA-C	5.28	119.04	110.22
9	r	906	ILE	N-CA-C	5.28	116.01	110.62
1	X	1510	PHE	N-CA-CB	5.28	119.94	111.91
3	a	958	TRP	N-CA-CB	5.28	119.04	110.17
3	a	992	ASP	CA-C-N	5.28	131.48	121.97
3	a	992	ASP	C-N-CA	5.28	131.48	121.97
4	b	494	THR	CA-CB-OG1	5.28	117.52	109.60
5	c	183	PHE	CB-CG-CD2	-5.28	111.72	120.70
7	e	163	ASN	OD1-CG-ND2	5.28	127.88	122.60
9	g	832	TYR	CA-C-N	5.28	131.63	121.54
9	g	832	TYR	C-N-CA	5.28	131.63	121.54
9	r	636	ILE	O-C-N	5.28	128.67	122.81
9	r	1059	GLN	CB-CA-C	-5.28	101.87	110.85
6	o	138	PRO	O-C-N	-5.28	117.19	123.10
9	r	891	ILE	O-C-N	5.28	127.38	121.94
1	X	973	THR	N-CA-CB	5.28	119.41	110.49
5	c	383	CYS	CA-C-N	5.28	127.78	120.29
5	c	383	CYS	C-N-CA	5.28	127.78	120.29
5	n	542	GLN	CB-CG-CD	-5.28	103.63	112.60
1	X	724	SER	O-C-N	-5.28	117.57	123.48
3	a	433	ILE	N-CA-C	5.28	116.78	109.29
3	a	443	LEU	O-C-N	-5.28	116.64	122.07
3	a	990	ASP	CA-CB-CG	5.28	117.88	112.60
3	a	1018	ILE	N-CA-C	-5.28	105.17	112.50
5	c	604	ASP	CA-CB-CG	5.28	117.88	112.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
7	e	241	ARG	NE-CZ-NH2	-5.28	114.45	119.20
9	g	1146	TYR	N-CA-CB	5.28	117.71	109.85
4	b	288	SER	CA-C-N	5.27	127.97	120.53
4	b	288	SER	C-N-CA	5.27	127.97	120.53
9	g	951	LEU	N-CA-C	-5.27	105.70	111.82
4	m	603	ASP	N-CA-CB	5.27	119.93	111.91
4	b	494	THR	N-CA-C	-5.27	105.12	112.03
4	m	262	ILE	CA-C-O	-5.27	114.56	120.25
7	p	178	PHE	N-CA-C	-5.27	106.43	112.92
9	r	437	TYR	N-CA-C	-5.27	104.14	111.52
9	r	523	ASP	CA-C-N	5.27	128.32	120.31
9	r	523	ASP	C-N-CA	5.27	128.32	120.31
3	a	555	LYS	O-C-N	5.27	129.08	122.23
4	b	293	LYS	N-CA-C	5.27	117.77	111.71
4	b	628	ALA	N-CA-CB	5.27	118.24	110.33
9	r	612	ASP	N-CA-C	-5.27	106.71	112.72
1	X	617	TYR	CA-C-N	5.27	127.61	120.65
1	X	617	TYR	C-N-CA	5.27	127.61	120.65
3	a	932	ASN	CA-C-N	5.27	132.24	122.70
3	a	932	ASN	C-N-CA	5.27	132.24	122.70
5	c	297	TYR	CB-CG-CD1	5.27	128.71	120.80
8	f	651	ILE	N-CA-C	-5.27	107.22	111.91
9	r	930	SER	N-CA-C	-5.27	107.39	112.97
9	r	1046	VAL	O-C-N	-5.27	116.76	121.87
1	X	140	LYS	N-CA-CB	5.27	118.33	110.22
3	l	338	ARG	CA-C-N	5.27	125.20	119.78
3	l	338	ARG	C-N-CA	5.27	125.20	119.78
1	X	281	GLN	N-CA-CB	5.27	118.84	111.15
5	c	609	LYS	N-CA-CB	5.27	119.39	110.49
4	m	556	ILE	CA-C-N	5.27	129.56	121.19
4	m	556	ILE	C-N-CA	5.27	129.56	121.19
4	m	567	LEU	N-CA-C	-5.27	106.53	113.17
9	r	1122	THR	CA-CB-OG1	5.27	117.50	109.60
1	X	1641	SER	CA-C-O	-5.26	115.29	120.82
3	a	179	GLU	CB-CA-C	-5.26	100.49	109.65
9	g	173	ILE	N-CA-CB	5.26	118.53	111.90
3	l	660	LYS	CA-C-N	5.26	128.11	120.79
3	l	660	LYS	C-N-CA	5.26	128.11	120.79
4	m	551	ASN	N-CA-C	-5.26	102.26	110.42
9	r	584	LYS	N-CA-C	5.26	118.52	110.20
9	r	610	LEU	CA-C-O	5.26	125.69	119.48
3	l	547	VAL	CB-CA-C	-5.26	104.96	112.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	q	642	ASN	OD1-CG-ND2	5.26	127.86	122.60
9	r	598	ILE	CB-CA-C	5.26	119.48	112.22
5	c	333	ARG	CA-C-O	5.26	126.53	120.90
5	c	625	LEU	N-CA-C	-5.26	106.54	113.17
8	f	621	GLN	CA-C-N	5.26	126.90	120.22
8	f	621	GLN	C-N-CA	5.26	126.90	120.22
9	g	542	ASN	N-CA-C	-5.26	106.54	113.17
3	l	369	ASN	OD1-CG-ND2	-5.26	117.34	122.60
7	p	325	ASP	CA-CB-CG	5.26	117.86	112.60
1	X	1546	SER	CA-C-N	5.26	127.76	120.29
1	X	1546	SER	C-N-CA	5.26	127.76	120.29
4	b	316	ALA	N-CA-C	-5.26	105.99	112.72
4	b	408	VAL	N-CA-C	-5.26	105.66	113.39
9	g	941	ILE	CA-C-O	5.26	123.96	118.96
3	l	104	GLN	N-CA-C	5.26	117.01	111.28
4	m	545	GLN	OE1-CD-NE2	5.26	127.86	122.60
8	q	690	PHE	CA-CB-CG	-5.26	108.54	113.80
9	r	813	GLY	CA-C-N	5.26	131.52	123.47
9	r	813	GLY	C-N-CA	5.26	131.52	123.47
3	a	888	VAL	N-CA-C	-5.26	106.31	111.88
3	a	1028	THR	N-CA-CB	5.26	119.12	110.39
4	b	427	LYS	CA-C-O	5.26	125.50	119.35
5	n	424	LEU	N-CA-CB	-5.26	102.88	110.56
9	r	1012	GLU	N-CA-C	-5.26	99.60	110.80
4	b	114	ILE	CA-C-N	5.26	127.85	120.28
4	b	114	ILE	C-N-CA	5.26	127.85	120.28
6	d	8	HIS	CA-CB-CG	-5.26	108.54	113.80
8	f	540	ASN	CA-C-N	5.26	131.71	121.41
8	f	540	ASN	C-N-CA	5.26	131.71	121.41
9	g	455	ILE	N-CA-CB	5.26	118.52	111.90
5	n	215	LEU	N-CA-CB	5.26	119.37	110.49
6	o	274	GLY	CA-C-O	5.26	123.82	119.04
8	q	652	LEU	CA-C-N	5.26	127.76	120.29
8	q	652	LEU	C-N-CA	5.26	127.76	120.29
1	X	1387	LEU	O-C-N	-5.25	115.21	122.46
7	e	10	ASP	CA-CB-CG	-5.25	107.35	112.60
8	f	640	SER	N-CA-C	-5.25	104.61	112.54
3	l	728	ILE	O-C-N	-5.25	116.00	122.57
4	m	186	ARG	NE-CZ-NH2	-5.25	114.47	119.20
5	n	341	GLN	CA-C-N	5.25	127.75	120.29
5	n	341	GLN	C-N-CA	5.25	127.75	120.29
1	X	902	GLU	CA-C-O	-5.25	115.29	121.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	900	VAL	N-CA-C	-5.25	105.20	112.50
6	d	112	TYR	N-CA-C	-5.25	101.43	109.41
9	g	1096	SER	N-CA-C	-5.25	106.71	113.01
3	l	97	LEU	N-CA-C	-5.25	102.51	110.39
3	l	330	SER	N-CA-C	-5.25	99.85	108.41
3	l	458	ASN	CA-CB-CG	-5.25	107.35	112.60
3	l	529	SER	N-CA-C	5.25	116.69	111.07
8	q	543	VAL	CA-C-O	-5.25	114.80	120.47
3	a	97	LEU	CA-C-O	-5.25	114.76	120.69
4	b	198	GLU	CA-C-N	5.25	131.56	121.54
4	b	198	GLU	C-N-CA	5.25	131.56	121.54
4	b	624	LEU	CA-C-O	-5.25	112.99	119.18
9	r	529	HIS	O-C-N	5.25	128.13	122.15
9	r	727	PHE	CA-C-O	5.25	126.00	119.97
1	X	827	PRO	N-CA-CB	5.25	108.76	103.25
3	a	810	ASP	CB-CA-C	-5.25	102.61	112.00
3	a	861	LEU	CA-C-N	5.25	132.79	122.61
3	a	861	LEU	C-N-CA	5.25	132.79	122.61
5	c	285	ARG	CG-CD-NE	-5.25	100.46	112.00
5	c	653	GLU	N-CA-C	-5.25	106.93	113.38
5	n	233	LEU	N-CA-CB	5.25	117.68	110.07
1	X	419	ASP	CA-C-N	5.25	127.31	120.28
1	X	419	ASP	C-N-CA	5.25	127.31	120.28
3	l	611	THR	O-C-N	-5.25	115.13	122.37
3	a	154	ASN	N-CA-CB	5.24	118.95	110.88
5	c	256	LYS	O-C-N	-5.24	116.56	122.12
7	e	327	LYS	CA-C-N	5.24	128.90	121.66
7	e	327	LYS	C-N-CA	5.24	128.90	121.66
9	g	584	LYS	CB-CG-CD	5.24	123.36	111.30
4	m	484	VAL	CA-CB-CG2	-5.24	101.48	110.40
9	r	303	HIS	CB-CA-C	-5.24	100.35	109.32
5	c	393	GLN	OE1-CD-NE2	5.24	127.84	122.60
7	e	62	ASP	CA-CB-CG	-5.24	107.36	112.60
9	g	1007	SER	N-CA-CB	5.24	119.35	110.49
3	a	542	ASP	CB-CA-C	-5.24	102.51	111.31
8	f	446	SER	O-C-N	-5.24	114.63	122.39
4	m	51	MET	CG-SD-CE	-5.24	89.37	100.90
5	n	584	ASN	CB-CG-ND2	-5.24	108.54	116.40
7	p	23	HIS	CE1-NE2-CD2	-5.24	103.76	109.00
7	p	186	SER	O-C-N	5.24	129.16	123.13
8	q	285	ASP	CA-C-N	5.24	127.73	120.29
8	q	285	ASP	C-N-CA	5.24	127.73	120.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	556	HIS	CE1-NE2-CD2	-5.24	103.76	109.00
3	a	321	THR	CA-CB-OG1	-5.24	101.74	109.60
8	f	246	THR	N-CA-CB	-5.24	102.23	110.30
8	f	350	VAL	CA-C-O	-5.24	115.10	120.71
4	m	550	HIS	ND1-CE1-NE2	5.24	113.64	108.40
3	a	520	LEU	O-C-N	5.24	128.76	122.79
4	b	647	ARG	CB-CA-C	-5.24	99.67	109.72
3	l	488	THR	CA-C-N	5.24	129.58	120.68
3	l	488	THR	C-N-CA	5.24	129.58	120.68
4	m	93	VAL	O-C-N	-5.24	117.41	123.07
4	m	256	GLY	CA-C-O	5.24	124.82	119.01
4	b	313	LEU	N-CA-C	-5.24	106.74	113.23
3	l	64	ASN	O-C-N	5.24	128.58	122.24
4	m	591	LEU	CA-C-N	5.23	129.80	122.79
4	m	591	LEU	C-N-CA	5.23	129.80	122.79
9	r	567	PHE	N-CA-CB	5.23	118.61	110.44
3	a	672	LYS	CA-C-N	5.23	127.29	120.28
3	a	672	LYS	C-N-CA	5.23	127.29	120.28
4	b	410	GLU	N-CA-CB	5.23	119.20	110.41
4	m	133	ASN	CA-CB-CG	5.23	117.83	112.60
4	m	559	PHE	CA-CB-CG	5.23	119.03	113.80
5	n	553	LEU	O-C-N	-5.23	116.68	122.07
8	q	235	GLN	N-CA-C	-5.23	101.34	109.24
1	X	717	VAL	N-CA-CB	5.23	120.24	110.77
1	X	1405	ASN	CA-C-N	5.23	127.62	120.77
1	X	1405	ASN	C-N-CA	5.23	127.62	120.77
3	a	606	LYS	N-CA-CB	5.23	119.33	110.49
5	c	614	ILE	N-CA-CB	-5.23	106.11	112.33
8	f	438	GLU	N-CA-C	-5.23	106.29	113.30
5	n	515	ILE	N-CA-CB	-5.23	105.66	111.41
9	r	938	ASN	CA-C-O	-5.23	114.68	120.33
4	b	222	GLU	CA-C-O	-5.23	112.95	119.28
8	f	120	TRP	N-CA-C	5.23	117.06	111.36
4	m	518	ASP	CA-CB-CG	5.23	117.83	112.60
9	g	123	PRO	CA-C-N	5.23	130.78	122.94
9	g	123	PRO	C-N-CA	5.23	130.78	122.94
1	X	818	ASN	O-C-N	5.22	128.47	122.25
3	a	762	MET	CA-C-O	-5.22	112.42	119.11
4	b	744	MET	CG-SD-CE	-5.22	89.41	100.90
9	g	325	PRO	O-C-N	5.22	128.93	123.03
3	a	185	GLY	CA-C-N	-5.22	115.43	122.95
3	a	185	GLY	C-N-CA	-5.22	115.43	122.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	641	ASP	CA-CB-CG	-5.22	107.38	112.60
5	c	253	ASP	N-CA-C	-5.22	106.14	112.88
5	c	263	GLU	CA-C-O	-5.22	115.32	120.70
9	g	96	TYR	N-CA-CB	5.22	121.24	111.53
9	g	897	ALA	CA-C-N	5.22	127.28	120.28
9	g	897	ALA	C-N-CA	5.22	127.28	120.28
5	n	409	LYS	N-CA-C	5.22	116.78	111.14
6	o	95	HIS	N-CA-C	-5.22	99.27	108.20
8	q	391	HIS	CA-C-N	5.22	129.56	120.68
8	q	391	HIS	C-N-CA	5.22	129.56	120.68
3	a	240	ASN	CB-CA-C	-5.22	101.08	110.37
9	g	306	LYS	N-CA-CB	5.22	117.71	109.83
9	g	691	TYR	CA-C-N	5.22	129.55	121.83
9	g	691	TYR	C-N-CA	5.22	129.55	121.83
3	l	574	LEU	O-C-N	5.22	127.45	122.07
4	m	664	VAL	CA-CB-CG1	5.22	119.27	110.40
8	q	46	ALA	CA-C-N	5.22	125.77	119.98
8	q	46	ALA	C-N-CA	5.22	125.77	119.98
8	q	256	LEU	CA-C-N	5.22	129.38	121.03
8	q	256	LEU	C-N-CA	5.22	129.38	121.03
9	r	1129	LEU	CA-C-N	5.22	128.04	120.79
9	r	1129	LEU	C-N-CA	5.22	128.04	120.79
4	b	703	ASP	CA-C-O	-5.22	115.82	121.87
9	g	776	ASN	CA-C-N	5.22	128.91	120.82
9	g	776	ASN	C-N-CA	5.22	128.91	120.82
3	l	364	GLN	CA-C-N	5.22	129.10	121.80
3	l	364	GLN	C-N-CA	5.22	129.10	121.80
7	p	28	SER	CA-C-O	5.22	127.98	121.46
8	q	324	VAL	CA-CB-CG2	-5.22	101.53	110.40
1	X	830	THR	O-C-N	-5.21	117.17	123.27
3	a	334	LEU	N-CA-C	-5.21	99.77	108.32
3	a	693	PHE	O-C-N	-5.21	116.17	122.48
6	o	196	LEU	CA-C-O	-5.21	115.35	120.98
8	q	553	ASN	OD1-CG-ND2	5.21	127.81	122.60
8	f	655	ILE	CA-C-N	5.21	127.58	120.54
8	f	655	ILE	C-N-CA	5.21	127.58	120.54
1	X	1012	VAL	CA-C-N	5.21	129.54	120.68
1	X	1012	VAL	C-N-CA	5.21	129.54	120.68
3	a	370	ASP	O-C-N	-5.21	115.66	122.59
3	a	875	LEU	CB-CA-C	-5.21	102.34	110.94
4	b	511	TYR	CA-C-O	-5.21	113.79	118.79
9	g	517	PRO	CA-C-O	-5.21	113.00	120.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	652	HIS	CE1-NE2-CD2	-5.21	103.79	109.00
3	l	958	TRP	N-CA-CB	5.21	119.30	110.49
1	X	910	ALA	O-C-N	-5.21	115.67	120.51
1	X	961	GLU	O-C-N	-5.21	116.05	122.25
1	X	1123	HIS	ND1-CE1-NE2	5.21	113.61	108.40
4	b	328	LEU	CA-C-N	5.21	128.93	120.60
4	b	328	LEU	C-N-CA	5.21	128.93	120.60
5	c	557	GLN	N-CA-CB	5.21	117.78	110.12
9	g	504	PHE	O-C-N	-5.21	116.46	122.09
9	g	785	HIS	CA-CB-CG	5.21	119.01	113.80
3	l	25	ASP	N-CA-C	-5.21	101.38	109.24
4	m	111	LEU	N-CA-C	5.21	116.96	111.28
5	n	320	VAL	N-CA-CB	5.21	117.62	110.54
7	p	8	HIS	CB-CG-CD2	-5.21	124.43	131.20
4	b	219	PRO	N-CA-CB	5.21	108.33	102.60
4	b	639	ARG	N-CA-C	-5.21	106.77	113.23
8	f	225	THR	CA-C-O	5.21	124.87	119.14
9	g	1092	PRO	N-CA-CB	-5.21	98.62	103.46
9	r	103	LYS	N-CA-C	5.21	118.66	112.72
1	X	1019	THR	N-CA-CB	5.21	118.23	110.22
5	c	413	PRO	N-CA-CB	5.21	108.72	103.25
3	l	546	THR	N-CA-C	-5.21	106.93	113.28
3	l	634	LEU	N-CA-C	5.21	118.89	112.54
1	X	198	MET	CB-CA-C	-5.20	101.92	110.72
3	a	71	HIS	N-CA-CB	5.20	118.13	109.60
3	a	112	GLU	CB-CA-C	5.20	118.22	109.48
4	b	523	LEU	CA-C-O	5.20	124.77	119.05
4	b	611	ILE	CB-CA-C	-5.20	105.22	112.04
9	g	374	SER	N-CA-C	-5.20	99.72	110.80
9	g	805	ALA	CA-C-O	-5.20	115.33	120.90
4	m	183	ASN	N-CA-C	-5.20	106.61	113.12
7	p	167	SER	N-CA-C	-5.20	100.69	109.07
8	q	621	GLN	O-C-N	5.20	128.08	122.15
9	r	941	ILE	CA-C-N	5.20	127.25	120.28
9	r	941	ILE	C-N-CA	5.20	127.25	120.28
1	X	967	LEU	N-CA-C	-5.20	106.62	113.17
7	e	8	HIS	CG-CD2-NE2	5.20	112.40	107.20
8	f	626	ASP	CA-C-N	5.20	131.48	121.54
8	f	626	ASP	C-N-CA	5.20	131.48	121.54
3	l	432	ILE	N-CA-C	-5.20	107.64	112.43
8	q	552	ARG	CG-CD-NE	-5.20	100.56	112.00
3	a	92	THR	N-CA-C	-5.20	99.93	108.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
3	a	618	SER	CA-C-N	5.20	127.52	120.65
3	a	618	SER	C-N-CA	5.20	127.52	120.65
3	a	741	LEU	N-CA-C	-5.20	106.71	113.16
4	b	667	VAL	O-C-N	5.20	126.77	122.09
9	g	115	LYS	N-CA-CB	5.20	118.50	110.60
9	g	588	ILE	O-C-N	5.20	128.86	122.05
9	g	981	ARG	NH1-CZ-NH2	5.20	126.06	119.30
9	g	1001	ASP	O-C-N	-5.20	115.87	122.27
3	l	954	ARG	CA-C-N	5.20	130.87	122.29
3	l	954	ARG	C-N-CA	5.20	130.87	122.29
4	m	304	ARG	CA-C-N	5.20	127.67	120.29
4	m	304	ARG	C-N-CA	5.20	127.67	120.29
8	q	391	HIS	N-CA-C	5.20	116.95	111.28
9	r	710	ILE	CA-C-N	5.20	129.78	122.09
9	r	710	ILE	C-N-CA	5.20	129.78	122.09
1	X	336	GLN	OE1-CD-NE2	5.20	127.80	122.60
4	b	715	GLU	CB-CA-C	-5.20	101.41	110.09
9	g	366	ILE	N-CA-CB	5.20	117.91	111.41
5	n	370	PHE	CA-CB-CG	5.20	119.00	113.80
5	n	432	GLU	CA-C-N	5.20	127.20	120.44
5	n	432	GLU	C-N-CA	5.20	127.20	120.44
3	a	121	VAL	CA-CB-CG2	5.20	119.23	110.40
8	f	408	ASP	O-C-N	5.20	127.63	122.12
3	a	279	TYR	N-CA-CB	5.20	119.32	111.06
9	g	156	ASN	OD1-CG-ND2	5.20	127.80	122.60
3	l	780	HIS	CA-C-O	-5.20	115.72	121.33
5	n	268	LEU	N-CA-CB	5.20	117.94	110.20
5	n	518	LEU	O-C-N	-5.20	116.11	122.34
7	p	318	ILE	N-CA-C	5.20	115.83	107.73
1	X	288	LEU	CA-C-N	5.19	131.46	121.54
1	X	288	LEU	C-N-CA	5.19	131.46	121.54
9	g	712	PHE	N-CA-CB	-5.19	101.11	110.88
3	l	93	ILE	CA-C-O	-5.19	116.37	121.67
5	n	440	GLN	N-CA-C	-5.19	106.45	112.89
1	X	1007	SER	CA-C-N	5.19	126.58	120.09
1	X	1007	SER	C-N-CA	5.19	126.58	120.09
3	a	153	GLN	N-CA-CB	5.19	121.18	111.52
4	b	324	ILE	CA-C-N	5.19	128.59	120.75
4	b	324	ILE	C-N-CA	5.19	128.59	120.75
5	c	348	CYS	N-CA-CB	5.19	119.27	110.49
7	e	78	ASP	N-CA-C	-5.19	106.25	112.59
9	g	247	LEU	N-CA-CB	5.19	119.26	110.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	1066	PHE	N-CA-C	-5.19	107.49	113.88
4	m	98	LEU	N-CA-C	-5.19	99.74	110.80
9	r	1052	ASN	CA-C-N	5.19	129.09	120.94
9	r	1052	ASN	C-N-CA	5.19	129.09	120.94
1	X	290	MET	CB-CA-C	-5.19	100.09	110.42
3	a	751	ARG	N-CA-C	5.19	121.86	110.80
6	d	11	LEU	CA-C-N	5.19	127.45	120.50
6	d	11	LEU	C-N-CA	5.19	127.45	120.50
7	e	23	HIS	CB-CG-CD2	-5.19	124.45	131.20
9	g	757	LYS	N-CA-CB	5.19	118.21	110.22
9	g	874	PHE	CA-C-N	5.19	127.66	120.29
9	g	874	PHE	C-N-CA	5.19	127.66	120.29
5	n	608	ASP	CA-C-N	5.19	131.45	121.54
5	n	608	ASP	C-N-CA	5.19	131.45	121.54
7	p	67	GLU	CB-CA-C	-5.19	102.17	110.79
1	X	1222	LEU	O-C-N	-5.19	115.85	122.34
3	a	151	HIS	CG-CD2-NE2	5.19	112.39	107.20
3	a	1000	TYR	CA-C-N	5.19	127.23	120.28
3	a	1000	TYR	C-N-CA	5.19	127.23	120.28
3	l	659	TYR	N-CA-CB	-5.19	102.47	110.20
8	q	70	LEU	N-CA-C	5.19	116.94	111.28
3	a	600	ASP	CA-CB-CG	5.19	117.79	112.60
3	a	787	ASN	CA-CB-CG	5.19	117.79	112.60
9	g	619	SER	N-CA-C	5.19	116.94	111.28
1	X	671	LEU	N-CA-C	-5.18	108.22	114.75
3	a	841	ALA	CB-CA-C	-5.18	102.74	110.88
5	n	487	HIS	CG-CD2-NE2	5.18	112.38	107.20
6	d	227	GLN	OE1-CD-NE2	-5.18	117.42	122.60
9	g	403	GLN	CB-CA-C	-5.18	104.68	112.09
3	l	925	LEU	N-CA-CB	5.18	119.77	110.80
9	r	679	ASP	N-CA-C	-5.18	99.32	108.23
3	a	878	HIS	ND1-CE1-NE2	5.18	113.58	108.40
3	l	143	ASN	CA-C-N	5.18	128.83	121.42
3	l	143	ASN	C-N-CA	5.18	128.83	121.42
5	n	179	LEU	N-CA-C	-5.18	99.77	110.80
8	q	620	LEU	CA-C-N	5.18	127.65	120.29
8	q	620	LEU	C-N-CA	5.18	127.65	120.29
9	r	1010	ASP	N-CA-CB	5.18	118.87	110.17
1	X	1215	VAL	N-CA-C	5.18	115.95	110.72
3	a	314	THR	CA-C-N	5.18	131.12	122.73
3	a	314	THR	C-N-CA	5.18	131.12	122.73
8	f	432	TYR	N-CA-C	-5.18	97.42	107.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	227	THR	N-CA-C	-5.18	99.52	108.69
3	l	386	LEU	O-C-N	-5.18	116.63	122.12
1	X	1531	SER	N-CA-C	5.18	116.92	111.28
4	b	338	VAL	CA-C-N	5.18	127.04	120.72
4	b	338	VAL	C-N-CA	5.18	127.04	120.72
5	c	266	CYS	N-CA-CB	5.18	118.27	110.30
5	n	303	VAL	CA-C-O	5.18	125.41	120.80
8	q	257	ASP	O-C-N	-5.18	116.11	121.60
4	b	604	ASP	N-CA-C	-5.17	106.28	112.59
4	b	696	GLU	O-C-N	5.17	127.40	122.07
7	e	67	GLU	CB-CG-CD	-5.17	103.80	112.60
8	f	443	GLU	N-CA-C	-5.17	106.65	113.17
9	g	177	ASP	N-CA-CB	5.17	119.95	111.31
4	m	82	ILE	N-CA-C	-5.17	100.88	108.85
9	r	789	ASN	N-CA-C	5.17	117.82	111.82
4	b	260	GLN	CA-C-N	5.17	130.44	122.42
4	b	260	GLN	C-N-CA	5.17	130.44	122.42
6	d	154	ALA	CB-CA-C	-5.17	104.43	110.17
3	a	526	ARG	CA-CB-CG	5.17	124.44	114.10
5	c	147	SER	CA-CB-OG	5.17	121.44	111.10
6	d	74	SER	O-C-N	-5.17	117.46	122.99
8	f	670	LYS	CA-C-N	5.17	127.63	120.29
8	f	670	LYS	C-N-CA	5.17	127.63	120.29
9	g	334	TRP	O-C-N	-5.17	117.27	123.06
1	X	179	LEU	N-CA-C	5.17	116.60	111.07
5	c	232	ASN	OD1-CG-ND2	5.17	127.77	122.60
6	d	16	VAL	CA-C-O	5.17	126.46	120.67
3	l	419	ILE	CB-CA-C	-5.17	105.28	111.85
3	a	508	LYS	CA-C-N	5.17	127.97	120.79
3	a	508	LYS	C-N-CA	5.17	127.97	120.79
7	e	91	GLU	CA-C-N	5.17	131.41	121.54
7	e	91	GLU	C-N-CA	5.17	131.41	121.54
9	g	262	ASN	N-CA-C	-5.17	105.65	112.94
3	l	761	ALA	N-CA-C	5.17	116.91	111.28
5	c	322	ILE	N-CA-C	-5.17	100.21	107.75
6	d	95	HIS	CE1-NE2-CD2	-5.17	103.83	109.00
5	n	197	VAL	N-CA-C	-5.17	101.53	108.35
5	n	351	ASP	N-CA-C	-5.17	102.13	110.14
1	X	1418	LEU	N-CA-CB	5.17	120.32	112.47
3	a	498	HIS	CE1-NE2-CD2	-5.17	103.83	109.00
3	l	708	ASN	N-CA-C	5.17	117.81	111.82
6	o	91	GLN	N-CA-C	5.17	117.66	109.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	890	GLN	O-C-N	-5.17	115.08	122.41
1	X	1004	LEU	N-CA-CB	5.16	118.49	110.80
3	a	11	LEU	CB-CA-C	-5.16	102.00	110.72
4	b	404	SER	N-CA-CB	-5.16	102.58	110.33
8	f	326	GLU	N-CA-C	5.16	118.84	112.54
3	l	1031	ARG	NE-CZ-NH1	-5.16	116.34	121.50
1	X	1565	ASN	CA-C-N	5.16	131.40	121.54
1	X	1565	ASN	C-N-CA	5.16	131.40	121.54
8	f	519	GLU	CA-C-N	5.16	128.34	121.01
8	f	519	GLU	C-N-CA	5.16	128.34	121.01
8	f	527	VAL	N-CA-C	-5.16	105.33	112.50
5	n	195	GLU	N-CA-C	5.16	119.29	112.89
4	b	242	THR	N-CA-C	-5.16	101.85	109.18
3	l	526	ARG	CG-CD-NE	-5.16	100.65	112.00
3	a	1017	TRP	CD2-CE2-CZ2	-5.16	117.24	122.40
4	b	513	PHE	N-CA-C	-5.16	100.68	108.46
5	c	762	LYS	CA-C-N	5.16	130.04	123.03
5	c	762	LYS	C-N-CA	5.16	130.04	123.03
4	m	264	CYS	CA-C-N	5.16	128.77	122.63
4	m	264	CYS	C-N-CA	5.16	128.77	122.63
1	X	1610	LYS	CA-C-N	5.15	127.70	120.28
1	X	1610	LYS	C-N-CA	5.15	127.70	120.28
3	l	752	HIS	ND1-CG-CD2	-5.15	100.95	106.10
4	m	397	ILE	CB-CA-C	-5.15	105.27	112.02
1	X	708	THR	CA-C-O	-5.15	114.28	120.10
9	g	929	LEU	CA-C-N	5.15	127.45	120.44
9	g	929	LEU	C-N-CA	5.15	127.45	120.44
3	l	738	ARG	CB-CG-CD	5.15	123.15	111.30
7	p	68	TYR	CA-CB-CG	-5.15	104.63	113.90
5	c	519	ARG	NE-CZ-NH2	-5.15	114.56	119.20
3	l	60	LEU	N-CA-C	-5.15	101.00	109.40
3	l	1011	ASP	CA-C-N	5.15	131.38	121.54
3	l	1011	ASP	C-N-CA	5.15	131.38	121.54
8	q	350	VAL	N-CA-C	-5.15	105.82	113.39
9	r	510	ASN	CA-CB-CG	5.15	117.75	112.60
9	r	1149	ASN	CA-C-O	-5.15	115.42	121.44
5	n	205	ASN	CA-C-N	5.15	124.76	119.56
5	n	205	ASN	C-N-CA	5.15	124.76	119.56
6	d	43	HIS	ND1-CE1-NE2	5.15	113.55	108.40
6	d	102	VAL	CB-CA-C	5.15	117.29	110.91
6	o	32	THR	N-CA-CB	5.15	120.31	111.00
8	q	685	SER	CB-CA-C	-5.15	100.17	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1449	GLU	CA-C-N	5.15	127.63	120.63
1	X	1449	GLU	C-N-CA	5.15	127.63	120.63
3	a	751	ARG	CG-CD-NE	-5.15	100.68	112.00
4	b	587	ASP	N-CA-C	5.15	121.76	110.80
8	f	682	LYS	N-CA-C	-5.15	101.77	109.95
9	g	133	ALA	CA-C-N	5.15	130.00	122.69
9	g	133	ALA	C-N-CA	5.15	130.00	122.69
9	g	425	VAL	CA-C-N	-5.15	116.57	122.95
9	g	425	VAL	C-N-CA	-5.15	116.57	122.95
3	l	626	HIS	CA-CB-CG	5.15	118.95	113.80
3	l	707	SER	CA-C-N	5.15	128.13	120.31
3	l	707	SER	C-N-CA	5.15	128.13	120.31
1	X	614	ILE	N-CA-C	-5.14	104.55	111.44
1	X	1086	ILE	N-CA-C	-5.14	106.13	111.58
4	b	694	VAL	CA-CB-CG2	5.14	119.15	110.40
3	l	566	ASN	CA-C-N	5.14	127.17	120.28
3	l	566	ASN	C-N-CA	5.14	127.17	120.28
7	p	289	GLN	OE1-CD-NE2	5.14	127.74	122.60
1	X	1074	LEU	O-C-N	-5.14	116.58	122.08
1	X	1444	LEU	CA-C-N	5.14	127.43	120.38
1	X	1444	LEU	C-N-CA	5.14	127.43	120.38
3	a	143	ASN	CA-C-O	-5.14	115.21	121.28
8	f	183	TYR	CA-C-O	-5.14	115.40	120.90
8	f	336	PRO	CA-C-N	5.14	127.59	120.29
8	f	336	PRO	C-N-CA	5.14	127.59	120.29
9	g	579	ILE	N-CA-C	-5.14	100.12	107.78
3	l	532	PHE	N-CA-CB	5.14	118.22	110.30
7	p	131	ASP	CA-C-O	5.14	126.00	120.55
4	m	173	TYR	CA-CB-CG	5.14	123.15	113.90
1	X	831	THR	O-C-N	-5.14	117.30	123.31
5	c	292	GLU	N-CA-CB	5.14	118.14	110.22
7	e	170	CYS	O-C-N	5.14	129.11	123.25
6	o	38	VAL	N-CA-CB	5.14	116.71	110.95
7	p	221	ALA	O-C-N	5.14	125.78	121.31
8	q	146	ASN	CA-C-N	5.14	127.43	120.44
8	q	146	ASN	C-N-CA	5.14	127.43	120.44
8	q	679	LYS	CA-C-O	5.14	125.90	119.78
9	r	1094	TYR	CA-C-N	5.14	127.04	120.56
9	r	1094	TYR	C-N-CA	5.14	127.04	120.56
5	n	632	GLU	N-CA-CB	5.14	119.17	110.49
1	X	956	PHE	CA-C-N	5.14	127.88	120.38
1	X	956	PHE	C-N-CA	5.14	127.88	120.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1338	GLU	CA-C-N	5.14	127.16	120.28
1	X	1338	GLU	C-N-CA	5.14	127.16	120.28
1	X	1462	ASN	N-CA-CB	5.14	117.67	110.12
5	c	306	ALA	CB-CA-C	-5.14	102.12	110.85
9	g	839	PHE	N-CA-C	-5.14	102.17	109.62
9	g	981	ARG	N-CA-C	-5.14	106.70	113.17
3	l	678	VAL	O-C-N	-5.14	116.54	121.83
4	m	155	LEU	N-CA-C	-5.14	106.52	112.89
5	n	281	GLU	CA-C-N	5.14	127.16	120.28
5	n	281	GLU	C-N-CA	5.14	127.16	120.28
5	n	283	LYS	CA-C-N	5.14	127.03	120.56
5	n	283	LYS	C-N-CA	5.14	127.03	120.56
8	q	552	ARG	N-CA-C	-5.14	106.32	112.59
9	r	596	CYS	CA-C-N	5.14	127.12	120.44
9	r	596	CYS	C-N-CA	5.14	127.12	120.44
9	r	828	THR	N-CA-C	5.14	117.78	111.82
9	r	1132	LYS	N-CA-C	5.14	116.57	111.07
3	a	952	ASN	OD1-CG-ND2	5.13	127.73	122.60
6	d	39	GLU	N-CA-C	-5.13	105.70	112.94
8	f	148	ILE	CA-CB-CG2	5.13	119.23	110.50
3	l	73	SER	CA-C-N	5.13	127.41	120.38
3	l	73	SER	C-N-CA	5.13	127.41	120.38
3	l	910	GLN	CA-C-N	5.13	128.12	120.31
3	l	910	GLN	C-N-CA	5.13	128.12	120.31
5	n	576	LEU	CA-C-O	5.13	124.47	119.08
8	q	49	LEU	CA-C-N	5.13	131.35	121.18
8	q	49	LEU	C-N-CA	5.13	131.35	121.18
7	e	134	LEU	N-CA-CB	5.13	118.00	110.35
9	g	1104	ILE	CA-CB-CG2	-5.13	101.77	110.50
3	a	525	LEU	CA-C-N	5.13	127.11	120.44
3	a	525	LEU	C-N-CA	5.13	127.11	120.44
3	a	839	GLU	CA-C-N	5.13	128.11	120.31
3	a	839	GLU	C-N-CA	5.13	128.11	120.31
4	b	617	THR	N-CA-C	-5.13	99.87	110.80
4	m	467	ASN	CA-CB-CG	-5.13	107.47	112.60
9	r	599	LYS	CA-CB-CG	5.13	124.36	114.10
9	r	516	LEU	N-CA-CB	5.13	119.50	110.37
9	g	68	ILE	N-CA-CB	5.13	118.36	111.90
6	o	135	THR	N-CA-C	-5.13	102.47	110.42
1	X	1256	GLU	CA-C-N	5.13	127.15	120.28
1	X	1256	GLU	C-N-CA	5.13	127.15	120.28
3	a	226	CYS	CB-CA-C	-5.13	100.15	109.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	611	SER	N-CA-C	-5.13	99.88	110.80
9	g	648	GLN	N-CA-C	5.13	117.61	111.71
1	X	948	LEU	N-CA-CB	5.12	120.45	112.25
9	g	125	ARG	N-CA-C	5.12	117.47	110.24
9	g	998	ASN	CB-CA-C	5.12	119.43	109.33
1	X	992	SER	N-CA-C	-5.12	99.89	110.80
1	X	1185	GLU	N-CA-C	-5.12	105.88	111.82
3	a	70	TYR	N-CA-C	5.12	117.44	108.52
5	c	194	ILE	CA-C-O	5.12	126.28	120.95
1	X	852	PHE	CA-C-N	5.12	127.65	120.28
1	X	852	PHE	C-N-CA	5.12	127.65	120.28
1	X	1202	SER	CA-C-N	5.12	128.57	120.89
1	X	1202	SER	C-N-CA	5.12	128.57	120.89
3	l	695	TYR	CA-C-O	5.12	125.72	119.78
9	r	1147	THR	O-C-N	5.12	129.23	122.93
1	X	1510	PHE	CA-CB-CG	-5.12	108.68	113.80
8	f	181	PHE	CA-CB-CG	5.12	118.92	113.80
6	o	229	ARG	CG-CD-NE	-5.12	100.74	112.00
1	X	263	SER	CA-C-N	5.12	127.45	120.54
1	X	263	SER	C-N-CA	5.12	127.45	120.54
1	X	1086	ILE	CB-CA-C	-5.12	105.49	111.94
1	X	1608	HIS	O-C-N	-5.12	116.70	121.36
6	d	98	HIS	CA-C-N	5.12	130.05	122.17
6	d	98	HIS	C-N-CA	5.12	130.05	122.17
9	g	532	LYS	N-CA-CB	5.12	117.74	110.16
7	p	63	TRP	O-C-N	-5.12	116.27	122.82
7	p	96	ARG	CB-CG-CD	5.12	123.07	111.30
9	r	607	SER	CA-C-O	5.12	124.15	118.52
1	X	1064	GLU	N-CA-C	-5.12	105.61	111.14
3	l	706	ASN	CA-C-N	5.12	127.65	120.28
3	l	706	ASN	C-N-CA	5.12	127.65	120.28
4	m	533	GLU	CA-C-N	5.12	128.69	120.30
4	m	533	GLU	C-N-CA	5.12	128.69	120.30
8	q	453	GLU	N-CA-C	-5.12	102.61	108.49
1	X	1633	ARG	CD-NE-CZ	-5.12	117.24	124.40
8	f	268	SER	N-CA-C	-5.12	103.11	111.04
4	m	120	ASP	CA-CB-CG	5.12	117.72	112.60
4	m	687	SER	CA-C-N	5.12	128.69	120.30
4	m	687	SER	C-N-CA	5.12	128.69	120.30
8	q	310	THR	N-CA-C	-5.12	99.91	110.80
3	a	1000	TYR	CB-CG-CD2	-5.11	113.13	120.80
4	b	318	GLY	O-C-N	5.11	127.15	122.19

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	b	696	GLU	CB-CG-CD	5.11	121.29	112.60
7	e	199	ASP	CA-C-N	5.11	125.63	120.00
7	e	199	ASP	C-N-CA	5.11	125.63	120.00
8	f	440	ASP	CA-CB-CG	5.11	117.71	112.60
9	r	1106	GLN	CA-C-N	5.11	127.55	120.29
9	r	1106	GLN	C-N-CA	5.11	127.55	120.29
1	X	1217	ARG	NE-CZ-NH1	-5.11	116.39	121.50
3	a	571	PHE	CA-CB-CG	-5.11	108.69	113.80
3	a	757	GLU	CB-CA-C	-5.11	102.30	110.79
9	g	122	VAL	N-CA-CB	5.11	118.20	111.40
1	X	684	LYS	CA-CB-CG	5.11	124.32	114.10
1	X	915	ASP	CA-C-N	-5.11	116.25	122.64
1	X	915	ASP	C-N-CA	-5.11	116.25	122.64
1	X	1318	LEU	N-CA-CB	5.11	118.09	110.22
4	b	505	ALA	CB-CA-C	-5.11	101.53	110.17
3	l	436	HIS	ND1-CE1-NE2	5.11	113.51	108.40
3	l	651	ILE	CB-CA-C	5.11	115.66	110.65
4	m	459	ASN	CA-CB-CG	-5.11	107.49	112.60
8	q	117	TYR	N-CA-CB	5.11	117.63	110.12
8	q	171	VAL	N-CA-C	-5.11	107.31	112.17
8	q	678	LEU	CA-C-N	5.11	130.96	122.73
8	q	678	LEU	C-N-CA	5.11	130.96	122.73
9	r	972	CYS	N-CA-CB	5.11	117.53	110.17
4	b	505	ALA	CA-C-O	5.11	125.40	119.32
7	e	20	TYR	N-CA-CB	5.11	118.20	110.28
8	f	315	LEU	CA-C-O	-5.11	113.16	120.16
9	r	722	PHE	CA-C-O	5.11	125.97	120.55
9	g	126	SER	N-CA-CB	5.11	120.37	111.13
3	l	968	ARG	CA-C-N	5.11	129.36	120.68
3	l	968	ARG	C-N-CA	5.11	129.36	120.68
4	m	545	GLN	CG-CD-OE1	-5.11	110.58	120.80
3	l	394	ASP	CA-CB-CG	5.11	117.70	112.60
8	q	230	GLU	N-CA-C	-5.11	106.46	113.30
3	a	563	GLU	N-CA-C	-5.10	102.20	110.32
1	X	1597	ARG	NH1-CZ-NH2	5.10	125.94	119.30
8	f	76	HIS	CE1-NE2-CD2	-5.10	103.90	109.00
9	g	995	THR	O-C-N	-5.10	117.16	123.44
3	l	885	VAL	CA-C-N	5.10	127.07	120.44
3	l	885	VAL	C-N-CA	5.10	127.07	120.44
7	p	91	GLU	N-CA-C	5.10	118.05	110.14
8	q	178	HIS	CA-C-O	5.10	126.16	120.80
1	X	1603	SER	CA-C-N	5.10	127.07	120.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	1603	SER	C-N-CA	5.10	127.07	120.44
5	c	524	ASP	N-CA-CB	5.10	118.08	110.22
9	g	781	TYR	N-CA-CB	5.10	117.62	110.12
8	q	395	CYS	CA-C-N	5.10	128.06	120.31
8	q	395	CYS	C-N-CA	5.10	128.06	120.31
3	a	497	MET	CA-C-N	5.10	131.28	121.54
3	a	497	MET	C-N-CA	5.10	131.28	121.54
3	a	931	ASP	CA-C-O	5.10	124.90	119.34
4	b	661	HIS	N-CA-C	-5.10	106.30	112.88
5	c	538	ILE	O-C-N	-5.10	116.04	121.80
5	c	601	GLU	O-C-N	-5.10	116.25	122.22
8	f	560	LYS	CB-CA-C	-5.10	101.57	110.09
3	l	141	SER	CA-C-N	5.10	131.28	121.54
3	l	141	SER	C-N-CA	5.10	131.28	121.54
4	m	519	ILE	N-CA-CB	-5.10	105.73	112.36
8	q	177	ASP	O-C-N	-5.10	115.60	122.43
1	X	1022	TYR	CB-CG-CD1	5.10	128.45	120.80
4	m	386	ILE	O-C-N	-5.10	116.20	122.57
1	X	1027	TRP	N-CA-C	-5.10	99.95	110.80
3	a	963	LYS	O-C-N	-5.10	116.67	122.23
8	f	661	PRO	N-CA-C	5.10	120.30	114.03
9	g	565	GLN	CB-CA-C	-5.10	101.38	110.70
3	l	422	ARG	O-C-N	-5.10	115.81	122.59
3	a	313	TYR	CB-CG-CD1	5.09	128.44	120.80
3	a	965	TYR	CA-CB-CG	5.09	123.07	113.90
4	m	204	PHE	N-CA-C	-5.09	105.42	110.97
5	n	326	GLY	N-CA-C	-5.09	108.59	115.21
1	X	704	ASP	CA-CB-CG	5.09	117.69	112.60
9	g	1082	ASP	CA-C-N	5.09	131.27	121.54
9	g	1082	ASP	C-N-CA	5.09	131.27	121.54
3	a	247	ASP	N-CA-C	-5.09	99.37	108.13
4	b	174	GLU	CA-C-O	-5.09	113.64	119.60
3	a	968	ARG	NE-CZ-NH2	5.09	123.78	119.20
9	g	133	ALA	CB-CA-C	-5.09	100.67	110.24
9	g	621	TYR	CA-CB-CG	-5.09	104.74	113.90
1	X	1230	VAL	CB-CA-C	5.09	119.01	112.14
3	a	138	LEU	N-CA-C	-5.09	107.20	113.41
4	b	572	SER	CA-C-N	5.09	128.04	120.31
4	b	572	SER	C-N-CA	5.09	128.04	120.31
1	X	1164	ASP	CA-CB-CG	5.09	117.69	112.60
1	X	1187	ILE	CB-CA-C	-5.09	103.87	112.16
5	c	251	ASP	CB-CA-C	-5.09	101.57	110.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	g	130	ASP	CA-C-N	5.09	127.93	120.71
9	g	130	ASP	C-N-CA	5.09	127.93	120.71
9	g	799	GLU	N-CA-C	-5.09	99.96	110.80
9	g	868	HIS	ND1-CE1-NE2	5.09	113.49	108.40
3	l	167	PHE	CA-C-N	5.09	128.09	120.87
3	l	167	PHE	C-N-CA	5.09	128.09	120.87
4	b	86	ASP	N-CA-C	-5.08	99.97	110.80
4	b	292	LEU	O-C-N	5.08	129.24	122.43
5	c	221	LEU	N-CA-C	-5.08	105.77	112.94
6	d	104	SER	O-C-N	5.08	129.47	123.27
3	l	336	LEU	CA-C-O	-5.08	115.06	120.40
3	l	808	TRP	CH2-CZ2-CE2	5.08	124.11	117.50
8	q	377	ASN	CB-CA-C	-5.08	101.85	110.19
3	a	902	THR	N-CA-C	-5.08	107.11	113.72
9	g	287	THR	N-CA-CB	5.08	118.15	110.42
3	l	144	THR	CA-C-N	5.08	130.76	122.07
3	l	144	THR	C-N-CA	5.08	130.76	122.07
4	m	587	ASP	N-CA-C	-5.08	99.97	110.80
8	q	645	ASP	N-CA-CB	5.08	119.08	110.49
1	X	390	ILE	N-CA-CB	5.08	115.22	109.99
8	f	478	ARG	NE-CZ-NH1	5.08	126.58	121.50
3	l	361	SER	N-CA-C	-5.08	106.92	113.02
4	m	348	GLN	OE1-CD-NE2	-5.08	117.52	122.60
6	o	213	SER	CA-C-O	5.08	124.52	119.49
8	q	715	LEU	N-CA-CB	5.08	118.05	110.22
9	r	1151	GLU	N-CA-CB	5.08	118.16	110.28
5	c	131	GLU	CA-C-N	5.08	126.96	120.56
5	c	131	GLU	C-N-CA	5.08	126.96	120.56
1	X	1090	THR	N-CA-C	5.08	116.50	111.07
5	c	573	VAL	CA-CB-CG1	5.08	119.03	110.40
6	d	156	ALA	O-C-N	5.08	129.01	123.22
7	e	11	LEU	CB-CA-C	-5.08	102.85	110.16
9	r	1083	LEU	O-C-N	5.08	128.34	122.09
1	X	822	ASN	OD1-CG-ND2	5.08	127.68	122.60
9	g	906	ILE	CA-CB-CG2	5.08	119.13	110.50
9	r	1135	SER	CA-CB-OG	5.08	121.25	111.10
1	X	715	THR	O-C-N	-5.08	116.61	122.09
1	X	1340	PHE	N-CA-C	5.08	116.81	111.28
7	e	230	LEU	O-C-N	5.08	129.79	123.19
9	g	292	PHE	CA-C-O	5.08	125.89	120.46
9	r	259	LYS	O-C-N	-5.08	115.77	122.42
1	X	784	THR	CA-C-N	5.07	130.83	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	X	784	THR	C-N-CA	5.07	130.83	121.70
4	b	92	PRO	N-CA-CB	5.07	107.83	103.27
4	b	527	VAL	CA-CB-CG1	-5.07	101.78	110.40
8	f	182	LYS	N-CA-C	5.07	116.50	111.07
3	l	122	ILE	CA-C-O	-5.07	115.10	120.48
3	l	592	LYS	O-C-N	-5.07	116.82	121.34
4	m	56	GLN	CA-C-N	5.07	126.18	119.84
4	m	56	GLN	C-N-CA	5.07	126.18	119.84
8	q	453	GLU	O-C-N	5.07	126.92	123.11
9	r	868	HIS	CB-CG-CD2	-5.07	124.60	131.20
9	g	1056	LYS	CA-C-N	5.07	127.34	120.44
9	g	1056	LYS	C-N-CA	5.07	127.34	120.44
3	l	423	ALA	N-CA-C	-5.07	106.34	112.88
1	X	1169	ALA	N-CA-CB	5.07	119.06	110.49
3	a	533	LEU	O-C-N	5.07	127.36	122.09
4	b	122	ARG	NE-CZ-NH1	5.07	126.57	121.50
4	b	504	ILE	N-CA-C	-5.07	107.35	112.17
4	b	572	SER	O-C-N	-5.07	115.16	122.36
5	c	142	ARG	CB-CA-C	-5.07	100.03	110.38
8	f	300	ASN	O-C-N	5.07	127.57	122.09
3	l	710	TYR	N-CA-C	-5.07	106.94	113.02
7	p	244	LYS	N-CA-C	-5.07	100.81	108.67
8	q	667	LEU	CA-C-N	5.07	127.49	120.29
8	q	667	LEU	C-N-CA	5.07	127.49	120.29
9	r	692	GLU	N-CA-CB	5.07	118.89	111.54
3	a	780	HIS	CE1-NE2-CD2	-5.07	103.93	109.00
8	q	437	ASN	OD1-CG-ND2	5.07	127.67	122.60
4	b	541	THR	CA-CB-OG1	5.07	117.20	109.60
9	g	338	PRO	N-CA-CB	5.07	108.57	103.25
9	g	714	TYR	CA-CB-CG	-5.07	104.78	113.90
9	g	735	LEU	CB-CA-C	-5.07	102.83	110.83
4	m	204	PHE	N-CA-CB	5.07	117.31	109.91
5	n	631	GLN	OE1-CD-NE2	-5.07	117.53	122.60
3	a	89	HIS	CG-CD2-NE2	5.07	112.27	107.20
6	d	63	HIS	O-C-N	-5.07	116.08	121.30
8	f	138	ASN	CA-C-N	5.07	131.50	122.13
8	f	138	ASN	C-N-CA	5.07	131.50	122.13
8	f	383	PRO	CA-C-N	5.07	127.52	120.63
8	f	383	PRO	C-N-CA	5.07	127.52	120.63
3	l	505	GLU	CA-C-O	5.07	125.82	120.10
4	m	669	LYS	N-CA-CB	5.07	119.05	110.49
4	m	724	MET	CB-CA-C	5.07	118.16	109.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
8	f	682	LYS	CG-CD-CE	5.06	122.95	111.30
9	g	372	SER	N-CA-C	-5.06	102.29	110.14
9	g	1118	SER	CA-C-O	-5.06	113.03	119.31
5	c	275	GLN	OE1-CD-NE2	5.06	127.66	122.60
3	l	88	TYR	N-CA-C	-5.06	106.79	113.17
5	n	584	ASN	N-CA-CB	5.06	118.55	110.65
8	q	417	ILE	CA-C-O	-5.06	115.29	120.71
1	X	1552	ASN	OD1-CG-ND2	-5.06	117.54	122.60
1	X	1092	SER	CA-C-O	-5.06	113.28	120.51
4	b	386	ILE	CA-C-N	5.06	131.20	121.54
4	b	386	ILE	C-N-CA	5.06	131.20	121.54
5	c	151	ALA	N-CA-C	-5.06	100.21	108.76
5	c	416	ASP	N-CA-C	-5.06	101.35	109.04
9	g	945	ARG	CA-C-O	-5.06	115.69	120.90
9	g	971	ILE	CA-CB-CG2	-5.06	101.90	110.50
9	g	1059	GLN	CB-CG-CD	-5.06	104.00	112.60
4	m	250	ASN	CA-C-O	-5.06	115.69	121.00
4	m	286	SER	N-CA-CB	5.06	118.12	110.28
8	q	677	LEU	N-CA-C	5.06	119.17	112.89
1	X	899	GLN	OE1-CD-NE2	5.06	127.66	122.60
3	a	580	PRO	N-CD-CG	5.06	110.78	103.20
3	l	860	GLU	N-CA-CB	5.06	118.12	110.28
7	p	49	ASP	N-CA-CB	5.06	119.04	110.49
9	r	777	ILE	CA-C-O	5.06	126.12	119.85
9	r	878	SER	CA-C-N	5.06	134.14	121.80
9	r	878	SER	C-N-CA	5.06	134.14	121.80
3	a	585	ASP	N-CA-CB	-5.06	102.69	110.12
3	a	717	ASN	CB-CA-C	5.06	117.02	109.13
5	c	199	ILE	CA-CB-CG1	5.06	119.00	110.40
3	l	585	ASP	CA-CB-CG	-5.06	107.54	112.60
9	r	996	VAL	CA-C-N	5.06	129.97	122.94
9	r	996	VAL	C-N-CA	5.06	129.97	122.94
1	X	156	THR	CA-CB-OG1	5.05	117.18	109.60
1	X	318	HIS	CE1-NE2-CD2	-5.05	103.95	109.00
8	f	387	ARG	NH1-CZ-NH2	5.05	125.87	119.30
9	g	427	THR	N-CA-CB	5.05	118.03	109.94
4	m	661	HIS	CA-C-N	5.05	130.90	122.66
4	m	661	HIS	C-N-CA	5.05	130.90	122.66
6	o	284	ASN	N-CA-C	-5.05	101.51	109.50
8	q	72	ALA	O-C-N	5.05	127.28	122.07
1	X	1509	GLN	OE1-CD-NE2	5.05	127.65	122.60
4	b	504	ILE	CB-CG1-CD1	5.05	124.41	113.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
6	d	284	ASN	CA-C-N	5.05	129.22	121.19
6	d	284	ASN	C-N-CA	5.05	129.22	121.19
8	f	319	SER	CA-C-N	5.05	130.87	121.62
8	f	319	SER	C-N-CA	5.05	130.87	121.62
4	m	615	VAL	O-C-N	5.05	129.09	122.12
3	a	577	PHE	CA-CB-CG	-5.05	108.75	113.80
4	b	609	GLN	N-CA-C	-5.05	105.82	112.94
9	g	80	PHE	N-CA-CB	5.05	117.97	110.49
9	g	220	VAL	CA-C-N	-5.05	115.83	122.85
9	g	220	VAL	C-N-CA	-5.05	115.83	122.85
3	l	93	ILE	N-CA-C	-5.05	101.43	108.80
6	o	236	GLN	N-CA-CB	5.05	118.85	110.52
9	r	433	LEU	CB-CA-C	-5.05	99.75	110.31
1	X	847	VAL	N-CA-C	5.05	119.84	109.34
5	c	338	LEU	CA-C-N	5.05	127.05	120.28
5	c	338	LEU	C-N-CA	5.05	127.05	120.28
5	n	337	GLU	CA-C-N	5.05	127.46	120.29
5	n	337	GLU	C-N-CA	5.05	127.46	120.29
6	o	215	THR	O-C-N	5.05	128.55	122.79
9	r	1080	SER	CA-C-O	5.05	126.73	121.38
5	c	373	LYS	N-CA-C	-5.05	106.71	112.92
9	g	662	ASN	CA-C-N	5.05	129.15	120.72
9	g	662	ASN	C-N-CA	5.05	129.15	120.72
9	g	1043	ARG	CD-NE-CZ	5.05	131.47	124.40
9	r	421	PRO	N-CA-C	-5.05	102.07	112.47
3	a	454	LYS	CA-C-N	5.05	129.77	121.39
3	a	454	LYS	C-N-CA	5.05	129.77	121.39
3	a	951	GLN	CA-C-N	5.05	127.46	120.29
3	a	951	GLN	C-N-CA	5.05	127.46	120.29
5	c	490	SER	N-CA-C	5.05	116.78	111.28
3	l	142	ALA	N-CA-CB	5.05	119.02	110.49
4	m	180	THR	CA-C-N	5.05	126.92	120.56
4	m	180	THR	C-N-CA	5.05	126.92	120.56
5	n	776	GLN	CB-CG-CD	-5.05	104.02	112.60
1	X	1231	GLU	N-CA-C	5.04	116.78	111.28
6	o	175	THR	N-CA-CB	5.04	118.92	110.85
1	X	323	TYR	CB-CG-CD1	5.04	128.36	120.80
5	c	497	LEU	CB-CA-C	5.04	117.83	110.26
3	l	947	SER	CA-C-N	5.04	127.85	121.85
3	l	947	SER	C-N-CA	5.04	127.85	121.85
8	q	32	PRO	N-CA-CB	5.04	107.73	103.19
4	b	216	ASP	N-CA-C	-5.04	100.06	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	c	273	VAL	CA-CB-CG2	-5.04	101.83	110.40
8	f	522	LEU	CA-C-N	5.04	127.82	119.35
8	f	522	LEU	C-N-CA	5.04	127.82	119.35
4	m	538	ILE	CA-C-O	5.04	126.51	121.17
6	o	264	LEU	CA-C-N	5.04	129.37	121.76
6	o	264	LEU	C-N-CA	5.04	129.37	121.76
1	X	719	ILE	CB-CA-C	5.04	118.94	112.14
1	X	1413	ASN	OD1-CG-ND2	5.04	127.64	122.60
5	c	539	PHE	CA-CB-CG	-5.04	108.76	113.80
7	e	239	ARG	N-CA-C	-5.04	101.49	109.96
3	l	541	PRO	N-CD-CG	5.04	110.76	103.20
9	r	582	GLU	CB-CG-CD	5.04	121.16	112.60
3	a	364	GLN	O-C-N	-5.04	117.32	123.16
5	c	379	PHE	CA-CB-CG	-5.04	108.76	113.80
5	n	155	THR	N-CA-C	5.04	119.27	113.18
1	X	1606	LEU	N-CA-C	5.04	117.42	111.33
4	b	193	ASP	CA-C-N	5.04	129.07	120.91
4	b	193	ASP	C-N-CA	5.04	129.07	120.91
8	f	702	TYR	N-CA-C	-5.04	100.08	110.80
3	l	893	HIS	CB-CG-CD2	5.04	137.75	131.20
9	r	1098	THR	CA-C-O	5.04	125.73	119.79
1	X	146	SER	CA-C-N	5.03	133.30	121.52
1	X	146	SER	C-N-CA	5.03	133.30	121.52
1	X	880	ASN	CB-CG-ND2	-5.03	108.85	116.40
4	b	172	PHE	CB-CG-CD2	5.03	129.26	120.70
7	e	59	VAL	CA-C-O	5.03	125.28	120.80
8	f	220	ASN	OD1-CG-ND2	5.03	127.63	122.60
8	f	705	PHE	CB-CA-C	5.03	119.12	110.81
3	l	1012	SER	N-CA-CB	5.03	119.00	110.49
5	n	649	LYS	CB-CA-C	5.03	115.99	109.80
1	X	1083	ALA	N-CA-CB	5.03	118.09	110.14
3	a	438	GLU	CA-C-N	5.03	132.06	123.05
3	a	438	GLU	C-N-CA	5.03	132.06	123.05
3	a	957	ASP	N-CA-CB	5.03	117.39	109.69
4	b	333	GLU	CA-C-O	-5.03	115.09	120.42
6	d	220	SER	CA-C-O	5.03	127.00	120.21
3	l	406	ARG	CA-C-N	5.03	131.27	121.41
3	l	406	ARG	C-N-CA	5.03	131.27	121.41
3	l	932	ASN	O-C-N	-5.03	115.93	122.37
8	q	394	ILE	N-CA-C	5.03	115.46	110.23
9	r	85	GLU	CB-CA-C	-5.03	100.74	110.35
9	r	1004	GLU	CA-C-N	5.03	127.02	120.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	r	1004	GLU	C-N-CA	5.03	127.02	120.28
1	X	1277	ILE	N-CA-C	-5.03	98.88	109.34
3	a	71	HIS	CG-CD2-NE2	5.03	112.23	107.20
8	f	408	ASP	CA-CB-CG	5.03	117.63	112.60
4	m	590	VAL	CA-CB-CG1	-5.03	101.85	110.40
8	q	604	VAL	N-CA-C	-5.03	107.65	111.62
3	a	349	LEU	CD1-CG-CD2	5.03	121.86	110.80
5	c	420	VAL	O-C-N	5.03	127.48	121.80
9	g	907	THR	CA-C-O	5.03	125.78	119.59
3	l	581	VAL	CA-CB-CG2	-5.03	101.85	110.40
6	o	44	LYS	N-CA-C	-5.03	100.97	109.07
9	r	1055	ASP	CA-CB-CG	5.03	117.63	112.60
1	X	1188	THR	CA-C-N	5.03	127.02	120.28
1	X	1188	THR	C-N-CA	5.03	127.02	120.28
3	l	544	MET	CB-CA-C	-5.03	99.91	109.66
4	m	296	PRO	CA-C-O	-5.03	115.73	121.56
6	o	48	THR	CA-C-O	5.03	125.74	120.36
8	q	289	HIS	N-CA-CB	5.03	117.25	109.91
8	q	605	SER	N-CA-C	-5.03	106.84	113.17
1	X	198	MET	CG-SD-CE	-5.03	89.84	100.90
1	X	1346	LYS	CA-C-N	5.03	131.26	121.41
1	X	1346	LYS	C-N-CA	5.03	131.26	121.41
3	a	955	SER	CA-C-N	5.03	131.26	121.41
3	a	955	SER	C-N-CA	5.03	131.26	121.41
7	e	59	VAL	N-CA-C	-5.03	107.65	111.62
8	f	577	GLU	CB-CG-CD	-5.03	104.06	112.60
9	g	138	CYS	CA-C-O	-5.03	115.27	120.70
9	g	916	SER	CA-C-N	5.03	127.02	120.28
9	g	916	SER	C-N-CA	5.03	127.02	120.28
5	n	412	LEU	N-CA-CB	5.03	116.81	110.23
6	o	65	LYS	N-CA-CB	5.03	118.98	110.49
8	q	106	GLU	N-CA-CB	5.03	117.51	110.12
9	r	917	LEU	N-CA-C	-5.03	105.71	111.14
9	r	1116	GLU	CB-CG-CD	-5.03	104.06	112.60
9	r	1117	ILE	N-CA-C	5.03	115.75	110.62
3	a	532	PHE	N-CA-C	5.02	118.56	112.23
3	a	637	PHE	CB-CG-CD1	-5.02	112.16	120.70
8	q	166	THR	CA-C-O	5.02	126.63	120.55
8	q	450	SER	O-C-N	-5.02	116.80	122.12
3	l	498	HIS	ND1-CE1-NE2	5.02	113.42	108.40
3	l	501	THR	N-CA-CB	5.02	119.27	110.98
4	m	712	THR	O-C-N	5.02	127.02	121.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	495	CYS	N-CA-CB	5.02	118.06	110.28
5	n	568	ALA	O-C-N	5.02	129.27	122.59
5	n	651	CYS	CA-C-O	-5.02	115.58	121.10
8	q	300	ASN	CA-C-N	5.02	127.42	120.29
8	q	300	ASN	C-N-CA	5.02	127.42	120.29
8	q	426	TYR	CB-CG-CD1	-5.02	113.27	120.80
3	a	563	GLU	N-CA-CB	5.02	118.59	110.41
4	b	365	ILE	CA-C-O	-5.02	113.22	119.95
5	c	167	LYS	N-CA-CB	5.02	117.86	110.33
5	c	508	LYS	CB-CG-CD	5.02	122.85	111.30
9	r	556	HIS	N-CA-CB	-5.02	103.56	111.39
1	X	292	THR	CB-CA-C	5.02	118.08	109.15
5	c	394	ILE	N-CA-C	-5.02	105.60	110.42
8	f	535	ARG	NH1-CZ-NH2	-5.02	112.77	119.30
9	g	1001	ASP	N-CA-C	-5.02	106.00	111.82
3	l	896	LEU	N-CA-C	-5.02	100.11	110.80
7	p	159	ILE	O-C-N	-5.02	115.38	121.10
8	q	156	CYS	CA-C-O	-5.02	114.87	120.54
8	q	666	GLU	N-CA-C	5.02	116.44	111.07
9	r	634	VAL	CA-C-O	5.02	126.03	120.46
1	X	1471	GLU	CA-C-O	-5.02	113.21	119.28
4	b	209	LEU	CA-C-N	5.02	127.94	120.31
4	b	209	LEU	C-N-CA	5.02	127.94	120.31
4	b	288	SER	CB-CA-C	-5.02	102.32	110.85
5	c	339	GLN	O-C-N	-5.02	116.80	122.12
6	d	66	PHE	CA-CB-CG	-5.02	108.78	113.80
6	d	191	ALA	CA-C-N	5.02	131.66	123.93
6	d	191	ALA	C-N-CA	5.02	131.66	123.93
9	g	348	LEU	O-C-N	-5.02	115.85	122.57
4	m	256	GLY	CA-C-N	5.02	130.65	122.07
4	m	256	GLY	C-N-CA	5.02	130.65	122.07
9	r	105	VAL	N-CA-C	-5.02	101.14	108.17
9	r	409	ASP	CB-CA-C	-5.02	103.80	111.83
9	r	831	LEU	CA-C-N	5.02	127.90	120.82
9	r	831	LEU	C-N-CA	5.02	127.90	120.82
4	m	257	LEU	CB-CA-C	5.02	118.09	109.51
9	r	1066	PHE	N-CA-C	-5.02	107.00	113.02
1	X	901	ILE	N-CA-C	5.01	117.32	111.05
5	c	628	VAL	N-CA-CB	5.01	119.50	111.23
9	g	1061	ILE	CA-C-O	5.01	125.04	119.42
3	l	511	ARG	NH1-CZ-NH2	-5.01	112.78	119.30
3	l	1034	LEU	N-CA-C	-5.01	106.85	113.17

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	m	370	LEU	O-C-N	5.01	129.26	122.59
4	m	610	ASP	N-CA-C	-5.01	105.89	112.41
5	n	286	ASN	CA-CB-CG	-5.01	107.59	112.60
5	n	571	ALA	N-CA-C	-5.01	107.16	113.28
9	r	641	VAL	CA-C-O	-5.01	114.51	120.78
9	r	731	GLU	CA-CB-CG	5.01	124.13	114.10
3	a	245	ILE	N-CA-C	-5.01	100.53	107.80
4	b	364	TYR	N-CA-CB	5.01	119.74	111.62
5	n	545	LYS	O-C-N	-5.01	116.81	122.12
9	r	983	VAL	CA-C-N	5.01	127.31	120.54
9	r	983	VAL	C-N-CA	5.01	127.31	120.54
1	X	399	VAL	N-CA-CB	5.01	117.74	110.52
1	X	754	TYR	N-CA-C	-5.01	101.46	109.23
3	a	693	PHE	CA-CB-CG	-5.01	108.79	113.80
4	b	403	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
5	c	317	HIS	CE1-NE2-CD2	-5.01	103.99	109.00
3	l	886	LEU	O-C-N	5.01	127.23	122.07
5	n	540	ASN	CB-CA-C	-5.01	101.36	110.63
8	q	70	LEU	CA-C-N	5.01	127.00	120.28
8	q	70	LEU	C-N-CA	5.01	127.00	120.28
8	q	474	ASN	N-CA-C	-5.01	104.50	110.41
1	X	1258	SER	CA-C-N	5.01	126.99	120.28
1	X	1258	SER	C-N-CA	5.01	126.99	120.28
3	a	68	ILE	CB-CA-C	5.01	118.04	111.33
3	a	975	ARG	CD-NE-CZ	-5.01	117.39	124.40
6	d	110	HIS	ND1-CE1-NE2	5.01	113.41	108.40
8	f	328	LEU	CA-C-O	5.01	125.76	120.10
9	g	378	PHE	CA-CB-CG	-5.01	108.79	113.80
9	g	442	LYS	O-C-N	-5.01	117.11	123.12
3	a	530	LYS	CB-CA-C	-5.01	102.48	110.79
3	l	391	SER	CA-C-N	5.01	127.92	120.31
3	l	391	SER	C-N-CA	5.01	127.92	120.31
5	n	364	SER	CA-C-N	5.01	124.62	119.56
5	n	364	SER	C-N-CA	5.01	124.62	119.56
6	o	52	HIS	ND1-CE1-NE2	5.01	113.41	108.40
4	b	473	LEU	N-CA-C	-5.01	107.34	113.50
3	l	403	ASP	CA-CB-CG	5.01	117.61	112.60
3	l	518	SER	N-CA-C	5.01	116.43	111.07
3	l	620	HIS	N-CA-C	5.01	116.74	111.28
3	l	769	ASN	CB-CG-OD1	-5.01	110.79	120.80
3	l	936	TYR	CA-C-O	-5.01	113.35	120.51
3	l	1025	VAL	CB-CA-C	-5.01	105.74	110.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
5	n	218	LYS	N-CA-C	-5.01	106.86	113.17
9	r	655	PHE	CA-CB-CG	-5.01	108.79	113.80
5	n	397	TYR	N-CA-C	-5.00	103.05	110.46
9	r	861	ILE	N-CA-C	-5.00	108.42	113.47
1	X	348	LYS	CB-CG-CD	5.00	122.81	111.30
1	X	1600	ALA	N-CA-CB	5.00	117.27	110.01
3	a	561	GLN	CA-CB-CG	5.00	124.11	114.10
8	f	76	HIS	CA-CB-CG	5.00	118.80	113.80
8	f	629	GLU	CB-CA-C	5.00	118.36	109.75
3	l	160	VAL	CA-C-O	-5.00	114.53	120.78
3	l	297	LEU	CA-C-O	-5.00	115.26	121.11
3	l	473	VAL	O-C-N	5.00	128.82	122.57
5	n	175	LEU	N-CA-C	-5.00	103.34	109.65
1	X	134	ARG	CA-C-O	-5.00	112.77	118.47
1	X	993	SER	N-CA-C	-5.00	101.02	109.07
1	X	1518	THR	CA-CB-OG1	5.00	117.10	109.60
1	X	1527	LYS	CA-CB-CG	5.00	124.10	114.10
3	a	657	LEU	CA-C-O	-5.00	115.25	120.55
4	b	352	THR	CA-C-O	-5.00	115.42	121.32
8	f	173	ASP	O-C-N	-5.00	115.61	122.46
9	g	622	ASN	CA-CB-CG	5.00	117.60	112.60
3	l	426	ILE	N-CA-C	-5.00	101.01	108.46
3	l	1017	TRP	CA-C-N	5.00	127.30	120.35
3	l	1017	TRP	C-N-CA	5.00	127.30	120.35
3	l	1030	LEU	N-CA-C	-5.00	106.96	113.16
5	n	258	ALA	O-C-N	5.00	127.42	122.12
8	q	613	ILE	CA-C-N	5.00	125.27	119.47
8	q	613	ILE	C-N-CA	5.00	125.27	119.47

All (10) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
1	X	793	LEU	CA
1	X	794	ILE	CA
1	X	1060	LEU	CA
1	X	1276	LYS	CA
1	X	1277	ILE	CA
1	X	1303	LEU	CA
1	X	1304	LYS	CA
8	f	576	ASN	CA
3	l	415	TYR	CA
8	q	482	ARG	CA

All (444) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	X	1008	THR	Peptide
1	X	1042	SER	Peptide
1	X	1060	LEU	Mainchain
1	X	1062	ARG	Sidechain
1	X	1170	ASP	Peptide
1	X	1196	TYR	Sidechain
1	X	1199	TYR	Sidechain
1	X	1233	PHE	Sidechain
1	X	1240	PHE	Sidechain
1	X	1260	TYR	Sidechain
1	X	1263	TYR	Sidechain
1	X	1304	LYS	Mainchain
1	X	1307	PHE	Sidechain
1	X	1308	TYR	Sidechain
1	X	1399	ASN	Peptide
1	X	1463	SER	Peptide
1	X	1490	ARG	Sidechain
1	X	150	GLN	Peptide
1	X	1524	TYR	Sidechain
1	X	1534	TYR	Sidechain
1	X	1536	TRP	Peptide
1	X	1566	TYR	Sidechain
1	X	1597	ARG	Sidechain
1	X	164	TYR	Sidechain
1	X	182	PHE	Sidechain
1	X	213	PHE	Peptide
1	X	322	HIS	Sidechain
1	X	327	PHE	Sidechain
1	X	330	TYR	Sidechain
1	X	369	LEU	Peptide
1	X	371	PHE	Sidechain
1	X	382	PHE	Sidechain
1	X	411	PHE	Sidechain
1	X	413	GLU	Peptide
1	X	430	ALA	Peptide
1	X	439	LEU	Peptide
1	X	440	ILE	Peptide
1	X	617	TYR	Sidechain
1	X	727	ASN	Peptide
1	X	728	ILE	Peptide
1	X	753	TYR	Sidechain
1	X	776	TYR	Sidechain

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Mol	Chain	Res	Type	Group
1	X	833	LYS	Peptide
1	X	835	LEU	Peptide
1	X	879	ILE	Peptide
1	X	884	LEU	Peptide
1	X	894	VAL	Peptide
1	X	906	TYR	Sidechain
1	X	927	LYS	Peptide
1	X	953	TYR	Sidechain
1	X	984	ASP	Peptide
3	a	1005	ASN	Peptide
3	a	1010	PHE	Peptide,Sidechain
3	a	1012	SER	Peptide
3	a	1014	TYR	Sidechain
3	a	1017	TRP	Peptide
3	a	1035	ARG	Peptide
3	a	173	PHE	Sidechain
3	a	177	PHE	Sidechain
3	a	193	HIS	Sidechain
3	a	204	TYR	Sidechain
3	a	220	TYR	Sidechain
3	a	223	VAL	Peptide
3	a	294	GLU	Peptide
3	a	342	LEU	Peptide
3	a	408	PHE	Sidechain
3	a	415	TYR	Sidechain
3	a	442	TYR	Sidechain
3	a	456	ALA	Peptide
3	a	466	TYR	Sidechain
3	a	479	TYR	Sidechain
3	a	516	PHE	Peptide
3	a	54	SER	Peptide
3	a	550	PHE	Sidechain
3	a	56	TYR	Sidechain
3	a	561	GLN	Peptide
3	a	591	MET	Peptide
3	a	593	PRO	Peptide
3	a	596	PHE	Peptide
3	a	6	ARG	Peptide
3	a	627	TYR	Sidechain
3	a	637	PHE	Peptide
3	a	642	LEU	Peptide
3	a	67	TYR	Sidechain

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Mol	Chain	Res	Type	Group
3	a	674	LEU	Peptide
3	a	686	PHE	Sidechain
3	a	688	PHE	Sidechain
3	a	695	TYR	Sidechain
3	a	701	TYR	Sidechain
3	a	717	ASN	Peptide
3	a	720	PHE	Peptide
3	a	727	TYR	Sidechain
3	a	734	HIS	Sidechain
3	a	748	PHE	Peptide
3	a	749	TYR	Peptide
3	a	751	ARG	Sidechain
3	a	760	PHE	Sidechain
3	a	769	ASN	Peptide
3	a	770	PHE	Sidechain
3	a	782	TYR	Peptide,Sidechain
3	a	806	SER	Peptide
3	a	815	PHE	Sidechain
3	a	821	HIS	Peptide
3	a	846	SER	Peptide
3	a	851	TYR	Peptide
3	a	862	GLN	Peptide
3	a	869	HIS	Sidechain
3	a	889	LEU	Peptide
3	a	892	GLY	Peptide
3	a	901	ARG	Sidechain
3	a	914	TYR	Peptide
3	a	945	VAL	Peptide
3	a	954	ARG	Sidechain
3	a	957	ASP	Peptide
3	a	958	TRP	Peptide
3	a	964	LEU	Peptide
3	a	970	LEU	Peptide
3	a	971	ASN	Peptide
3	a	975	ARG	Peptide
3	a	995	ARG	Sidechain
4	b	102	LYS	Peptide
4	b	173	TYR	Sidechain
4	b	179	LEU	Peptide
4	b	267	ARG	Sidechain
4	b	271	LEU	Peptide
4	b	344	ARG	Sidechain

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Mol	Chain	Res	Type	Group
4	b	354	TYR	Sidechain
4	b	364	TYR	Sidechain
4	b	374	TYR	Sidechain
4	b	406	LEU	Peptide
4	b	464	TYR	Sidechain
4	b	482	TRP	Peptide
4	b	490	ALA	Peptide
4	b	54	ASN	Peptide
4	b	576	PHE	Sidechain
4	b	619	SER	Mainchain
4	b	634	TYR	Sidechain
4	b	639	ARG	Sidechain
4	b	641	ASP	Peptide
4	b	647	ARG	Sidechain
4	b	655	PHE	Peptide,Sidechain
4	b	657	TYR	Peptide
4	b	673	PRO	Peptide
4	b	676	LEU	Peptide
4	b	687	SER	Peptide
4	b	704	GLU	Peptide
4	b	737	PHE	Peptide
4	b	81	PHE	Sidechain
4	b	88	TYR	Sidechain
5	c	142	ARG	Sidechain
5	c	143	ARG	Sidechain
5	c	148	TYR	Sidechain
5	c	189	TYR	Sidechain
5	c	200	GLU	Peptide
5	c	207	TYR	Peptide
5	c	225	GLU	Peptide
5	c	248	TYR	Sidechain
5	c	267	ARG	Sidechain
5	c	300	LEU	Peptide
5	c	391	TYR	Sidechain
5	c	397	TYR	Sidechain
5	c	414	TYR	Sidechain
5	c	425	TYR	Sidechain
5	c	446	ASP	Peptide
5	c	456	THR	Peptide
5	c	459	PHE	Sidechain
5	c	509	ARG	Sidechain
5	c	548	TYR	Sidechain

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Mol	Chain	Res	Type	Group
5	c	579	ARG	Sidechain
5	c	583	SER	Peptide
5	c	634	ILE	Peptide
5	c	645	TYR	Peptide
5	c	648	TYR	Peptide
5	c	649	LYS	Peptide
5	c	650	HIS	Peptide
5	c	783	ARG	Sidechain
6	d	112	TYR	Sidechain
6	d	131	LYS	Peptide
6	d	221	TYR	Sidechain
6	d	229	ARG	Sidechain
6	d	8	HIS	Sidechain
7	e	112	TYR	Sidechain
7	e	113	SER	Peptide
7	e	174	CYS	Peptide
7	e	196	ARG	Sidechain
7	e	305	GLY	Peptide
7	e	323	GLY	Peptide
7	e	324	ASP	Peptide
7	e	332	LYS	Peptide
7	e	68	TYR	Peptide
8	f	163	ARG	Sidechain
8	f	259	TYR	Sidechain
8	f	269	GLY	Peptide
8	f	335	HIS	Sidechain
8	f	391	HIS	Sidechain
8	f	432	TYR	Sidechain
8	f	482	ARG	Peptide,Sidechain
8	f	653	TYR	Sidechain
8	f	676	LYS	Peptide
8	f	683	PHE	Sidechain
8	f	686	GLU	Peptide
8	f	714	TYR	Sidechain
8	f	73	ARG	Sidechain
8	f	99	TYR	Sidechain
9	g	1044	ARG	Sidechain
9	g	106	TYR	Sidechain
9	g	1060	HIS	Sidechain
9	g	1094	TYR	Sidechain
9	g	1099	TYR	Sidechain
9	g	1102	PHE	Sidechain

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Mol	Chain	Res	Type	Group
9	g	112	SER	Peptide
9	g	113	THR	Peptide
9	g	118	PRO	Peptide
9	g	120	ILE	Peptide
9	g	142	PHE	Peptide
9	g	145	THR	Peptide
9	g	146	MET	Peptide
9	g	175	TYR	Sidechain
9	g	234	ARG	Sidechain
9	g	271	ARG	Sidechain
9	g	284	TYR	Sidechain
9	g	316	ILE	Peptide
9	g	352	TYR	Sidechain
9	g	361	TYR	Sidechain
9	g	378	PHE	Peptide
9	g	380	THR	Peptide
9	g	420	PHE	Peptide
9	g	437	TYR	Sidechain
9	g	441	ARG	Sidechain
9	g	447	VAL	Peptide
9	g	466	TYR	Sidechain
9	g	477	PHE	Sidechain
9	g	497	HIS	Peptide
9	g	503	TYR	Sidechain
9	g	526	SER	Peptide
9	g	574	ASN	Peptide
9	g	579	ILE	Peptide
9	g	621	TYR	Peptide
9	g	627	GLU	Peptide
9	g	628	HIS	Peptide
9	g	654	VAL	Peptide
9	g	659	PRO	Peptide
9	g	692	GLU	Peptide
9	g	709	PHE	Sidechain
9	g	713	ASP	Peptide
9	g	714	TYR	Sidechain
9	g	750	TYR	Sidechain
9	g	790	HIS	Peptide
9	g	797	LEU	Peptide
9	g	843	PHE	Sidechain
9	g	845	PHE	Sidechain
9	g	881	LYS	Peptide

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Mol	Chain	Res	Type	Group
9	g	89	TYR	Sidechain
9	g	936	LYS	Peptide
9	g	945	ARG	Sidechain
9	g	949	TYR	Sidechain
9	g	96	TYR	Sidechain
9	g	981	ARG	Sidechain
3	l	1	MET	Peptide
3	l	1010	PHE	Sidechain
3	l	156	TYR	Sidechain
3	l	199	PHE	Peptide
3	l	204	TYR	Sidechain
3	l	212	PHE	Sidechain
3	l	264	ASP	Peptide
3	l	283	TYR	Sidechain
3	l	295	ASN	Peptide
3	l	338	ARG	Peptide
3	l	348	TYR	Sidechain
3	l	415	TYR	Sidechain
3	l	466	TYR	Sidechain
3	l	484	TYR	Sidechain
3	l	485	LYS	Peptide
3	l	490	VAL	Mainchain
3	l	495	TYR	Sidechain
3	l	571	PHE	Sidechain
3	l	601	PHE	Sidechain
3	l	627	TYR	Sidechain
3	l	628	ARG	Sidechain
3	l	659	TYR	Sidechain
3	l	688	PHE	Sidechain
3	l	698	LEU	Peptide
3	l	70	TYR	Sidechain
3	l	710	TYR	Sidechain
3	l	72	PHE	Sidechain
3	l	720	PHE	Peptide,Sidechain
3	l	724	PHE	Sidechain
3	l	725	ARG	Sidechain
3	l	75	ARG	Sidechain
3	l	751	ARG	Sidechain
3	l	769	ASN	Peptide
3	l	798	LYS	Peptide
3	l	81	PHE	Sidechain
3	l	824	PHE	Sidechain

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Mol	Chain	Res	Type	Group
3	l	825	TYR	Sidechain
3	l	851	TYR	Peptide
3	l	862	GLN	Peptide
3	l	880	ARG	Peptide
3	l	883	GLU	Peptide
3	l	887	ASP	Peptide
3	l	916	ARG	Sidechain
3	l	924	ARG	Peptide
3	l	929	HIS	Sidechain
3	l	941	ASP	Peptide
3	l	965	TYR	Peptide
3	l	984	TYR	Sidechain
3	l	992	ASP	Peptide
4	m	158	PHE	Sidechain
4	m	189	TYR	Sidechain
4	m	190	PHE	Peptide
4	m	218	GLU	Peptide
4	m	239	VAL	Peptide
4	m	244	TYR	Sidechain
4	m	245	PHE	Sidechain
4	m	255	ARG	Sidechain
4	m	265	ILE	Peptide
4	m	344	ARG	Sidechain
4	m	362	LEU	Peptide
4	m	511	TYR	Peptide
4	m	528	GLU	Peptide
4	m	545	GLN	Peptide
4	m	564	LYS	Peptide
4	m	571	TYR	Sidechain
4	m	593	ALA	Peptide
4	m	625	ALA	Peptide
4	m	629	VAL	Mainchain
4	m	652	LEU	Peptide
4	m	655	PHE	Peptide
4	m	657	TYR	Peptide
4	m	658	LEU	Peptide
4	m	659	PRO	Peptide
4	m	662	TYR	Peptide
4	m	675	PHE	Peptide
4	m	69	PHE	Sidechain
4	m	717	ASP	Peptide
4	m	87	LYS	Peptide

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Mol	Chain	Res	Type	Group
5	n	148	TYR	Sidechain
5	n	153	PHE	Sidechain
5	n	163	ASP	Peptide
5	n	181	ARG	Sidechain
5	n	217	PHE	Sidechain
5	n	246	TYR	Sidechain
5	n	248	TYR	Sidechain
5	n	250	THR	Peptide
5	n	305	ARG	Sidechain
5	n	323	SER	Peptide
5	n	324	TYR	Sidechain
5	n	325	LEU	Peptide
5	n	333	ARG	Sidechain
5	n	397	TYR	Sidechain
5	n	425	TYR	Sidechain
5	n	441	ARG	Sidechain
5	n	483	PHE	Sidechain
5	n	492	PHE	Sidechain
5	n	496	PHE	Peptide,Sidechain
5	n	498	ASN	Peptide
5	n	551	ASN	Peptide
5	n	552	TYR	Sidechain
5	n	607	ARG	Sidechain
5	n	611	SER	Peptide
5	n	629	GLU	Peptide
5	n	648	TYR	Peptide
5	n	649	LYS	Peptide
6	o	108	ALA	Peptide
6	o	110	HIS	Peptide
6	o	140	ILE	Peptide
6	o	187	TYR	Peptide,Sidechain
6	o	194	TYR	Sidechain
6	o	20	TYR	Sidechain
6	o	273	GLY	Peptide
6	o	288	LYS	Peptide
6	o	67	GLY	Peptide
6	o	75	TYR	Sidechain
7	p	112	TYR	Sidechain
7	p	116	PHE	Sidechain
7	p	120	HIS	Sidechain
7	p	164	HIS	Sidechain
7	p	17	TYR	Sidechain

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Mol	Chain	Res	Type	Group
7	p	194	TYR	Sidechain
7	p	196	ARG	Sidechain
7	p	20	TYR	Sidechain
7	p	226	ARG	Sidechain
7	p	27	CYS	Peptide
7	p	309	SER	Peptide
7	p	32	HIS	Sidechain
8	q	11	ARG	Sidechain
8	q	180	PHE	Sidechain
8	q	248	TYR	Sidechain
8	q	279	TYR	Peptide
8	q	344	ARG	Sidechain
8	q	387	ARG	Sidechain
8	q	42	PHE	Sidechain
8	q	426	TYR	Sidechain
8	q	453	GLU	Peptide
8	q	469	ARG	Sidechain
8	q	506	ILE	Peptide
8	q	576	ASN	Mainchain
8	q	587	TYR	Sidechain
8	q	597	TYR	Sidechain
8	q	604	VAL	Peptide
8	q	623	PHE	Sidechain
8	q	73	ARG	Sidechain
8	q	97	HIS	Peptide
8	q	99	TYR	Sidechain
9	r	1094	TYR	Sidechain
9	r	1099	TYR	Sidechain
9	r	1102	PHE	Sidechain
9	r	144	ALA	Mainchain
9	r	203	SER	Mainchain
9	r	259	LYS	Mainchain
9	r	297	LEU	Mainchain
9	r	340	GLN	Mainchain
9	r	352	TYR	Mainchain
9	r	389	SER	Mainchain
9	r	403	GLN	Mainchain
9	r	431	SER	Mainchain
9	r	539	PHE	Sidechain
9	r	570	PHE	Sidechain
9	r	577	TYR	Sidechain
9	r	621	TYR	Sidechain

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Mol	Chain	Res	Type	Group
9	r	678	TYR	Sidechain
9	r	690	ARG	Sidechain
9	r	691	TYR	Sidechain
9	r	712	PHE	Sidechain
9	r	72	LEU	Mainchain
9	r	732	GLU	Peptide
9	r	753	PHE	Sidechain
9	r	790	HIS	Sidechain
9	r	80	PHE	Mainchain
9	r	835	PHE	Peptide
9	r	850	TYR	Peptide
9	r	853	LYS	Peptide
9	r	862	PHE	Peptide
9	r	867	GLN	Peptide
9	r	882	TYR	Sidechain
9	r	89	TYR	Mainchain
9	r	890	GLN	Peptide

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	X	9208	0	9538	158	0
2	Y	315	0	65	0	0
2	Z	315	0	65	0	0
3	a	8279	0	8125	34	0
3	l	8279	0	8121	40	0
4	b	5424	0	5397	16	0
4	m	5384	0	5361	11	0
5	c	4520	0	4539	16	0
5	n	4505	0	4521	21	0
6	d	2160	0	2096	9	0
6	o	2160	0	2096	14	0
7	e	2438	0	2378	5	0
7	p	2438	0	2378	8	0
8	f	5261	0	5261	30	0
8	q	5254	0	5252	23	0
9	g	8627	0	8539	47	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
9	r	8575	0	8472	1256	0
All	All	83142	0	82204	1659	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 10.

All (1659) 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)
9:r:334:TRP:CZ3	9:r:336:SER:HB2	1.23	1.67
9:r:284:TYR:CG	9:r:292:PHE:HZ	1.12	1.66
9:r:207:LYS:HG2	9:r:229:PHE:CD2	1.16	1.65
9:r:284:TYR:HB3	9:r:292:PHE:CZ	1.27	1.65
9:r:284:TYR:CD2	9:r:292:PHE:CZ	1.82	1.64
9:r:92:MET:HB2	9:r:460:TYR:CE1	1.12	1.62
9:r:284:TYR:CD2	9:r:292:PHE:CE2	1.76	1.62
9:r:142:PHE:CE1	9:r:160:GLU:HG2	1.13	1.60
9:r:98:LEU:HD11	9:r:105:VAL:CG1	1.31	1.59
9:r:115:LYS:C	9:r:118:PRO:HD2	1.18	1.57
9:r:276:LEU:HD22	9:r:343:SER:CB	1.15	1.56
9:r:268:VAL:HG13	9:r:340:GLN:CB	1.30	1.54
9:r:284:TYR:CB	9:r:292:PHE:CZ	1.84	1.54
9:r:442:LYS:HD2	9:r:520:ILE:CG2	1.06	1.53
9:r:86:LEU:HD11	9:r:101:ASP:CG	1.30	1.53
9:r:104:LYS:HD3	9:r:106:TYR:CE2	1.39	1.53
9:r:284:TYR:HD2	9:r:292:PHE:CE2	0.84	1.52
9:r:426:ILE:CG2	9:r:428:GLN:HE21	1.22	1.52
9:r:403:GLN:CG	9:r:413:VAL:HG11	1.27	1.52
9:r:334:TRP:CH2	9:r:336:SER:HB2	1.41	1.51
9:r:268:VAL:HG13	9:r:340:GLN:CG	1.10	1.51
1:X:745:HIS:CE1	1:X:749:ILE:HG22	1.41	1.50
9:r:429:VAL:CG1	9:r:443:TRP:HE1	1.23	1.50
9:r:442:LYS:CA	9:r:522:LEU:N	1.75	1.50
3:l:207:SER:CB	3:l:236:VAL:HG22	1.43	1.49
9:r:276:LEU:CD2	9:r:343:SER:CB	1.88	1.49
9:r:429:VAL:HG22	9:r:443:TRP:CZ2	1.45	1.48
9:r:142:PHE:CE1	9:r:160:GLU:CG	1.97	1.47
9:r:416:ILE:CG2	9:r:428:GLN:C	1.83	1.46
9:r:98:LEU:CD2	9:r:138:CYS:SG	2.02	1.46
9:r:467:VAL:CG2	9:r:477:PHE:HE2	1.25	1.45
9:r:442:LYS:HB2	9:r:523:ASP:N	1.24	1.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:268:VAL:CG1	9:r:340:GLN:CB	1.95	1.44
9:r:115:LYS:O	9:r:118:PRO:CD	1.66	1.44
9:r:321:GLN:HB3	9:r:331:LEU:CD2	1.44	1.43
9:r:442:LYS:CD	9:r:520:ILE:HG23	0.95	1.43
9:r:207:LYS:CB	9:r:229:PHE:CE2	2.01	1.43
9:r:268:VAL:CG1	9:r:340:GLN:HG2	1.47	1.42
9:r:403:GLN:HG2	9:r:413:VAL:CG1	1.48	1.42
9:r:429:VAL:HG22	9:r:443:TRP:CE2	1.55	1.41
9:r:268:VAL:CG1	9:r:340:GLN:HA	1.47	1.41
9:r:352:TYR:CE1	9:r:356:CYS:CB	1.94	1.41
9:r:467:VAL:CG2	9:r:477:PHE:CE2	2.04	1.40
9:r:207:LYS:NZ	9:r:227:ARG:HE	1.06	1.40
9:r:86:LEU:CD2	9:r:101:ASP:HA	1.49	1.40
9:r:352:TYR:CE1	9:r:356:CYS:HB2	1.29	1.39
9:r:442:LYS:CB	9:r:523:ASP:H	1.33	1.39
9:r:276:LEU:CD2	9:r:343:SER:HB3	1.48	1.38
9:r:143:PRO:CD	9:r:159:ASP:O	1.71	1.38
9:r:429:VAL:CG2	9:r:443:TRP:CZ2	2.08	1.37
3:l:207:SER:HG	3:l:246:TRP:CD1	1.42	1.36
9:r:67:TYR:O	9:r:500:GLN:CB	1.72	1.35
9:r:207:LYS:CG	9:r:229:PHE:CD2	1.84	1.35
9:r:429:VAL:HG13	9:r:443:TRP:NE1	1.40	1.35
9:r:478:PHE:CE2	9:r:497:HIS:CE1	2.15	1.34
9:r:442:LYS:HG3	9:r:521:SER:N	1.42	1.34
9:r:268:VAL:CG1	9:r:340:GLN:CA	2.05	1.33
9:r:416:ILE:HG23	9:r:428:GLN:C	1.40	1.33
9:r:212:LEU:HD21	9:r:272:ASN:CB	1.57	1.33
9:r:228:ILE:N	9:r:248:LEU:HD22	1.40	1.33
9:r:142:PHE:HE1	9:r:160:GLU:CG	1.35	1.32
1:X:319:PRO:HD2	1:X:357:ASP:OD2	1.22	1.32
9:r:291:ILE:CG2	9:r:309:ASP:OD1	1.77	1.32
9:r:104:LYS:NZ	9:r:106:TYR:OH	1.64	1.31
3:l:207:SER:HB2	3:l:236:VAL:CG2	1.60	1.31
9:r:86:LEU:CD1	9:r:101:ASP:CB	2.09	1.31
9:r:129:ASN:OD1	9:r:166:ILE:CD1	1.78	1.31
9:r:268:VAL:CG1	9:r:340:GLN:CG	1.96	1.31
9:r:426:ILE:HG22	9:r:428:GLN:NE2	1.43	1.30
9:r:442:LYS:HD2	9:r:520:ILE:CB	1.54	1.30
9:r:67:TYR:N	9:r:501:ALA:HB2	1.42	1.30
9:r:442:LYS:HE3	9:r:444:GLU:OE2	1.18	1.29
9:r:212:LEU:CD2	9:r:272:ASN:HB2	1.60	1.29

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:334:TRP:CH2	9:r:336:SER:CB	2.14	1.29
9:r:321:GLN:CB	9:r:331:LEU:HD22	1.63	1.28
9:r:426:ILE:CG2	9:r:428:GLN:NE2	1.91	1.28
9:r:284:TYR:CB	9:r:292:PHE:HZ	1.28	1.28
9:r:444:GLU:OE2	9:r:520:ILE:CD1	1.80	1.27
9:r:478:PHE:CD2	9:r:497:HIS:CE1	2.22	1.27
9:r:183:ASN:O	9:r:198:LEU:HD12	1.18	1.27
9:r:207:LYS:CB	9:r:229:PHE:CD2	2.16	1.27
9:r:86:LEU:CD1	9:r:101:ASP:HB2	1.61	1.27
1:X:775:PHE:CE2	1:X:811:ASP:O	1.88	1.26
9:r:152:ALA:HA	9:r:155:PRO:CD	1.64	1.26
9:r:263:THR:CG2	9:r:264:ASN:N	1.90	1.26
9:r:288:ASN:O	9:r:338:PRO:HD2	1.31	1.26
9:r:352:TYR:CD1	9:r:358:GLU:O	1.89	1.26
9:r:291:ILE:HG23	9:r:309:ASP:OD1	1.29	1.25
9:r:334:TRP:CZ3	9:r:336:SER:CB	2.18	1.25
9:r:267:VAL:CG1	9:r:271:ARG:HH11	1.47	1.25
9:r:276:LEU:HD11	9:r:404:MET:CE	1.66	1.25
9:r:67:TYR:O	9:r:500:GLN:HB3	1.06	1.24
9:r:228:ILE:N	9:r:248:LEU:CD2	1.98	1.24
9:r:442:LYS:CG	9:r:521:SER:H	1.49	1.24
9:r:143:PRO:HD2	9:r:159:ASP:C	1.63	1.23
9:r:396:LYS:C	9:r:397:PRO:CD	2.11	1.23
9:r:147:ASP:HA	9:r:150:PRO:CD	1.69	1.23
9:r:174:TYR:CE2	9:r:233:ILE:HG13	1.73	1.23
9:r:284:TYR:CG	9:r:292:PHE:CZ	1.97	1.23
9:r:284:TYR:HB3	9:r:292:PHE:CE1	1.74	1.23
9:r:300:THR:O	9:r:300:THR:CG2	1.76	1.22
9:r:348:LEU:HD22	9:r:399:ILE:CD1	1.69	1.22
9:r:98:LEU:CD1	9:r:105:VAL:CG1	2.15	1.22
9:r:92:MET:CA	9:r:460:TYR:CZ	2.22	1.22
9:r:129:ASN:ND2	9:r:166:ILE:HG12	1.52	1.22
9:r:442:LYS:CA	9:r:522:LEU:H	1.44	1.22
9:r:267:VAL:HG11	9:r:271:ARG:NH1	1.55	1.21
9:r:438:SER:O	9:r:439:MET:HG2	1.41	1.21
9:r:207:LYS:NZ	9:r:227:ARG:NE	1.87	1.20
9:r:361:TYR:CE2	9:r:397:PRO:HG3	1.77	1.20
9:r:403:GLN:CG	9:r:413:VAL:CG1	2.08	1.19
9:r:442:LYS:HA	9:r:521:SER:C	1.67	1.19
9:r:418:VAL:HG21	9:r:465:LEU:CD2	1.70	1.19
9:r:467:VAL:HG23	9:r:477:PHE:CE2	1.69	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:352:TYR:HE1	9:r:356:CYS:CB	1.35	1.18
9:r:442:LYS:HA	9:r:522:LEU:N	0.86	1.18
9:r:86:LEU:HD13	9:r:101:ASP:CB	1.72	1.18
9:r:92:MET:HB3	9:r:460:TYR:OH	1.00	1.17
9:r:98:LEU:HD22	9:r:138:CYS:SG	1.75	1.17
9:r:210:LEU:HD11	9:r:270:LEU:HD12	1.17	1.17
9:r:261:PHE:CE2	9:r:286:THR:O	1.84	1.17
9:r:429:VAL:CG2	9:r:443:TRP:HZ2	1.47	1.17
9:r:115:LYS:C	9:r:118:PRO:CD	2.12	1.17
9:r:210:LEU:HD21	9:r:270:LEU:CD1	1.73	1.17
9:r:284:TYR:CE2	9:r:344:SER:HB2	1.80	1.17
9:r:286:THR:HG22	9:r:287:THR:N	1.43	1.17
9:r:410:THR:CG2	9:r:411:ASN:N	2.05	1.17
9:r:68:ILE:CA	9:r:500:GLN:HG3	1.75	1.16
9:r:115:LYS:O	9:r:118:PRO:HD2	1.03	1.16
9:r:410:THR:HG22	9:r:411:ASN:N	1.26	1.15
9:r:467:VAL:HG21	9:r:477:PHE:CE2	1.71	1.15
9:r:86:LEU:HD11	9:r:101:ASP:CB	1.72	1.15
9:r:338:PRO:N	9:r:338:PRO:CD	2.08	1.15
9:r:99:VAL:HG23	9:r:108:TRP:HZ3	1.10	1.14
9:r:247:LEU:HD21	9:r:293:GLN:CD	1.71	1.14
9:r:165:ILE:HG13	9:r:221:LEU:HD13	1.23	1.14
9:r:276:LEU:CD2	9:r:343:SER:HB2	1.62	1.14
9:r:324:TYR:CE1	9:r:360:TYR:CB	2.31	1.14
1:X:745:HIS:CE1	1:X:749:ILE:CG2	2.32	1.13
9:r:129:ASN:OD1	9:r:166:ILE:HD11	0.95	1.13
9:r:357:ASN:O	9:r:390:ILE:N	1.79	1.13
9:r:68:ILE:HA	9:r:500:GLN:HG3	1.14	1.13
9:r:416:ILE:HG22	9:r:428:GLN:O	1.37	1.13
1:X:813:ILE:HG23	1:X:816:ALA:HB3	1.14	1.12
9:r:207:LYS:HB3	9:r:229:PHE:CD2	1.81	1.13
9:r:403:GLN:CD	9:r:413:VAL:HG11	1.73	1.12
9:r:472:MET:HB2	9:r:475:LEU:HD11	1.19	1.13
9:r:89:TYR:OH	9:r:107:ILE:HG12	1.48	1.12
9:r:227:ARG:HD3	9:r:252:PHE:HB2	1.23	1.12
9:r:147:ASP:HA	9:r:150:PRO:HD3	1.16	1.12
9:r:222:SER:OG	9:r:270:LEU:CD1	1.96	1.12
9:r:399:ILE:HG23	9:r:417:LEU:HD21	1.31	1.12
1:X:319:PRO:HD2	1:X:357:ASP:CG	1.74	1.12
9:r:68:ILE:HG21	9:r:70:LYS:CE	1.79	1.12
9:r:319:SER:CB	9:r:381:TYR:CE2	2.33	1.12

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:325:PRO:O	9:r:325:PRO:HG2	1.35	1.11
9:r:143:PRO:HD2	9:r:159:ASP:O	1.33	1.11
9:r:418:VAL:HG21	9:r:465:LEU:HD22	1.26	1.11
9:r:137:ARG:HD3	9:r:167:ILE:HG13	1.31	1.11
9:r:210:LEU:HD21	9:r:270:LEU:CG	1.81	1.11
9:r:321:GLN:NE2	9:r:334:TRP:HB3	1.64	1.11
9:r:472:MET:CB	9:r:475:LEU:HD11	1.82	1.10
9:r:429:VAL:CG1	9:r:443:TRP:NE1	2.01	1.10
9:r:68:ILE:HA	9:r:500:GLN:CG	1.81	1.10
9:r:104:LYS:CD	9:r:106:TYR:CE2	2.33	1.10
9:r:280:THR:HG22	9:r:281:ARG:N	1.34	1.10
9:r:429:VAL:HG12	9:r:440:ARG:HB3	1.24	1.10
1:X:323:TYR:OH	1:X:359:LEU:HB3	1.51	1.10
9:r:267:VAL:CG1	9:r:271:ARG:NH1	2.10	1.10
9:r:268:VAL:CB	9:r:340:GLN:HG2	1.79	1.09
9:r:98:LEU:CD1	9:r:105:VAL:HG13	1.81	1.09
9:r:263:THR:HG22	9:r:264:ASN:N	1.12	1.09
9:r:371:SER:HB2	9:r:374:SER:O	1.49	1.09
1:X:813:ILE:HG23	1:X:816:ALA:CB	1.82	1.09
1:X:813:ILE:CG2	1:X:816:ALA:HB3	1.83	1.09
9:r:143:PRO:HD2	9:r:159:ASP:CA	1.82	1.09
9:r:467:VAL:HG23	9:r:477:PHE:HE2	0.94	1.09
9:g:774:PHE:CZ	9:g:777:ILE:HD13	1.85	1.09
9:r:268:VAL:HG22	9:r:340:GLN:HG3	1.25	1.09
9:r:319:SER:HB3	9:r:381:TYR:CE2	1.88	1.09
9:r:368:PHE:HE1	9:r:375:PHE:CD1	1.71	1.09
9:r:444:GLU:OE2	9:r:520:ILE:HD13	1.30	1.09
9:r:67:TYR:N	9:r:501:ALA:CB	2.16	1.08
9:r:123:PRO:CD	9:r:123:PRO:N	2.17	1.08
9:r:267:VAL:HG12	9:r:267:VAL:O	1.45	1.08
9:r:412:GLU:HA	9:r:478:PHE:CE1	1.87	1.08
9:r:429:VAL:HG13	9:r:443:TRP:CD1	1.88	1.08
9:r:442:LYS:CE	9:r:444:GLU:OE2	2.02	1.08
9:r:227:ARG:C	9:r:248:LEU:CD2	2.22	1.08
9:r:268:VAL:HG12	9:r:340:GLN:HA	1.09	1.08
9:r:267:VAL:HG13	9:r:271:ARG:HH11	1.14	1.07
9:r:324:TYR:HE1	9:r:360:TYR:HB3	1.16	1.07
9:r:86:LEU:O	9:r:456:ILE:HG23	1.53	1.07
9:r:139:ILE:HD11	9:r:219:ILE:CG2	1.84	1.07
9:r:228:ILE:H	9:r:248:LEU:CG	1.50	1.07
9:r:348:LEU:HD22	9:r:399:ILE:HD11	1.29	1.07

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:478:PHE:CE2	9:r:497:HIS:HE1	1.58	1.07
1:X:684:LYS:CG	1:X:744:LEU:HB2	1.83	1.07
9:r:86:LEU:CD1	9:r:101:ASP:CG	2.23	1.06
9:r:152:ALA:HA	9:r:155:PRO:HD2	1.12	1.06
9:r:346:LEU:HD21	9:r:417:LEU:HD22	1.31	1.06
9:r:98:LEU:HD21	9:r:138:CYS:SG	1.93	1.06
9:r:152:ALA:CA	9:r:155:PRO:HD2	1.84	1.06
9:r:442:LYS:CG	9:r:521:SER:N	2.11	1.06
9:r:207:LYS:HZ2	9:r:227:ARG:NE	1.51	1.06
9:r:225:MET:SD	9:r:260:ILE:CG1	2.43	1.06
9:r:321:GLN:HE21	9:r:334:TRP:HB2	1.19	1.06
9:r:271:ARG:HG2	9:r:343:SER:HA	1.30	1.06
9:r:324:TYR:HE1	9:r:360:TYR:CB	1.65	1.06
3:l:207:SER:O	3:l:236:VAL:HG23	1.56	1.06
9:r:167:ILE:O	9:r:208:CYS:HB2	1.55	1.06
9:r:342:GLU:OE2	9:r:401:ILE:CB	2.01	1.06
3:l:207:SER:OG	3:l:246:TRP:HD1	1.37	1.05
9:r:67:TYR:C	9:r:500:GLN:HB2	1.80	1.05
9:r:288:ASN:O	9:r:338:PRO:CD	2.03	1.05
9:r:320:LEU:HD23	9:r:381:TYR:CD1	1.90	1.05
9:r:321:GLN:HE21	9:r:334:TRP:CB	1.68	1.05
9:g:1016:PHE:CZ	9:r:253:LYS:NZ	2.25	1.05
9:r:227:ARG:HB3	9:r:248:LEU:HD21	1.10	1.05
9:r:316:ILE:HB	9:r:381:TYR:OH	1.56	1.05
9:r:86:LEU:HD13	9:r:101:ASP:HB2	1.05	1.05
9:r:86:LEU:O	9:r:456:ILE:CG2	2.04	1.05
9:r:321:GLN:NE2	9:r:334:TRP:CB	2.19	1.05
9:r:416:ILE:HD11	9:r:441:ARG:O	1.55	1.05
3:l:207:SER:O	3:l:236:VAL:CG2	2.03	1.05
9:r:280:THR:CG2	9:r:281:ARG:N	2.13	1.05
9:r:442:LYS:CD	9:r:520:ILE:CG2	1.85	1.05
9:r:261:PHE:CD2	9:r:286:THR:O	2.09	1.04
9:r:284:TYR:HD2	9:r:292:PHE:CZ	1.45	1.04
9:r:210:LEU:CD1	9:r:270:LEU:HD12	1.88	1.04
9:r:136:PRO:N	9:r:136:PRO:CD	2.21	1.03
9:r:276:LEU:HD22	9:r:343:SER:HB2	1.18	1.03
9:r:296:GLN:HB2	9:r:307:LEU:HD11	1.36	1.03
9:r:416:ILE:CB	9:r:428:GLN:O	2.06	1.03
9:r:170:SER:HB3	9:r:203:SER:HB2	1.36	1.03
9:r:352:TYR:HE1	9:r:356:CYS:HB3	1.19	1.03
9:r:391:THR:OG1	9:r:392:ASP:N	1.72	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:321:GLN:HB3	9:r:331:LEU:HD22	1.04	1.03
9:r:442:LYS:HD3	9:r:520:ILE:HG23	1.08	1.02
9:r:143:PRO:CD	9:r:143:PRO:N	2.22	1.02
9:r:397:PRO:CD	9:r:397:PRO:N	2.17	1.02
9:r:399:ILE:CG2	9:r:417:LEU:HD11	1.89	1.02
9:r:421:PRO:N	9:r:421:PRO:CD	2.21	1.02
9:r:368:PHE:CZ	9:r:375:PHE:CE1	2.46	1.02
9:r:430:ASN:H	9:r:440:ARG:NE	1.55	1.02
9:r:268:VAL:HG13	9:r:340:GLN:CA	1.78	1.02
9:r:276:LEU:HD23	9:r:343:SER:HB3	1.34	1.02
9:r:430:ASN:N	9:r:440:ARG:HE	1.58	1.02
9:r:227:ARG:CB	9:r:248:LEU:HD21	1.78	1.02
9:r:286:THR:CG2	9:r:287:THR:N	2.21	1.02
9:g:1016:PHE:CE2	9:r:253:LYS:NZ	2.28	1.01
9:r:67:TYR:C	9:r:500:GLN:CB	2.31	1.01
9:r:412:GLU:HA	9:r:478:PHE:CZ	1.94	1.01
9:r:145:THR:OG1	9:r:146:MET:N	1.60	1.01
9:r:210:LEU:HD21	9:r:270:LEU:HD12	1.34	1.01
9:r:183:ASN:O	9:r:198:LEU:CD1	2.09	1.01
9:r:429:VAL:CG2	9:r:443:TRP:CE2	2.36	1.01
1:X:745:HIS:ND1	1:X:749:ILE:HG22	1.76	1.00
9:r:227:ARG:HH12	9:r:249:ASN:HA	1.24	1.00
9:r:240:PRO:CD	9:r:240:PRO:N	2.22	1.00
9:r:76:TYR:CD2	9:r:78:SER:N	2.27	1.00
9:r:142:PHE:CD1	9:r:160:GLU:HG2	1.96	1.00
9:r:444:GLU:CG	9:r:519:GLU:O	2.08	1.00
9:r:447:VAL:HG21	9:r:508:ASN:OD1	1.60	1.00
9:r:104:LYS:CD	9:r:106:TYR:HE2	1.72	1.00
9:r:225:MET:SD	9:r:260:ILE:HG12	2.00	1.00
9:r:129:ASN:HD21	9:r:166:ILE:HG12	1.21	1.00
9:r:276:LEU:HD23	9:r:343:SER:O	1.62	1.00
9:r:276:LEU:HD11	9:r:404:MET:HE2	1.42	0.99
9:r:426:ILE:HG21	9:r:428:GLN:NE2	1.72	0.99
9:r:442:LYS:HG2	9:r:520:ILE:HA	1.44	0.99
9:r:68:ILE:CG2	9:r:70:LYS:HE3	1.91	0.99
9:r:416:ILE:CG2	9:r:428:GLN:O	0.69	0.99
9:r:401:ILE:HG12	9:r:417:LEU:HD13	1.38	0.99
1:X:380:THR:HG22	1:X:411:PHE:O	1.61	0.99
9:r:401:ILE:CG1	9:r:417:LEU:HD13	1.92	0.99
9:r:341:ASP:OD1	9:r:347:PHE:CE1	2.15	0.99
9:r:86:LEU:HD22	9:r:101:ASP:HA	1.03	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:98:LEU:CD1	9:r:105:VAL:HG12	1.91	0.99
9:r:334:TRP:HE1	9:r:351:ILE:HB	1.18	0.99
9:r:352:TYR:CD1	9:r:356:CYS:HB2	1.98	0.99
9:r:115:LYS:O	9:r:118:PRO:CG	2.10	0.99
9:r:139:ILE:HD13	9:r:211:MET:HG3	1.42	0.99
9:r:368:PHE:CE1	9:r:375:PHE:CD1	2.49	0.99
9:r:429:VAL:CG1	9:r:440:ARG:HB3	1.91	0.99
9:r:68:ILE:HG21	9:r:70:LYS:HE3	1.02	0.98
9:r:69:VAL:HG23	9:r:504:PHE:CZ	1.98	0.98
9:r:359:THR:HG1	9:r:395:PHE:HE1	1.00	0.98
9:r:429:VAL:HG22	9:r:443:TRP:NE1	1.77	0.98
3:l:207:SER:OG	3:l:246:TRP:CD1	2.10	0.98
9:r:209:ASP:HB2	9:r:223:THR:CA	1.90	0.98
9:r:393:THR:O	9:r:394:LYS:CB	2.12	0.98
9:r:227:ARG:CD	9:r:252:PHE:HB2	1.93	0.98
9:r:247:LEU:HD21	9:r:293:GLN:OE1	1.63	0.98
9:r:320:LEU:CD2	9:r:381:TYR:CD1	2.46	0.98
9:r:247:LEU:HD22	9:r:293:GLN:HB3	1.45	0.98
9:r:442:LYS:CB	9:r:522:LEU:H	1.75	0.98
9:r:86:LEU:HD22	9:r:101:ASP:CA	1.92	0.98
9:r:228:ILE:H	9:r:248:LEU:CB	1.77	0.98
9:r:327:ALA:O	9:r:330:THR:OG1	1.80	0.98
9:r:152:ALA:CA	9:r:155:PRO:CD	2.41	0.98
9:r:122:VAL:HG23	9:r:124:PHE:CE2	1.99	0.98
9:r:418:VAL:CG2	9:r:465:LEU:HD22	1.94	0.98
9:r:324:TYR:CE1	9:r:360:TYR:HB2	1.99	0.98
9:r:224:ASN:O	9:r:260:ILE:HG23	1.62	0.97
9:r:99:VAL:HG23	9:r:108:TRP:CZ3	1.99	0.97
9:r:161:THR:HG22	9:r:176:GLU:O	1.64	0.97
9:r:319:SER:HB2	9:r:381:TYR:CE2	1.98	0.97
9:r:207:LYS:HB3	9:r:229:PHE:HD2	1.23	0.97
9:r:368:PHE:CE1	9:r:375:PHE:CE1	2.53	0.97
9:r:429:VAL:CG2	9:r:443:TRP:NE1	2.28	0.97
9:r:98:LEU:HD11	9:r:105:VAL:HG12	1.47	0.97
9:r:267:VAL:CG1	9:r:267:VAL:O	2.12	0.97
8:f:27:ASN:N	8:f:435:PHE:CE1	2.32	0.97
9:r:352:TYR:CD2	9:r:390:ILE:HD13	2.00	0.97
9:r:426:ILE:HG22	9:r:428:GLN:HE21	0.81	0.97
9:r:263:THR:HG22	9:r:264:ASN:CA	1.94	0.96
9:r:342:GLU:OE2	9:r:401:ILE:HB	1.15	0.96
9:r:352:TYR:HD1	9:r:358:GLU:O	1.42	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:478:PHE:HE2	9:r:497:HIS:CE1	1.66	0.96
9:r:382:ARG:NH2	9:r:443:TRP:CZ2	2.33	0.96
9:r:118:PRO:CD	9:r:118:PRO:N	2.27	0.96
9:r:368:PHE:CZ	9:r:375:PHE:HE1	1.82	0.96
9:r:398:LYS:HB2	9:r:420:PHE:CZ	2.01	0.96
9:r:403:GLN:CD	9:r:413:VAL:CG1	2.36	0.96
9:r:129:ASN:CG	9:r:166:ILE:HD11	1.91	0.95
9:r:268:VAL:HG11	9:r:340:GLN:CB	1.91	0.95
3:l:207:SER:CB	3:l:236:VAL:H	1.77	0.95
1:X:684:LYS:HG2	1:X:744:LEU:HB2	1.43	0.95
9:r:429:VAL:HB	9:r:440:ARG:HG3	1.48	0.95
9:r:129:ASN:CG	9:r:166:ILE:CD1	2.39	0.95
9:r:399:ILE:HG22	9:r:417:LEU:HD11	1.45	0.95
9:r:199:PRO:N	9:r:199:PRO:CD	2.29	0.95
9:r:284:TYR:CZ	9:r:344:SER:HB2	2.01	0.94
9:r:418:VAL:CG1	9:r:425:VAL:HG13	1.97	0.94
9:r:227:ARG:C	9:r:248:LEU:HD22	1.88	0.94
9:r:268:VAL:CG1	9:r:340:GLN:HB2	1.97	0.94
9:r:92:MET:CB	9:r:460:TYR:CZ	0.91	0.94
9:r:348:LEU:CD2	9:r:399:ILE:HD11	1.96	0.94
9:r:442:LYS:HA	9:r:522:LEU:CA	1.89	0.94
9:r:96:TYR:CZ	9:r:160:GLU:OE2	2.20	0.94
9:r:174:TYR:CD2	9:r:233:ILE:HG13	2.02	0.94
9:r:444:GLU:HG2	9:r:519:GLU:O	1.67	0.94
9:r:228:ILE:N	9:r:248:LEU:CG	2.10	0.94
9:r:276:LEU:HD22	9:r:343:SER:HB3	1.09	0.94
9:r:325:PRO:O	9:r:325:PRO:CG	1.93	0.94
9:r:208:CYS:C	9:r:223:THR:HA	1.93	0.93
9:r:268:VAL:HG13	9:r:340:GLN:HG2	0.94	0.93
9:r:429:VAL:HA	9:r:440:ARG:HD2	1.49	0.93
9:r:143:PRO:HD2	9:r:159:ASP:HA	1.51	0.93
9:r:208:CYS:O	9:r:223:THR:HA	1.66	0.93
9:r:361:TYR:HE2	9:r:397:PRO:HG3	1.27	0.93
9:r:291:ILE:HG21	9:r:309:ASP:CG	1.94	0.93
9:r:401:ILE:HG12	9:r:417:LEU:CD1	1.98	0.93
1:X:318:HIS:HB3	1:X:357:ASP:OD2	1.69	0.93
9:r:76:TYR:HD2	9:r:78:SER:H	0.94	0.93
9:r:334:TRP:NE1	9:r:351:ILE:HB	1.35	0.93
9:r:416:ILE:HG21	9:r:428:GLN:O	1.14	0.93
9:r:86:LEU:CD2	9:r:101:ASP:CA	2.46	0.92
9:r:284:TYR:CD2	9:r:292:PHE:HE2	1.42	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:286:THR:HG22	9:r:287:THR:H	1.18	0.92
9:r:147:ASP:CA	9:r:150:PRO:CD	2.47	0.92
9:r:393:THR:O	9:r:394:LYS:HG3	1.69	0.92
9:r:86:LEU:HD21	9:r:101:ASP:HA	1.50	0.92
9:r:207:LYS:HG3	9:r:227:ARG:HB3	1.51	0.92
9:r:210:LEU:HD21	9:r:270:LEU:HG	1.50	0.92
9:r:122:VAL:HG21	9:r:178:ILE:HG12	1.49	0.92
9:r:429:VAL:CB	9:r:443:TRP:HE1	1.82	0.92
9:r:478:PHE:CE2	9:r:497:HIS:ND1	2.37	0.92
9:r:226:GLY:O	9:r:248:LEU:CD1	2.16	0.92
9:r:393:THR:O	9:r:394:LYS:CG	2.17	0.92
1:X:380:THR:CG2	1:X:411:PHE:O	2.18	0.92
1:X:684:LYS:HG3	1:X:744:LEU:HB2	1.52	0.92
9:r:418:VAL:HG13	9:r:425:VAL:HG13	1.52	0.92
9:r:209:ASP:HB2	9:r:223:THR:C	1.94	0.91
9:r:276:LEU:HD22	9:r:343:SER:OG	1.70	0.91
9:r:280:THR:CG2	9:r:281:ARG:H	1.79	0.91
3:l:207:SER:HB2	3:l:236:VAL:H	1.35	0.91
9:r:122:VAL:CG2	9:r:124:PHE:CE2	2.53	0.91
9:r:368:PHE:HZ	9:r:375:PHE:HE1	1.10	0.91
9:r:210:LEU:HD11	9:r:222:SER:OG	1.70	0.91
9:r:416:ILE:HG21	9:r:428:GLN:N	1.86	0.91
1:X:775:PHE:HE2	1:X:811:ASP:O	1.45	0.91
9:r:210:LEU:CD2	9:r:270:LEU:HD12	2.00	0.91
9:r:382:ARG:HE	9:r:443:TRP:HZ2	1.14	0.91
9:r:210:LEU:HD11	9:r:270:LEU:CD1	2.00	0.91
9:r:247:LEU:CD2	9:r:293:GLN:CD	2.44	0.91
1:X:745:HIS:HE1	1:X:749:ILE:HG22	1.33	0.91
9:r:90:ILE:HG22	9:r:91:ASP:N	1.85	0.91
9:r:139:ILE:HD11	9:r:219:ILE:HG21	1.51	0.90
9:r:98:LEU:HD13	9:r:107:ILE:CG1	2.01	0.90
9:r:228:ILE:CA	9:r:248:LEU:HD22	2.02	0.90
9:r:68:ILE:HG12	9:r:500:GLN:CG	2.02	0.90
9:r:211:MET:SD	9:r:219:ILE:HD12	2.11	0.90
9:r:346:LEU:CD2	9:r:417:LEU:HD22	2.01	0.90
9:r:400:PHE:O	9:r:417:LEU:HD12	1.71	0.90
9:r:438:SER:O	9:r:439:MET:CG	2.19	0.90
9:r:104:LYS:HD3	9:r:106:TYR:CZ	2.07	0.90
9:r:263:THR:CG2	9:r:265:SER:H	1.85	0.90
9:r:115:LYS:HB3	9:r:118:PRO:HD3	1.54	0.90
9:r:139:ILE:CD1	9:r:219:ILE:CG2	2.49	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:393:THR:O	9:r:394:LYS:HB2	1.71	0.90
9:r:321:GLN:HB3	9:r:331:LEU:HD21	1.53	0.89
9:r:276:LEU:HD11	9:r:404:MET:HE1	1.53	0.89
9:r:334:TRP:NE1	9:r:351:ILE:CB	2.30	0.89
9:r:129:ASN:ND2	9:r:166:ILE:CG1	2.34	0.89
1:X:319:PRO:CD	1:X:357:ASP:OD2	2.16	0.89
9:r:143:PRO:HD3	9:r:159:ASP:O	1.72	0.89
9:r:76:TYR:CE1	9:r:119:TYR:CE2	2.41	0.89
9:r:122:VAL:HG23	9:r:124:PHE:HE2	1.35	0.89
9:r:222:SER:OG	9:r:270:LEU:HD11	1.70	0.89
9:r:227:ARG:HD3	9:r:252:PHE:CB	2.02	0.89
9:r:429:VAL:CG2	9:r:443:TRP:HE1	1.85	0.89
9:r:86:LEU:HD22	9:r:100:ASN:O	1.72	0.89
9:r:268:VAL:CA	9:r:340:GLN:HG2	2.03	0.89
9:r:478:PHE:HD2	9:r:497:HIS:CE1	1.80	0.89
9:r:207:LYS:HZ3	9:r:227:ARG:HE	1.21	0.88
9:r:263:THR:HG22	9:r:264:ASN:H	1.11	0.88
9:r:410:THR:CG2	9:r:411:ASN:H	1.74	0.88
9:r:98:LEU:HD23	9:r:138:CYS:SG	2.12	0.88
9:r:268:VAL:HG22	9:r:340:GLN:CG	2.03	0.88
9:r:165:ILE:HG22	9:r:166:ILE:N	1.88	0.88
9:r:442:LYS:CG	9:r:520:ILE:HA	2.04	0.88
9:r:426:ILE:HG21	9:r:428:GLN:HE21	1.26	0.88
9:r:92:MET:HB2	9:r:460:TYR:CZ	0.70	0.88
9:r:382:ARG:NE	9:r:443:TRP:CZ2	2.41	0.88
9:r:478:PHE:CD2	9:r:497:HIS:ND1	2.40	0.88
9:r:268:VAL:HG11	9:r:340:GLN:HB2	1.51	0.88
9:r:68:ILE:CB	9:r:500:GLN:HG3	2.03	0.87
9:r:291:ILE:HG21	9:r:309:ASP:OD1	1.75	0.87
9:r:165:ILE:CG1	9:r:221:LEU:HD13	2.03	0.87
9:r:346:LEU:HD23	9:r:401:ILE:HD11	1.55	0.87
9:r:68:ILE:CG1	9:r:500:GLN:HG3	2.04	0.87
9:r:92:MET:HB2	9:r:460:TYR:CD1	1.92	0.87
9:r:73:GLN:HB2	9:r:110:ILE:HG23	1.55	0.86
9:r:98:LEU:HD11	9:r:105:VAL:HG13	0.87	0.86
9:r:416:ILE:HG21	9:r:428:GLN:C	1.69	0.86
9:r:429:VAL:HG13	9:r:443:TRP:HE1	0.97	0.86
1:X:319:PRO:CD	1:X:357:ASP:CG	2.49	0.86
9:r:219:ILE:CG1	9:r:231:ILE:HB	2.05	0.86
9:r:467:VAL:HG21	9:r:477:PHE:CZ	2.09	0.86
9:r:226:GLY:O	9:r:248:LEU:HD12	1.74	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:380:THR:CB	1:X:411:PHE:HB3	2.05	0.86
9:r:316:ILE:CB	9:r:381:TYR:OH	2.23	0.86
9:g:1012:GLU:O	9:r:249:ASN:ND2	2.09	0.86
9:r:167:ILE:O	9:r:208:CYS:CB	2.22	0.86
9:r:276:LEU:CD1	9:r:404:MET:CE	2.52	0.86
9:r:401:ILE:CG1	9:r:417:LEU:CD1	2.53	0.86
9:r:382:ARG:NE	9:r:443:TRP:CH2	2.44	0.86
9:r:267:VAL:HG13	9:r:271:ARG:HD2	1.58	0.86
9:r:263:THR:CG2	9:r:264:ASN:H	1.69	0.85
1:X:1096:ILE:HG23	1:X:1097:LEU:HD22	1.58	0.85
9:r:432:LYS:HE2	9:r:440:ARG:HB2	1.56	0.85
8:f:27:ASN:N	8:f:435:PHE:CD1	2.44	0.85
9:r:319:SER:HB3	9:r:381:TYR:CD2	2.11	0.85
9:r:403:GLN:OE1	9:r:413:VAL:HG13	1.74	0.85
9:r:280:THR:HG22	9:r:281:ARG:H	1.03	0.85
9:r:442:LYS:CG	9:r:520:ILE:HG23	2.06	0.85
9:r:413:VAL:HG12	9:r:414:THR:N	1.89	0.85
9:r:423:ALA:O	9:r:449:LEU:HG	1.77	0.85
9:r:412:GLU:CA	9:r:478:PHE:CE1	2.59	0.85
9:r:76:TYR:HD2	9:r:78:SER:N	1.70	0.85
1:X:743:ILE:HG12	1:X:805:LEU:HB2	1.59	0.84
9:r:403:GLN:CB	9:r:414:THR:O	2.25	0.84
9:r:442:LYS:CA	9:r:522:LEU:CA	2.46	0.84
9:r:67:TYR:N	9:r:501:ALA:CA	2.40	0.84
9:r:152:ALA:HA	9:r:155:PRO:HD3	1.57	0.84
1:X:745:HIS:ND1	1:X:749:ILE:CG2	2.36	0.84
9:g:774:PHE:CZ	9:g:777:ILE:CD1	2.61	0.84
9:r:371:SER:CB	9:r:374:SER:O	2.26	0.84
9:r:124:PHE:CZ	9:r:178:ILE:HG13	2.13	0.83
9:r:447:VAL:HG21	9:r:508:ASN:CG	2.02	0.83
9:g:1016:PHE:HZ	9:r:253:LYS:HZ1	1.23	0.83
9:r:207:LYS:HG2	9:r:229:PHE:CG	2.10	0.83
9:r:399:ILE:CG2	9:r:417:LEU:HD21	2.07	0.83
9:r:228:ILE:C	9:r:248:LEU:HD22	2.03	0.83
9:r:291:ILE:CG2	9:r:309:ASP:CG	2.50	0.83
9:r:412:GLU:CA	9:r:478:PHE:HE1	1.92	0.83
9:r:268:VAL:CG2	9:r:340:GLN:HG3	2.05	0.83
9:r:139:ILE:CD1	9:r:219:ILE:HG22	2.07	0.83
9:r:340:GLN:OE1	9:r:399:ILE:HB	1.77	0.83
9:r:377:ILE:HD11	9:r:378:PHE:CE2	2.14	0.83
9:r:247:LEU:CD2	9:r:293:GLN:CB	2.57	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:414:THR:HG22	9:r:441:ARG:HG2	1.59	0.83
9:r:324:TYR:CE1	9:r:360:TYR:HB3	2.05	0.82
9:r:115:LYS:CB	9:r:118:PRO:CD	2.56	0.82
9:r:129:ASN:HD21	9:r:166:ILE:CG1	1.90	0.82
9:r:115:LYS:CB	9:r:118:PRO:HD3	2.09	0.82
9:r:403:GLN:NE2	9:r:406:ASN:HB3	1.94	0.82
9:r:287:THR:OG1	9:r:289:LYS:N	2.10	0.82
9:r:372:SER:O	9:r:373:ASN:HB2	1.77	0.82
9:r:403:GLN:HB3	9:r:414:THR:O	1.79	0.82
1:X:776:TYR:O	1:X:781:ASP:HB2	1.79	0.82
9:r:115:LYS:O	9:r:118:PRO:HG2	1.78	0.82
9:r:92:MET:HB3	9:r:460:TYR:CZ	1.00	0.82
9:r:267:VAL:HG11	9:r:271:ARG:HH12	1.44	0.82
9:r:271:ARG:HG2	9:r:343:SER:CA	2.09	0.82
9:r:284:TYR:CE2	9:r:344:SER:CB	2.63	0.82
9:r:403:GLN:HB3	9:r:415:SER:HA	1.60	0.82
9:r:418:VAL:HG13	9:r:425:VAL:CG1	2.09	0.82
9:r:284:TYR:CB	9:r:292:PHE:CE1	2.48	0.82
9:r:76:TYR:CG	9:r:77:SER:N	2.47	0.81
9:r:104:LYS:HD3	9:r:106:TYR:HE2	0.99	0.81
9:r:122:VAL:HG21	9:r:178:ILE:CG1	2.10	0.81
9:r:139:ILE:HD12	9:r:219:ILE:HG22	1.62	0.81
9:r:360:TYR:HB3	9:r:383:LEU:HD11	1.62	0.81
9:r:211:MET:HE2	9:r:221:LEU:HD13	1.63	0.81
9:r:410:THR:HG22	9:r:411:ASN:H	1.02	0.81
9:r:442:LYS:HG3	9:r:520:ILE:C	2.05	0.81
9:r:442:LYS:CG	9:r:520:ILE:CA	2.58	0.81
9:r:271:ARG:HG2	9:r:343:SER:H	1.42	0.81
1:X:1096:ILE:HD11	1:X:1214:PHE:HE1	1.44	0.81
9:r:312:ILE:O	9:r:316:ILE:HG12	1.80	0.81
9:r:346:LEU:HD11	9:r:363:LEU:HB3	1.61	0.81
9:r:448:SER:O	9:r:453:ILE:HG23	1.80	0.81
1:X:745:HIS:HA	1:X:749:ILE:HB	1.63	0.81
9:r:288:ASN:C	9:r:338:PRO:HD2	2.05	0.80
9:r:442:LYS:HB2	9:r:523:ASP:CA	2.10	0.80
9:r:263:THR:CG2	9:r:265:SER:N	2.44	0.80
9:r:321:GLN:CB	9:r:331:LEU:CD2	2.33	0.80
9:r:207:LYS:HZ2	9:r:227:ARG:HE	0.83	0.80
9:r:220:VAL:CG1	9:r:228:ILE:HG23	2.11	0.80
9:r:429:VAL:HG23	9:r:443:TRP:HZ2	1.41	0.80
9:r:271:ARG:HG2	9:r:343:SER:N	1.95	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:429:VAL:HG11	9:r:443:TRP:HE1	1.44	0.80
9:r:69:VAL:HG23	9:r:504:PHE:HZ	1.44	0.80
9:r:359:THR:OG1	9:r:390:ILE:HG22	1.82	0.80
9:r:429:VAL:HB	9:r:440:ARG:CG	2.11	0.80
9:r:324:TYR:HB2	9:r:326:PHE:CE2	2.16	0.80
9:r:334:TRP:HZ3	9:r:336:SER:HB2	1.41	0.80
9:r:72:LEU:HB3	9:r:474:VAL:HG12	1.65	0.79
9:r:225:MET:SD	9:r:260:ILE:HD11	2.22	0.79
9:r:248:LEU:HD12	9:r:251:PRO:HD2	1.63	0.79
9:r:96:TYR:CE1	9:r:160:GLU:OE2	2.36	0.79
9:r:222:SER:CB	9:r:270:LEU:HD11	2.13	0.79
9:r:268:VAL:CG2	9:r:340:GLN:CG	2.59	0.79
9:r:92:MET:HB3	9:r:460:TYR:HH	0.98	0.79
9:r:122:VAL:CG2	9:r:124:PHE:HE2	1.93	0.79
9:r:183:ASN:C	9:r:198:LEU:HD12	2.07	0.79
9:r:418:VAL:HG21	9:r:465:LEU:HD21	1.65	0.79
9:r:276:LEU:HD21	9:r:343:SER:HB2	1.62	0.79
9:r:68:ILE:HG12	9:r:500:GLN:HG2	1.64	0.79
9:r:268:VAL:HG12	9:r:268:VAL:O	1.79	0.79
1:X:684:LYS:CG	1:X:744:LEU:CB	2.59	0.79
9:r:287:THR:O	9:r:338:PRO:HG2	1.82	0.78
9:r:139:ILE:CG2	9:r:211:MET:O	2.32	0.78
9:r:416:ILE:HG22	9:r:417:LEU:O	1.84	0.78
9:r:472:MET:HB2	9:r:475:LEU:CD1	2.07	0.78
9:r:247:LEU:HD22	9:r:293:GLN:CB	2.13	0.78
9:r:274:PRO:O	9:r:280:THR:HG23	1.83	0.78
9:r:382:ARG:NH2	9:r:443:TRP:CH2	2.51	0.78
9:r:67:TYR:HB2	9:r:504:PHE:HE2	1.48	0.78
9:r:442:LYS:HD3	9:r:523:ASP:HB2	1.63	0.78
3:a:903:ASN:HD22	3:a:951:GLN:HE22	1.31	0.78
9:r:142:PHE:HE1	9:r:160:GLU:CD	1.92	0.78
9:r:228:ILE:H	9:r:248:LEU:HB2	1.47	0.78
1:X:222:GLU:OE2	1:X:361:LYS:CG	2.32	0.78
9:r:139:ILE:CD1	9:r:211:MET:HG3	2.14	0.78
9:r:92:MET:CB	9:r:460:TYR:OH	1.78	0.77
9:r:320:LEU:CD2	9:r:381:TYR:CE1	2.68	0.77
9:r:424:VAL:HG12	9:r:447:VAL:HA	1.65	0.77
9:r:143:PRO:CD	9:r:159:ASP:C	2.39	0.77
9:r:268:VAL:CB	9:r:340:GLN:CG	2.50	0.77
9:r:324:TYR:CZ	9:r:362:ILE:HD11	2.19	0.77
9:r:139:ILE:HG21	9:r:211:MET:C	2.09	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:442:LYS:HG2	9:r:521:SER:H	1.47	0.77
9:r:67:TYR:N	9:r:501:ALA:N	2.33	0.77
9:r:170:SER:CB	9:r:203:SER:HB2	2.14	0.77
9:r:142:PHE:CE1	9:r:160:GLU:CD	2.62	0.77
9:r:167:ILE:O	9:r:208:CYS:SG	2.43	0.77
9:r:222:SER:OG	9:r:270:LEU:HD12	1.85	0.77
9:r:152:ALA:HB1	9:r:157:ASP:HB3	1.65	0.77
9:r:170:SER:HB3	9:r:203:SER:CB	2.13	0.77
9:r:292:PHE:HE2	9:r:294:THR:OG1	1.68	0.77
9:r:334:TRP:HE1	9:r:351:ILE:CB	1.94	0.77
9:r:341:ASP:OD1	9:r:347:PHE:CZ	2.38	0.77
9:r:68:ILE:HG12	9:r:500:GLN:HG3	1.64	0.76
9:r:416:ILE:HD12	9:r:427:THR:HG22	1.66	0.76
9:r:441:ARG:HH11	9:r:522:LEU:HD21	1.48	0.76
3:l:207:SER:CA	3:l:236:VAL:HG22	2.16	0.76
9:r:99:VAL:CG2	9:r:108:TRP:HZ3	1.95	0.76
9:r:286:THR:HG23	9:r:291:ILE:O	1.85	0.76
9:r:326:PHE:HB3	9:r:330:THR:OG1	1.84	0.76
9:r:167:ILE:HA	9:r:208:CYS:HB3	1.67	0.76
1:X:684:LYS:HG2	1:X:744:LEU:CB	2.16	0.76
9:g:774:PHE:O	9:g:778:ASN:ND2	2.19	0.76
1:X:1057:LYS:NZ	1:X:1158:TYR:OH	2.19	0.76
9:r:340:GLN:OE1	9:r:399:ILE:CB	2.34	0.76
9:r:398:LYS:CB	9:r:420:PHE:CZ	2.69	0.75
9:r:442:LYS:CE	9:r:523:ASP:HB2	2.16	0.75
9:r:290:GLY:HA2	9:r:312:ILE:HD11	1.67	0.75
9:r:348:LEU:CG	9:r:399:ILE:HD11	2.16	0.75
9:r:359:THR:OG1	9:r:395:PHE:HE1	1.69	0.75
9:r:67:TYR:HB2	9:r:504:PHE:CE2	2.21	0.75
9:r:451:ASN:HD22	9:r:546:ILE:HD12	1.52	0.75
9:r:76:TYR:CD2	9:r:77:SER:N	2.54	0.75
9:r:271:ARG:CG	9:r:343:SER:H	1.99	0.75
9:r:271:ARG:CG	9:r:343:SER:HA	2.15	0.75
9:r:263:THR:HG22	9:r:265:SER:N	2.01	0.75
9:r:209:ASP:HB2	9:r:223:THR:HA	1.68	0.75
9:r:259:LYS:NZ	9:r:291:ILE:HG13	2.02	0.75
9:r:418:VAL:CG2	9:r:465:LEU:CD2	2.55	0.75
9:g:774:PHE:CE2	9:g:777:ILE:HD13	2.21	0.74
3:l:207:SER:CB	3:l:236:VAL:CG2	2.39	0.74
9:r:319:SER:CB	9:r:381:TYR:HE2	1.94	0.74
9:r:210:LEU:HG	9:r:222:SER:HB2	1.67	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:442:LYS:CD	9:r:523:ASP:HB2	2.17	0.74
9:r:225:MET:SD	9:r:260:ILE:CD1	2.74	0.74
9:r:442:LYS:CG	9:r:520:ILE:C	2.61	0.74
3:l:207:SER:HB2	3:l:236:VAL:HG22	0.77	0.74
9:r:227:ARG:HH11	9:r:252:PHE:HB2	1.51	0.74
9:r:266:SER:O	9:r:270:LEU:O	2.04	0.74
9:r:321:GLN:HB2	9:r:331:LEU:HD22	1.69	0.74
9:r:276:LEU:HD13	9:r:404:MET:SD	2.27	0.74
9:r:363:LEU:HG	9:r:384:ASN:HD21	1.53	0.74
9:r:416:ILE:HG12	9:r:429:VAL:HG12	1.69	0.74
9:r:270:LEU:CD2	9:r:285:ILE:HG13	2.18	0.74
9:r:300:THR:O	9:r:300:THR:HG22	0.96	0.74
9:r:86:LEU:HD11	9:r:101:ASP:OD2	1.87	0.73
9:r:141:THR:HB	9:r:161:THR:OG1	1.87	0.73
9:r:227:ARG:NH1	9:r:252:PHE:HB2	2.04	0.73
9:r:291:ILE:HG21	9:r:309:ASP:OD2	1.88	0.73
8:f:8:GLN:HE21	8:f:68:TRP:HH2	1.35	0.73
9:r:442:LYS:HD2	9:r:520:ILE:CA	2.16	0.73
9:r:444:GLU:HG3	9:r:519:GLU:O	1.87	0.73
9:r:207:LYS:HZ1	9:r:227:ARG:NH2	1.86	0.73
9:r:258:SER:HB3	9:r:289:LYS:HD3	1.70	0.73
9:r:276:LEU:HD21	9:r:404:MET:HE1	1.70	0.73
1:X:375:TYR:O	1:X:378:VAL:HG12	1.88	0.73
9:r:167:ILE:O	9:r:167:ILE:HG22	1.88	0.73
9:r:90:ILE:CG2	9:r:91:ASP:N	2.50	0.73
9:r:142:PHE:CZ	9:r:160:GLU:HG2	2.14	0.73
9:r:111:HIS:CE1	9:r:119:TYR:CD1	2.76	0.73
9:r:98:LEU:CD1	9:r:107:ILE:CG1	2.67	0.72
9:r:334:TRP:CH2	9:r:336:SER:OG	2.41	0.72
9:r:334:TRP:HH2	9:r:336:SER:OG	1.72	0.72
9:r:270:LEU:HD23	9:r:285:ILE:HA	1.71	0.72
9:r:286:THR:CG2	9:r:287:THR:H	1.93	0.72
9:r:403:GLN:HG2	9:r:413:VAL:HG11	0.73	0.72
9:r:448:SER:OG	9:r:455:ILE:HG13	1.90	0.72
1:X:318:HIS:HA	1:X:357:ASP:OD1	1.89	0.72
9:r:96:TYR:CD1	9:r:109:ASN:HA	2.24	0.72
9:r:68:ILE:CG1	9:r:500:GLN:CG	2.64	0.72
9:r:250:LYS:HD2	9:r:306:LYS:NZ	2.05	0.72
9:r:165:ILE:CG2	9:r:166:ILE:N	2.53	0.72
9:r:416:ILE:HG21	9:r:428:GLN:CA	2.19	0.72
9:r:399:ILE:HG23	9:r:417:LEU:CD2	2.15	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:442:LYS:HA	9:r:522:LEU:H	0.96	0.71
9:r:75:ASP:OD1	9:r:76:TYR:O	2.09	0.71
9:r:416:ILE:HD11	9:r:441:ARG:C	2.14	0.71
9:r:348:LEU:HD22	9:r:399:ILE:CG1	2.20	0.71
9:r:403:GLN:OE1	9:r:413:VAL:CG1	2.36	0.71
9:r:207:LYS:HZ1	9:r:227:ARG:NE	1.89	0.71
9:r:210:LEU:CD2	9:r:270:LEU:HG	2.18	0.71
9:r:340:GLN:CD	9:r:399:ILE:HB	2.14	0.71
9:r:399:ILE:HG23	9:r:417:LEU:HD11	1.70	0.71
9:r:442:LYS:HG2	9:r:520:ILE:CA	2.18	0.71
9:r:98:LEU:HD13	9:r:107:ILE:HG12	1.72	0.71
9:r:96:TYR:CD2	9:r:142:PHE:CZ	2.79	0.71
9:r:429:VAL:CG1	9:r:440:ARG:CB	2.68	0.71
9:r:263:THR:HG21	9:r:265:SER:H	1.56	0.71
9:r:324:TYR:CE1	9:r:360:TYR:CG	2.78	0.71
9:r:247:LEU:CD2	9:r:293:GLN:HB3	2.17	0.71
9:r:292:PHE:CE2	9:r:294:THR:OG1	2.44	0.71
9:r:212:LEU:HD21	9:r:272:ASN:HB2	0.77	0.71
9:r:250:LYS:CD	9:r:306:LYS:NZ	2.54	0.71
1:X:690:LEU:HG	1:X:745:HIS:HE1	1.56	0.70
9:r:291:ILE:HG22	9:r:292:PHE:N	2.06	0.70
9:r:86:LEU:CD1	9:r:101:ASP:CA	2.68	0.70
9:r:86:LEU:HD13	9:r:101:ASP:CA	2.20	0.70
9:r:410:THR:HG22	9:r:411:ASN:CA	2.19	0.70
1:X:319:PRO:HG3	1:X:358:VAL:O	1.92	0.70
9:r:396:LYS:C	9:r:397:PRO:HD3	2.16	0.70
9:r:442:LYS:HB2	9:r:523:ASP:H	0.55	0.70
9:r:324:TYR:CZ	9:r:360:TYR:HB2	2.26	0.70
1:X:774:ILE:HB	1:X:806:PHE:CE1	2.27	0.70
9:r:270:LEU:CD2	9:r:285:ILE:CG1	2.70	0.70
9:r:276:LEU:CD1	9:r:404:MET:SD	2.79	0.70
9:r:363:LEU:HD21	9:r:417:LEU:HD23	1.72	0.70
9:r:260:ILE:HG22	9:r:261:PHE:N	2.07	0.70
9:r:151:LEU:O	9:r:155:PRO:CD	2.39	0.70
9:g:774:PHE:CE1	9:g:777:ILE:CD1	2.75	0.69
9:r:137:ARG:HB3	9:r:165:ILE:O	1.92	0.69
9:r:341:ASP:CG	9:r:347:PHE:CE1	2.69	0.69
9:r:403:GLN:HB2	9:r:414:THR:O	1.91	0.69
9:r:442:LYS:CD	9:r:520:ILE:CA	2.70	0.69
9:r:247:LEU:HD21	9:r:293:GLN:CB	2.21	0.69
9:r:413:VAL:CG1	9:r:414:THR:N	2.54	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:68:ILE:CG2	9:r:70:LYS:CE	2.61	0.69
9:r:124:PHE:CE1	9:r:181:ILE:HG22	2.27	0.69
9:r:207:LYS:NZ	9:r:227:ARG:NH2	2.39	0.69
9:r:90:ILE:HD11	9:r:466:TYR:CD2	2.28	0.69
3:l:244:LYS:HZ3	3:l:246:TRP:HE1	1.40	0.69
9:r:227:ARG:HB3	9:r:248:LEU:CD2	2.05	0.69
9:r:247:LEU:H	9:r:295:TRP:HE1	1.37	0.69
1:X:318:HIS:CB	1:X:357:ASP:OD2	2.41	0.69
9:r:352:TYR:CE1	9:r:358:GLU:O	2.45	0.69
9:r:430:ASN:C	9:r:432:LYS:H	2.00	0.69
6:o:247:LEU:HD12	6:o:247:LEU:H	1.58	0.69
9:r:96:TYR:HD1	9:r:109:ASN:HA	1.57	0.69
9:r:98:LEU:CD1	9:r:107:ILE:HG13	2.23	0.69
9:r:261:PHE:HD1	9:r:288:ASN:H	1.35	0.69
9:r:442:LYS:HE2	9:r:523:ASP:HB2	1.74	0.69
9:r:444:GLU:CD	9:r:520:ILE:HD13	2.15	0.69
9:r:84:ASP:CG	9:r:470:LYS:HD3	2.18	0.69
9:r:86:LEU:O	9:r:456:ILE:HG21	1.89	0.69
1:X:380:THR:HG21	1:X:411:PHE:CB	2.24	0.69
1:X:380:THR:HG21	1:X:411:PHE:HB3	1.75	0.69
9:r:271:ARG:CD	9:r:343:SER:H	2.06	0.69
9:r:320:LEU:CD2	9:r:381:TYR:HD1	2.06	0.69
9:r:324:TYR:HB2	9:r:326:PHE:CD2	2.29	0.68
9:r:353:ASP:OD1	9:r:356:CYS:SG	2.45	0.68
9:r:361:TYR:HE2	9:r:397:PRO:CG	2.03	0.68
9:r:377:ILE:HG13	9:r:378:PHE:CD2	2.28	0.68
9:r:418:VAL:HG21	9:r:465:LEU:CD1	2.23	0.68
9:r:444:GLU:OE2	9:r:520:ILE:HD11	1.87	0.68
9:r:76:TYR:HE1	9:r:119:TYR:CE2	2.10	0.68
9:r:143:PRO:CD	9:r:159:ASP:HA	2.21	0.68
9:r:320:LEU:HD21	9:r:381:TYR:CD1	2.26	0.68
3:l:207:SER:HB3	3:l:236:VAL:H	1.57	0.68
9:r:67:TYR:CD2	9:r:444:GLU:OE1	2.46	0.68
9:r:444:GLU:HG2	9:r:519:GLU:C	2.17	0.68
9:r:447:VAL:CG2	9:r:508:ASN:ND2	2.56	0.68
8:f:704:LEU:HD23	8:f:704:LEU:H	1.58	0.68
9:r:89:TYR:O	9:r:89:TYR:CD2	2.46	0.68
9:r:472:MET:HB3	9:r:475:LEU:HD11	1.75	0.68
9:r:68:ILE:CG2	9:r:70:LYS:CD	2.71	0.68
9:r:68:ILE:HD12	9:r:497:HIS:CD2	2.29	0.68
9:r:263:THR:HG21	9:r:265:SER:N	2.08	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:319:SER:O	9:r:323:LEU:HG	1.93	0.68
9:r:139:ILE:CG2	9:r:211:MET:C	2.66	0.68
9:r:360:TYR:HB3	9:r:383:LEU:CD1	2.22	0.68
9:r:252:PHE:O	9:r:252:PHE:CD2	2.46	0.67
9:r:430:ASN:O	9:r:432:LYS:N	2.26	0.67
9:r:68:ILE:HG21	9:r:70:LYS:CD	2.24	0.67
1:X:381:VAL:O	1:X:384:GLU:OE1	2.12	0.67
9:r:207:LYS:CG	9:r:229:PHE:CE2	0.71	0.67
9:r:403:GLN:CB	9:r:413:VAL:CG1	2.73	0.67
1:X:684:LYS:HG3	1:X:744:LEU:CB	2.21	0.67
9:r:86:LEU:HD21	9:r:101:ASP:OD1	1.94	0.67
9:r:111:HIS:HE1	9:r:120:ILE:H	1.40	0.67
9:r:401:ILE:HG13	9:r:417:LEU:CD1	2.24	0.67
9:r:442:LYS:CG	9:r:520:ILE:CG2	2.69	0.67
9:r:216:PRO:HD3	9:r:299:ALA:HB2	1.77	0.67
3:l:207:SER:HB2	3:l:236:VAL:N	2.08	0.67
9:r:141:THR:HA	9:r:213:ASN:ND2	2.09	0.67
9:r:215:GLU:CB	9:r:299:ALA:HB2	2.25	0.67
9:r:227:ARG:NH1	9:r:249:ASN:HA	2.06	0.67
9:r:290:GLY:CA	9:r:312:ILE:HD11	2.24	0.67
9:r:320:LEU:HD21	9:r:381:TYR:CE1	2.30	0.67
9:r:152:ALA:C	9:r:155:PRO:HD2	2.20	0.67
9:r:270:LEU:HD23	9:r:285:ILE:HG13	1.77	0.67
9:r:67:TYR:C	9:r:500:GLN:HB3	2.00	0.67
9:r:68:ILE:HA	9:r:500:GLN:CB	2.24	0.67
9:r:69:VAL:CG2	9:r:504:PHE:CZ	2.75	0.67
9:r:416:ILE:CD1	9:r:427:THR:HG22	2.25	0.67
5:n:385:LEU:HD13	5:n:406:HIS:CD2	2.29	0.66
9:r:207:LYS:HG2	9:r:229:PHE:CE2	0.45	0.66
9:r:210:LEU:CD2	9:r:270:LEU:CG	2.66	0.66
9:r:219:ILE:HG13	9:r:231:ILE:HB	1.76	0.66
9:r:348:LEU:HB2	9:r:399:ILE:HG13	1.76	0.66
9:r:396:LYS:CA	9:r:397:PRO:CD	2.73	0.66
9:r:442:LYS:CB	9:r:523:ASP:N	2.14	0.66
1:X:908:VAL:HG21	1:X:967:LEU:HD11	1.77	0.66
9:r:442:LYS:CD	9:r:520:ILE:CB	2.45	0.66
1:X:380:THR:HB	1:X:411:PHE:HB3	1.77	0.66
9:r:320:LEU:HD23	9:r:381:TYR:HD1	1.60	0.66
9:r:122:VAL:HG21	9:r:124:PHE:CE2	2.30	0.66
9:r:290:GLY:HA2	9:r:338:PRO:HG3	1.76	0.66
9:r:418:VAL:CG1	9:r:425:VAL:CG1	2.70	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:403:GLN:HG2	9:r:413:VAL:HG12	1.69	0.66
9:r:361:TYR:CE2	9:r:397:PRO:CG	2.68	0.66
9:r:363:LEU:CD2	9:r:417:LEU:HD23	2.25	0.66
9:r:416:ILE:HG13	9:r:441:ARG:H	1.58	0.66
9:r:442:LYS:CD	9:r:520:ILE:HA	2.26	0.66
9:r:443:TRP:N	9:r:521:SER:N	2.42	0.66
1:X:380:THR:CG2	1:X:411:PHE:HB3	2.24	0.66
4:b:79:MET:HE1	7:e:45:TRP:CH2	2.31	0.66
9:r:268:VAL:HG11	9:r:340:GLN:CA	2.08	0.66
9:r:330:THR:O	9:r:333:ILE:HG12	1.95	0.66
9:g:1012:GLU:O	9:r:253:LYS:NZ	2.29	0.66
9:r:219:ILE:HG12	9:r:231:ILE:HB	1.78	0.66
9:r:68:ILE:CD1	9:r:497:HIS:CD2	2.79	0.65
9:r:69:VAL:HG22	9:r:477:PHE:CD1	2.31	0.65
9:r:79:GLY:C	9:r:81:SER:H	2.03	0.65
9:r:167:ILE:CA	9:r:208:CYS:HB3	2.26	0.65
9:r:252:PHE:O	9:r:252:PHE:CG	2.48	0.65
9:r:276:LEU:CD2	9:r:343:SER:O	2.39	0.65
9:r:270:LEU:HD21	9:r:285:ILE:CG1	2.26	0.65
1:X:323:TYR:HE1	1:X:359:LEU:HG	1.61	0.65
9:r:263:THR:HB	9:r:269:SER:HB2	1.78	0.65
9:r:270:LEU:CD2	9:r:285:ILE:CB	2.75	0.65
1:X:1097:LEU:HD22	1:X:1097:LEU:H	1.61	0.65
9:g:1016:PHE:HE2	9:r:253:LYS:NZ	1.90	0.65
3:l:207:SER:HB2	3:l:236:VAL:CB	2.25	0.65
9:r:68:ILE:CG2	9:r:70:LYS:HD3	2.26	0.65
9:r:68:ILE:HG13	9:r:497:HIS:HA	1.77	0.65
9:r:98:LEU:CD2	9:r:138:CYS:CB	2.72	0.65
9:r:165:ILE:HG13	9:r:221:LEU:CD1	2.15	0.65
9:r:367:ILE:HG22	9:r:369:ASP:H	1.60	0.65
9:r:363:LEU:CD2	9:r:417:LEU:CD2	2.74	0.65
4:m:71:LEU:HD22	7:p:313:ASN:HA	1.79	0.65
8:f:7:TYR:CD1	8:f:61:ASN:OD1	2.50	0.65
9:r:96:TYR:CE2	9:r:160:GLU:OE2	2.49	0.65
9:r:352:TYR:CE2	9:r:390:ILE:HD13	2.31	0.65
9:r:416:ILE:CG2	9:r:428:GLN:CA	2.73	0.65
9:r:431:SER:O	9:r:433:LEU:N	2.21	0.65
9:r:444:GLU:OE1	9:r:501:ALA:HB1	1.96	0.65
9:r:450:ARG:HG3	9:r:545:TYR:OH	1.97	0.64
9:r:433:LEU:O	9:r:433:LEU:HG	1.96	0.64
9:r:382:ARG:CZ	9:r:443:TRP:CH2	2.80	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:740:ASN:O	1:X:743:ILE:HB	1.97	0.64
9:r:270:LEU:CD2	9:r:285:ILE:HB	2.27	0.64
9:r:444:GLU:OE2	9:r:501:ALA:HB1	1.98	0.64
9:r:115:LYS:CA	9:r:118:PRO:HD2	2.20	0.64
9:r:259:LYS:C	9:r:287:THR:HG21	2.22	0.64
9:r:263:THR:HG22	9:r:264:ASN:C	2.23	0.64
9:r:267:VAL:HG13	9:r:271:ARG:NH1	1.93	0.64
9:r:348:LEU:HD22	9:r:399:ILE:HD13	1.76	0.64
9:r:134:VAL:HG12	9:r:136:PRO:N	2.11	0.64
8:f:377:ASN:O	8:f:381:ASP:HB3	1.97	0.64
9:r:398:LYS:HB2	9:r:420:PHE:CE2	2.32	0.64
9:r:137:ARG:HD3	9:r:167:ILE:CG1	2.19	0.64
9:r:207:LYS:HG3	9:r:227:ARG:CB	2.28	0.64
9:r:429:VAL:HG21	9:r:443:TRP:CZ2	2.24	0.64
9:r:444:GLU:CD	9:r:501:ALA:HB1	2.23	0.64
9:r:227:ARG:C	9:r:248:LEU:HD21	2.13	0.64
1:X:743:ILE:HA	1:X:805:LEU:HD12	1.80	0.63
1:X:1095:GLU:O	1:X:1119:ASN:ND2	2.31	0.63
9:r:346:LEU:CD2	9:r:401:ILE:HD11	2.26	0.63
9:r:227:ARG:NH1	9:r:248:LEU:O	2.30	0.63
9:r:444:GLU:HA	9:r:519:GLU:O	1.97	0.63
9:r:444:GLU:CA	9:r:519:GLU:O	2.47	0.63
9:r:99:VAL:CG2	9:r:108:TRP:CZ3	2.77	0.63
9:r:403:GLN:HE22	9:r:463:LYS:HD3	1.62	0.63
9:r:416:ILE:HD12	9:r:427:THR:CG2	2.28	0.63
9:r:71:THR:HA	9:r:475:LEU:HD23	1.79	0.63
1:X:1057:LYS:CE	1:X:1158:TYR:OH	2.47	0.63
9:r:261:PHE:CD1	9:r:288:ASN:N	2.41	0.63
9:r:228:ILE:HB	9:r:248:LEU:HB2	1.79	0.63
9:r:448:SER:C	9:r:453:ILE:HG23	2.23	0.63
1:X:966:GLY:H	1:X:969:ILE:HG22	1.62	0.63
9:r:84:ASP:OD1	9:r:470:LYS:CG	2.47	0.62
9:r:225:MET:SD	9:r:260:ILE:HG13	2.34	0.62
9:r:451:ASN:O	9:r:452:ASP:HB2	1.98	0.62
9:r:544:LYS:HA	9:r:633:THR:CG2	2.28	0.62
9:r:206:GLU:O	9:r:223:THR:HG21	1.80	0.62
9:r:92:MET:O	9:r:92:MET:HG2	1.97	0.62
9:r:98:LEU:HD23	9:r:138:CYS:CB	2.30	0.62
9:r:352:TYR:CE2	9:r:390:ILE:CD1	2.83	0.62
9:r:451:ASN:ND2	9:r:546:ILE:HD12	2.14	0.62
9:r:211:MET:CE	9:r:221:LEU:HD13	2.28	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:226:GLY:O	9:r:248:LEU:HD13	1.99	0.62
9:r:348:LEU:HB2	9:r:399:ILE:CG1	2.30	0.62
9:r:372:SER:O	9:r:373:ASN:CB	2.48	0.62
9:r:207:LYS:CB	9:r:229:PHE:HE2	1.69	0.62
9:r:410:THR:CG2	9:r:412:GLU:H	2.13	0.62
9:r:220:VAL:CG1	9:r:228:ILE:CG2	2.77	0.62
9:r:166:ILE:O	9:r:208:CYS:SG	2.48	0.61
9:r:166:ILE:HG22	9:r:168:LYS:H	1.65	0.61
9:r:207:LYS:NZ	9:r:227:ARG:CZ	2.63	0.61
9:r:348:LEU:HB2	9:r:399:ILE:CD1	2.30	0.61
1:X:801:LYS:O	1:X:804:GLN:HB2	2.01	0.61
9:r:210:LEU:CG	9:r:270:LEU:HD12	2.30	0.61
9:r:247:LEU:CD2	9:r:293:GLN:HB2	2.29	0.61
9:r:438:SER:O	9:r:439:MET:CB	2.47	0.61
9:r:442:LYS:HE3	9:r:444:GLU:CD	2.19	0.61
9:r:84:ASP:OD1	9:r:470:LYS:HG3	2.01	0.61
9:r:263:THR:HG22	9:r:265:SER:H	1.58	0.61
1:X:318:HIS:CD2	1:X:357:ASP:OD1	2.53	0.61
1:X:775:PHE:CZ	1:X:812:SER:HA	2.35	0.61
1:X:1095:GLU:OE2	1:X:1095:GLU:HA	2.00	0.61
9:r:67:TYR:HD2	9:r:444:GLU:OE1	1.80	0.61
9:r:167:ILE:O	9:r:167:ILE:CG2	2.47	0.61
9:r:207:LYS:HA	9:r:227:ARG:HB2	1.82	0.61
5:n:331:ARG:HH22	8:q:216:GLN:HG3	1.66	0.61
9:r:391:THR:OG1	9:r:393:THR:N	2.33	0.61
9:r:423:ALA:O	9:r:449:LEU:CG	2.49	0.61
8:f:432:TYR:CE1	8:f:435:PHE:HB2	2.35	0.61
9:r:86:LEU:HB3	9:r:100:ASN:O	2.00	0.61
9:r:215:GLU:HB2	9:r:299:ALA:HB2	1.83	0.61
9:r:270:LEU:HD21	9:r:285:ILE:HD12	1.83	0.61
9:r:116:ASP:N	9:r:118:PRO:HD2	2.06	0.61
3:l:207:SER:C	3:l:236:VAL:CG2	2.74	0.60
9:r:68:ILE:CA	9:r:500:GLN:CG	2.57	0.60
9:r:450:ARG:N	9:r:453:ILE:HG22	2.15	0.60
1:X:1548:ILE:HD11	1:X:1616:ILE:HD13	1.82	0.60
8:q:27:ASN:OD1	8:q:27:ASN:N	2.34	0.60
9:r:324:TYR:CE1	9:r:383:LEU:HD13	2.36	0.60
8:f:355:LEU:HD22	8:f:355:LEU:H	1.65	0.60
9:r:442:LYS:HG2	9:r:521:SER:N	2.05	0.60
1:X:740:ASN:HA	1:X:743:ILE:HD12	1.83	0.60
1:X:777:ASP:HA	1:X:781:ASP:HB2	1.81	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:111:HIS:NE2	9:r:119:TYR:CE1	2.68	0.60
9:r:139:ILE:HD11	9:r:219:ILE:CB	2.31	0.60
9:r:267:VAL:HG13	9:r:271:ARG:CD	2.29	0.60
9:r:377:ILE:CG1	9:r:378:PHE:CD2	2.83	0.60
9:r:248:LEU:HA	9:r:251:PRO:CD	2.31	0.60
9:r:96:TYR:CE2	9:r:142:PHE:CZ	2.89	0.60
9:r:183:ASN:C	9:r:198:LEU:CD1	2.72	0.60
9:r:352:TYR:CE2	9:r:353:ASP:O	2.54	0.60
9:g:774:PHE:CE2	9:g:777:ILE:CD1	2.84	0.60
9:r:258:SER:HB3	9:r:289:LYS:CD	2.31	0.60
9:r:447:VAL:CG2	9:r:508:ASN:HD21	2.14	0.60
8:f:7:TYR:HD1	8:f:61:ASN:OD1	1.84	0.60
9:r:447:VAL:HG21	9:r:508:ASN:ND2	2.16	0.60
6:d:15:ALA:HB1	6:d:24:LEU:HD11	1.84	0.60
9:r:274:PRO:CG	9:r:275:ILE:N	2.62	0.60
9:r:411:ASN:HA	9:r:441:ARG:HH22	1.66	0.60
1:X:690:LEU:HG	1:X:745:HIS:CE1	2.37	0.59
4:m:280:VAL:HG12	4:m:280:VAL:O	2.01	0.59
9:r:115:LYS:HB2	9:r:118:PRO:HG3	1.84	0.59
9:r:260:ILE:CG2	9:r:261:PHE:N	2.64	0.59
9:r:363:LEU:HD21	9:r:417:LEU:CD2	2.31	0.59
9:r:382:ARG:NE	9:r:443:TRP:HH2	1.96	0.59
9:r:393:THR:C	9:r:394:LYS:HG3	2.27	0.59
9:r:166:ILE:HG22	9:r:167:ILE:N	2.16	0.59
9:r:390:ILE:O	9:r:390:ILE:HG13	2.03	0.59
9:r:416:ILE:CG2	9:r:428:GLN:N	2.54	0.59
3:a:272:LYS:H	3:a:272:LYS:HD2	1.66	0.59
9:r:287:THR:OG1	9:r:288:ASN:N	2.09	0.59
9:r:430:ASN:C	9:r:430:ASN:OD1	2.43	0.59
1:X:323:TYR:CE1	1:X:359:LEU:HG	2.38	0.59
9:r:348:LEU:CD2	9:r:399:ILE:CD1	2.58	0.59
1:X:813:ILE:O	1:X:813:ILE:HG22	2.02	0.59
8:q:75:TRP:HE1	8:q:392:LEU:HD21	1.67	0.59
9:r:124:PHE:CE2	9:r:178:ILE:HG13	2.37	0.59
9:r:244:LEU:HD22	9:r:248:LEU:HD23	1.84	0.59
9:r:274:PRO:HG2	9:r:275:ILE:N	2.17	0.59
4:b:710:TYR:CZ	4:b:714:ILE:HD12	2.37	0.59
9:r:86:LEU:CD1	9:r:101:ASP:HA	2.32	0.59
9:r:89:TYR:HH	9:r:107:ILE:HG12	1.66	0.59
9:r:292:PHE:HE2	9:r:294:THR:HG1	1.39	0.59
1:X:813:ILE:HG22	1:X:817:PRO:HD3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:92:MET:C	9:r:460:TYR:CE2	2.60	0.59
9:r:115:LYS:HB2	9:r:118:PRO:CD	2.33	0.59
9:r:167:ILE:HG23	9:r:208:CYS:O	2.03	0.59
9:r:268:VAL:HG11	9:r:339:LEU:O	2.03	0.59
9:r:310:VAL:HG13	9:r:375:PHE:CD2	2.38	0.59
9:r:467:VAL:CB	9:r:477:PHE:HE2	2.09	0.58
1:X:859:ILE:HD13	1:X:910:ALA:HB2	1.85	0.58
9:r:76:TYR:CE2	9:r:77:SER:HB2	2.38	0.58
9:r:348:LEU:HB2	9:r:399:ILE:HD11	1.84	0.58
1:X:1160:ILE:HB	1:X:1161:PRO:HD3	1.86	0.58
6:d:233:ILE:HG21	6:d:289:TRP:CH2	2.38	0.58
9:r:250:LYS:HD3	9:r:306:LYS:NZ	2.17	0.58
9:g:1016:PHE:HZ	9:r:253:LYS:NZ	1.84	0.58
9:r:98:LEU:HD13	9:r:107:ILE:CD1	2.34	0.58
9:r:111:HIS:NE2	9:r:119:TYR:CD1	2.71	0.58
9:r:159:ASP:OD1	9:r:160:GLU:HG3	2.04	0.58
9:r:173:ILE:HG12	9:r:198:LEU:HD23	1.83	0.58
9:r:98:LEU:HD23	9:r:138:CYS:HB3	1.86	0.58
9:r:290:GLY:CA	9:r:338:PRO:HG3	2.33	0.58
1:X:222:GLU:OE2	1:X:361:LYS:HD3	2.04	0.58
9:r:128:ASP:O	9:r:129:ASN:OD1	2.22	0.58
9:r:259:LYS:HZ3	9:r:291:ILE:HG13	1.67	0.58
9:r:416:ILE:HG23	9:r:429:VAL:N	2.12	0.58
9:r:435:SER:HB3	9:r:438:SER:HB3	1.86	0.58
9:r:115:LYS:HB3	9:r:118:PRO:CD	2.26	0.57
9:r:268:VAL:CG1	9:r:268:VAL:O	2.45	0.57
9:r:382:ARG:NE	9:r:443:TRP:HZ2	1.93	0.57
9:r:141:THR:HG21	9:r:217:ALA:HA	1.86	0.57
9:r:207:LYS:CG	9:r:229:PHE:HE2	0.59	0.57
1:X:222:GLU:OE2	1:X:361:LYS:HG2	2.03	0.57
9:r:129:ASN:CG	9:r:166:ILE:CG1	2.74	0.57
9:r:174:TYR:CE2	9:r:233:ILE:CG1	2.68	0.57
9:r:212:LEU:HD21	9:r:272:ASN:HB3	1.77	0.57
6:d:140:ILE:HB	8:q:165:ASN:HD21	1.69	0.57
5:n:428:ASN:HD22	5:n:463:ARG:HE	1.52	0.57
9:r:115:LYS:CA	9:r:118:PRO:CD	2.81	0.57
9:r:382:ARG:HD3	9:r:432:LYS:HB2	1.86	0.57
1:X:803:LEU:O	1:X:803:LEU:HG	2.03	0.57
9:r:139:ILE:HG21	9:r:212:LEU:N	2.19	0.57
9:r:216:PRO:HD3	9:r:299:ALA:CB	2.33	0.57
9:r:216:PRO:HB3	9:r:299:ALA:HB1	1.85	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:129:ASN:CG	9:r:166:ILE:HG12	2.25	0.57
9:r:453:ILE:HA	9:r:471:GLN:HG2	1.85	0.57
1:X:775:PHE:CD2	1:X:811:ASP:O	2.55	0.57
1:X:1007:SER:HA	1:X:1195:GLN:HE22	1.69	0.57
7:e:25:ALA:H	7:e:63:TRP:HE1	1.52	0.57
8:f:8:GLN:NE2	8:f:68:TRP:HH2	2.03	0.57
9:r:89:TYR:CE2	9:r:98:LEU:N	2.73	0.57
9:r:361:TYR:CD1	9:r:386:PHE:HD2	2.23	0.57
9:r:122:VAL:HG21	9:r:124:PHE:CZ	2.40	0.57
8:f:377:ASN:HB2	8:f:380:ILE:HG12	1.86	0.57
9:r:73:GLN:CB	9:r:110:ILE:HG23	2.31	0.57
4:m:557:ALA:HB2	4:m:621:ARG:HH22	1.70	0.56
9:r:270:LEU:HD21	9:r:285:ILE:HG13	1.84	0.56
4:m:108:VAL:O	4:m:108:VAL:HG22	2.05	0.56
9:r:418:VAL:HG11	9:r:465:LEU:HD21	1.87	0.56
1:X:360:GLN:HE21	1:X:399:VAL:HG21	1.69	0.56
1:X:1096:ILE:HG21	1:X:1217:ARG:CZ	2.35	0.56
8:f:363:VAL:HA	8:f:374:GLU:OE1	2.06	0.56
9:r:79:GLY:C	9:r:81:SER:N	2.62	0.56
9:r:106:TYR:CE1	9:r:123:PRO:HB3	2.40	0.56
9:r:174:TYR:CD2	9:r:233:ILE:CG1	2.83	0.56
9:r:206:GLU:O	9:r:223:THR:CG2	2.51	0.56
9:r:358:GLU:HA	9:r:389:SER:HA	1.88	0.56
9:r:132:ILE:HG22	9:r:133:ALA:O	2.06	0.56
9:r:222:SER:CB	9:r:270:LEU:CD1	2.77	0.56
9:r:270:LEU:HD21	9:r:285:ILE:CD1	2.35	0.56
1:X:813:ILE:CG2	1:X:817:PRO:HD3	2.35	0.56
5:n:138:ILE:HG23	6:o:75:TYR:CE1	2.41	0.56
5:n:142:ARG:HH12	6:o:103:ASN:HA	1.70	0.56
9:r:382:ARG:CZ	9:r:443:TRP:CZ2	2.89	0.56
9:r:368:PHE:HZ	9:r:375:PHE:CE1	1.94	0.56
9:r:403:GLN:NE2	9:r:463:LYS:HD3	2.20	0.56
9:r:111:HIS:CE1	9:r:119:TYR:HA	2.40	0.56
9:r:113:THR:HG22	9:r:115:LYS:H	1.71	0.56
9:r:310:VAL:CG1	9:r:375:PHE:CD2	2.60	0.56
9:r:170:SER:HB3	9:r:203:SER:H	1.71	0.56
9:r:291:ILE:CG2	9:r:292:PHE:N	2.68	0.56
9:r:341:ASP:OD1	9:r:347:PHE:CD1	2.59	0.56
9:r:106:TYR:CD1	9:r:123:PRO:HB3	2.41	0.56
9:r:210:LEU:HB2	9:r:266:SER:HA	1.87	0.56
8:q:8:GLN:HE21	8:q:53:LEU:HD21	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:155:PRO:O	9:r:155:PRO:HG2	2.03	0.55
9:r:139:ILE:HG22	9:r:211:MET:O	2.05	0.55
9:r:147:ASP:CA	9:r:150:PRO:HD2	2.33	0.55
1:X:1057:LYS:HE2	1:X:1158:TYR:OH	2.06	0.55
9:g:774:PHE:CD1	9:g:777:ILE:HD12	2.41	0.55
9:g:1016:PHE:CZ	9:r:253:LYS:CE	2.90	0.55
9:r:216:PRO:CB	9:r:299:ALA:HB1	2.37	0.55
1:X:318:HIS:CD2	1:X:357:ASP:CG	2.85	0.55
9:g:69:VAL:HG13	9:g:477:PHE:CD1	2.42	0.55
9:g:262:ASN:H	9:g:262:ASN:HD22	1.55	0.55
9:r:75:ASP:OD1	9:r:75:ASP:C	2.50	0.55
9:r:174:TYR:C	9:r:198:LEU:HG	2.30	0.55
9:r:326:PHE:CE1	9:r:353:ASP:HB3	2.42	0.55
8:f:217:GLU:HG2	8:f:240:HIS:CD2	2.42	0.55
9:r:76:TYR:CE2	9:r:78:SER:N	2.66	0.55
9:r:210:LEU:CD1	9:r:222:SER:OG	2.52	0.55
9:r:227:ARG:NH1	9:r:252:PHE:CB	2.69	0.55
1:X:1096:ILE:HG21	1:X:1217:ARG:NH1	2.22	0.55
1:X:1304:LYS:HD2	1:X:1306:ASN:HD22	1.72	0.55
9:r:339:LEU:CD1	9:r:397:PRO:HG2	2.36	0.55
9:r:416:ILE:CG2	9:r:428:GLN:H	2.20	0.55
5:c:782:LEU:HD23	5:c:782:LEU:H	1.72	0.55
9:r:152:ALA:C	9:r:155:PRO:CD	2.78	0.55
9:r:210:LEU:CB	9:r:266:SER:HA	2.36	0.55
9:r:443:TRP:N	9:r:521:SER:C	2.64	0.55
1:X:319:PRO:HG3	1:X:358:VAL:C	2.32	0.55
3:l:354:LEU:HD13	3:l:463:ILE:HD11	1.89	0.55
1:X:813:ILE:HG23	1:X:816:ALA:HB2	1.85	0.54
4:b:79:MET:HE1	7:e:45:TRP:CZ2	2.42	0.54
9:r:147:ASP:CA	9:r:150:PRO:HD3	2.09	0.54
9:r:348:LEU:CB	9:r:399:ILE:HD11	2.37	0.54
1:X:745:HIS:HD1	1:X:749:ILE:CG2	2.16	0.54
9:r:68:ILE:HG22	9:r:70:LYS:HG2	1.90	0.54
4:b:265:ILE:HG22	4:b:270:LEU:HB2	1.90	0.54
3:l:460:ALA:HA	3:l:473:VAL:HG11	1.89	0.54
9:r:416:ILE:HG23	9:r:429:VAL:CA	2.37	0.54
7:p:58:ILE:HD12	7:p:58:ILE:H	1.73	0.54
9:r:86:LEU:HD21	9:r:101:ASP:CA	2.29	0.54
9:r:152:ALA:O	9:r:155:PRO:HD2	2.06	0.54
9:r:313:TYR:O	9:r:317:LEU:HB2	2.07	0.54
9:r:363:LEU:HD22	9:r:417:LEU:CD2	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:365:THR:OG1	9:r:380:THR:OG1	2.24	0.54
9:r:412:GLU:C	9:r:478:PHE:HE1	2.15	0.54
9:r:91:ASP:OD1	9:r:91:ASP:C	2.50	0.54
9:r:98:LEU:HD12	9:r:107:ILE:HG13	1.89	0.54
5:c:638:ILE:HD11	5:c:766:LYS:H	1.73	0.54
9:r:76:TYR:CE1	9:r:119:TYR:HE2	2.18	0.54
9:r:166:ILE:HG22	9:r:168:LYS:N	2.22	0.54
9:r:377:ILE:CD1	9:r:378:PHE:CE2	2.88	0.54
9:r:412:GLU:HA	9:r:478:PHE:HZ	1.64	0.54
1:X:360:GLN:C	1:X:362:LEU:H	2.16	0.54
9:r:98:LEU:HD13	9:r:107:ILE:HD11	1.89	0.54
9:r:543:GLY:O	9:r:633:THR:HG22	2.08	0.54
5:c:179:LEU:HD22	5:c:446:ASP:HB2	1.90	0.53
5:c:190:LEU:HD21	5:c:527:LEU:HD11	1.91	0.53
9:r:319:SER:HB2	9:r:381:TYR:CZ	2.42	0.53
3:a:959:GLU:OE2	3:a:959:GLU:HA	2.07	0.53
9:r:104:LYS:CD	9:r:106:TYR:CZ	2.83	0.53
9:r:380:THR:HG21	9:r:434:ASP:HB2	1.89	0.53
5:n:192:LYS:HZ1	5:n:196:LYS:HE2	1.74	0.53
9:r:201:ASN:HB2	9:r:240:PRO:HG2	1.90	0.53
9:r:339:LEU:HD13	9:r:397:PRO:HD2	1.90	0.53
9:r:429:VAL:CA	9:r:440:ARG:HD2	2.30	0.53
9:r:334:TRP:HZ3	9:r:336:SER:CB	2.09	0.53
1:X:360:GLN:NE2	1:X:399:VAL:HG21	2.23	0.53
4:m:452:GLU:HA	4:m:458:ARG:HH21	1.74	0.53
9:r:67:TYR:O	9:r:500:GLN:C	2.51	0.53
9:r:142:PHE:HE1	9:r:160:GLU:HG3	1.56	0.53
9:r:167:ILE:CA	9:r:208:CYS:CB	2.86	0.53
9:r:175:TYR:CA	9:r:198:LEU:HG	2.39	0.53
9:r:247:LEU:HD21	9:r:293:GLN:HB2	1.86	0.53
1:X:1096:ILE:HD11	1:X:1214:PHE:CE1	2.34	0.53
8:q:237:ILE:HG22	8:q:239:LYS:H	1.74	0.53
9:r:215:GLU:HB3	9:r:299:ALA:HB2	1.89	0.53
6:o:258:TRP:HA	6:o:258:TRP:CE3	2.44	0.53
9:r:164:LEU:HB3	9:r:173:ILE:HG22	1.89	0.53
9:r:348:LEU:HD13	9:r:399:ILE:HD11	1.91	0.53
8:f:700:LYS:HZ1	9:g:929:LEU:HD22	1.74	0.53
9:r:249:ASN:HD21	9:r:253:LYS:HE3	1.74	0.53
1:X:829:ASN:HD22	1:X:830:THR:H	1.55	0.52
9:r:207:LYS:HG3	9:r:229:PHE:HE2	0.42	0.52
9:r:216:PRO:HG3	9:r:299:ALA:HA	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:270:LEU:HD23	9:r:285:ILE:CG1	2.39	0.52
9:r:401:ILE:HG21	9:r:404:MET:HG2	1.92	0.52
9:r:447:VAL:CG2	9:r:508:ASN:CG	2.78	0.52
9:g:154:ASN:H	9:g:155:PRO:CD	2.21	0.52
9:r:270:LEU:HD23	9:r:285:ILE:CB	2.38	0.52
9:r:380:THR:CG2	9:r:434:ASP:HB2	2.39	0.52
1:X:1089:SER:HA	1:X:1217:ARG:HH21	1.74	0.52
9:r:391:THR:OG1	9:r:392:ASP:C	2.53	0.52
9:r:413:VAL:HG12	9:r:414:THR:C	2.34	0.52
9:r:320:LEU:HG	9:r:381:TYR:CE1	2.44	0.52
1:X:318:HIS:HD2	1:X:357:ASP:CG	2.17	0.52
3:a:903:ASN:ND2	3:a:951:GLN:HE22	2.04	0.52
9:r:94:ILE:HG13	9:r:96:TYR:H	1.74	0.52
9:r:216:PRO:HB3	9:r:299:ALA:O	2.09	0.52
9:r:228:ILE:N	9:r:248:LEU:HB2	2.19	0.52
9:r:290:GLY:N	9:r:338:PRO:HG3	2.23	0.52
9:r:812:SER:H	9:r:849:GLU:HG2	1.75	0.52
1:X:213:PHE:CD2	1:X:301:ALA:HB3	2.45	0.52
8:f:30:GLN:OE1	8:f:30:GLN:HA	2.05	0.52
8:f:542:ARG:HH11	8:f:545:ALA:HB3	1.74	0.52
9:r:324:TYR:CB	9:r:326:PHE:CE2	2.91	0.52
9:r:903:LEU:HA	9:r:906:ILE:HD12	1.91	0.52
1:X:222:GLU:OE2	1:X:361:LYS:CD	2.58	0.52
9:r:90:ILE:HG22	9:r:91:ASP:C	2.35	0.52
9:r:119:TYR:CZ	9:r:121:THR:OG1	2.62	0.52
9:r:442:LYS:CG	9:r:522:LEU:H	2.21	0.52
1:X:793:LEU:HD23	1:X:794:ILE:H	1.75	0.52
3:a:928:ALA:HB3	3:a:929:HIS:CD2	2.45	0.52
8:f:616:LEU:HD23	8:f:616:LEU:H	1.75	0.52
9:r:139:ILE:CD1	9:r:219:ILE:HB	2.40	0.52
9:r:399:ILE:HD12	9:r:417:LEU:HD21	1.92	0.52
1:X:1633:ARG:HE	1:X:1634:LEU:H	1.57	0.52
9:r:73:GLN:HG3	9:r:111:HIS:H	1.74	0.52
9:r:227:ARG:HD2	9:r:248:LEU:HG	1.92	0.52
9:r:227:ARG:HB3	9:r:229:PHE:CE2	2.45	0.52
9:r:348:LEU:HD11	9:r:419:MET:HE3	1.91	0.52
3:a:4:LEU:HD21	3:a:342:LEU:HD23	1.92	0.51
5:c:284:ILE:HG23	5:c:293:GLN:HE22	1.73	0.51
9:r:215:GLU:HB3	9:r:299:ALA:CB	2.41	0.51
9:r:270:LEU:HD22	9:r:285:ILE:HB	1.92	0.51
9:r:348:LEU:CD1	9:r:399:ILE:HD11	2.40	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:1160:ILE:N	1:X:1161:PRO:CD	2.73	0.51
4:b:116:ARG:HH22	4:b:528:GLU:HA	1.75	0.51
9:r:115:LYS:HB2	9:r:118:PRO:CG	2.41	0.51
9:r:416:ILE:HG22	9:r:417:LEU:N	2.24	0.51
9:r:442:LYS:CA	9:r:523:ASP:N	2.73	0.51
1:X:777:ASP:HA	1:X:781:ASP:CB	2.39	0.51
1:X:1489:PRO:HG3	8:q:582:GLU:OE2	2.10	0.51
4:b:597:LYS:HG3	4:b:632:GLN:HE21	1.76	0.51
9:r:139:ILE:CD1	9:r:219:ILE:CB	2.88	0.51
1:X:685:TYR:HE1	1:X:744:LEU:HG	1.76	0.51
9:g:66:ARG:HE	9:g:441:ARG:HE	1.59	0.51
8:q:8:GLN:C	8:q:10:GLU:H	2.19	0.51
9:r:467:VAL:HG23	9:r:477:PHE:CD2	2.39	0.51
3:a:89:HIS:CG	3:a:90:GLY:H	2.28	0.51
9:r:86:LEU:HD11	9:r:101:ASP:OD1	1.97	0.51
9:r:96:TYR:CD2	9:r:142:PHE:HZ	2.27	0.51
9:r:270:LEU:HD23	9:r:285:ILE:CA	2.39	0.51
4:m:578:ALA:H	4:m:665:LEU:HD23	1.76	0.51
9:r:167:ILE:C	9:r:208:CYS:SG	2.93	0.51
9:r:207:LYS:HG3	9:r:229:PHE:CE2	1.12	0.51
9:r:247:LEU:HD21	9:r:293:GLN:CG	2.39	0.51
9:r:366:ILE:HB	9:r:368:PHE:CE2	2.46	0.51
9:r:174:TYR:O	9:r:198:LEU:HG	2.11	0.51
3:l:146:ASN:C	3:l:149:TRP:HE1	2.19	0.51
9:r:348:LEU:CD2	9:r:399:ILE:HG12	2.41	0.51
9:r:248:LEU:HA	9:r:251:PRO:HD3	1.93	0.51
1:X:774:ILE:HB	1:X:806:PHE:CD1	2.46	0.50
9:g:1012:GLU:O	9:r:253:LYS:CE	2.59	0.50
3:l:207:SER:C	3:l:236:VAL:HG22	2.36	0.50
9:r:432:LYS:NZ	9:r:437:TYR:HA	2.26	0.50
9:r:462:SER:O	9:r:463:LYS:HB2	2.11	0.50
9:r:544:LYS:HA	9:r:633:THR:HG22	1.93	0.50
1:X:1055:GLN:HG2	1:X:1064:GLU:HB3	1.93	0.50
9:r:450:ARG:N	9:r:453:ILE:CG2	2.74	0.50
5:c:454:ILE:HD13	5:c:469:THR:HG23	1.94	0.50
6:o:97:VAL:O	6:o:98:HIS:CG	2.65	0.50
9:r:170:SER:HA	9:r:208:CYS:SG	2.52	0.50
9:r:321:GLN:HE22	9:r:331:LEU:C	2.15	0.50
9:r:423:ALA:O	9:r:424:VAL:HG13	2.12	0.50
1:X:806:PHE:HA	1:X:811:ASP:CB	2.41	0.50
9:g:174:TYR:O	9:g:198:LEU:HD12	2.11	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:207:LYS:HG3	9:r:248:LEU:HD21	1.93	0.50
9:r:220:VAL:HG11	9:r:228:ILE:HG23	1.92	0.50
9:r:346:LEU:HD23	9:r:417:LEU:HD13	1.94	0.50
9:g:89:TYR:CE2	9:g:139:ILE:HA	2.46	0.50
3:l:21:ASN:HD22	3:l:24:VAL:HG11	1.77	0.50
7:p:23:HIS:CE1	7:p:37:LYS:HD2	2.46	0.50
9:r:280:THR:HG22	9:r:281:ARG:CA	2.34	0.50
9:r:168:LYS:O	9:r:168:LYS:HG2	2.11	0.50
9:r:216:PRO:CD	9:r:299:ALA:CB	2.90	0.50
9:r:403:GLN:OE1	9:r:463:LYS:HB3	2.11	0.50
9:r:426:ILE:CG2	9:r:428:GLN:HE22	2.13	0.50
9:r:229:PHE:CE2	9:r:248:LEU:HD21	2.47	0.50
9:r:416:ILE:HG23	9:r:429:VAL:HA	1.93	0.50
1:X:1173:TRP:CG	1:X:1174:ASN:H	2.29	0.50
9:r:68:ILE:HD13	9:r:70:LYS:HE3	1.93	0.50
9:r:124:PHE:HZ	9:r:178:ILE:HG13	1.70	0.50
9:r:321:GLN:CD	9:r:334:TRP:HB3	2.35	0.50
9:r:377:ILE:CG1	9:r:378:PHE:CE2	2.95	0.50
1:X:1484:LYS:H	8:q:632:LYS:HD2	1.76	0.49
9:r:68:ILE:N	9:r:500:GLN:CB	2.74	0.49
9:r:165:ILE:HG22	9:r:166:ILE:O	2.11	0.49
9:r:174:TYR:CD2	9:r:199:PRO:HD2	2.46	0.49
9:r:451:ASN:O	9:r:452:ASP:CB	2.60	0.49
8:f:43:ARG:CB	8:f:43:ARG:HH11	2.25	0.49
9:r:167:ILE:C	9:r:208:CYS:CB	2.83	0.49
9:r:348:LEU:HD22	9:r:399:ILE:HG12	1.92	0.49
9:r:414:THR:HG22	9:r:441:ARG:CG	2.38	0.49
9:r:68:ILE:N	9:r:500:GLN:HB2	2.23	0.49
9:r:210:LEU:CG	9:r:222:SER:HB2	2.39	0.49
9:r:321:GLN:CD	9:r:331:LEU:HD22	2.37	0.49
1:X:357:ASP:OD1	1:X:357:ASP:N	2.44	0.49
1:X:1160:ILE:H	1:X:1161:PRO:CD	2.25	0.49
9:r:134:VAL:HG21	9:r:137:ARG:HH12	1.77	0.49
9:r:170:SER:CB	9:r:203:SER:H	2.25	0.49
9:r:258:SER:HB3	9:r:289:LYS:CG	2.43	0.49
9:r:442:LYS:CB	9:r:521:SER:H	2.22	0.49
6:o:52:HIS:CE1	6:o:80:LEU:HD12	2.47	0.49
9:r:94:ILE:CD1	9:r:96:TYR:CD1	2.84	0.49
9:r:210:LEU:HD22	9:r:270:LEU:HB2	1.95	0.49
9:r:320:LEU:CG	9:r:381:TYR:CE1	2.95	0.49
9:g:125:ARG:HE	9:g:181:ILE:CG2	2.24	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:100:ASN:HD21	9:r:133:ALA:CB	2.25	0.49
9:r:324:TYR:CZ	9:r:362:ILE:CD1	2.92	0.49
9:r:324:TYR:OH	9:r:362:ILE:CD1	2.61	0.49
9:r:401:ILE:HG12	9:r:417:LEU:HD12	1.88	0.49
9:r:432:LYS:HZ2	9:r:437:TYR:HA	1.77	0.49
9:r:468:LEU:HD12	9:r:473:GLY:C	2.38	0.49
6:d:103:ASN:HD22	6:d:149:ASN:HA	1.77	0.49
9:g:1012:GLU:O	9:r:253:LYS:HE3	2.12	0.49
9:r:80:PHE:O	9:r:81:SER:O	2.30	0.49
9:r:124:PHE:CZ	9:r:178:ILE:CG1	2.90	0.49
9:r:124:PHE:HZ	9:r:178:ILE:CG1	2.26	0.49
9:r:207:LYS:HZ1	9:r:227:ARG:CZ	2.25	0.49
9:r:209:ASP:O	9:r:222:SER:N	2.35	0.49
9:r:396:LYS:N	9:r:397:PRO:HD3	2.27	0.49
9:r:412:GLU:O	9:r:478:PHE:HE1	1.94	0.49
1:X:380:THR:HG22	1:X:380:THR:O	2.11	0.49
4:b:623:THR:HA	4:b:653:ILE:HG22	1.94	0.49
5:n:573:VAL:HA	5:n:596:ARG:HH22	1.78	0.49
9:r:222:SER:HB3	9:r:270:LEU:HD11	1.89	0.49
9:r:860:LEU:HD23	9:r:860:LEU:H	1.77	0.49
1:X:1096:ILE:CG2	1:X:1217:ARG:NH1	2.76	0.49
4:b:320:SER:HB2	4:b:329:ARG:HH12	1.78	0.49
5:n:294:ILE:HG13	5:n:309:LEU:HD23	1.94	0.49
9:r:288:ASN:O	9:r:338:PRO:HD3	2.07	0.49
8:f:466:ASN:HD21	8:f:476:LEU:HD21	1.78	0.48
9:r:229:PHE:CE2	9:r:248:LEU:CD2	2.96	0.48
9:r:469:THR:OG1	9:r:475:LEU:HD12	2.12	0.48
9:r:478:PHE:CD2	9:r:497:HIS:HE1	1.88	0.48
1:X:774:ILE:CB	1:X:806:PHE:CE1	2.94	0.48
5:c:651:CYS:H	6:d:133:ASN:HA	1.78	0.48
9:r:79:GLY:O	9:r:81:SER:N	2.46	0.48
9:r:89:TYR:O	9:r:89:TYR:CG	2.66	0.48
9:r:259:LYS:HZ2	9:r:291:ILE:HG13	1.74	0.48
9:r:309:ASP:OD1	9:r:309:ASP:C	2.53	0.48
9:r:363:LEU:HD22	9:r:417:LEU:HD22	1.93	0.48
9:r:418:VAL:HG21	9:r:465:LEU:HD13	1.93	0.48
3:l:757:GLU:HB2	3:l:780:HIS:CE1	2.48	0.48
9:r:421:PRO:O	9:r:455:ILE:HD12	2.13	0.48
9:r:429:VAL:HG21	9:r:432:LYS:HG3	1.95	0.48
9:r:452:ASP:O	9:r:470:LYS:HD2	2.14	0.48
8:q:664:LEU:O	8:q:668:HIS:CD2	2.66	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:67:TYR:O	9:r:504:PHE:CZ	2.66	0.48
9:r:68:ILE:CA	9:r:500:GLN:CB	2.89	0.48
9:r:134:VAL:CG2	9:r:137:ARG:HH12	2.26	0.48
9:r:284:TYR:CD2	9:r:294:THR:OG1	2.66	0.48
4:m:197:VAL:HG22	4:m:204:PHE:CE2	2.49	0.48
9:r:165:ILE:HG21	9:r:221:LEU:CD1	2.43	0.48
9:r:363:LEU:CD1	9:r:417:LEU:HD23	2.43	0.48
1:X:360:GLN:HE21	1:X:399:VAL:CG2	2.25	0.48
1:X:935:VAL:HG11	1:X:955:PHE:HB2	1.95	0.48
9:r:73:GLN:CD	9:r:110:ILE:HG23	2.34	0.48
9:r:286:THR:HG22	9:r:287:THR:CA	2.36	0.48
9:r:413:VAL:O	9:r:441:ARG:NE	2.43	0.48
9:r:430:ASN:C	9:r:432:LYS:N	2.67	0.48
9:r:250:LYS:HD2	9:r:306:LYS:HZ3	1.79	0.48
9:r:549:MET:HB2	9:r:629:LEU:H	1.78	0.48
9:r:68:ILE:HD11	9:r:497:HIS:CD2	2.49	0.48
9:r:80:PHE:O	9:r:81:SER:C	2.54	0.48
9:r:227:ARG:HD3	9:r:252:PHE:CG	2.49	0.48
1:X:803:LEU:HD12	1:X:807:LEU:HD23	1.95	0.48
9:g:274:PRO:O	9:g:280:THR:HA	2.14	0.48
9:r:69:VAL:HG23	9:r:504:PHE:CE2	2.47	0.48
9:r:100:ASN:HD21	9:r:133:ALA:HB1	1.78	0.48
9:r:151:LEU:O	9:r:155:PRO:N	2.46	0.48
9:r:446:ILE:HG21	9:r:477:PHE:HE1	1.79	0.48
5:n:497:LEU:HD13	5:n:502:ALA:HB1	1.95	0.48
9:r:96:TYR:CE1	9:r:109:ASN:CG	2.92	0.48
9:r:276:LEU:CD1	9:r:404:MET:HE1	2.32	0.48
9:r:430:ASN:H	9:r:440:ARG:HE	0.74	0.48
5:c:394:ILE:HD12	5:c:394:ILE:H	1.78	0.47
9:r:206:GLU:O	9:r:227:ARG:HB2	2.14	0.47
9:r:340:GLN:OE1	9:r:399:ILE:CG1	2.62	0.47
9:r:670:THR:HG21	9:r:743:LEU:HD13	1.96	0.47
3:a:319:ILE:H	3:a:319:ILE:HD12	1.79	0.47
8:f:142:SER:H	8:f:204:ASP:HB2	1.78	0.47
9:r:429:VAL:CG1	9:r:443:TRP:CD1	2.71	0.47
9:r:442:LYS:CA	9:r:521:SER:H	2.26	0.47
9:g:534:THR:O	9:g:538:ILE:HG22	2.14	0.47
9:r:98:LEU:CD1	9:r:107:ILE:HG12	2.39	0.47
9:r:254:LEU:HD12	9:r:259:LYS:CE	2.43	0.47
8:q:459:LYS:HA	8:q:516:TRP:HE1	1.78	0.47
9:r:84:ASP:O	9:r:85:GLU:HB2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:334:TRP:HH2	9:r:336:SER:HG	1.63	0.47
9:r:339:LEU:HD13	9:r:397:PRO:HG2	1.94	0.47
9:r:83:ASP:C	9:r:83:ASP:OD1	2.54	0.47
9:r:276:LEU:HD22	9:r:343:SER:HG	1.73	0.47
9:r:412:GLU:CA	9:r:478:PHE:CZ	2.84	0.47
1:X:271:LEU:HD13	1:X:378:VAL:HA	1.97	0.47
5:n:321:LEU:HA	5:n:324:TYR:CE2	2.50	0.47
9:r:460:TYR:C	9:r:460:TYR:CD2	2.92	0.47
1:X:390:ILE:HD12	1:X:390:ILE:H	1.80	0.47
3:a:207:SER:OG	3:a:214:ARG:NE	2.48	0.47
9:g:1000:SER:HB3	9:g:1101:ARG:HH12	1.80	0.47
3:l:290:LEU:HD23	3:l:331:ILE:HG21	1.97	0.47
9:r:348:LEU:CD2	9:r:399:ILE:CG1	2.89	0.47
3:a:887:ASP:HA	3:a:890:ARG:HB3	1.97	0.47
9:g:774:PHE:CE1	9:g:777:ILE:HD12	2.49	0.47
9:g:774:PHE:CG	9:g:777:ILE:HD12	2.50	0.47
9:r:286:THR:CG2	9:r:291:ILE:O	2.58	0.47
9:r:850:TYR:CZ	9:r:854:HIS:CE1	3.03	0.47
1:X:1480:GLN:HB3	8:q:631:ILE:O	2.15	0.47
9:g:870:VAL:HG22	9:g:874:PHE:CZ	2.49	0.47
5:n:515:ILE:HD11	5:n:541:ALA:HB1	1.97	0.47
9:r:242:LEU:HD12	9:r:242:LEU:O	2.15	0.47
9:r:593:ILE:HG23	9:r:680:GLY:HA2	1.97	0.47
9:g:542:ASN:HD22	9:g:567:PHE:HB2	1.80	0.47
9:r:400:PHE:CE2	9:r:458:SER:HB3	2.49	0.47
1:X:403:ILE:O	1:X:403:ILE:HG22	2.15	0.46
3:a:177:PHE:CD2	3:a:223:VAL:HG21	2.50	0.46
9:g:1012:GLU:C	9:r:253:LYS:NZ	2.73	0.46
8:q:453:GLU:HG3	8:q:454:ASP:H	1.80	0.46
9:r:369:ASP:OD1	9:r:370:SER:N	2.48	0.46
6:d:58:ARG:HH22	6:d:150:SER:HB3	1.80	0.46
6:o:258:TRP:HA	6:o:258:TRP:HE3	1.80	0.46
9:r:227:ARG:HD3	9:r:252:PHE:CD1	2.50	0.46
9:r:1124:ASN:HD21	9:r:1127:ASN:H	1.62	0.46
1:X:359:LEU:N	1:X:359:LEU:HD13	2.30	0.46
9:r:391:THR:HB	9:r:392:ASP:H	1.10	0.46
9:r:86:LEU:CD2	9:r:100:ASN:O	2.53	0.46
9:r:165:ILE:HG22	9:r:166:ILE:C	2.40	0.46
9:r:261:PHE:CE2	9:r:285:ILE:HG12	2.51	0.46
1:X:745:HIS:CD2	1:X:750:PHE:HA	2.49	0.46
9:r:174:TYR:HD2	9:r:199:PRO:HD2	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:206:GLU:O	9:r:223:THR:CB	2.63	0.46
9:r:209:ASP:HB3	9:r:222:SER:HB2	1.98	0.46
9:r:220:VAL:HG11	9:r:228:ILE:CG2	2.46	0.46
9:r:334:TRP:CH2	9:r:336:SER:CA	2.94	0.46
1:X:743:ILE:O	1:X:743:ILE:HG23	2.15	0.46
9:r:104:LYS:CE	9:r:106:TYR:OH	2.60	0.46
9:r:442:LYS:HD3	9:r:523:ASP:CB	2.38	0.46
9:r:393:THR:HB	9:r:394:LYS:H	1.23	0.46
3:l:528:ILE:HG22	3:l:532:PHE:CE2	2.51	0.46
5:n:280:ILE:HD12	5:n:296:LEU:HD22	1.98	0.46
9:r:209:ASP:HB3	9:r:222:SER:CB	2.37	0.46
9:r:249:ASN:ND2	9:r:253:LYS:HE3	2.30	0.46
9:r:259:LYS:HZ3	9:r:291:ILE:CG1	2.29	0.46
9:r:280:THR:CG2	9:r:281:ARG:HG3	2.46	0.46
1:X:900:ILE:HG22	1:X:929:MET:HG2	1.98	0.46
1:X:954:ILE:HD12	1:X:957:THR:HB	1.97	0.46
9:g:104:LYS:HB2	9:g:106:TYR:CE1	2.51	0.46
9:r:72:LEU:HD23	9:r:466:TYR:CD1	2.51	0.46
9:r:166:ILE:CG2	9:r:167:ILE:N	2.77	0.46
9:r:702:ASP:HA	9:r:774:PHE:CD2	2.50	0.46
3:a:385:SER:O	3:a:389:LEU:HG	2.16	0.46
6:o:185:TRP:CZ3	6:o:196:LEU:HB2	2.51	0.46
7:p:115:LYS:HG3	7:p:171:LEU:HB2	1.98	0.46
9:r:393:THR:OG1	9:r:394:LYS:N	2.29	0.46
1:X:685:TYR:CE1	1:X:744:LEU:HG	2.52	0.45
3:a:96:HIS:CE1	3:a:97:LEU:O	2.69	0.45
3:l:853:LEU:HD23	3:l:853:LEU:H	1.81	0.45
5:n:453:LEU:HD11	5:n:463:ARG:NH1	2.31	0.45
9:r:165:ILE:CB	9:r:221:LEU:HD13	2.46	0.45
4:m:406:LEU:HD23	4:m:409:MET:HE3	1.98	0.45
9:r:165:ILE:HG21	9:r:221:LEU:HD11	1.98	0.45
9:r:321:GLN:NE2	9:r:331:LEU:HA	2.30	0.45
4:b:121:ASP:HB2	4:b:140:HIS:CD2	2.52	0.45
4:b:186:ARG:HA	4:b:190:PHE:CG	2.52	0.45
9:r:96:TYR:CE2	9:r:142:PHE:CE1	3.03	0.45
9:r:147:ASP:C	9:r:150:PRO:CD	2.89	0.45
9:r:152:ALA:O	9:r:155:PRO:CD	2.64	0.45
9:r:316:ILE:CG2	9:r:381:TYR:OH	2.64	0.45
9:r:432:LYS:HZ2	9:r:437:TYR:CA	2.29	0.45
5:c:190:LEU:HD22	5:c:489:HIS:CD2	2.50	0.45
9:g:1016:PHE:HZ	9:r:253:LYS:CE	2.25	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:o:49:LEU:HD21	6:o:89:TRP:HB2	1.98	0.45
9:r:86:LEU:HD22	9:r:100:ASN:C	2.40	0.45
9:r:321:GLN:NE2	9:r:334:TRP:HB2	1.96	0.45
9:r:326:PHE:HE1	9:r:353:ASP:HB3	1.82	0.45
1:X:368:ILE:HG22	1:X:368:ILE:O	2.17	0.45
1:X:1160:ILE:CB	1:X:1161:PRO:HD3	2.45	0.45
3:a:924:ARG:H	3:a:968:ARG:CB	2.30	0.45
4:b:97:ARG:HG3	4:b:171:ARG:HH12	1.80	0.45
9:r:136:PRO:HB3	9:r:265:SER:HA	1.97	0.45
9:r:399:ILE:HG23	9:r:417:LEU:CD1	2.43	0.45
1:X:793:LEU:CD2	1:X:794:ILE:H	2.29	0.45
8:f:377:ASN:H	8:f:380:ILE:HG13	1.82	0.45
9:r:164:LEU:HB3	9:r:173:ILE:CG2	2.47	0.45
9:r:214:CYS:HA	9:r:272:ASN:ND2	2.32	0.45
9:r:258:SER:O	9:r:289:LYS:HG2	2.17	0.45
9:r:446:ILE:HG21	9:r:477:PHE:CE1	2.51	0.45
1:X:271:LEU:HD22	1:X:378:VAL:HB	1.99	0.45
1:X:813:ILE:HD12	1:X:816:ALA:HB2	1.98	0.45
9:g:774:PHE:CE2	9:g:777:ILE:HG21	2.52	0.45
9:r:416:ILE:HG13	9:r:441:ARG:N	2.30	0.45
9:r:423:ALA:O	9:r:424:VAL:CG1	2.65	0.45
9:r:585:LEU:HD23	9:r:585:LEU:H	1.82	0.45
3:l:803:HIS:CG	3:l:804:GLY:H	2.35	0.45
9:r:214:CYS:HA	9:r:272:ASN:HD21	1.82	0.45
5:n:333:ARG:HA	5:n:362:SER:HA	1.99	0.45
8:f:678:LEU:HD12	8:f:686:GLU:CD	2.41	0.44
9:g:1019:LEU:HD13	9:g:1065:VAL:HG23	2.00	0.44
1:X:1057:LYS:HA	1:X:1057:LYS:HD2	1.57	0.44
9:r:157:ASP:OD2	9:r:158:GLN:O	2.36	0.44
9:r:393:THR:OG1	9:r:394:LYS:HG3	2.18	0.44
9:r:447:VAL:HG23	9:r:508:ASN:ND2	2.32	0.44
9:r:790:HIS:CE1	9:r:814:LEU:HB2	2.52	0.44
3:l:5:SER:HB2	3:l:495:TYR:HB3	1.99	0.44
1:X:222:GLU:OE2	1:X:361:LYS:HG3	2.15	0.44
1:X:740:ASN:CA	1:X:743:ILE:HD12	2.48	0.44
8:f:589:HIS:CE1	8:f:630:LEU:HD22	2.53	0.44
3:l:366:LEU:HD13	3:l:378:TRP:CE2	2.53	0.44
8:q:445:CYS:O	8:q:449:LEU:HG	2.18	0.44
9:r:258:SER:O	9:r:289:LYS:CG	2.66	0.44
9:r:418:VAL:HG12	9:r:425:VAL:HG13	1.95	0.44
9:r:972:CYS:HA	9:r:1010:ASP:CB	2.48	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:g:362:ILE:HD12	9:g:383:LEU:HA	1.99	0.44
3:l:207:SER:OG	3:l:236:VAL:HG22	2.06	0.44
9:r:89:TYR:CD1	9:r:98:LEU:O	2.71	0.44
1:X:318:HIS:HA	1:X:357:ASP:CG	2.41	0.44
9:r:228:ILE:C	9:r:248:LEU:CD2	2.85	0.44
9:r:432:LYS:HE2	9:r:440:ARG:CB	2.38	0.44
1:X:360:GLN:C	1:X:362:LEU:N	2.75	0.44
5:c:294:ILE:HD11	5:c:310:ALA:HA	1.99	0.44
9:g:703:THR:HG23	9:g:709:PHE:HB2	2.00	0.44
9:g:924:LEU:HD13	9:g:951:LEU:HG	1.99	0.44
6:o:226:SER:H	6:o:257:LEU:HD12	1.83	0.44
8:q:7:TYR:HB2	8:q:8:GLN:H	1.52	0.44
9:r:137:ARG:CB	9:r:165:ILE:O	2.64	0.44
9:r:369:ASP:OD1	9:r:369:ASP:C	2.60	0.44
9:r:396:LYS:O	9:r:397:PRO:CD	2.59	0.44
3:a:942:ILE:HD13	3:a:942:ILE:HG21	1.82	0.44
5:c:265:HIS:CD2	5:c:394:ILE:HG21	2.52	0.44
9:r:137:ARG:HH11	9:r:167:ILE:HG13	1.83	0.44
9:r:391:THR:HG23	9:r:394:LYS:HD2	2.00	0.44
9:r:451:ASN:HD22	9:r:546:ILE:CD1	2.27	0.44
4:b:242:THR:HG22	4:b:243:GLN:H	1.83	0.43
7:p:215:ILE:HG21	7:p:218:ILE:HD11	2.00	0.43
8:q:141:THR:O	8:q:142:SER:HB2	2.18	0.43
9:r:175:TYR:HA	9:r:198:LEU:HG	2.00	0.43
9:r:276:LEU:CD2	9:r:404:MET:HE1	2.45	0.43
9:r:544:LYS:HA	9:r:633:THR:CB	2.47	0.43
1:X:742:LEU:C	1:X:744:LEU:H	2.25	0.43
1:X:803:LEU:HD23	1:X:803:LEU:C	2.43	0.43
1:X:908:VAL:HG21	1:X:967:LEU:CD1	2.46	0.43
4:b:186:ARG:HA	4:b:190:PHE:CD2	2.54	0.43
5:c:158:MET:HA	5:c:175:LEU:HD12	2.00	0.43
9:r:68:ILE:HG22	9:r:70:LYS:CD	2.47	0.43
9:r:137:ARG:CD	9:r:165:ILE:O	2.66	0.43
9:r:308:ILE:HG12	9:r:373:ASN:O	2.17	0.43
9:r:403:GLN:HB2	9:r:413:VAL:CG1	2.46	0.43
3:a:107:THR:HA	3:a:166:LEU:HB3	2.00	0.43
8:f:64:SER:HB2	8:f:68:TRP:CZ2	2.53	0.43
8:f:541:GLY:HA2	8:f:655:ILE:HD12	2.01	0.43
7:p:191:ALA:HB3	7:p:208:LEU:HD11	2.01	0.43
1:X:684:LYS:HE2	1:X:744:LEU:HB3	1.99	0.43
1:X:780:HIS:O	1:X:780:HIS:CG	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:X:380:THR:HG21	1:X:411:PHE:HB2	1.99	0.43
6:d:63:HIS:CD2	6:d:109:PRO:HA	2.53	0.43
6:o:247:LEU:HD22	6:o:250:GLU:HA	2.00	0.43
9:r:73:GLN:HB2	9:r:110:ILE:CG2	2.38	0.43
9:r:288:ASN:C	9:r:338:PRO:CD	2.78	0.43
9:r:423:ALA:C	9:r:424:VAL:HG13	2.43	0.43
1:X:813:ILE:HG22	1:X:817:PRO:CD	2.48	0.43
3:a:188:LYS:HG2	3:a:194:TYR:CE2	2.53	0.43
3:a:921:THR:HG22	3:a:930:SER:HA	2.00	0.43
3:a:1001:LEU:HD23	3:a:1031:ARG:HH12	1.84	0.43
4:b:356:SER:HB3	4:b:381:ALA:HB2	1.99	0.43
9:r:250:LYS:HD3	9:r:306:LYS:HZ2	1.82	0.43
9:r:472:MET:SD	9:r:547:PRO:HG2	2.58	0.43
1:X:1558:GLN:HE21	1:X:1562:ASN:HD21	1.67	0.43
9:r:205:GLY:O	9:r:206:GLU:HB2	2.19	0.43
9:r:308:ILE:HG13	9:r:309:ASP:N	2.34	0.43
9:r:361:TYR:CE1	9:r:386:PHE:CE2	3.06	0.43
8:f:355:LEU:H	8:f:355:LEU:CD2	2.32	0.43
3:l:855:GLU:HA	3:l:861:LEU:HD13	2.00	0.43
9:r:424:VAL:C	9:r:455:ILE:HD11	2.44	0.43
9:r:719:ASN:HA	9:r:722:PHE:CD2	2.53	0.43
3:a:68:ILE:HD13	3:a:139:PHE:CE1	2.54	0.43
6:o:12:ILE:HD12	6:o:12:ILE:H	1.84	0.43
7:p:58:ILE:HD12	7:p:58:ILE:N	2.33	0.43
1:X:380:THR:HG21	1:X:411:PHE:O	2.11	0.43
3:l:454:LYS:HD2	3:l:454:LYS:HA	1.82	0.43
5:n:335:LEU:HD21	8:q:201:LYS:HE2	2.00	0.43
8:q:8:GLN:C	8:q:10:GLU:N	2.77	0.43
9:r:216:PRO:CD	9:r:299:ALA:HB1	2.49	0.43
9:r:418:VAL:CG2	9:r:465:LEU:HD21	2.39	0.43
9:r:432:LYS:CE	9:r:440:ARG:HB2	2.39	0.43
9:r:442:LYS:CG	9:r:523:ASP:H	2.19	0.43
9:r:443:TRP:N	9:r:521:SER:H	2.14	0.43
1:X:381:VAL:HA	1:X:414:ASN:CB	2.49	0.42
3:a:186:LEU:HD12	3:a:186:LEU:HA	1.93	0.42
8:f:50:ALA:HA	8:f:65:SER:HB3	2.01	0.42
5:n:623:LEU:HD13	5:n:665:ILE:HB	2.01	0.42
9:r:105:VAL:HG12	9:r:107:ILE:HG13	2.01	0.42
9:r:142:PHE:CE1	9:r:160:GLU:OE2	2.72	0.42
9:r:326:PHE:CD1	9:r:330:THR:HB	2.54	0.42
9:r:366:ILE:HG22	9:r:367:ILE:N	2.34	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:r:401:ILE:CG1	9:r:417:LEU:HD12	2.46	0.42
9:r:403:GLN:HE21	9:r:406:ASN:H	1.67	0.42
9:r:454:ASP:OD1	9:r:455:ILE:N	2.51	0.42
3:a:329:TRP:HB3	3:a:355:TRP:HB3	2.01	0.42
9:r:266:SER:OG	9:r:267:VAL:N	2.51	0.42
9:r:293:GLN:HG2	9:r:309:ASP:CB	2.48	0.42
9:r:348:LEU:CB	9:r:399:ILE:CG1	2.97	0.42
9:r:424:VAL:HG13	9:r:449:LEU:HD11	2.01	0.42
1:X:799:ALA:O	1:X:803:LEU:HB3	2.19	0.42
1:X:860:ALA:HB2	1:X:957:THR:HG21	2.02	0.42
3:a:235:ILE:HG22	3:a:243:LEU:HD22	2.01	0.42
3:a:762:MET:HA	3:a:765:PHE:HB3	2.01	0.42
9:g:627:GLU:HB3	9:g:630:THR:H	1.84	0.42
9:r:84:ASP:CG	9:r:470:LYS:CD	2.91	0.42
9:r:384:ASN:HB3	9:r:428:GLN:CD	2.44	0.42
1:X:347:THR:O	1:X:350:ALA:HB3	2.20	0.42
1:X:900:ILE:H	1:X:900:ILE:HD12	1.83	0.42
3:l:329:TRP:CD2	3:l:355:TRP:HB3	2.54	0.42
7:p:115:LYS:CG	7:p:171:LEU:HB2	2.50	0.42
9:r:451:ASN:ND2	9:r:546:ILE:CD1	2.82	0.42
3:a:590:GLN:HA	3:a:590:GLN:OE1	2.18	0.42
6:o:66:PHE:CE2	6:o:69:ILE:HD12	2.54	0.42
9:r:363:LEU:HD11	9:r:417:LEU:HD23	2.01	0.42
9:r:416:ILE:HG22	9:r:428:GLN:H	1.84	0.42
1:X:1594:ASP:HB2	1:X:1597:ARG:HE	1.84	0.42
3:a:838:GLN:HB3	3:a:878:HIS:CE1	2.53	0.42
3:a:981:LEU:O	3:a:981:LEU:HD23	2.19	0.42
4:b:522:MET:HE3	4:b:538:ILE:HG21	2.01	0.42
5:n:644:PHE:O	5:n:644:PHE:CD1	2.72	0.42
9:r:67:TYR:CE2	9:r:444:GLU:OE1	2.72	0.42
9:r:248:LEU:O	9:r:248:LEU:HG	2.19	0.42
9:r:361:TYR:CD1	9:r:386:PHE:CD2	3.06	0.42
1:X:213:PHE:CE2	1:X:301:ALA:HB3	2.55	0.42
1:X:259:SER:HA	8:q:145:LEU:HD11	2.02	0.42
1:X:740:ASN:CB	1:X:743:ILE:HD12	2.50	0.42
1:X:774:ILE:CG2	1:X:806:PHE:CE1	3.03	0.42
3:l:1019:LEU:HD23	3:l:1019:LEU:HA	1.96	0.42
9:r:247:LEU:CD2	9:r:293:GLN:OE1	2.50	0.42
9:r:391:THR:OG1	9:r:392:ASP:CA	2.63	0.42
1:X:803:LEU:HA	1:X:807:LEU:HB2	2.00	0.42
8:f:481:GLN:HA	8:f:533:LEU:HD11	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:l:1018:ILE:HG21	3:l:1018:ILE:HD13	1.80	0.42
9:r:104:LYS:CE	9:r:106:TYR:HE2	2.31	0.42
9:r:220:VAL:HG13	9:r:228:ILE:CG2	2.48	0.42
9:r:316:ILE:HD12	9:r:320:LEU:HD11	2.01	0.42
9:r:702:ASP:OD1	9:r:774:PHE:HD2	2.03	0.42
1:X:1450:LEU:HD23	1:X:1450:LEU:HA	1.93	0.42
3:a:10:ASN:HD21	3:a:12:LEU:HB2	1.84	0.42
5:c:320:VAL:HG21	8:f:242:LEU:HD11	2.02	0.42
7:e:77:TYR:HA	7:e:110:SER:HB2	2.01	0.42
9:r:250:LYS:CD	9:r:306:LYS:HZ2	2.30	0.42
4:b:180:THR:HG21	4:b:390:TRP:CD2	2.55	0.42
9:r:215:GLU:HB2	9:r:216:PRO:HD3	1.79	0.42
1:X:618:LEU:HD23	1:X:618:LEU:HA	1.96	0.41
9:r:158:GLN:HG2	9:r:179:ASN:HB2	2.02	0.41
9:r:254:LEU:HD12	9:r:259:LYS:HE3	2.02	0.41
9:r:403:GLN:HE21	9:r:406:ASN:HB3	1.77	0.41
9:r:942:ASN:HA	9:r:945:ARG:HE	1.84	0.41
3:a:924:ARG:H	3:a:968:ARG:HB2	1.85	0.41
4:m:668:ALA:HB2	4:m:695:ILE:HD12	2.03	0.41
9:r:340:GLN:OE1	9:r:399:ILE:HG13	2.19	0.41
9:r:442:LYS:HD3	9:r:523:ASP:O	2.20	0.41
5:n:293:GLN:OE1	5:n:293:GLN:HA	2.21	0.41
9:r:280:THR:O	9:r:281:ARG:HB2	2.20	0.41
9:r:472:MET:HB3	9:r:475:LEU:HD21	2.01	0.41
9:r:1081:VAL:HG21	9:r:1127:ASN:HA	2.03	0.41
1:X:319:PRO:CG	1:X:358:VAL:O	2.66	0.41
1:X:742:LEU:C	1:X:744:LEU:N	2.78	0.41
3:l:672:LYS:HA	3:l:675:LEU:HB3	2.03	0.41
9:r:147:ASP:OD1	9:r:150:PRO:HD3	2.21	0.41
9:r:268:VAL:HA	9:r:340:GLN:HG2	1.93	0.41
9:r:282:LEU:HD23	9:r:296:GLN:HA	2.02	0.41
9:r:285:ILE:HG22	9:r:295:TRP:HZ3	1.84	0.41
1:X:858:LEU:HD12	1:X:867:ASP:H	1.84	0.41
7:e:243:PHE:CD1	7:e:296:LEU:HD13	2.56	0.41
9:r:104:LYS:CD	9:r:106:TYR:OH	2.69	0.41
9:r:206:GLU:O	9:r:223:THR:OG1	2.33	0.41
9:r:263:THR:HG23	9:r:264:ASN:H	1.73	0.41
9:r:423:ALA:O	9:r:449:LEU:CD2	2.68	0.41
9:r:429:VAL:HG21	9:r:443:TRP:CE2	2.46	0.41
9:r:442:LYS:HG2	9:r:520:ILE:C	2.40	0.41
1:X:965:ASP:HB2	1:X:979:ASN:H	1.84	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:g:760:ILE:HG22	9:g:761:ASN:HD22	1.85	0.41
9:r:68:ILE:HG21	9:r:70:LYS:HD3	1.95	0.41
9:r:167:ILE:HG23	9:r:208:CYS:HB2	2.02	0.41
9:g:109:ASN:O	9:g:111:HIS:CE1	2.74	0.41
9:g:173:ILE:HG22	9:g:198:LEU:HB2	2.01	0.41
3:l:83:PRO:O	3:l:87:ALA:HA	2.21	0.41
4:m:466:LEU:HD22	4:m:488:LEU:HD21	2.02	0.41
9:r:73:GLN:HG2	9:r:74:THR:O	2.20	0.41
9:r:222:SER:OG	9:r:270:LEU:HD13	2.09	0.41
9:r:441:ARG:HG3	9:r:441:ARG:NH1	2.36	0.41
3:l:962:LYS:H	3:l:965:TYR:H	1.68	0.41
9:r:90:ILE:HG23	9:r:96:TYR:O	2.21	0.41
9:r:92:MET:O	9:r:92:MET:CG	2.63	0.41
9:r:142:PHE:CZ	9:r:160:GLU:CD	2.98	0.41
9:r:230:PHE:HE1	9:r:297:LEU:CD1	2.33	0.41
9:r:460:TYR:CD2	9:r:460:TYR:O	2.74	0.41
1:X:264:LEU:HD22	1:X:375:TYR:CZ	2.56	0.41
1:X:774:ILE:HB	1:X:806:PHE:HE1	1.80	0.41
1:X:833:LYS:HA	1:X:895:HIS:CE1	2.56	0.41
8:q:106:GLU:HG3	8:q:298:ILE:HD11	2.02	0.41
8:q:126:LEU:HD23	8:q:126:LEU:H	1.86	0.41
8:q:240:HIS:CE1	8:q:243:TRP:CE3	3.09	0.41
9:r:228:ILE:O	9:r:248:LEU:CD2	2.69	0.41
9:r:291:ILE:HD13	9:r:311:ASN:HA	2.03	0.41
9:r:449:LEU:C	9:r:453:ILE:HG22	2.46	0.41
9:r:544:LYS:HA	9:r:633:THR:HB	2.02	0.41
9:r:1040:LEU:HD23	9:r:1043:ARG:HH21	1.84	0.41
6:d:246:THR:C	6:d:247:LEU:HD12	2.46	0.41
9:g:879:ALA:HB1	9:g:880:PRO:HD2	2.03	0.41
9:r:228:ILE:N	9:r:248:LEU:CB	2.60	0.41
9:r:442:LYS:CA	9:r:521:SER:C	2.60	0.41
3:a:109:THR:HG21	3:a:168:TYR:H	1.86	0.40
3:a:777:PHE:HB3	3:a:828:LEU:HD11	2.03	0.40
5:c:149:THR:HG1	6:d:258:TRP:CD1	2.39	0.40
3:l:422:ARG:NH2	3:l:479:TYR:CD2	2.88	0.40
9:r:142:PHE:HE1	9:r:160:GLU:OE2	2.04	0.40
9:r:421:PRO:HD2	9:r:424:VAL:HG23	2.03	0.40
9:r:679:ASP:OD1	9:r:683:GLU:HG2	2.21	0.40
1:X:1344:PHE:H	1:X:1347:GLY:HA3	1.86	0.40
3:a:488:THR:HG22	3:a:489:THR:H	1.87	0.40
5:c:332:ILE:HA	5:c:335:LEU:HB3	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:g:269:SER:O	9:g:270:LEU:HD23	2.21	0.40
8:q:256:LEU:HD23	8:q:256:LEU:HA	1.96	0.40
9:r:174:TYR:O	9:r:199:PRO:HD2	2.21	0.40
9:r:293:GLN:HG2	9:r:309:ASP:HB2	2.03	0.40
9:r:399:ILE:CG2	9:r:417:LEU:CD1	2.79	0.40
9:r:624:THR:HA	9:r:628:HIS:CD2	2.56	0.40
1:X:1618:PRO:HG3	1:X:1627:LEU:HD12	2.03	0.40
3:l:287:LEU:H	3:l:287:LEU:HD23	1.86	0.40
9:r:155:PRO:O	9:r:156:ASN:HB2	2.21	0.40
9:r:442:LYS:HB2	9:r:523:ASP:CB	2.51	0.40
9:r:442:LYS:HD3	9:r:520:ILE:CG2	2.01	0.40
1:X:782:VAL:O	1:X:782:VAL:HG23	2.20	0.40
5:c:246:TYR:CE1	5:c:248:TYR:HB2	2.56	0.40
8:f:364:GLU:HG3	8:f:374:GLU:HG3	2.04	0.40
4:m:360:PHE:HB3	4:m:370:LEU:HD13	2.02	0.40
5:n:138:ILE:HG23	6:o:75:TYR:CD1	2.56	0.40
9:r:76:TYR:CD2	9:r:76:TYR:C	2.90	0.40
9:r:210:LEU:HD12	9:r:210:LEU:C	2.46	0.40
9:r:224:ASN:O	9:r:260:ILE:CG2	2.51	0.40
9:r:285:ILE:HG22	9:r:293:GLN:HB2	2.03	0.40
3:a:266:ASP:HB3	3:a:267:PRO:HD2	2.04	0.40
3:a:266:ASP:H	3:a:269:HIS:CE1	2.40	0.40
9:g:831:LEU:HD22	9:g:831:LEU:N	2.37	0.40
5:n:182:LYS:HD3	5:n:182:LYS:H	1.87	0.40
5:n:294:ILE:HG23	5:n:306:ALA:HB1	2.03	0.40
9:r:104:LYS:CE	9:r:106:TYR:CE2	3.02	0.40
9:r:227:ARG:HH11	9:r:252:PHE:CB	2.26	0.40
9:r:448:SER:OG	9:r:455:ILE:CG1	2.65	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	X	1099/1655 (66%)	839 (76%)	171 (16%)	89 (8%)	1 9
3	a	996/1037 (96%)	825 (83%)	114 (11%)	57 (6%)	1 14
3	l	991/1037 (96%)	809 (82%)	115 (12%)	67 (7%)	1 11
4	b	667/744 (90%)	545 (82%)	80 (12%)	42 (6%)	1 13
4	m	662/744 (89%)	531 (80%)	81 (12%)	50 (8%)	1 10
5	c	551/712 (77%)	474 (86%)	53 (10%)	24 (4%)	2 17
5	n	549/712 (77%)	488 (89%)	48 (9%)	13 (2%)	4 27
6	d	270/297 (91%)	229 (85%)	35 (13%)	6 (2%)	5 29
6	o	270/297 (91%)	231 (86%)	28 (10%)	11 (4%)	2 18
7	e	303/349 (87%)	263 (87%)	30 (10%)	10 (3%)	3 21
7	p	303/349 (87%)	265 (88%)	30 (10%)	8 (3%)	4 25
8	f	635/726 (88%)	554 (87%)	55 (9%)	26 (4%)	2 18
8	q	634/726 (87%)	546 (86%)	66 (10%)	22 (4%)	3 20
9	g	1052/1157 (91%)	847 (80%)	137 (13%)	68 (6%)	1 12
9	r	1048/1157 (91%)	917 (88%)	88 (8%)	43 (4%)	2 18
All	All	10030/11699 (86%)	8363 (83%)	1131 (11%)	536 (5%)	2 15

All (536) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	X	136	ASN
1	X	217	GLN
1	X	370	SER
1	X	408	PRO
1	X	430	ALA
1	X	431	LYS
1	X	440	ILE
1	X	728	ILE
1	X	748	HIS
1	X	764	LYS
1	X	794	ILE
1	X	826	SER
1	X	871	SER
1	X	878	PHE
1	X	930	ALA
1	X	1030	SER
1	X	1042	SER
1	X	1046	LYS

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Mol	Chain	Res	Type
1	X	1050	SER
1	X	1057	LYS
1	X	1171	ARG
1	X	1239	ASP
1	X	1240	PHE
1	X	1252	LEU
1	X	1304	LYS
1	X	1429	HIS
3	a	207	SER
3	a	230	HIS
3	a	294	GLU
3	a	424	GLN
3	a	543	SER
3	a	750	LEU
3	a	798	LYS
3	a	881	MET
3	a	886	LEU
3	a	993	VAL
4	b	199	GLU
4	b	216	ASP
4	b	344	ARG
4	b	424	CYS
4	b	457	TYR
4	b	615	VAL
4	b	677	LEU
4	b	687	SER
4	b	741	GLN
5	c	147	SER
5	c	323	SER
5	c	377	SER
5	c	398	SER
5	c	520	ALA
5	c	628	VAL
5	c	648	TYR
8	f	228	ALA
8	f	440	ASP
8	f	551	GLU
8	f	557	GLU
8	f	559	CYS
8	f	611	SER
8	f	633	THR
9	g	94	ILE

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Mol	Chain	Res	Type
9	g	117	THR
9	g	146	MET
9	g	154	ASN
9	g	159	ASP
9	g	265	SER
9	g	280	THR
9	g	578	LYS
9	g	688	THR
9	g	705	LYS
9	g	713	ASP
9	g	714	TYR
9	g	1011	ASP
9	g	1015	LEU
9	g	1083	LEU
3	l	55	GLU
3	l	105	ARG
3	l	142	ALA
3	l	180	ASP
3	l	346	ALA
3	l	416	GLY
3	l	456	ALA
3	l	476	PHE
3	l	600	ASP
3	l	716	GLU
3	l	729	ILE
3	l	769	ASN
3	l	806	SER
3	l	994	ILE
3	l	1003	VAL
3	l	1012	SER
3	l	1019	LEU
4	m	227	VAL
4	m	369	GLU
4	m	401	LYS
4	m	492	SER
4	m	507	LEU
4	m	553	ILE
4	m	580	CYS
4	m	587	ASP
4	m	625	ALA
4	m	669	LYS
4	m	710	TYR

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Mol	Chain	Res	Type
4	m	718	LYS
5	n	179	LEU
5	n	228	SER
5	n	530	LEU
5	n	583	SER
5	n	609	LYS
5	n	611	SER
6	o	98	HIS
6	o	286	GLU
7	p	189	GLU
7	p	336	SER
8	q	142	SER
8	q	542	ARG
8	q	612	ASN
8	q	645	ASP
9	r	210	LEU
9	r	216	PRO
9	r	304	PRO
9	r	394	LYS
9	r	397	PRO
9	r	421	PRO
9	r	439	MET
9	r	515	ASN
9	r	628	HIS
9	r	630	THR
9	r	631	THR
9	r	712	PHE
9	r	716	ASN
9	r	734	SER
9	r	797	LEU
9	r	830	SER
9	r	841	LYS
9	r	879	ALA
9	r	912	LYS
9	r	1013	GLU
9	r	1126	ASP
1	X	163	ASP
1	X	164	TYR
1	X	276	ASN
1	X	381	VAL
1	X	405	SER
1	X	417	THR

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Mol	Chain	Res	Type
1	X	445	LEU
1	X	729	HIS
1	X	755	ASN
1	X	810	MET
1	X	862	ARG
1	X	880	ASN
1	X	897	LYS
1	X	898	VAL
1	X	921	SER
1	X	926	ALA
1	X	938	ASP
1	X	940	SER
1	X	977	ALA
1	X	984	ASP
1	X	985	GLU
1	X	992	SER
1	X	1032	ILE
1	X	1040	VAL
1	X	1060	LEU
1	X	1061	THR
1	X	1092	SER
1	X	1173	TRP
1	X	1277	ILE
1	X	1307	PHE
1	X	1399	ASN
1	X	1427	SER
1	X	1478	ILE
1	X	1542	ALA
3	a	55	GLU
3	a	210	ARG
3	a	211	PHE
3	a	219	ASP
3	a	261	SER
3	a	347	SER
3	a	359	THR
3	a	494	PHE
3	a	497	MET
3	a	600	ASP
3	a	715	THR
3	a	736	ASN
3	a	751	ARG
3	a	837	SER

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Mol	Chain	Res	Type
3	a	882	PHE
3	a	884	GLU
3	a	885	VAL
3	a	917	ASP
3	a	975	ARG
3	a	1011	ASP
3	a	1013	ALA
4	b	86	ASP
4	b	98	LEU
4	b	118	LEU
4	b	122	ARG
4	b	165	GLN
4	b	323	ASP
4	b	377	MET
4	b	381	ALA
4	b	516	ASN
4	b	526	CYS
4	b	591	LEU
4	b	595	VAL
4	b	603	ASP
4	b	710	TYR
4	b	740	CYS
5	c	224	MET
5	c	345	THR
5	c	348	CYS
5	c	530	LEU
5	c	651	CYS
6	d	219	ARG
7	e	92	GLU
7	e	106	ASP
7	e	162	ALA
7	e	338	GLU
8	f	232	ASN
8	f	515	GLU
8	f	627	THR
8	f	635	LEU
8	f	702	TYR
9	g	152	ALA
9	g	218	GLY
9	g	550	LEU
9	g	661	GLN
9	g	799	GLU

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Mol	Chain	Res	Type
9	g	811	LEU
9	g	819	GLN
9	g	856	LYS
9	g	885	VAL
9	g	938	ASN
9	g	1007	SER
9	g	1084	LEU
9	g	1143	GLU
9	g	1150	TYR
3	l	12	LEU
3	l	21	ASN
3	l	63	SER
3	l	86	ASP
3	l	116	GLN
3	l	250	SER
3	l	328	ILE
3	l	454	LYS
3	l	794	LEU
3	l	836	ASN
3	l	881	MET
3	l	889	LEU
3	l	929	HIS
3	l	953	LEU
3	l	962	LYS
3	l	974	GLU
3	l	1002	MET
4	m	222	GLU
4	m	413	ASP
4	m	542	LEU
4	m	601	ALA
4	m	628	ALA
4	m	641	ASP
4	m	654	GLU
4	m	670	PHE
4	m	692	ILE
4	m	693	GLU
4	m	698	LYS
4	m	706	SER
4	m	738	LYS
5	n	222	ASP
5	n	567	LEU
5	n	607	ARG

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Mol	Chain	Res	Type
6	o	11	LEU
6	o	65	LYS
6	o	191	ALA
7	p	301	ASP
8	q	55	ASN
8	q	157	ASP
8	q	280	SER
8	q	471	PRO
8	q	557	GLU
8	q	576	ASN
8	q	632	LYS
8	q	638	LEU
9	r	80	PHE
9	r	269	SER
9	r	514	PHE
9	r	637	ASN
9	r	705	LYS
9	r	827	THR
9	r	835	PHE
9	r	932	LEU
9	r	974	ARG
9	r	1016	PHE
9	r	1055	ASP
1	X	280	ALA
1	X	419	ASP
1	X	662	THR
1	X	796	SER
1	X	809	PRO
1	X	866	ARG
1	X	1027	TRP
1	X	1041	ASN
1	X	1124	ASP
1	X	1172	SER
1	X	1320	GLU
1	X	1477	ALA
3	a	20	PRO
3	a	283	TYR
3	a	370	ASP
3	a	423	ALA
3	a	454	LYS
3	a	606	LYS
3	a	687	SER

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Mol	Chain	Res	Type
3	a	861	LEU
3	a	1012	SER
4	b	272	PRO
4	b	387	THR
4	b	456	SER
4	b	464	TYR
4	b	594	ILE
4	b	718	LYS
5	c	302	ASP
5	c	393	GLN
5	c	609	LYS
6	d	51	GLY
7	e	39	ASP
7	e	93	CYS
8	f	142	SER
8	f	426	TYR
8	f	433	ALA
8	f	469	ARG
9	g	70	LYS
9	g	160	GLU
9	g	209	ASP
9	g	239	LYS
9	g	412	GLU
9	g	423	ALA
9	g	438	SER
9	g	494	VAL
9	g	607	SER
9	g	631	THR
9	g	655	PHE
9	g	709	PHE
9	g	866	GLN
3	l	16	GLU
3	l	22	ASN
3	l	54	SER
3	l	62	LEU
3	l	172	GLN
3	l	295	ASN
3	l	420	PHE
3	l	436	HIS
3	l	443	LEU
3	l	649	GLN
3	l	717	ASN

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Mol	Chain	Res	Type
3	l	736	ASN
3	l	797	LEU
3	l	857	GLN
3	l	880	ARG
3	l	967	PHE
3	l	971	ASN
4	m	55	ASP
4	m	98	LEU
4	m	511	TYR
4	m	517	ASP
4	m	518	ASP
4	m	544	ASN
4	m	656	PRO
4	m	689	ALA
4	m	720	LEU
5	n	349	SER
5	n	656	ALA
6	o	43	HIS
6	o	187	TYR
6	o	192	GLN
7	p	158	SER
8	q	97	HIS
8	q	206	ILE
8	q	373	THR
8	q	578	ASP
8	q	683	PHE
8	q	699	ASP
9	r	199	PRO
9	r	622	ASN
9	r	773	ASN
9	r	833	GLU
9	r	1052	ASN
1	X	416	LEU
1	X	646	LEU
1	X	765	PHE
1	X	822	ASN
1	X	836	GLY
1	X	1028	THR
1	X	1120	LYS
1	X	1290	SER
1	X	1540	LYS
3	a	114	GLU

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Mol	Chain	Res	Type
3	a	126	GLY
3	a	173	PHE
3	a	269	HIS
3	a	395	LEU
3	a	716	GLU
3	a	817	VAL
3	a	847	LYS
3	a	928	ALA
3	a	967	PHE
3	a	996	LYS
3	a	1017	TRP
4	b	555	SER
4	b	592	ASN
4	b	658	LEU
4	b	664	VAL
4	b	742	ALA
5	c	288	SER
5	c	301	ASN
5	c	778	GLU
6	d	201	GLU
7	e	120	HIS
8	f	230	GLU
8	f	272	PRO
8	f	522	LEU
8	f	548	GLN
8	f	678	LEU
9	g	144	ALA
9	g	454	ASP
9	g	546	ILE
9	g	937	ASP
9	g	1016	PHE
3	l	437	ASN
3	l	440	GLU
3	l	687	SER
3	l	781	ASP
3	l	879	PHE
3	l	958	TRP
4	m	193	ASP
4	m	581	MET
5	n	551	ASN
6	o	255	ASP
7	p	163	ASN

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Mol	Chain	Res	Type
7	p	217	SER
1	X	991	LYS
3	a	190	ASP
3	a	1026	THR
4	b	63	ASP
4	b	342	ASN
4	b	383	VAL
4	b	521	TRP
5	c	247	PRO
5	c	321	LEU
5	c	413	PRO
5	c	611	SER
6	d	55	PRO
6	d	289	TRP
7	e	31	GLN
7	e	188	LEU
7	e	289	GLN
8	f	154	LYS
8	f	429	ILE
8	f	453	GLU
9	g	86	LEU
9	g	93	GLN
9	g	148	GLU
9	g	161	THR
9	g	217	ALA
9	g	247	LEU
9	g	251	PRO
9	g	444	GLU
9	g	509	ALA
9	g	833	GLU
9	g	1032	GLU
3	l	114	GLU
3	l	327	ALA
3	l	786	ILE
4	m	593	ALA
4	m	675	PHE
7	p	66	PRO
7	p	94	SER
8	q	164	GLU
8	q	441	CYS
9	r	123	PRO
9	r	431	SER

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Mol	Chain	Res	Type
9	r	1079	PRO
1	X	407	ALA
1	X	691	SER
1	X	780	HIS
1	X	1472	SER
3	a	203	SER
3	a	894	GLU
3	a	945	VAL
8	f	33	ILE
9	g	245	GLY
9	g	355	SER
9	g	639	PRO
3	l	149	TRP
4	m	57	PRO
4	m	75	SER
4	m	191	ILE
4	m	390	TRP
4	m	588	ASP
4	m	594	ILE
4	m	627	TYR
4	m	659	PRO
8	q	628	PHE
9	r	687	LYS
1	X	743	ILE
5	c	775	GLY
9	g	274	PRO
4	m	219	PRO
4	m	512	PRO
5	n	654	VAL
6	o	51	GLY
6	o	202	GLY
9	r	546	ILE
9	g	396	LYS
9	g	548	PRO
3	l	648	GLY
4	b	402	ILE
5	c	776	GLN
8	f	470	LEU
9	g	758	ILE
3	l	192	VAL
4	m	595	VAL
1	X	778	VAL

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Mol	Chain	Res	Type
1	X	813	ILE
4	b	673	PRO
9	g	132	ILE
9	g	815	VAL
3	l	807	ILE
3	l	817	VAL
8	q	520	GLY
9	r	274	PRO
4	b	653	ILE
6	d	155	PRO
9	g	613	ILE
3	l	169	VAL
3	l	171	PRO
4	m	217	GLY

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	X	1072/1557 (69%)	986 (92%)	86 (8%)	11	31
3	a	945/972 (97%)	894 (95%)	51 (5%)	20	41
3	l	945/972 (97%)	909 (96%)	36 (4%)	29	50
4	b	606/670 (90%)	581 (96%)	25 (4%)	27	49
4	m	602/670 (90%)	572 (95%)	30 (5%)	22	43
5	c	513/646 (79%)	491 (96%)	22 (4%)	26	47
5	n	511/646 (79%)	494 (97%)	17 (3%)	33	55
6	d	233/252 (92%)	222 (95%)	11 (5%)	23	45
6	o	233/252 (92%)	220 (94%)	13 (6%)	19	40
7	e	269/305 (88%)	258 (96%)	11 (4%)	27	49
7	p	269/305 (88%)	257 (96%)	12 (4%)	24	46
8	f	594/669 (89%)	552 (93%)	42 (7%)	13	35
8	q	593/669 (89%)	560 (94%)	33 (6%)	19	40

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	g	997/1088 (92%)	949 (95%)	48 (5%)	23 44
9	r	991/1088 (91%)	966 (98%)	25 (2%)	42 63
All	All	9373/10761 (87%)	8911 (95%)	462 (5%)	24 43

All (462) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	X	141	LEU
1	X	145	ILE
1	X	155	ILE
1	X	197	LEU
1	X	198	MET
1	X	203	LYS
1	X	217	GLN
1	X	259	SER
1	X	266	THR
1	X	276	ASN
1	X	358	VAL
1	X	359	LEU
1	X	360	GLN
1	X	361	LYS
1	X	362	LEU
1	X	378	VAL
1	X	379	ILE
1	X	386	SER
1	X	406	LYS
1	X	414	ASN
1	X	415	PHE
1	X	434	LEU
1	X	663	MET
1	X	676	LEU
1	X	682	LEU
1	X	725	LEU
1	X	743	ILE
1	X	744	LEU
1	X	745	HIS
1	X	753	TYR
1	X	763	GLN
1	X	773	LEU
1	X	778	VAL
1	X	781	ASP

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Mol	Chain	Res	Type
1	X	794	ILE
1	X	795	ILE
1	X	803	LEU
1	X	804	GLN
1	X	805	LEU
1	X	822	ASN
1	X	831	THR
1	X	833	LYS
1	X	858	LEU
1	X	879	ILE
1	X	885	VAL
1	X	903	LEU
1	X	923	LEU
1	X	933	LYS
1	X	944	GLN
1	X	945	ASP
1	X	973	THR
1	X	1009	PRO
1	X	1021	THR
1	X	1027	TRP
1	X	1040	VAL
1	X	1055	GLN
1	X	1056	LYS
1	X	1057	LYS
1	X	1060	LEU
1	X	1065	THR
1	X	1069	ILE
1	X	1094	SER
1	X	1095	GLU
1	X	1096	ILE
1	X	1123	HIS
1	X	1160	ILE
1	X	1220	VAL
1	X	1237	ASN
1	X	1252	LEU
1	X	1254	ARG
1	X	1277	ILE
1	X	1315	VAL
1	X	1333	SER
1	X	1352	LEU
1	X	1400	PRO
1	X	1406	VAL

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Mol	Chain	Res	Type
1	X	1427	SER
1	X	1431	ILE
1	X	1459	LYS
1	X	1490	ARG
1	X	1491	LEU
1	X	1501	SER
1	X	1521	PHE
1	X	1527	LYS
1	X	1534	TYR
1	X	1567	GLN
3	a	12	LEU
3	a	22	ASN
3	a	23	THR
3	a	58	ASN
3	a	68	ILE
3	a	110	ILE
3	a	130	THR
3	a	136	SER
3	a	137	PHE
3	a	148	GLU
3	a	150	PHE
3	a	188	LYS
3	a	202	ASN
3	a	204	TYR
3	a	259	MET
3	a	293	LEU
3	a	302	THR
3	a	319	ILE
3	a	321	THR
3	a	349	LEU
3	a	356	LYS
3	a	424	GLN
3	a	430	ASN
3	a	455	THR
3	a	462	SER
3	a	472	LEU
3	a	480	ASN
3	a	513	LEU
3	a	546	THR
3	a	551	THR
3	a	558	LEU
3	a	564	ILE

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Mol	Chain	Res	Type
3	a	567	LEU
3	a	575	ASN
3	a	715	THR
3	a	724	PHE
3	a	728	ILE
3	a	741	LEU
3	a	780	HIS
3	a	787	ASN
3	a	800	GLU
3	a	807	ILE
3	a	842	LEU
3	a	861	LEU
3	a	913	ILE
3	a	935	LEU
3	a	945	VAL
3	a	965	TYR
3	a	974	GLU
3	a	1012	SER
3	a	1014	TYR
4	b	58	ILE
4	b	107	TYR
4	b	132	VAL
4	b	162	VAL
4	b	203	GLU
4	b	205	ILE
4	b	239	VAL
4	b	241	GLU
4	b	242	THR
4	b	265	ILE
4	b	277	THR
4	b	292	LEU
4	b	354	TYR
4	b	373	GLU
4	b	405	ILE
4	b	407	PRO
4	b	420	THR
4	b	494	THR
4	b	508	LEU
4	b	538	ILE
4	b	575	LEU
4	b	598	ASN
4	b	609	GLN

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Mol	Chain	Res	Type
4	b	611	ILE
4	b	622	GLN
5	c	149	THR
5	c	162	LYS
5	c	164	ILE
5	c	165	VAL
5	c	183	PHE
5	c	203	LYS
5	c	205	ASN
5	c	233	LEU
5	c	249	LYS
5	c	262	LYS
5	c	299	LEU
5	c	325	LEU
5	c	332	ILE
5	c	350	ILE
5	c	352	LYS
5	c	407	LEU
5	c	446	ASP
5	c	458	ARG
5	c	469	THR
5	c	567	LEU
5	c	596	ARG
5	c	652	ARG
6	d	66	PHE
6	d	88	ARG
6	d	135	THR
6	d	141	ILE
6	d	180	ASN
6	d	217	LEU
6	d	230	THR
6	d	238	ASN
6	d	246	THR
6	d	256	VAL
6	d	265	SER
7	e	11	LEU
7	e	17	TYR
7	e	59	VAL
7	e	212	LYS
7	e	213	SER
7	e	218	ILE
7	e	236	LYS

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Mol	Chain	Res	Type
7	e	246	THR
7	e	289	GLN
7	e	317	THR
7	e	341	CYS
8	f	8	GLN
8	f	9	THR
8	f	10	GLU
8	f	30	GLN
8	f	31	ASN
8	f	37	ASN
8	f	40	ARG
8	f	43	ARG
8	f	104	LEU
8	f	126	LEU
8	f	142	SER
8	f	148	ILE
8	f	166	THR
8	f	168	VAL
8	f	172	LYS
8	f	188	ILE
8	f	237	ILE
8	f	292	GLN
8	f	317	LEU
8	f	323	THR
8	f	343	ILE
8	f	355	LEU
8	f	363	VAL
8	f	373	THR
8	f	374	GLU
8	f	376	SER
8	f	407	VAL
8	f	408	ASP
8	f	419	LEU
8	f	452	LEU
8	f	506	ILE
8	f	548	GLN
8	f	575	GLU
8	f	576	ASN
8	f	581	LEU
8	f	606	LEU
8	f	617	ILE
8	f	642	ASN

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Mol	Chain	Res	Type
8	f	663	LEU
8	f	667	LEU
8	f	676	LYS
8	f	682	LYS
9	g	117	THR
9	g	167	ILE
9	g	173	ILE
9	g	176	GLU
9	g	213	ASN
9	g	219	ILE
9	g	242	LEU
9	g	262	ASN
9	g	316	ILE
9	g	359	THR
9	g	387	MET
9	g	413	VAL
9	g	427	THR
9	g	463	LYS
9	g	507	ILE
9	g	520	ILE
9	g	522	LEU
9	g	529	HIS
9	g	550	LEU
9	g	584	LYS
9	g	616	LYS
9	g	617	THR
9	g	631	THR
9	g	657	LEU
9	g	698	PRO
9	g	703	THR
9	g	746	VAL
9	g	758	ILE
9	g	772	ASP
9	g	775	ILE
9	g	814	LEU
9	g	815	VAL
9	g	819	GLN
9	g	831	LEU
9	g	891	ILE
9	g	960	ILE
9	g	962	ASN
9	g	971	ILE

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Mol	Chain	Res	Type
9	g	985	ASN
9	g	994	THR
9	g	1011	ASP
9	g	1058	LEU
9	g	1065	VAL
9	g	1084	LEU
9	g	1127	ASN
9	g	1145	ASN
9	g	1147	THR
9	g	1152	THR
3	l	70	TYR
3	l	77	THR
3	l	99	ASN
3	l	105	ARG
3	l	108	LEU
3	l	109	THR
3	l	162	VAL
3	l	172	GLN
3	l	244	LYS
3	l	245	ILE
3	l	249	THR
3	l	271	ARG
3	l	282	LEU
3	l	285	ASN
3	l	289	THR
3	l	315	PHE
3	l	344	VAL
3	l	352	ILE
3	l	437	ASN
3	l	449	ILE
3	l	464	THR
3	l	465	LEU
3	l	486	LEU
3	l	488	THR
3	l	562	PHE
3	l	608	ASP
3	l	613	ILE
3	l	619	LEU
3	l	649	GLN
3	l	664	LEU
3	l	667	LEU
3	l	679	LEU

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Mol	Chain	Res	Type
3	l	718	SER
3	l	889	LEU
3	l	942	ILE
3	l	972	LYS
4	m	52	THR
4	m	58	ILE
4	m	94	ARG
4	m	125	ASN
4	m	135	ASN
4	m	154	GLU
4	m	186	ARG
4	m	201	ARG
4	m	407	PRO
4	m	433	ILE
4	m	478	ASP
4	m	488	LEU
4	m	504	ILE
4	m	514	VAL
4	m	515	THR
4	m	520	GLU
4	m	542	LEU
4	m	552	ILE
4	m	554	GLU
4	m	588	ASP
4	m	592	ASN
4	m	603	ASP
4	m	615	VAL
4	m	616	VAL
4	m	624	LEU
4	m	647	ARG
4	m	662	TYR
4	m	673	PRO
4	m	683	MET
4	m	730	ASN
5	n	167	LYS
5	n	177	THR
5	n	182	LYS
5	n	192	LYS
5	n	197	VAL
5	n	262	LYS
5	n	350	ILE
5	n	388	THR

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Mol	Chain	Res	Type
5	n	445	LEU
5	n	452	TYR
5	n	474	THR
5	n	501	LYS
5	n	526	ILE
5	n	585	ASN
5	n	592	LEU
5	n	593	LYS
5	n	637	LEU
6	o	18	ASP
6	o	32	THR
6	o	33	ILE
6	o	43	HIS
6	o	56	VAL
6	o	63	HIS
6	o	66	PHE
6	o	136	THR
6	o	155	PRO
6	o	220	SER
6	o	230	THR
6	o	246	THR
6	o	247	LEU
7	p	80	THR
7	p	86	GLU
7	p	146	ARG
7	p	183	LEU
7	p	188	LEU
7	p	192	ILE
7	p	212	LYS
7	p	229	GLN
7	p	230	LEU
7	p	320	SER
7	p	334	THR
7	p	342	MET
8	q	7	TYR
8	q	8	GLN
8	q	27	ASN
8	q	30	GLN
8	q	31	ASN
8	q	124	VAL
8	q	147	SER
8	q	161	PRO

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Mol	Chain	Res	Type
8	q	172	LYS
8	q	180	PHE
8	q	188	ILE
8	q	206	ILE
8	q	213	CYS
8	q	220	ASN
8	q	223	ILE
8	q	267	LEU
8	q	313	LEU
8	q	380	ILE
8	q	382	LYS
8	q	438	GLU
8	q	460	LYS
8	q	469	ARG
8	q	523	TYR
8	q	575	GLU
8	q	576	ASN
8	q	582	GLU
8	q	603	SER
8	q	615	THR
8	q	633	THR
8	q	646	SER
8	q	679	LYS
8	q	682	LYS
8	q	701	ILE
9	r	70	LYS
9	r	104	LYS
9	r	297	LEU
9	r	515	ASN
9	r	516	LEU
9	r	569	THR
9	r	585	LEU
9	r	588	ILE
9	r	618	LEU
9	r	626	ASN
9	r	632	LYS
9	r	639	PRO
9	r	645	ILE
9	r	687	LYS
9	r	773	ASN
9	r	790	HIS
9	r	812	SER

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Mol	Chain	Res	Type
9	r	851	LEU
9	r	870	VAL
9	r	932	LEU
9	r	964	LEU
9	r	969	VAL
9	r	1003	VAL
9	r	1087	LYS
9	r	1152	THR

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (291) such sidechains are listed below:

Mol	Chain	Res	Type
1	X	136	ASN
1	X	150	GLN
1	X	201	ASN
1	X	210	ASN
1	X	217	GLN
1	X	218	ASN
1	X	219	GLN
1	X	276	ASN
1	X	318	HIS
1	X	322	HIS
1	X	360	GLN
1	X	414	ASN
1	X	418	ASN
1	X	636	GLN
1	X	692	ASN
1	X	780	HIS
1	X	829	ASN
1	X	895	HIS
1	X	979	ASN
1	X	1093	ASN
1	X	1119	ASN
1	X	1182	ASN
1	X	1193	ASN
1	X	1195	GLN
1	X	1232	HIS
1	X	1249	GLN
1	X	1306	ASN
1	X	1423	ASN
1	X	1429	HIS
1	X	1493	ASN

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Mol	Chain	Res	Type
1	X	1528	GLN
1	X	1539	ASN
1	X	1558	GLN
1	X	1608	HIS
1	X	1648	GLN
3	a	96	HIS
3	a	99	ASN
3	a	111	GLN
3	a	116	GLN
3	a	132	GLN
3	a	153	GLN
3	a	200	ASN
3	a	230	HIS
3	a	242	HIS
3	a	269	HIS
3	a	322	ASN
3	a	343	ASN
3	a	369	ASN
3	a	393	HIS
3	a	430	ASN
3	a	436	HIS
3	a	458	ASN
3	a	474	ASN
3	a	496	ASN
3	a	522	ASN
3	a	556	ASN
3	a	561	GLN
3	a	584	ASN
3	a	588	ASN
3	a	621	GLN
3	a	670	GLN
3	a	756	GLN
3	a	780	HIS
3	a	827	GLN
3	a	835	ASN
3	a	857	GLN
3	a	878	HIS
3	a	903	ASN
3	a	910	GLN
3	a	929	HIS
3	a	952	ASN
3	a	1016	GLN

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Mol	Chain	Res	Type
4	b	56	GLN
4	b	78	ASN
4	b	141	ASN
4	b	153	ASN
4	b	213	ASN
4	b	251	GLN
4	b	260	GLN
4	b	315	GLN
4	b	342	ASN
4	b	403	HIS
4	b	432	ASN
4	b	467	ASN
4	b	545	GLN
4	b	550	HIS
4	b	609	GLN
4	b	632	GLN
4	b	644	GLN
5	c	134	ASN
5	c	265	HIS
5	c	293	GLN
5	c	328	ASN
5	c	353	ASN
5	c	406	HIS
5	c	423	GLN
5	c	460	ASN
5	c	480	GLN
5	c	489	HIS
5	c	536	GLN
5	c	585	ASN
5	c	590	ASN
5	c	631	GLN
5	c	647	GLN
5	c	663	GLN
6	d	91	GLN
6	d	98	HIS
6	d	103	ASN
6	d	144	HIS
6	d	192	GLN
6	d	238	ASN
6	d	240	GLN
6	d	267	ASN
6	d	276	ASN

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Mol	Chain	Res	Type
7	e	8	HIS
7	e	23	HIS
7	e	130	ASN
7	e	211	HIS
7	e	289	GLN
7	e	293	GLN
7	e	300	HIS
8	f	8	GLN
8	f	55	ASN
8	f	61	ASN
8	f	220	ASN
8	f	273	ASN
8	f	274	GLN
8	f	300	ASN
8	f	305	ASN
8	f	325	GLN
8	f	329	ASN
8	f	400	ASN
8	f	428	ASN
8	f	461	GLN
8	f	466	ASN
8	f	586	GLN
8	f	589	HIS
9	g	73	GLN
9	g	100	ASN
9	g	129	ASN
9	g	201	ASN
9	g	241	GLN
9	g	262	ASN
9	g	264	ASN
9	g	321	GLN
9	g	337	HIS
9	g	340	GLN
9	g	373	ASN
9	g	403	GLN
9	g	471	GLN
9	g	555	GLN
9	g	565	GLN
9	g	566	ASN
9	g	601	ASN
9	g	620	ASN
9	g	628	HIS

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Mol	Chain	Res	Type
9	g	662	ASN
9	g	671	ASN
9	g	711	ASN
9	g	716	ASN
9	g	761	ASN
9	g	763	GLN
9	g	796	ASN
9	g	819	GLN
9	g	854	HIS
9	g	890	GLN
9	g	901	ASN
9	g	948	GLN
9	g	962	ASN
9	g	1059	GLN
9	g	1134	HIS
3	l	21	ASN
3	l	58	ASN
3	l	89	HIS
3	l	99	ASN
3	l	143	ASN
3	l	154	ASN
3	l	200	ASN
3	l	269	HIS
3	l	318	ASN
3	l	322	ASN
3	l	364	GLN
3	l	383	ASN
3	l	430	ASN
3	l	477	GLN
3	l	481	HIS
3	l	487	ASN
3	l	496	ASN
3	l	575	ASN
3	l	584	ASN
3	l	658	HIS
3	l	694	ASN
3	l	734	HIS
3	l	769	ASN
3	l	780	HIS
3	l	871	HIS
3	l	878	HIS
3	l	932	ASN

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Mol	Chain	Res	Type
3	l	952	ASN
3	l	988	GLN
3	l	1005	ASN
4	m	135	ASN
4	m	140	HIS
4	m	153	ASN
4	m	343	GLN
4	m	388	ASN
4	m	392	GLN
4	m	598	ASN
4	m	632	GLN
4	m	661	HIS
5	n	209	GLN
5	n	252	ASN
5	n	317	HIS
5	n	353	ASN
5	n	393	GLN
5	n	406	HIS
5	n	428	ASN
5	n	443	ASN
5	n	487	HIS
5	n	489	HIS
5	n	523	ASN
5	n	525	HIS
5	n	540	ASN
5	n	551	ASN
5	n	558	ASN
5	n	585	ASN
5	n	589	ASN
5	n	627	ASN
6	o	8	HIS
6	o	52	HIS
6	o	86	ASN
6	o	95	HIS
6	o	98	HIS
6	o	144	HIS
6	o	240	GLN
7	p	23	HIS
7	p	32	HIS
7	p	99	ASN
7	p	105	ASN
7	p	130	ASN

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Mol	Chain	Res	Type
7	p	164	HIS
7	p	211	HIS
8	q	8	GLN
8	q	27	ASN
8	q	30	GLN
8	q	76	HIS
8	q	111	GLN
8	q	118	GLN
8	q	146	ASN
8	q	240	HIS
8	q	307	GLN
8	q	509	HIS
8	q	528	HIS
8	q	540	ASN
8	q	554	ASN
8	q	561	ASN
8	q	586	GLN
8	q	621	GLN
8	q	668	HIS
8	q	706	GLN
9	r	100	ASN
9	r	111	HIS
9	r	288	ASN
9	r	321	GLN
9	r	337	HIS
9	r	428	GLN
9	r	451	ASN
9	r	497	HIS
9	r	508	ASN
9	r	515	ASN
9	r	524	GLN
9	r	601	ASN
9	r	620	ASN
9	r	628	HIS
9	r	637	ASN
9	r	668	ASN
9	r	761	ASN
9	r	773	ASN
9	r	785	HIS
9	r	789	ASN
9	r	790	HIS
9	r	796	ASN

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Mol	Chain	Res	Type
9	r	816	GLN
9	r	854	HIS
9	r	858	ASN
9	r	890	GLN
9	r	1027	ASN
9	r	1074	ASN
9	r	1127	ASN
9	r	1134	HIS
9	r	1149	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 oligosaccharides 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
3	l	4
5	c	2
5	n	2

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Mol	Chain	Number of breaks
9	r	1
3	a	1
9	g	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	877:GLU	C	878:SER	N	16.07
1	l	207:SER	C	208:LEU	N	14.63
1	l	206:LYS	C	207:SER	N	13.72
1	a	486:LEU	C	487:ASN	N	6.43
1	c	533:PRO	C	535:SER	N	5.54
1	g	807:PHE	C	808:TYR	N	5.07
1	n	665:ILE	C	760:VAL	N	4.73
1	l	486:LEU	C	487:ASN	N	4.13
1	n	533:PRO	C	535:SER	N	4.10
1	l	460:ALA	C	461:SER	N	4.03
1	c	665:ILE	C	760:VAL	N	3.49

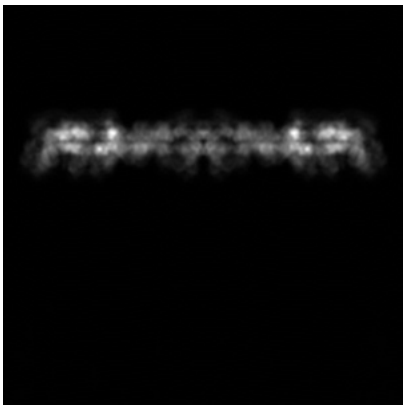
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-24231. These allow visual inspection of the internal detail of the map and identification of artifacts.

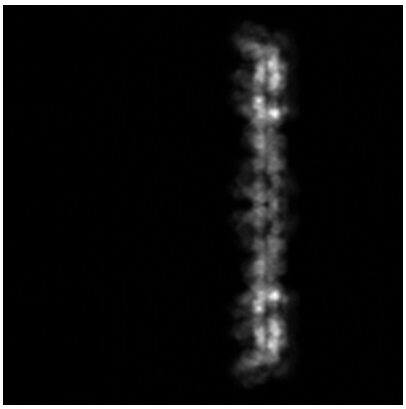
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

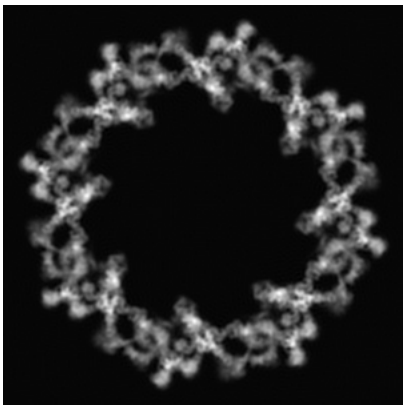
6.1.1 Primary map



X

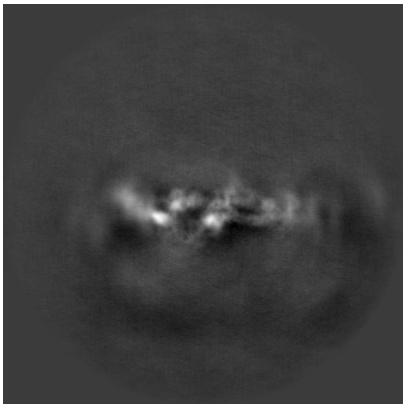


Y

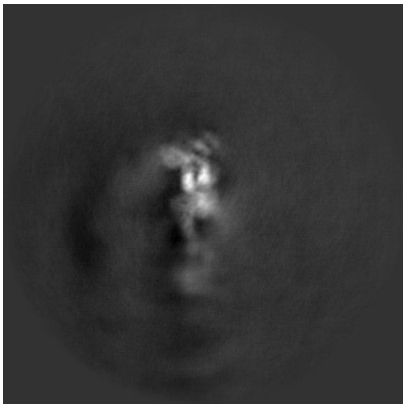


Z

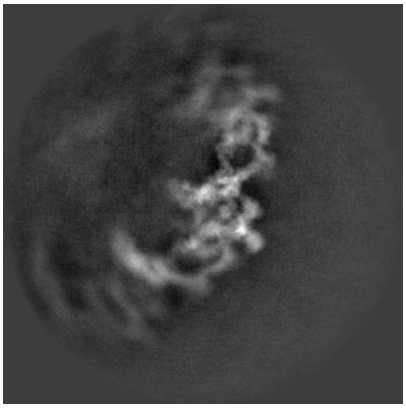
6.1.2 Raw map



X



Y



Z

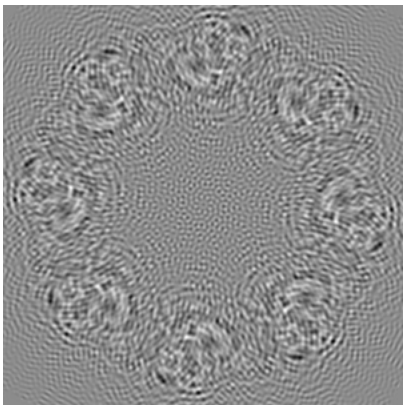
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

6.2.1 Primary map

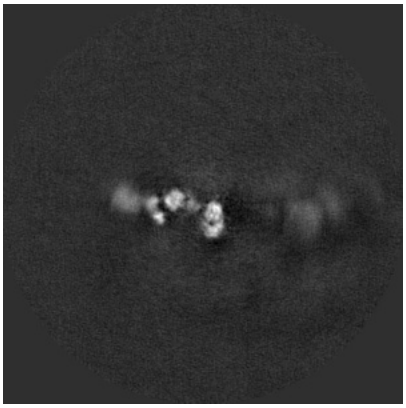
X Index: 240

Y Index: 240

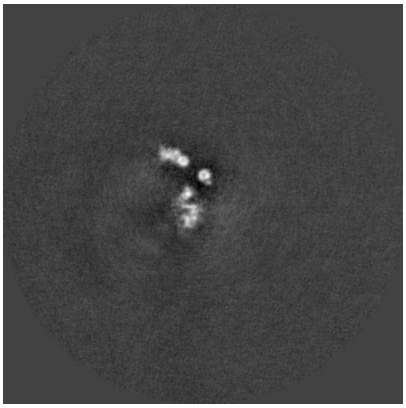


Z Index: 240

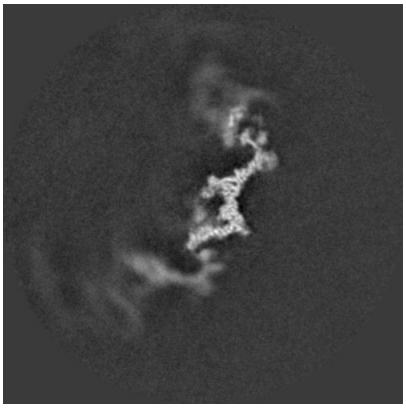
6.2.2 Raw map



X Index: 150



Y Index: 150

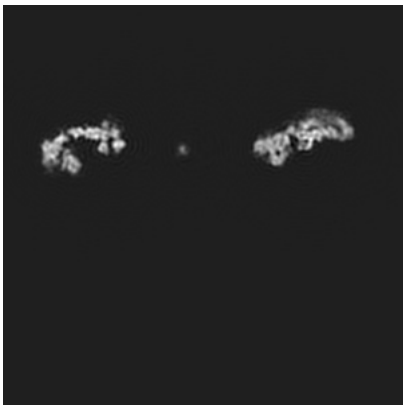


Z Index: 150

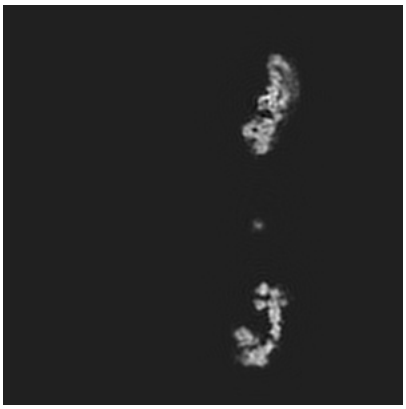
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

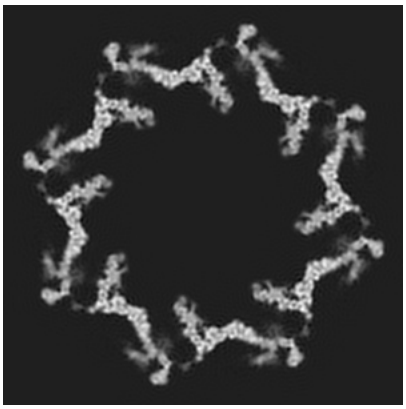
6.3.1 Primary map



X Index: 351

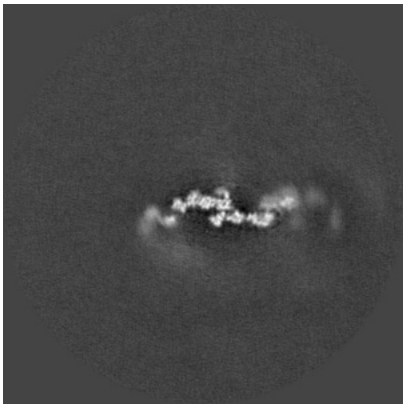


Y Index: 129

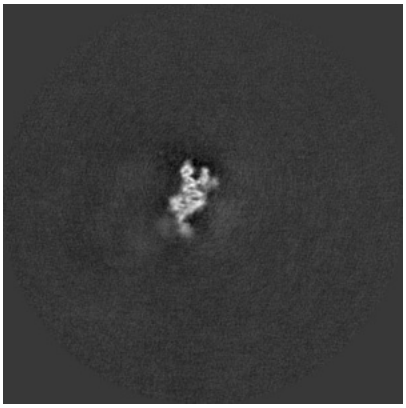


Z Index: 309

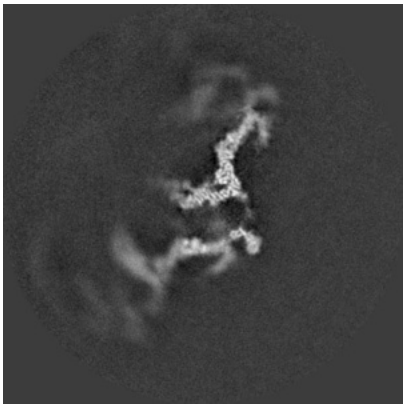
6.3.2 Raw map



X Index: 170



Y Index: 158

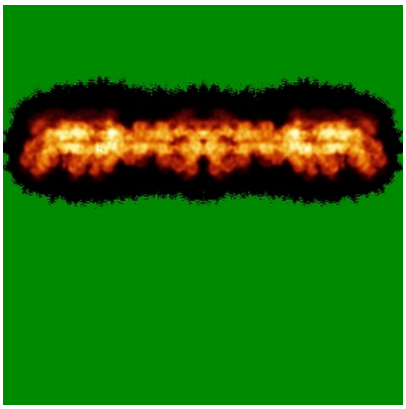


Z Index: 140

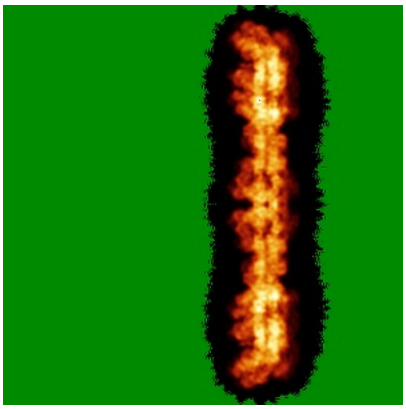
The images above show the largest variance slices of the map in three orthogonal directions.

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

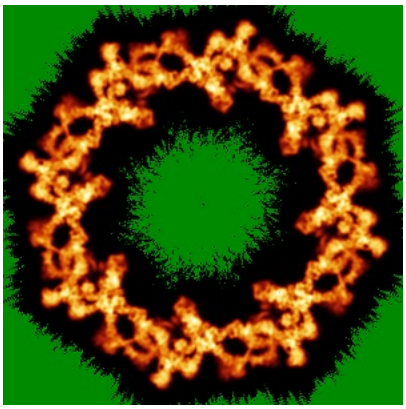
6.4.1 Primary map



X

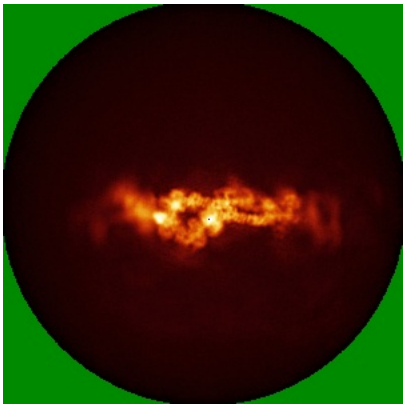


Y

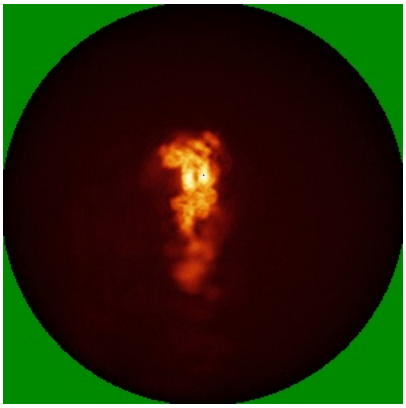


Z

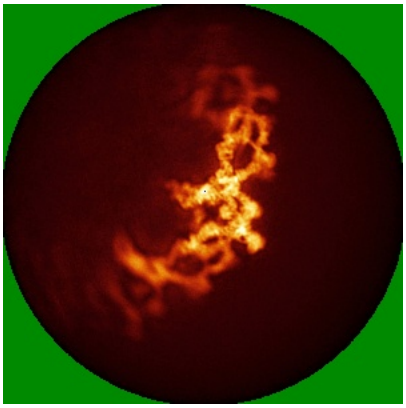
6.4.2 Raw map



X



Y

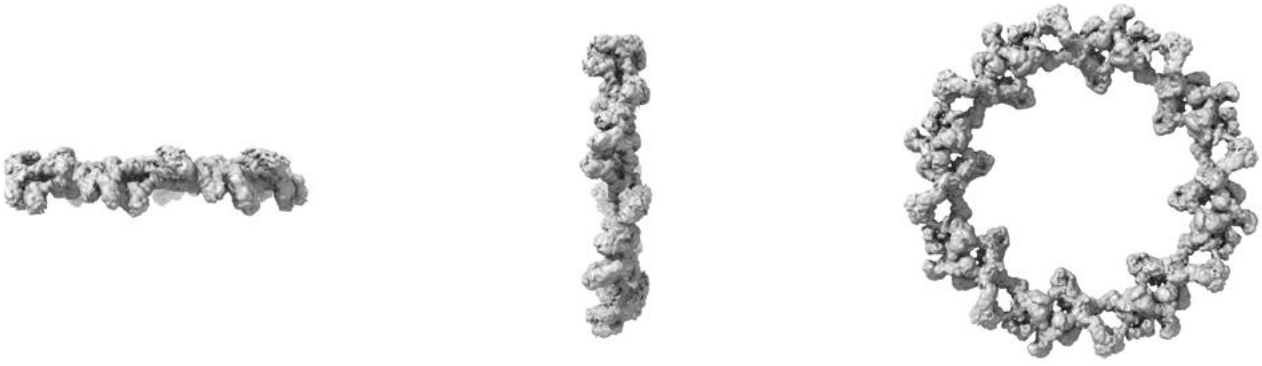


Z

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)

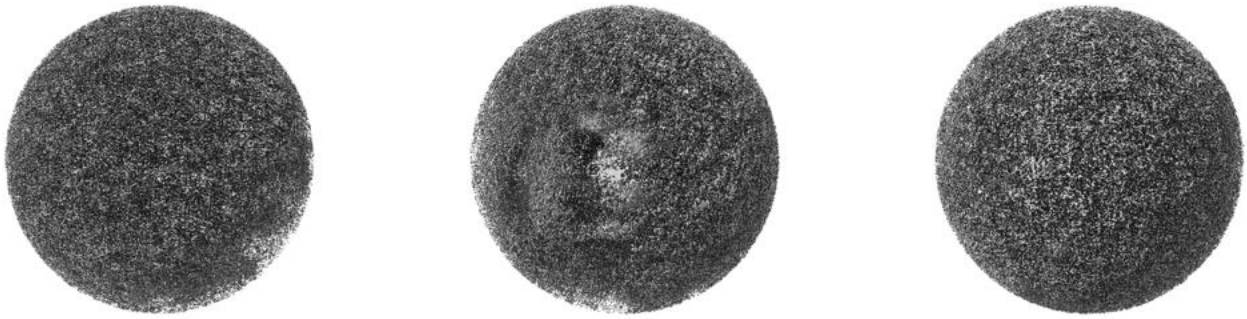
6.5.1 Primary map



X Y Z

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

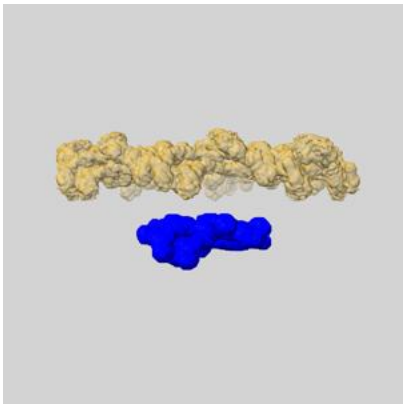
6.6 Mask visualisation (i)

This section shows the 3D surface view of the primary map at 50% transparency overlaid with the specified mask at 0% transparency

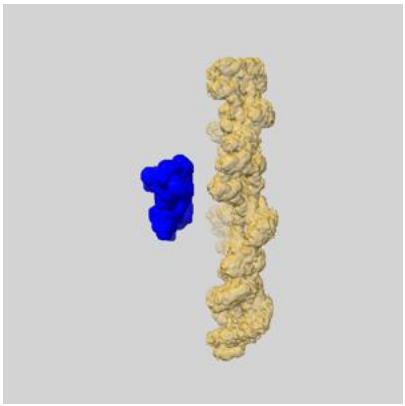
A mask typically either:

- Encompasses the whole structure
- Separates out a domain, a functional unit, a monomer or an area of interest from a larger structure

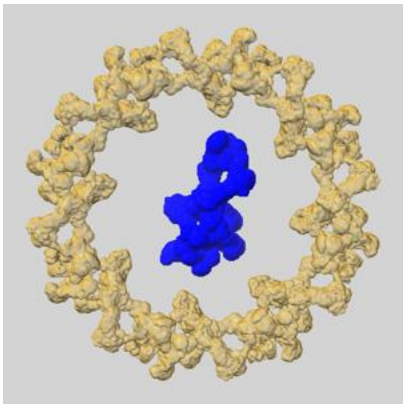
6.6.1 emd_24231_msk_1.map (i)



X



Y

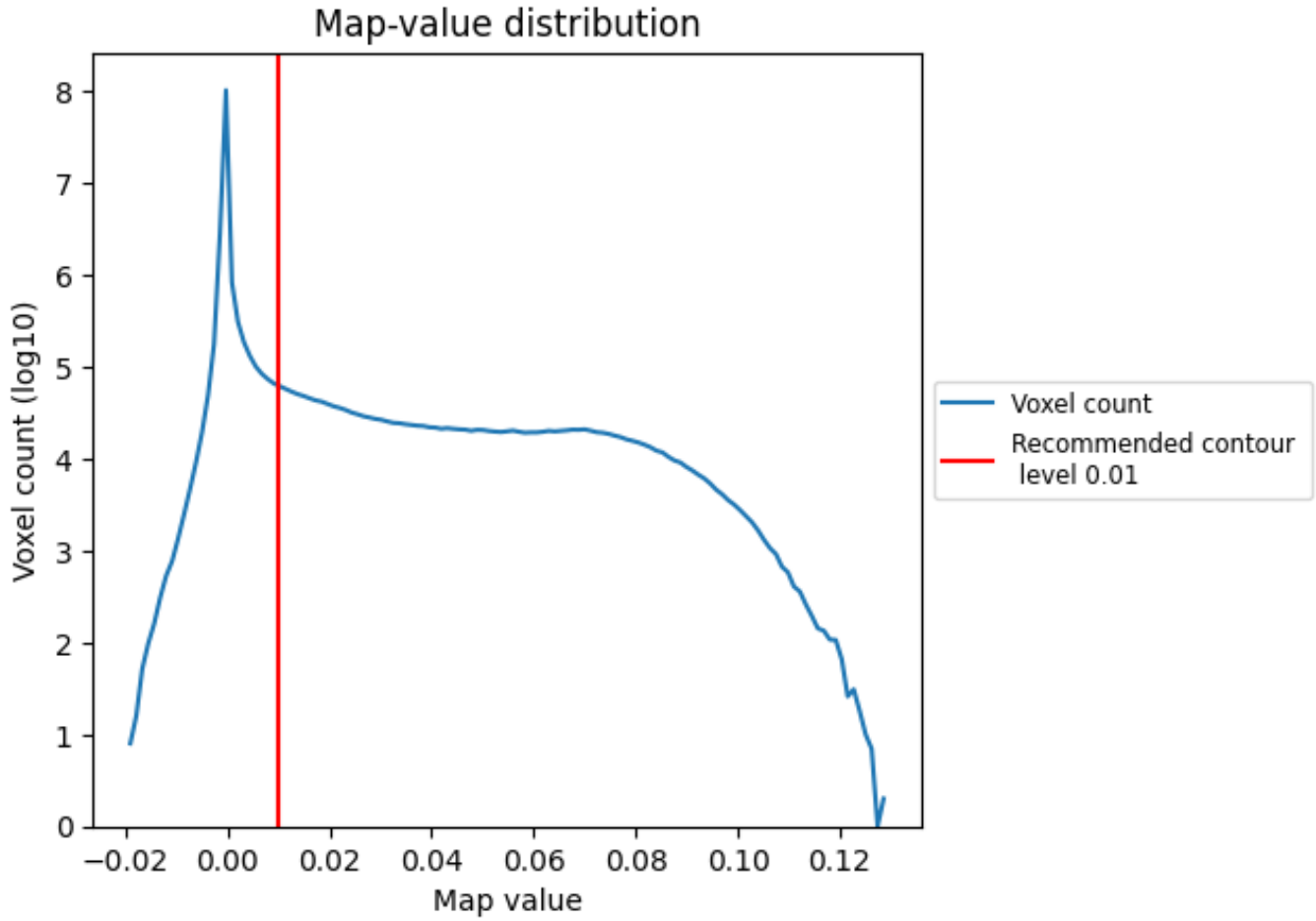


Z

7 Map analysis

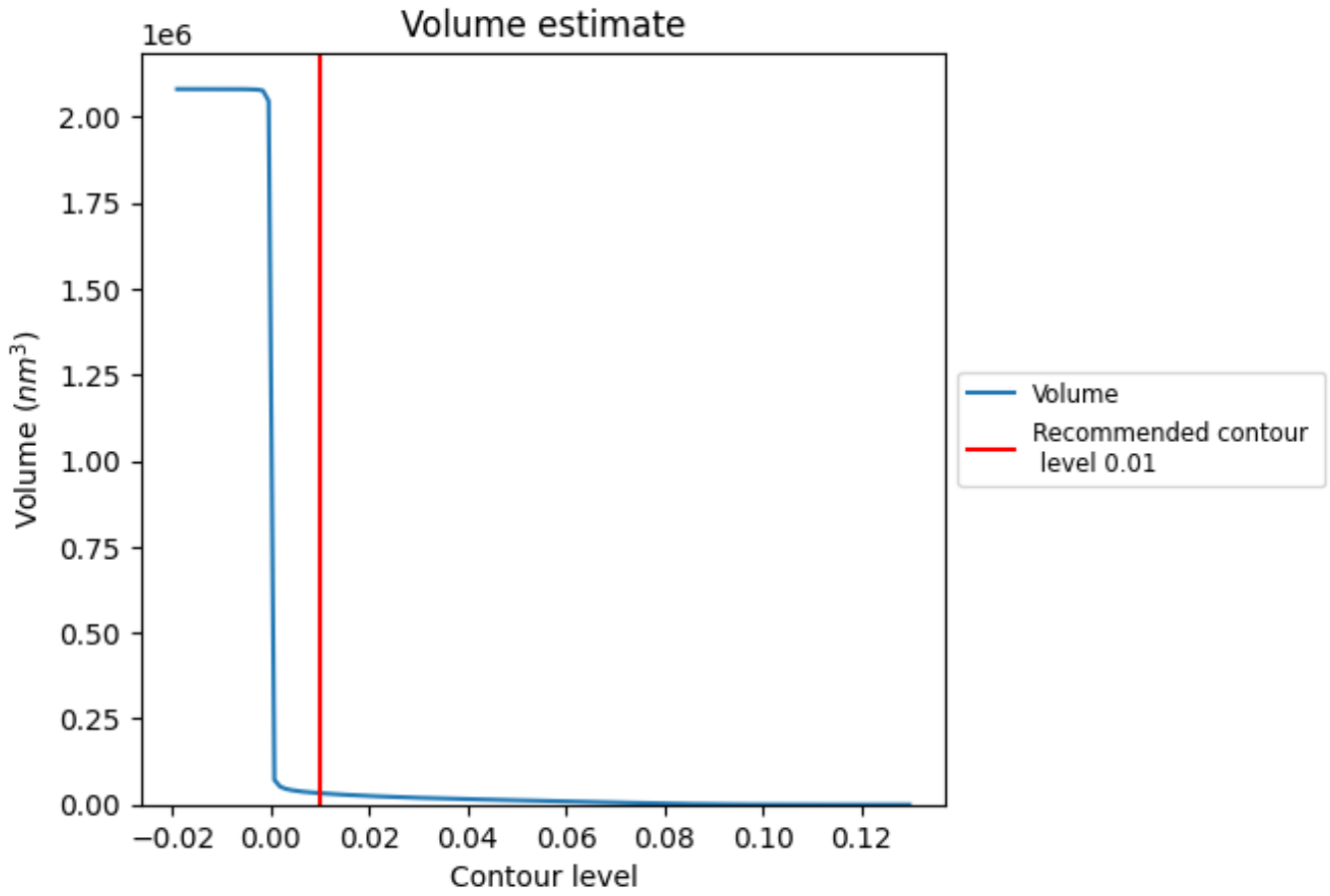
This section contains the results of statistical analysis of the map.

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.

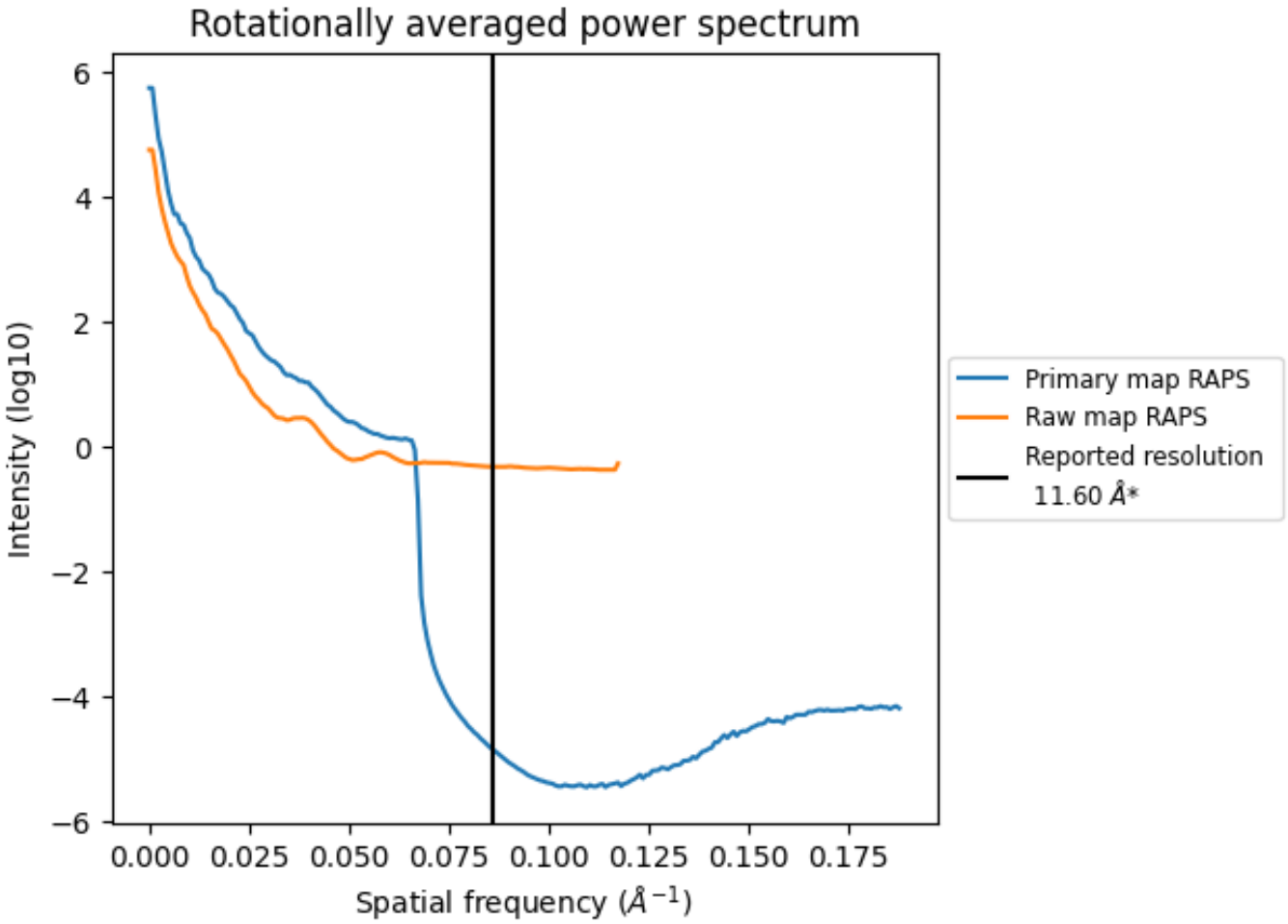
7.2 Volume estimate



The volume at the recommended contour level is 33303 nm^3; this corresponds to an approximate mass of 30083 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)

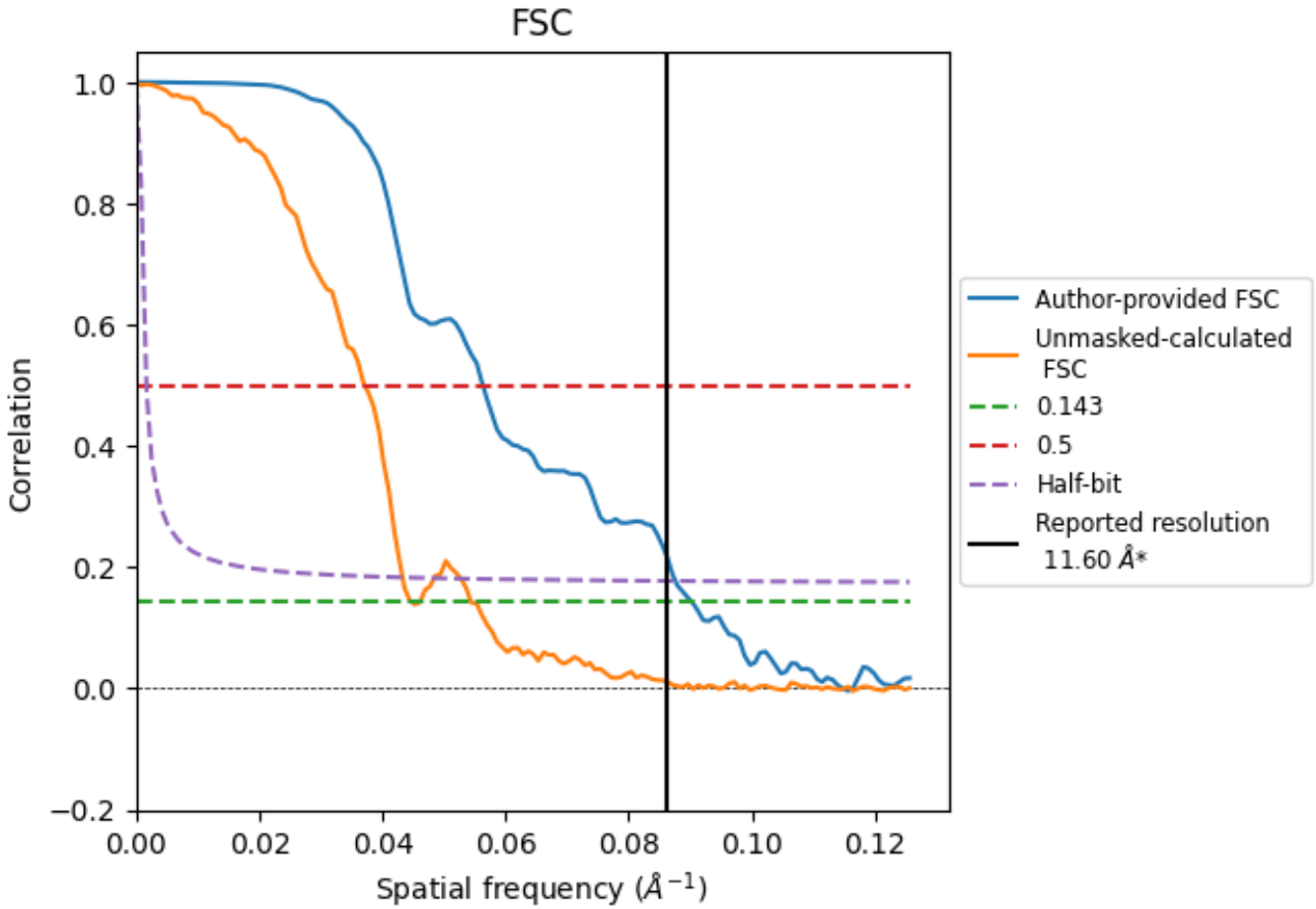


*Reported resolution corresponds to spatial frequency of 0.086 Å^{-1}

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 0.086 Å^{-1}

8.2 Resolution estimates (i)

Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	11.60	-	-
Author-provided FSC curve	11.09	17.76	11.42
Unmasked-calculated*	22.37	26.95	23.15

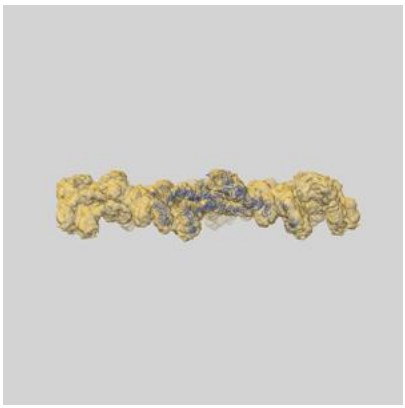
*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 22.37 differs from the reported value 11.6 by more than 10 %

9 Map-model fit

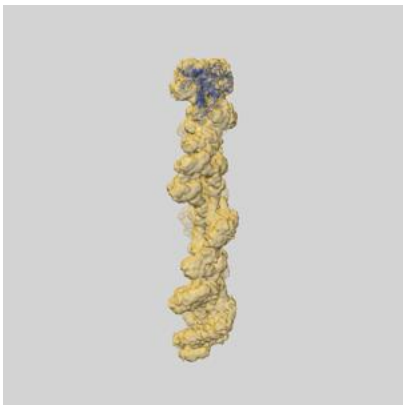
This section contains information regarding the fit between EMDB map EMD-24231 and PDB model 7N84. Per-residue inclusion information can be found in section 3 on page 6.

9.1 Map-model overlays

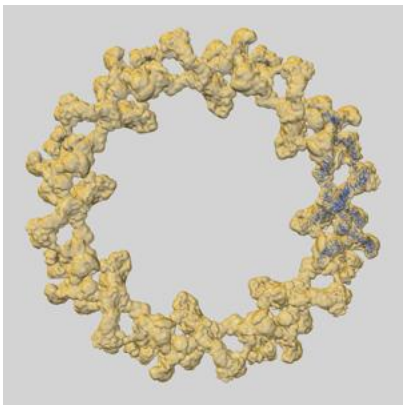
9.1.1 Map-model overlay



X

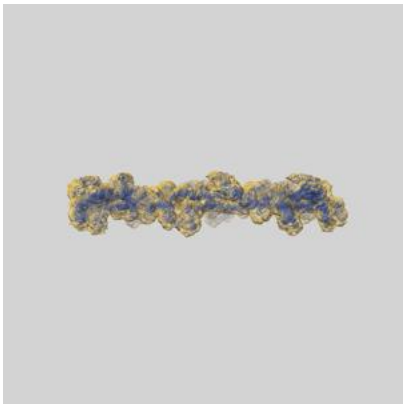


Y

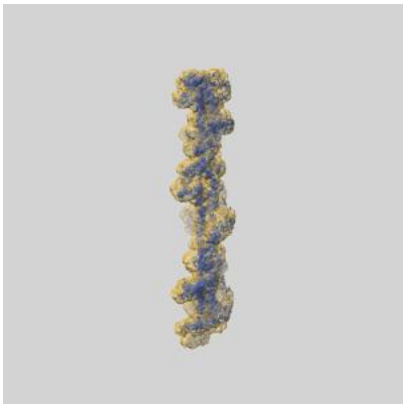


Z

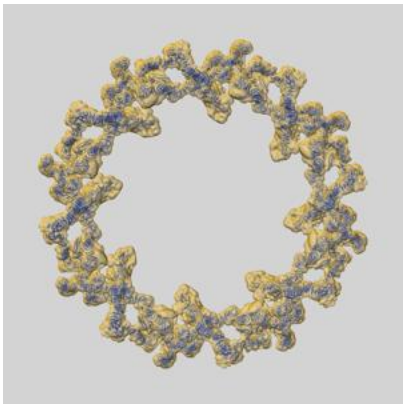
9.1.2 Map-model assembly overlay



X



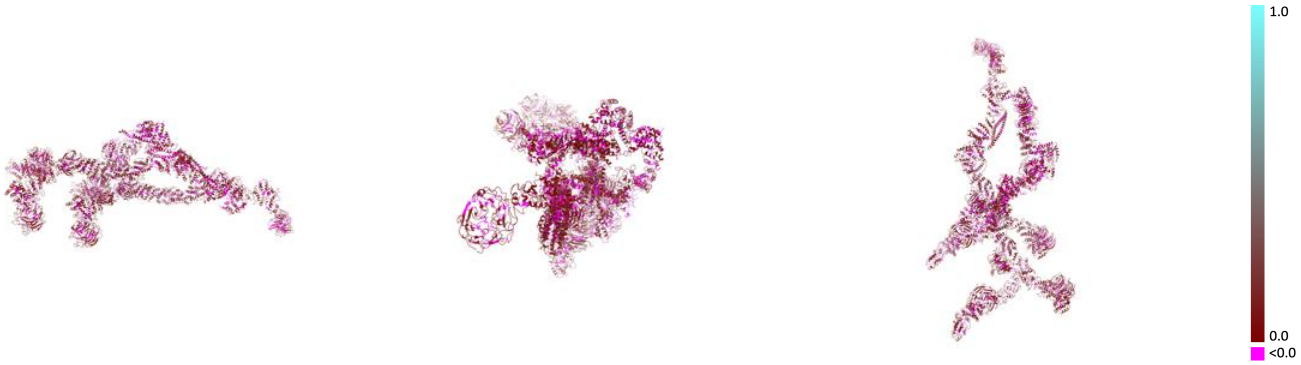
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.01 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

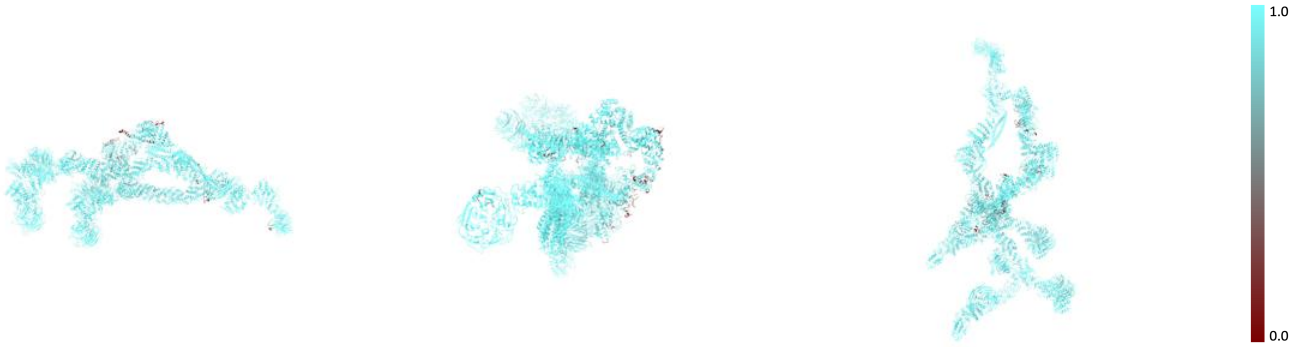
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

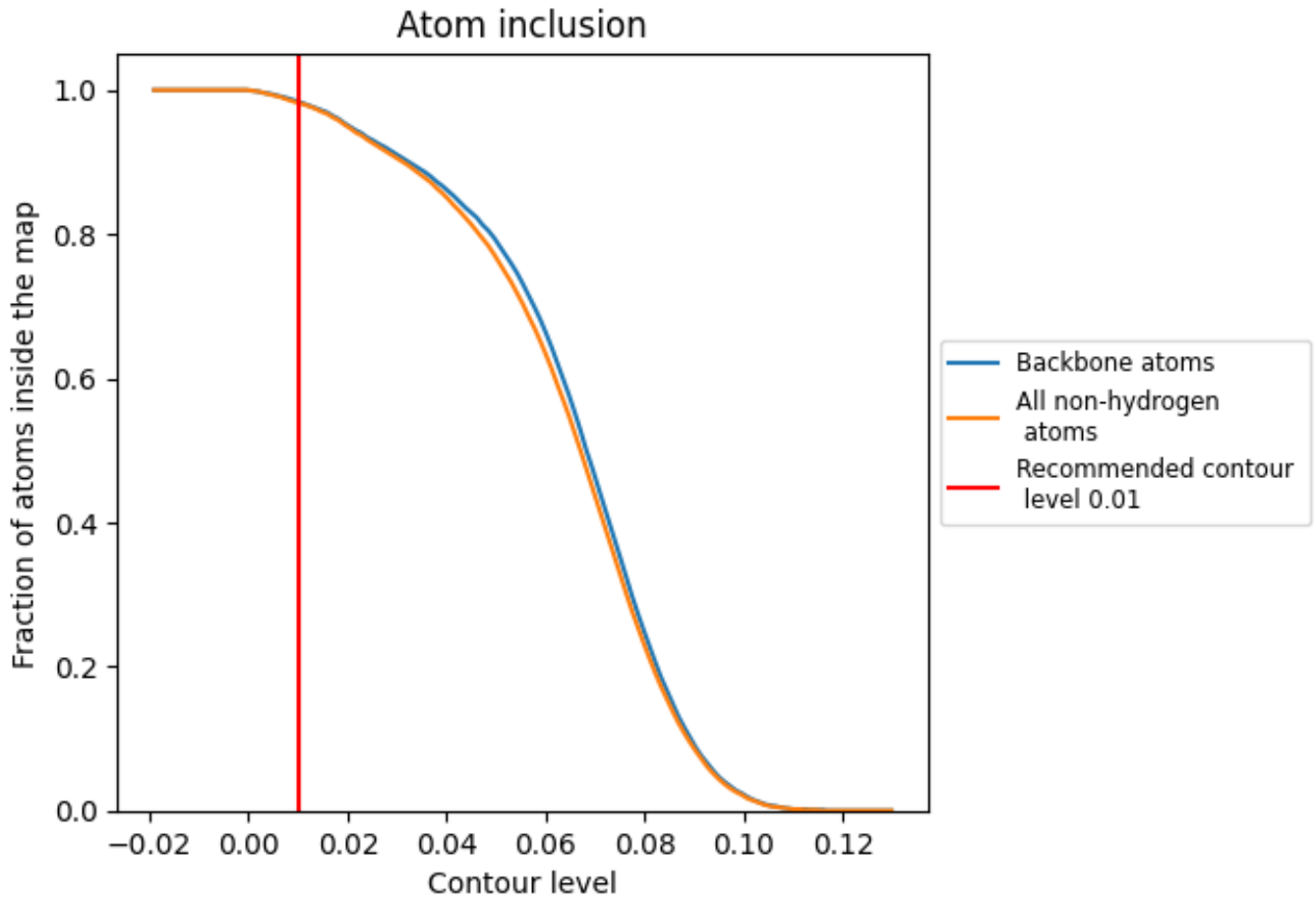
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.01).

9.4 Atom inclusion (i)



At the recommended contour level, 98% of all backbone atoms, 98% 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 (0.01) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.9820	0.0630
X	0.8870	0.0340
Y	0.9870	0.0690
Z	1.0000	0.0680
a	1.0000	0.0700
b	1.0000	0.0610
c	1.0000	0.0820
d	1.0000	0.0660
e	1.0000	0.0680
f	1.0000	0.0760
g	0.9910	0.0490
l	1.0000	0.0700
m	1.0000	0.0700
n	1.0000	0.0860
o	1.0000	0.0690
p	1.0000	0.0620
q	1.0000	0.0770
r	0.9610	0.0520