Full wwPDB EM Validation Report ⓘ

Nov 26, 2022 – 01:59 PM EST

PDB ID	:	5IY6
EMDB ID	:	EMD-3307
Title	:	Human holo-PIC in the closed state
Authors	:	He, Y.; Yan, C.; Fang, J.; Inouye, C.; Tjian, R.; Ivanov, I.; Nogales, E.
Deposited on	:	2016-03-24
Resolution	:	7.20 Å(reported)

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

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

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

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

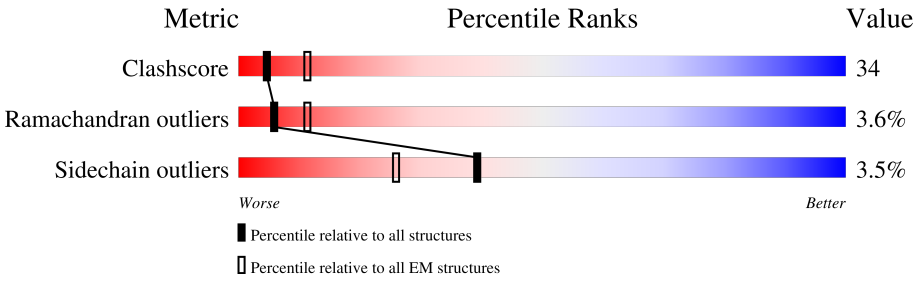
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 7.20 Å.

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



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

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

Mol	Chain	Length	Quality of chain
1	A	1970	24% 41% 31% · 26%
2	B	1174	22% 50% 46% · ·
3	C	275	10% 46% 50% ·
4	D	142	21% 65% 26% 9%
5	E	210	22% 50% 46% · ·
6	F	127	15% 35% 32% · 32%
7	G	172	18% 65% 32% · ·
8	H	150	18% 47% 46% 6% ·

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Mol	Chain	Length	Quality of chain
9	I	125	20% 41% 50% 9%
10	J	67	19% 55% 42%
11	K	117	12% 55% 45%
12	L	58	26% 47% 5% 21%
13	M	316	14% 48% 30% 18%
14	N	376	7% 15% 14% 70%
15	O	109	9% 48% 43% 9%
16	P	339	6% 29% 24% 45%
17	Q	439	11% 21% 18% 59%
18	R	291	14% 31% 19% 43%
19	S	517	12% 18% 9% 73%
20	T	249	30% 49% 35% 6% 11%
21	U	301	18% 31% 21% 5% 44%
22	V	782	25% 38% 18% 39%
23	W	760	29% 59% 23% 12%
24	0	395	11% 32% 14% 52%
25	1	71	61% 17% 61% 8% 13%
26	2	462	23% 21% 35% 41%
27	3	308	18% 15% 42% 5% 37%
28	X	65	45% 34% 18%
29	Y	65	12% 38% 43% 17%

2 Entry composition

There are 31 unique types of molecules in this entry. The entry contains 61839 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 DNA-directed RNA polymerase II subunit RPB1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1454	11515	7234	2058	2150	73	0	0

- Molecule 2 is a protein called DNA-directed RNA polymerase II subunit RPB2.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
2	B	1165	9317	5878	1637	1738	64	0	0

- Molecule 3 is a protein called DNA-directed RNA polymerase II subunit RPB3.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
3	C	275	2213	1386	380	440	7	0	0

- Molecule 4 is a protein called DNA-directed RNA polymerase II subunit RPB4.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
4	D	129	1062	665	179	214	4	0	0

- Molecule 5 is a protein called DNA-directed RNA polymerase II subunit RPB5.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
5	E	210	1723	1088	301	325	9	0	0

- Molecule 6 is a protein called DNA-directed RNA polymerase II subunit RPB6.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
6	F	86	689	437	120	127	5	0	0

- Molecule 7 is a protein called DNA-directed RNA polymerase II subunit RPB7.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	G	171	Total	C	N	O	S	0	0
			1351	875	219	249	8		

- Molecule 8 is a protein called DNA-directed RNA polymerase II subunit RPB8.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	150	Total	C	N	O	S	0	0
			1205	764	196	239	6		

- Molecule 9 is a protein called DNA-directed RNA polymerase II subunit RPB9.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	125	Total	C	N	O	S	0	0
			1013	626	177	198	12		

- Molecule 10 is a protein called DNA-directed RNA polymerase II subunit RPB10.

Mol	Chain	Residues	Atoms					AltConf	Trace
10	J	67	Total	C	N	O	S	0	0
			533	345	90	92	6		

- Molecule 11 is a protein called DNA-directed RNA polymerase II subunit RPB11-a.

Mol	Chain	Residues	Atoms					AltConf	Trace
11	K	117	Total	C	N	O	S	0	0
			937	604	154	177	2		

- Molecule 12 is a protein called DNA-directed RNA polymerase II subunit RPB12.

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	46	Total	C	N	O	S	0	0
			388	241	75	66	6		

- Molecule 13 is a protein called Transcription initiation factor IIB.

Mol	Chain	Residues	Atoms					AltConf	Trace
13	M	260	Total	C	N	O	S	0	0
			2018	1265	360	376	17		

- Molecule 14 is a protein called Transcription initiation factor IIA subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	N	113	Total	C	N	O	S	0	0
			930	585	152	189	4		

- Molecule 15 is a protein called Transcription initiation factor IIA subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	O	99	Total	C	N	O	S	0	0
			806	510	142	151	3		

- Molecule 16 is a protein called TATA-box-binding protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
16	P	185	Total	C	N	O	S	0	0
			1462	946	257	252	7		

- Molecule 17 is a protein called General transcription factor IIE subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	Q	180	Total	C	N	O	S	0	0
			1484	938	262	273	11		

- Molecule 18 is a protein called Transcription initiation factor IIE subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	R	165	Total	C	N	O	S	0	0
			1357	865	235	253	4		

- Molecule 19 is a protein called General transcription factor IIF subunit 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	S	138	Total	C	N	O	S	0	0
			1138	719	208	208	3		

- Molecule 20 is a protein called General transcription factor IIF subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	T	222	Total	C	N	O	S	0	0
			1788	1127	320	338	3		

- Molecule 21 is a protein called Transcription elongation factor A protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	U	170	Total	C	N	O	S	0	0
			1343	818	247	263	15		

- Molecule 22 is a protein called TFIIH basal transcription factor complex helicase XPB subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	V	475	Total	C	N	O	S	0	0
			3855	2454	663	712	26		

- Molecule 23 is a protein called TFIIH basal transcription factor complex helicase XPD subunit.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	W	665	Total	C	N	O	S	0	0
			5348	3415	932	975	26		

- Molecule 24 is a protein called General transcription factor IIH subunit 2.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	0	188	Total	C	N	O	S	0	0
			1479	935	258	276	10		

- Molecule 25 is a protein called General transcription factor IIH subunit 5.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	1	62	Total	C	N	O	S	0	0
			491	317	77	93	4		

- Molecule 26 is a protein called General transcription factor IIH subunit 4.

Mol	Chain	Residues	Atoms					AltConf	Trace
26	2	274	Total	C	N	O	S	0	0
			2196	1417	377	392	10		

- Molecule 27 is a protein called General transcription factor IIH subunit 3.

Mol	Chain	Residues	Atoms					AltConf	Trace
27	3	193	Total	C	N	O	S	0	0
			1526	978	252	284	12		

- Molecule 28 is a DNA chain called SCP-X.

Mol	Chain	Residues	Atoms					AltConf	Trace
28	X	65	Total	C	N	O	P	0	0
			1343	633	261	385	64		

- Molecule 29 is a DNA chain called SCP-Y.

Mol	Chain	Residues	Atoms					AltConf	Trace
29	Y	65	Total	C	N	O	P	0	0
			1316	625	236	391	64		

- Molecule 30 is MAGNESIUM ION (three-letter code: MG) (formula: Mg).

Mol	Chain	Residues	Atoms		AltConf
30	A	1	Total	Mg	0
			1	1	
30	B	1	Total	Mg	0
			1	1	

- Molecule 31 is ZINC ION (three-letter code: ZN) (formula: Zn).

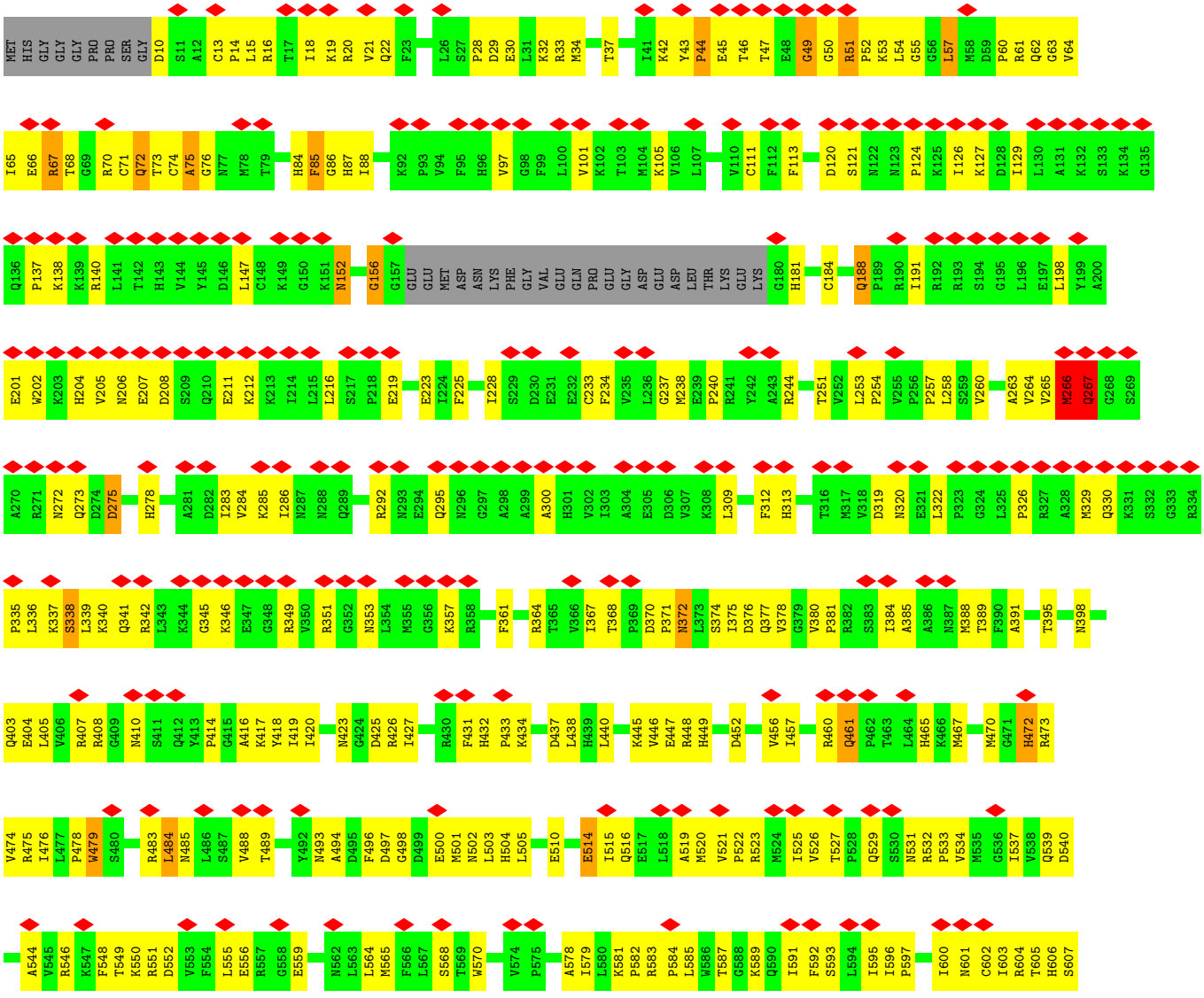
Mol	Chain	Residues	Atoms		AltConf
31	A	2	Total	Zn	0
			2	2	
31	B	1	Total	Zn	0
			1	1	
31	C	1	Total	Zn	0
			1	1	
31	I	2	Total	Zn	0
			2	2	
31	J	1	Total	Zn	0
			1	1	
31	L	1	Total	Zn	0
			1	1	
31	M	1	Total	Zn	0
			1	1	
31	Q	1	Total	Zn	0
			1	1	
31	U	1	Total	Zn	0
			1	1	

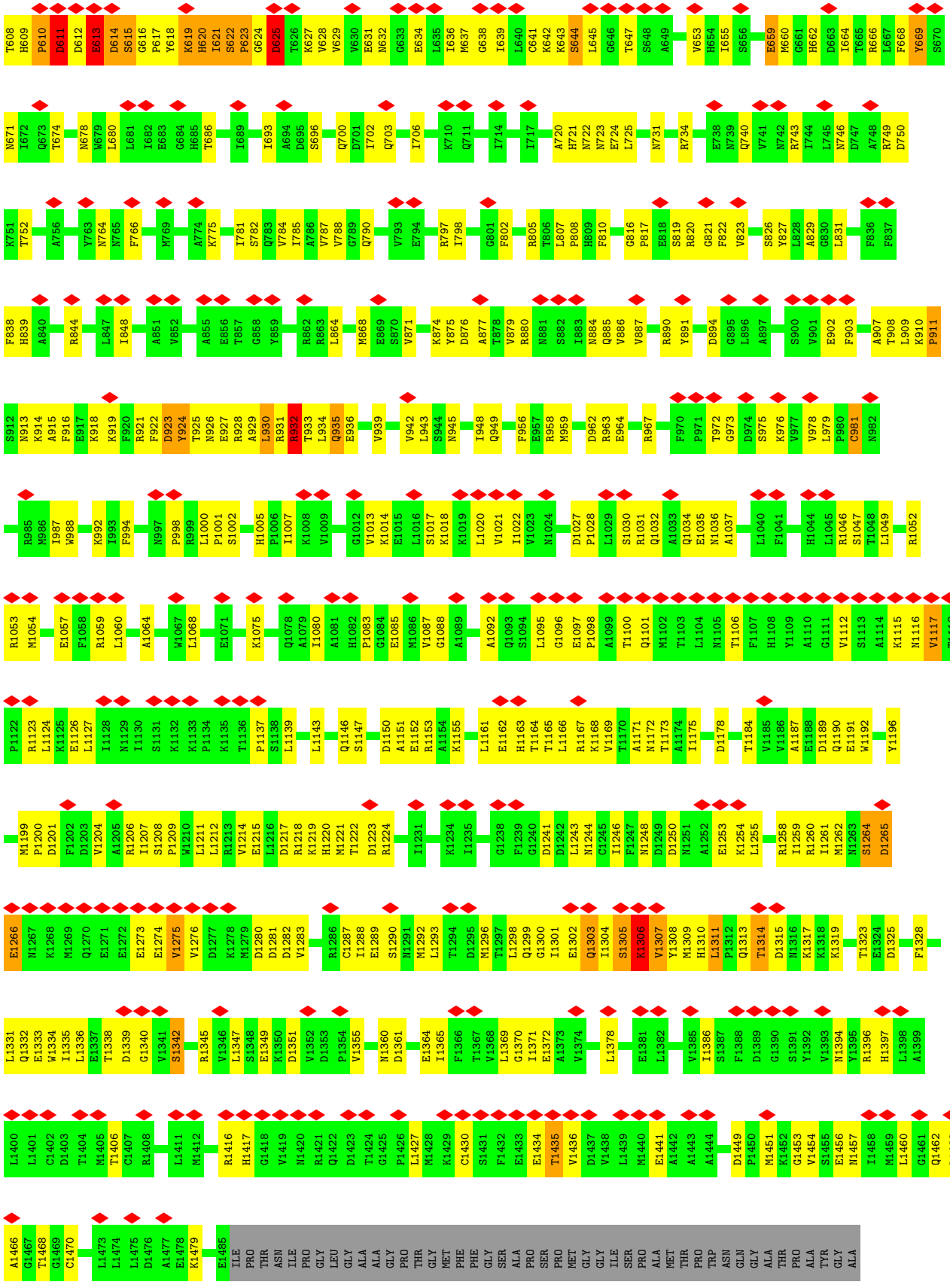
3 Residue-property plots (i)

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: DNA-directed RNA polymerase II subunit RPB1

Chain A:

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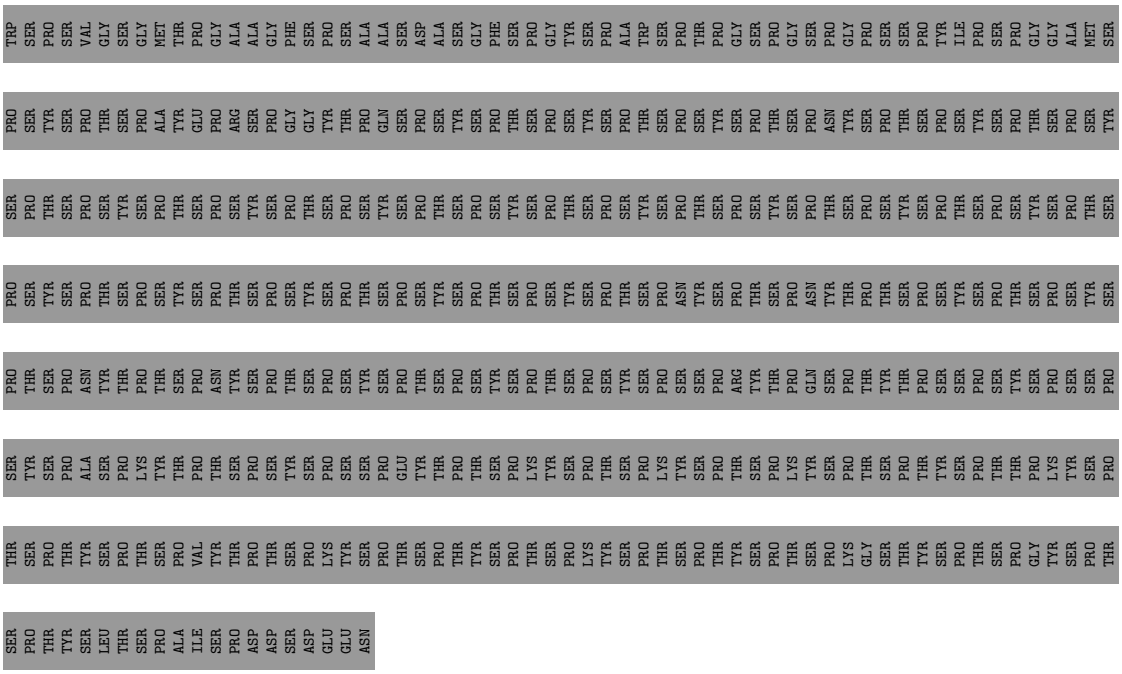
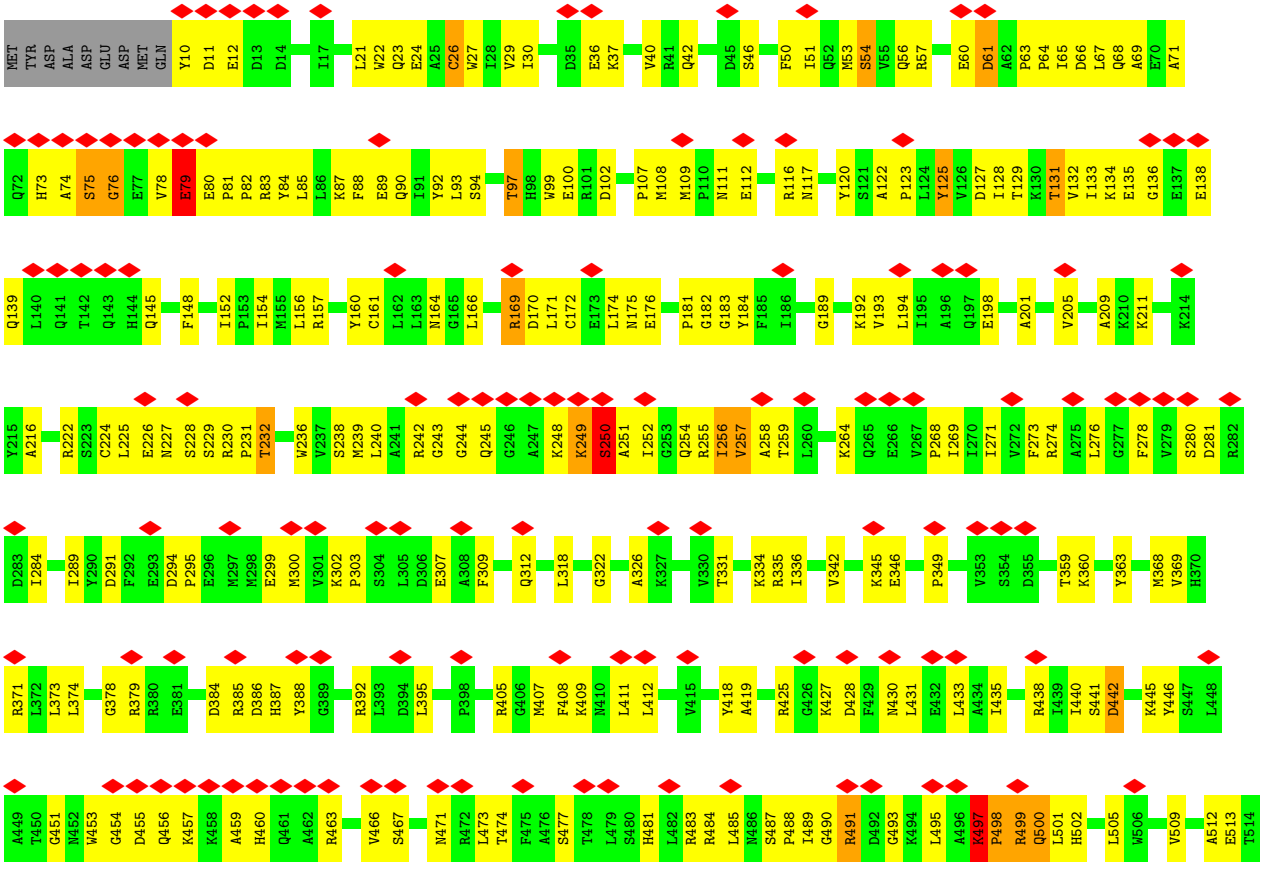
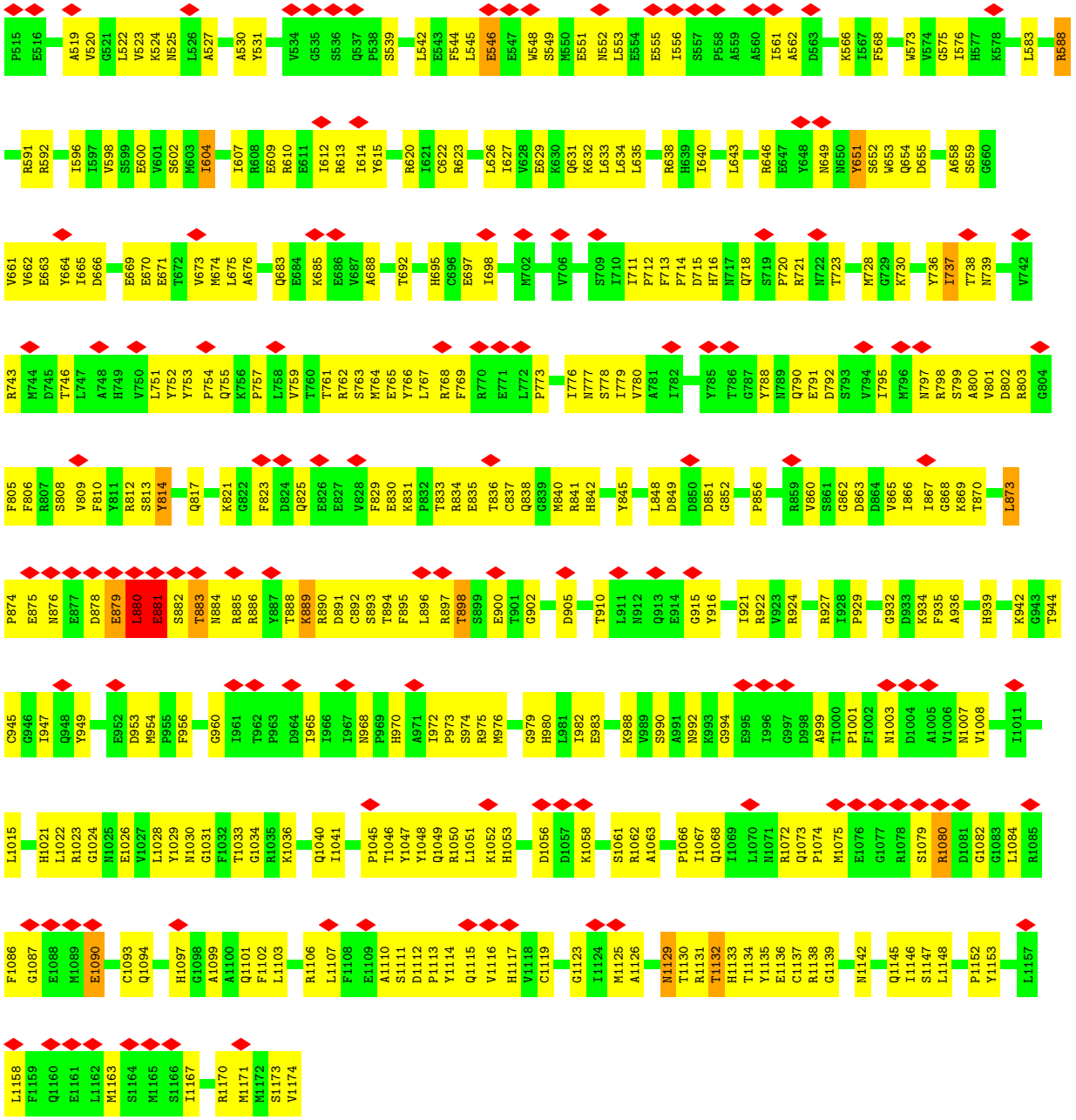
N671 I672 Q673 T674 N678 W679 L680 L681 I682 E683 G684 H685 T686 I689 I693 A694 D695 S696 Q700 D701 I702 Q703 I706 K710 Q711 I714 I717 A720 H721 N722 N723 E724 L725 N731 R734 E738 N739 Q740 V741 N742 R743 I744 L745 N746 D747 A748 R749 D750
K751 T752 A756 Y763 N764 N765 F766 M769 A774 K775 I781 S782 Q783 V784 I785 A786 V787 V788 G789 Q790 V793 E794 R797 I798 G801 F802 R805 T806 L807 P808 H809 F810 G816 P817 E818 S819 R820 G821 F822 V823 S826 Y827 L828 A829 G830 L831 F836 F837
F838 H839 A840 R844 L847 I848 A851 V852 A855 E856 T857 G858 Y859 R862 R863 L864 M868 E869 S870 V871 K874 Y875 D876 A877 T878 V879 R880 N881 S882 I883 N884 Q885 V886 V887 R890 Y891 D894 G895 L896 A897 S900 V901 E902 F903 A907 T908 L909 K910 P911
S912 N913 K914 A915 F916 E917 K918 K919 F920 R921 F922 D923 Y924 T925 N926 E927 R928 A929 L930 R931 R932 T933 L934 Q935 E936 V939 V942 L943 S944 N945 I948 Q949 F956 E957 R958 M959 D962 R963 E964 R967 F970 P971 T972 G973 D974 S975 K976 V977 V978 L979 P980 C981 N982
R985 M986 I987 W988 K992 I993 F994 N997 P998 R999 L1000 P1001 S1002 H1005 P1006 I1007 K1008 V1009 G1012 V1013 K1014 E1015 L1016 S1017 K1018 K1019 L1020 V1021 I1022 V1023 N1024 D1027 P1028 L1029 S1030 R1031 Q1032 A1033 Q1034 E1035 N1036 A1037 L1040 F1041 H1044 L1045 R1046 S1047 T1048 L1049 R1052
R1053 M1054 E1057 F1058 R1059 L1060 A1064 W1067 L1068 E1071 K1075 Q1078 A1079 I1080 A1081 H1082 P1083 G1084 E1085 M1086 V1087 G1088 A1089 A1092 Q1093 S1094 L1095 G1096 E1097 P1098 A1099 T1100 Q1101 M1102 T1103 L1104 N1105 T1106 F1107 H1108 Y1109 A1110 G1111 V1112 S1113 A1114 K1115 N1116 V1117 T1118 L1119 G1120 V1121
P1122 R1123 L1124 K1125 E1126 L1127 I1128 N1129 I1130 S1131 K1132 K1133 P1134 K1135 T1136 P1137 S1138 L1139 L1143 Q1146 S1147 D1150 A1151 E1152 R1153 A1154 K1155 L1161 E1162 H1163 T1164 T1165 L1166 R1167 K1168 V1169 T1170 A1171 N1172 T1173 A1174 I1175 D1178 T1184 V1185 V1186 A1187 E1188 D1189 Q1190 E1191 W1192 Y1196
M1199 P1200 D1201 F1202 D1203 V1204 A1205 R1206 I1207 S1208 P1209 W1210 L1211 L1212 R1213 V1214 E1215 L1216 D1217 R1218 K1219 H1220 M1221 T1222 D1223 R1224 T1231 K1234 I1235 G1238 F1239 G1240 D1241 D1242 L1243 N1244 C1245 I1246 F1247 N1248 D1249 D1250 N1251 A1252 E1253 K1254 L1255 R1258 I1259 R1260 I1261 M1262 N1263 S1264 D1265
E1266 N1267 K1268 M1269 Q1270 E1271 E1272 E1273 E1274 V1275 V1276 D1277 K1278 M1279 D1280 D1281 D1282 V1283 R1286 C1287 I1288 E1289 S1290 N1291 M1292 L1293 T1294 D1295 M1296 T1297 L1298 Q1299 G1300 I1301 E1302 Q1303 I1304 S1305 K1306 V1307 Y1308 M1309 H1310 L1311 P1312 Q1313 T1314 D1315 N1316 K1317 K1318 K1319 T1323 E1324 D1325 F1328
L1331 Q1332 E1333 W1334 I1335 L1336 E1337 T1338 D1339 G1340 V1341 S1342 R1345 V1346 L1347 S1348 E1349 K1350 D1351 V1352 D1353 P1354 V1355 N1360 D1361 E1364 I1365 F1366 T1367 V1368 L1369 G1370 I1371 E1372 A1373 V1374 L1378 E1381 L1382 V1385 I1386 S1387 F1388 D1389 G1390 S1391 Y1392 V1393 N1394 Y1395 R1396 H1397 L1398 A1399
L1400 L1401 C1402 D1403 T1404 M1405 T1406 C1407 R1408 L1411 M1412 R1416 H1417 G1418 V1419 N1420 R1421 Q1422 D1423 T1424 G1425 P1426 L1427 M1428 K1429 C1430 S1431 F1432 E1433 E1434 T1435 V1436 D1437 V1438 L1439 M1440 E1441 A1442 A1443 A1444 D1449 P1450 M1451 K1452 G1453 V1454 S1455 E1456 N1457 I1458 M1459 L1460 G1461 Q1462 L1463 A1464 P1465
A1466 G1467 T1468 G1469 C1470 L1473 L1474 L1475 D1476 A1477 E1478 K1479 E1485 ILE PRO THR ASN ILE PRO GLY LEU GLY ALA ALA GLY PRO THR GLY MET PHE PHE GLY SER ALA PRO SER PRO MET GLY GLY ILE SER PRO ALA MET THR PRO TRP ASN GLN GLY ALA THR PRO ALA TYR GLY ALA



• Molecule 2: DNA-directed RNA polymerase II subunit RPB2

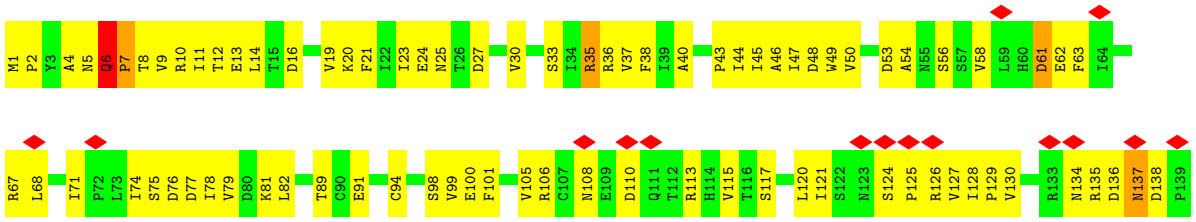
Chain B:

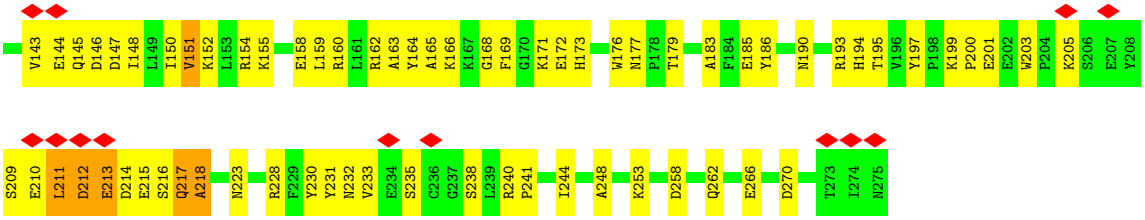




• Molecule 3: DNA-directed RNA polymerase II subunit RPB3

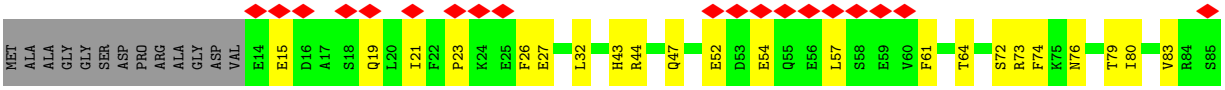
Chain C:

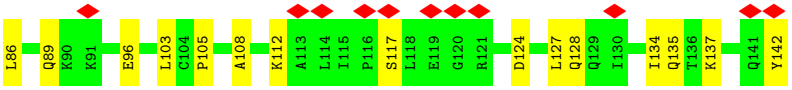




• Molecule 4: DNA-directed RNA polymerase II subunit RPB4

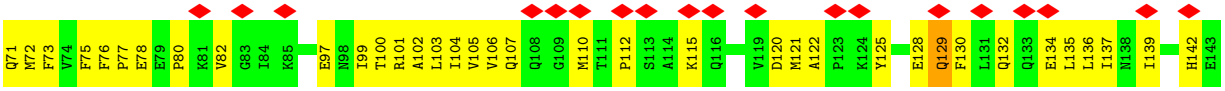
Chain D:

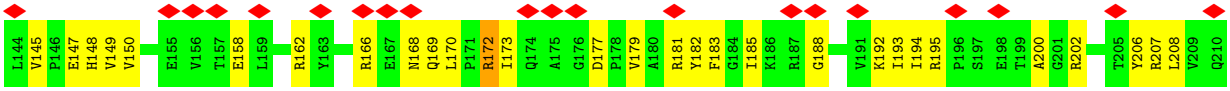




• Molecule 5: DNA-directed RNA polymerase II subunit RPB5

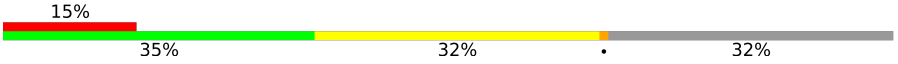
Chain E:

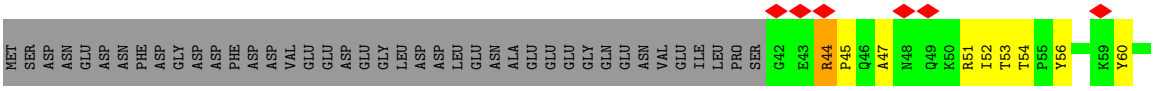


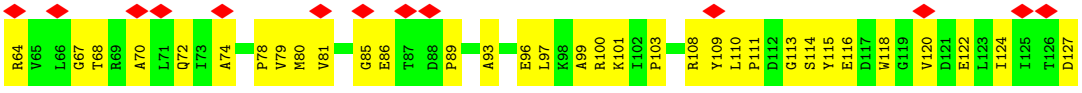


• Molecule 6: DNA-directed RNA polymerase II subunit RPB6

Chain F:

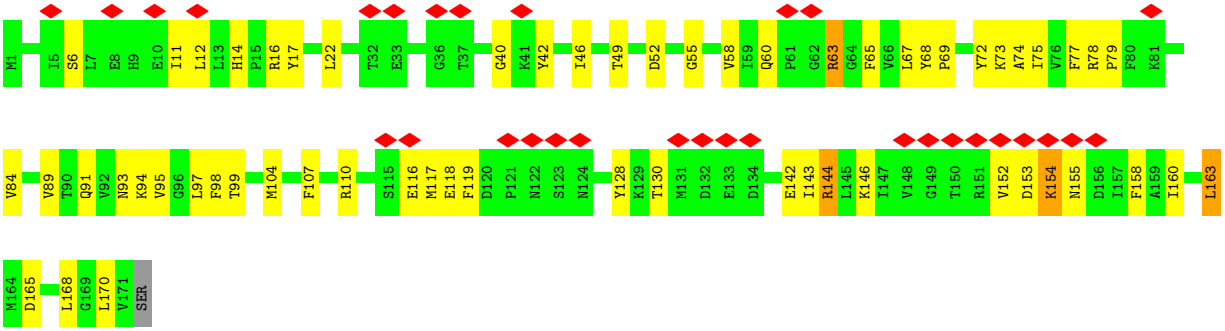






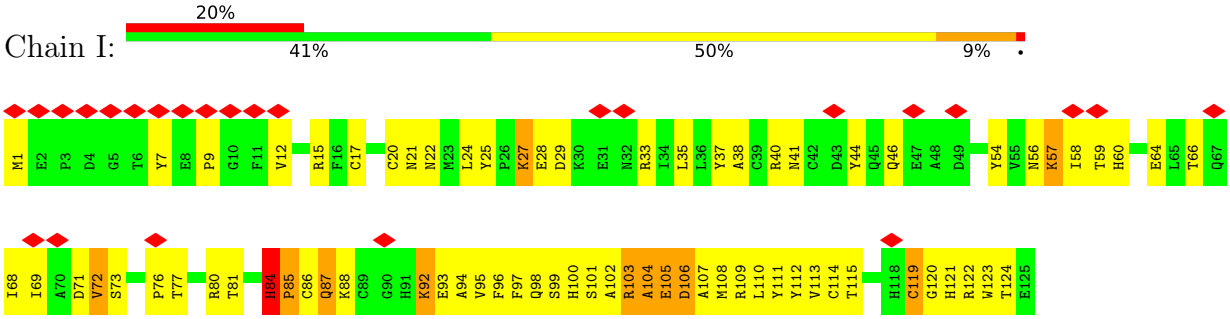
• Molecule 7: DNA-directed RNA polymerase II subunit RPB7

Chain G:

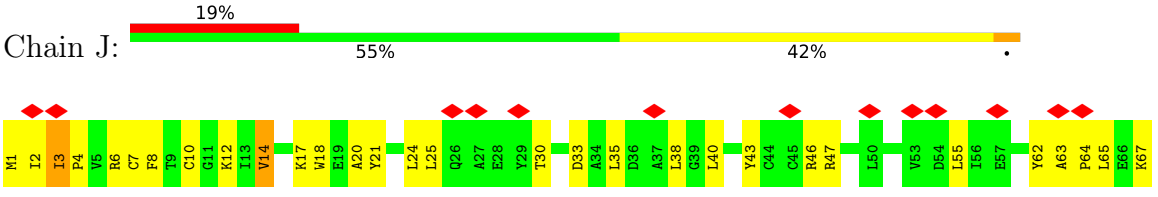


• Molecule 8: DNA-directed RNA polymerase II subunit RPB8

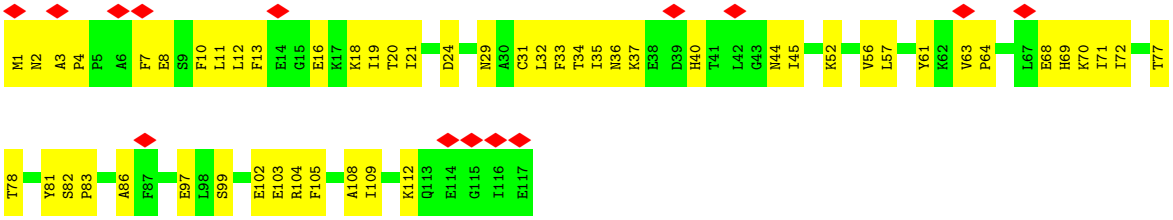
• Molecule 9: DNA-directed RNA polymerase II subunit RPB9



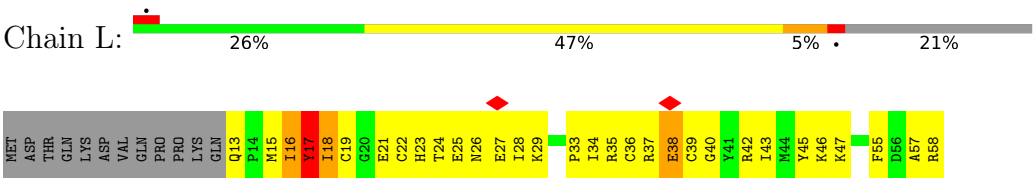
• Molecule 10: DNA-directed RNA polymerase II subunit RPB10



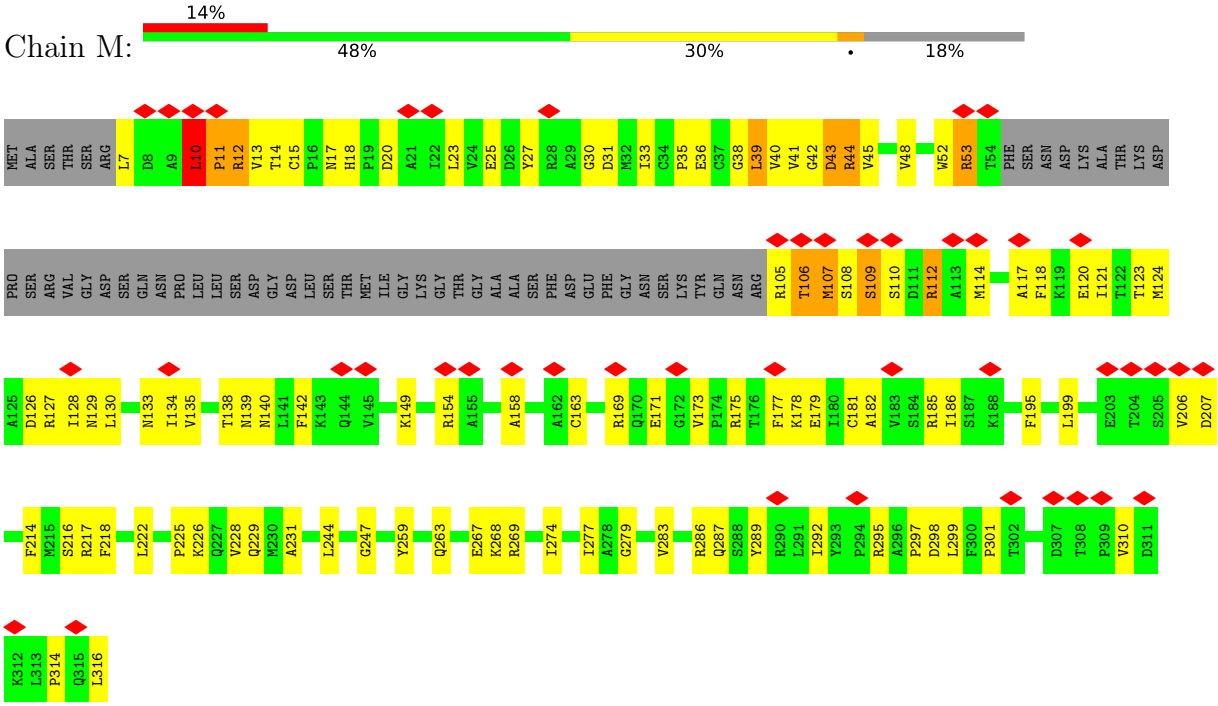
• Molecule 11: DNA-directed RNA polymerase II subunit RPB11-a



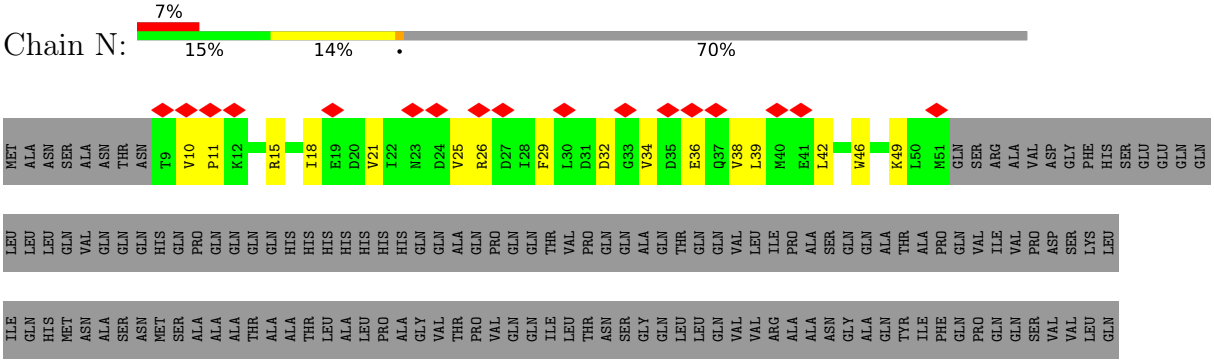
• Molecule 12: DNA-directed RNA polymerase II subunit RPB12

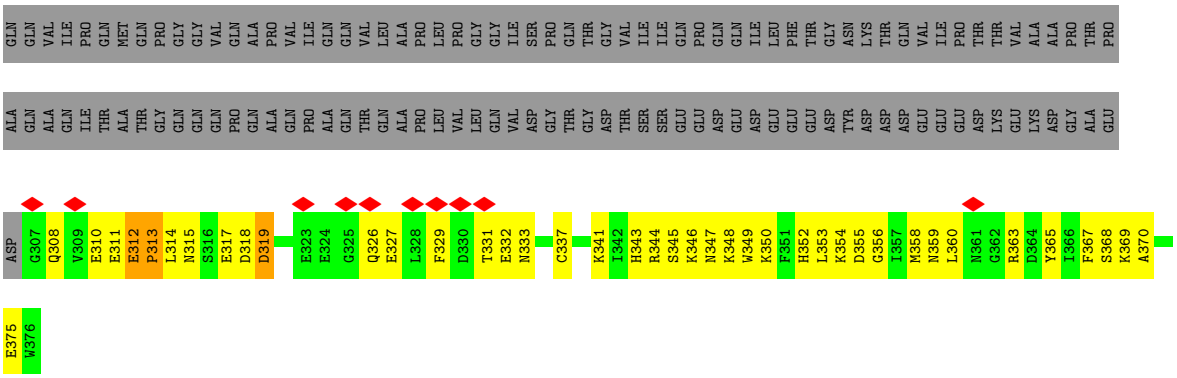


• Molecule 13: Transcription initiation factor IIB



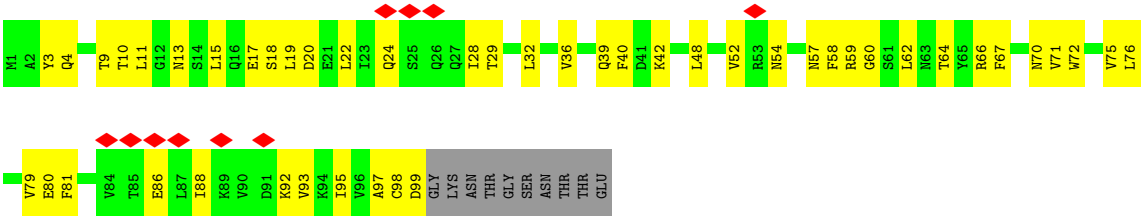
• Molecule 14: Transcription initiation factor IIA subunit 1





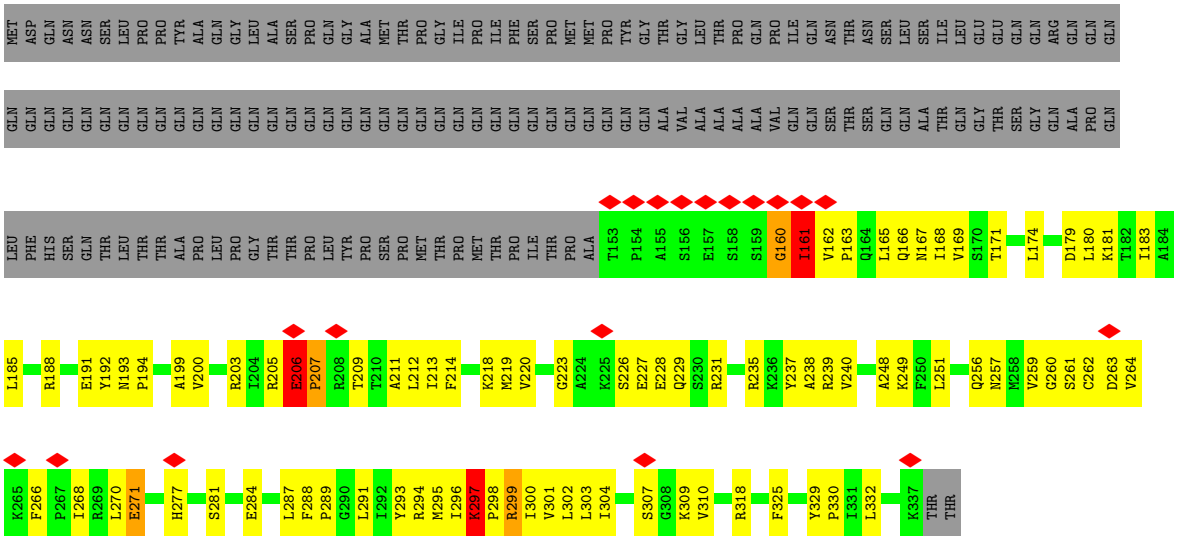
• Molecule 15: Transcription initiation factor IIA subunit 2

Chain O:



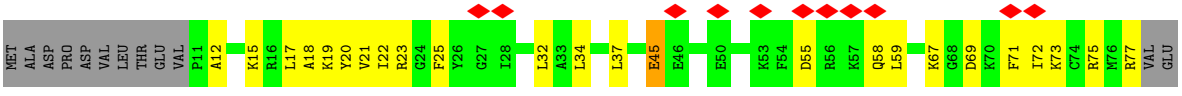
• Molecule 16: TATA-box-binding protein

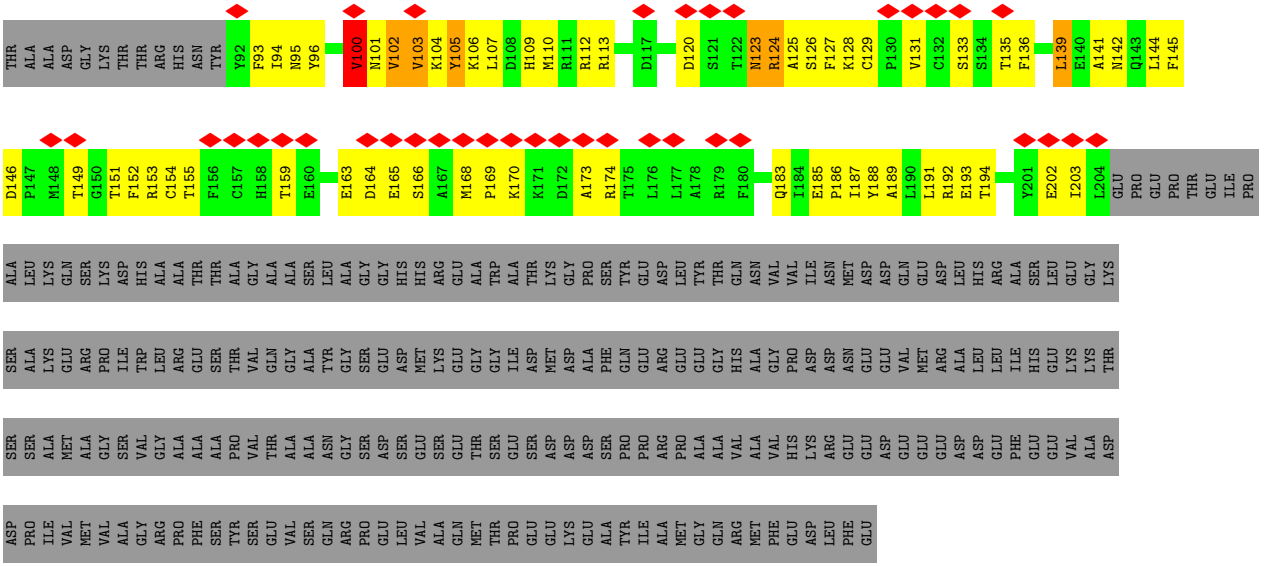
Chain P:



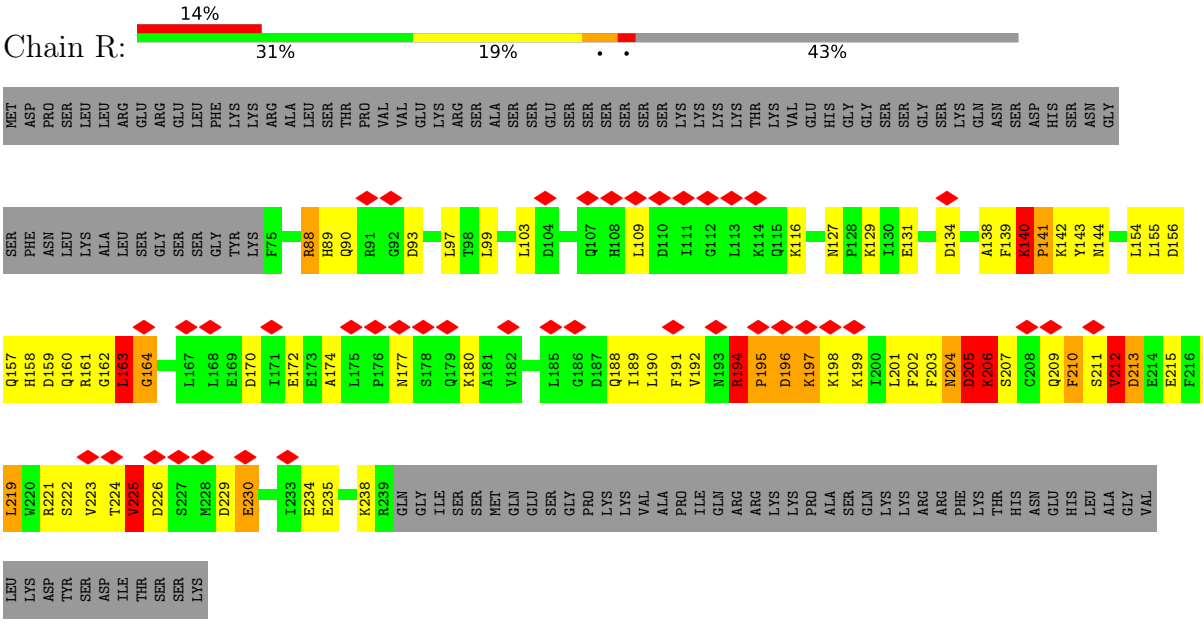
• Molecule 17: General transcription factor IIE subunit 1

Chain Q:

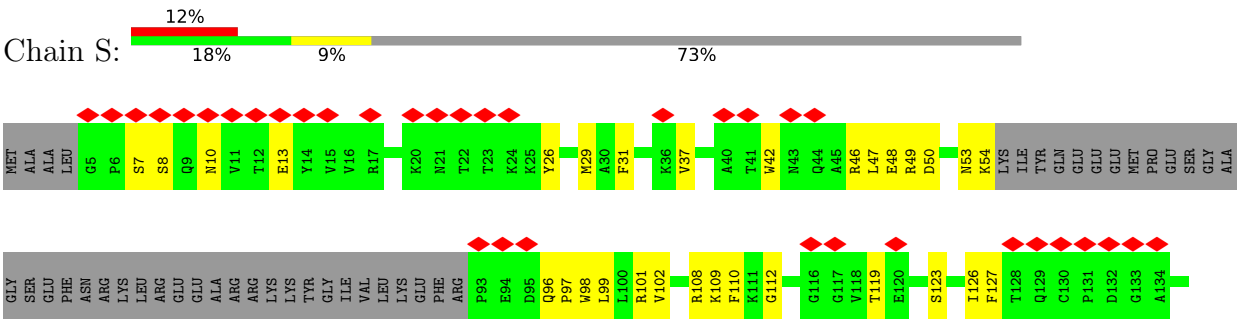


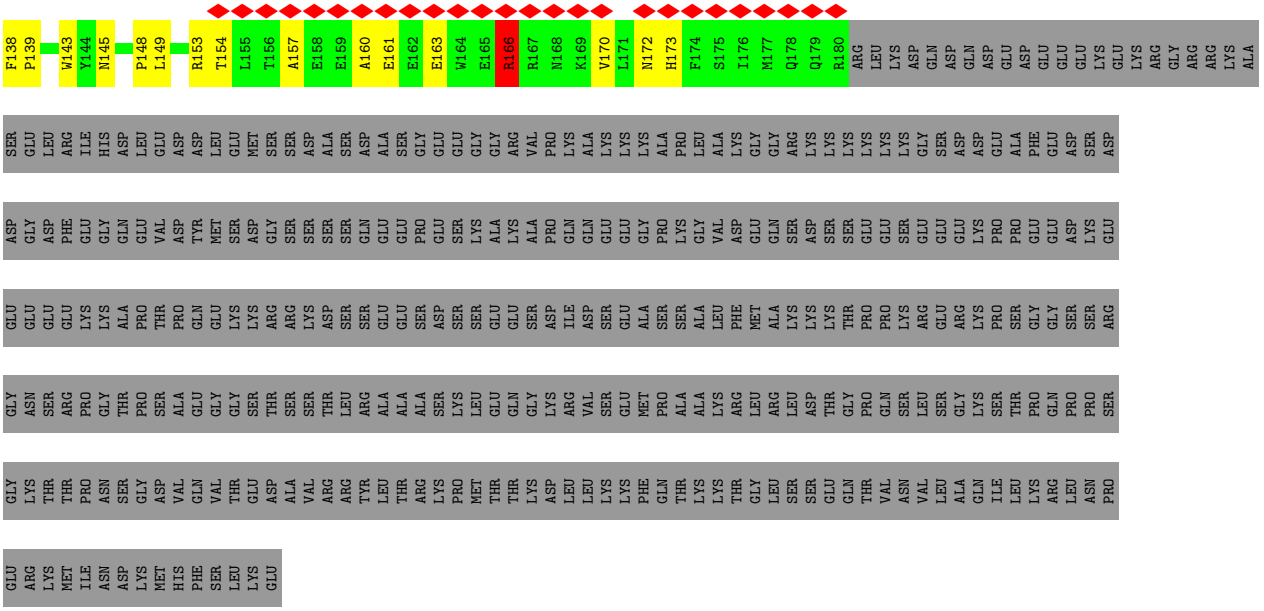


• Molecule 18: Transcription initiation factor IIE subunit beta



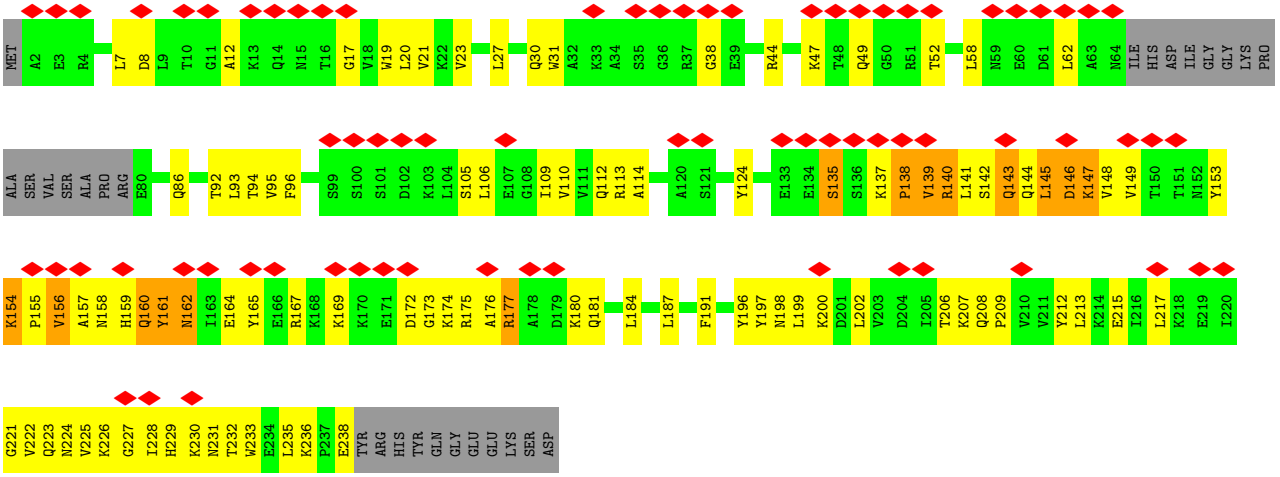
• Molecule 19: General transcription factor IIF subunit 1





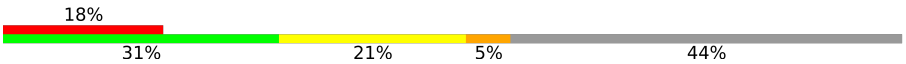
• Molecule 20: General transcription factor IIF subunit 2

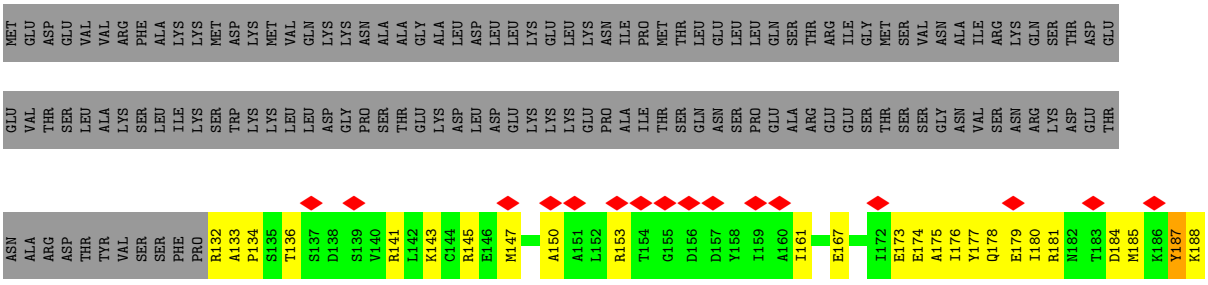
Chain T:



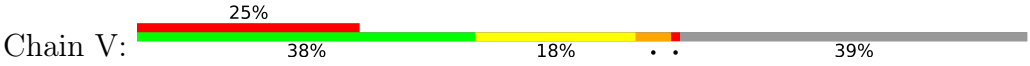
• Molecule 21: Transcription elongation factor A protein 1

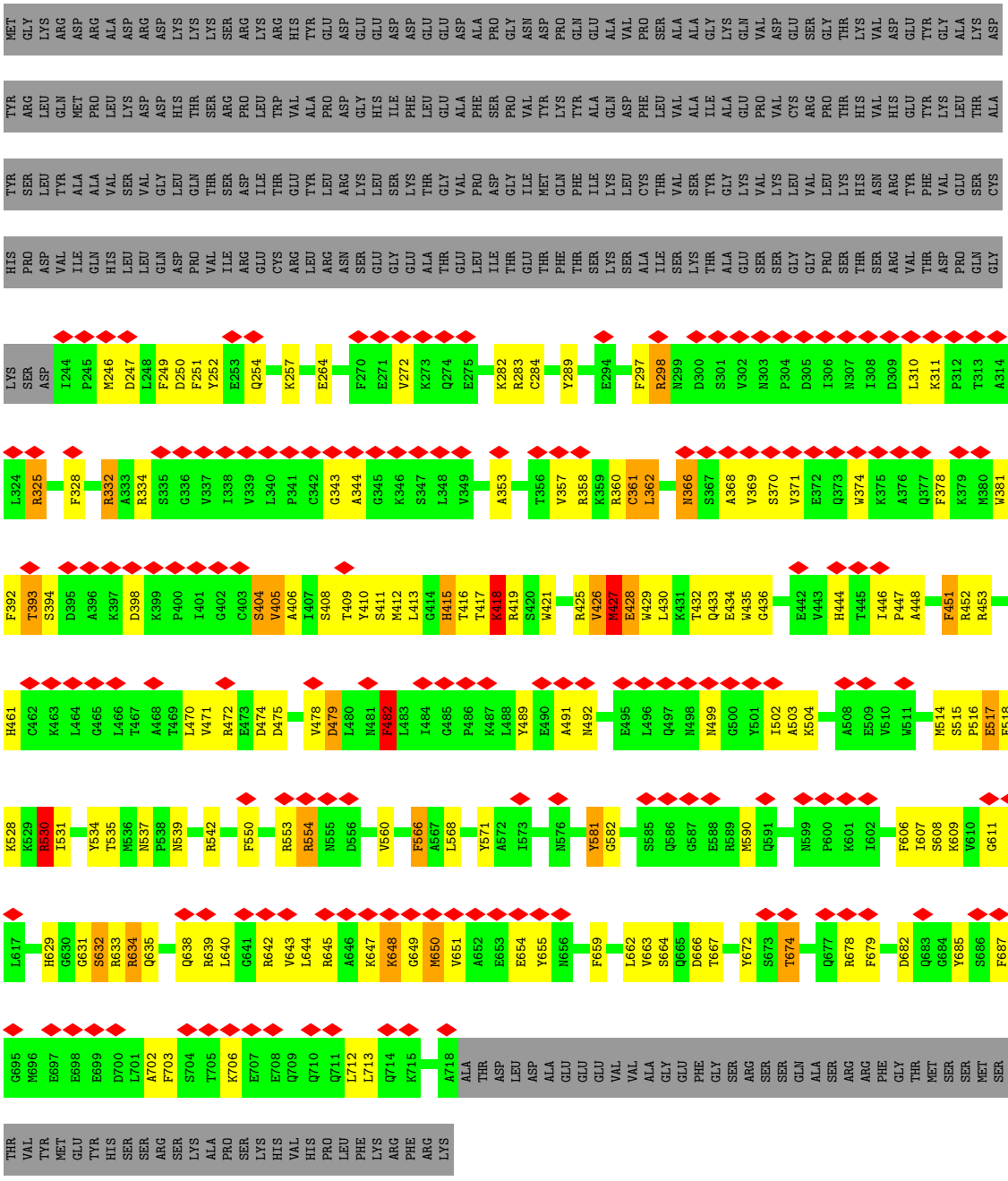
Chain U:





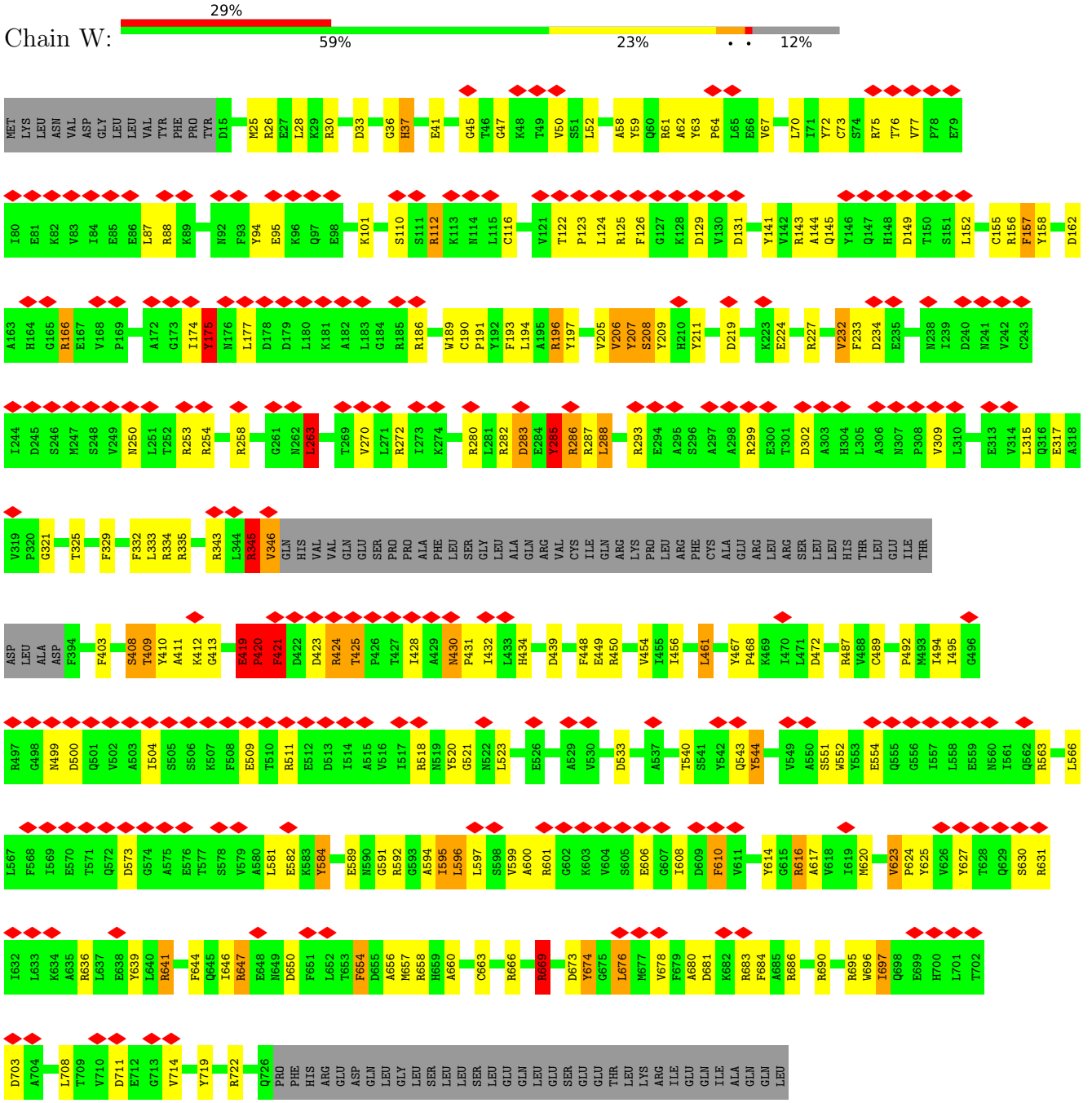
• Molecule 22: TFIIH basal transcription factor complex helicase XPB subunit





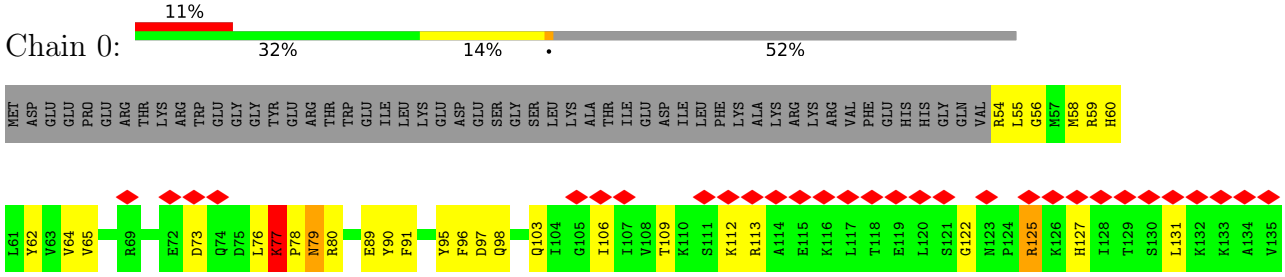
• Molecule 23: TFIIH basal transcription factor complex helicase XPD subunit

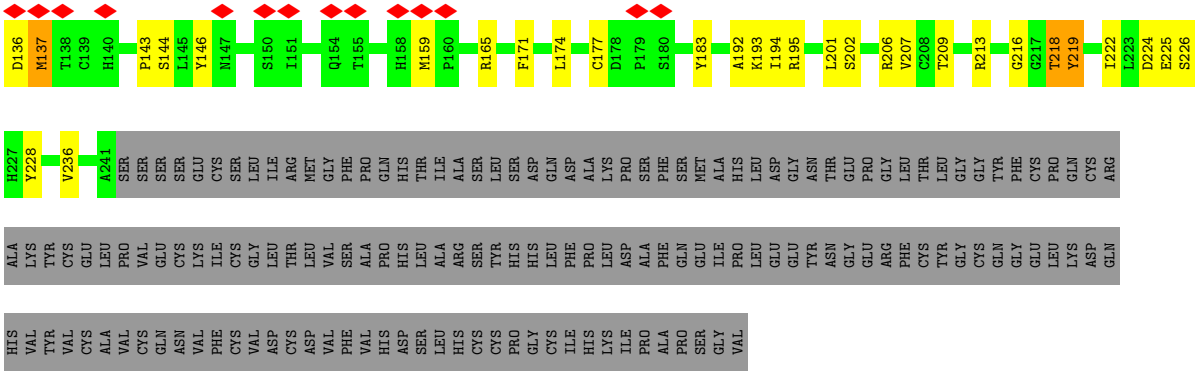
Chain W:



• Molecule 24: General transcription factor IIH subunit 2

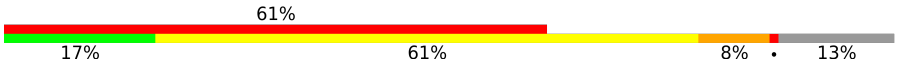
Chain 0:

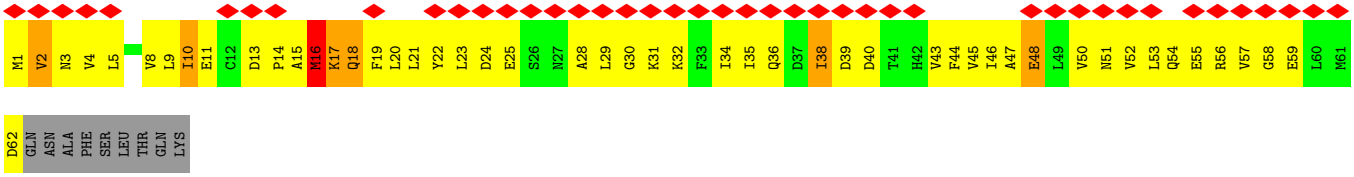




• Molecule 25: General transcription factor IIH subunit 5

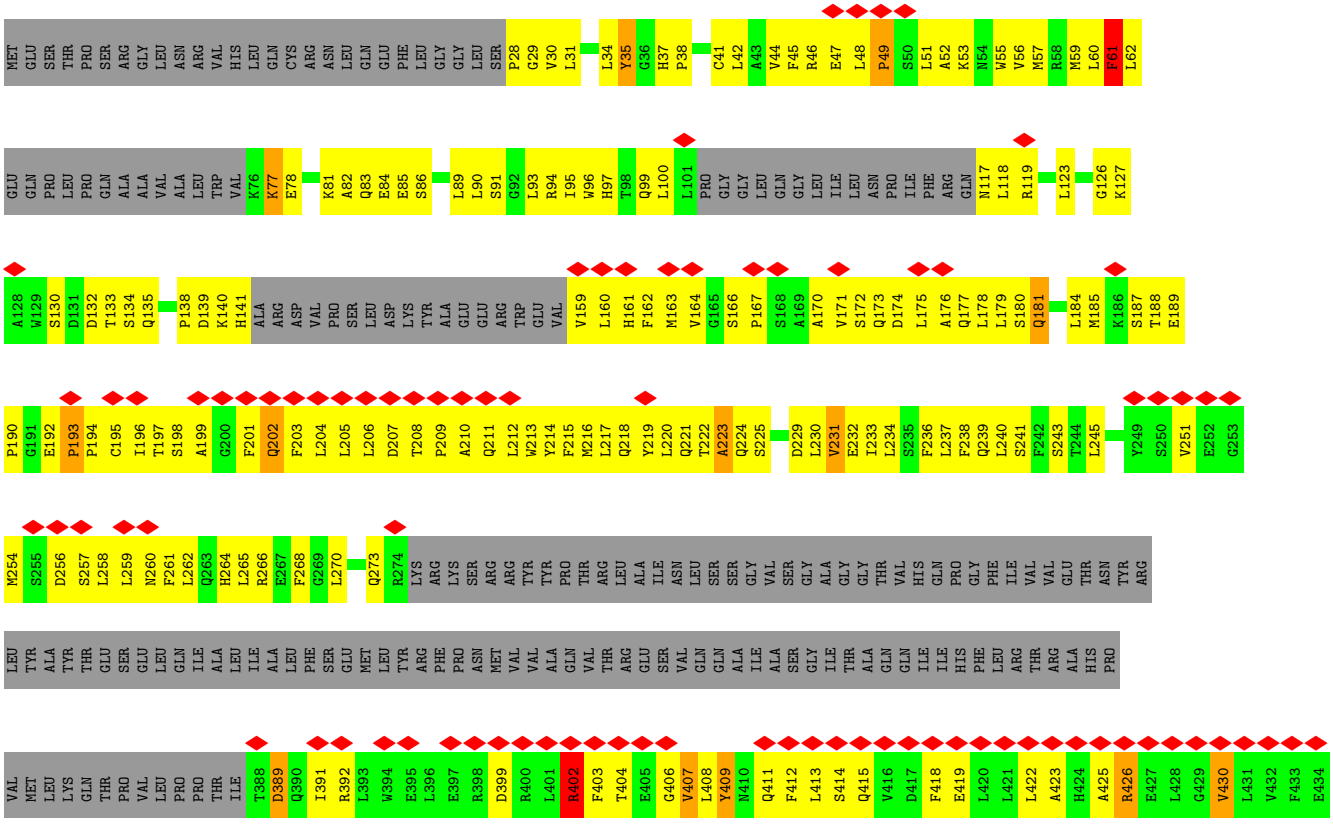
Chain 1:

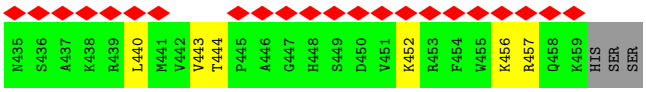




• Molecule 26: General transcription factor IIH subunit 4

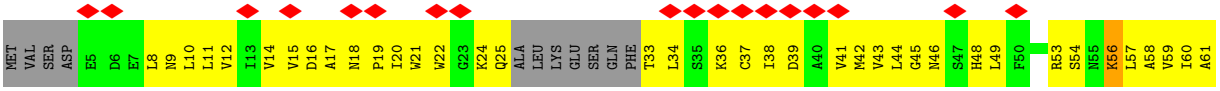
Chain 2:

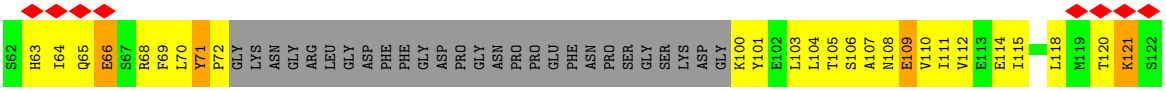


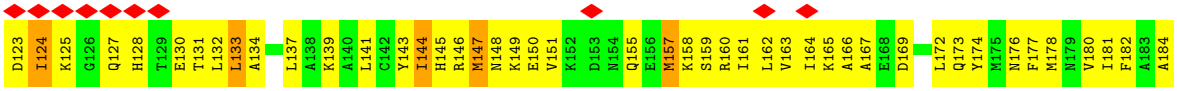


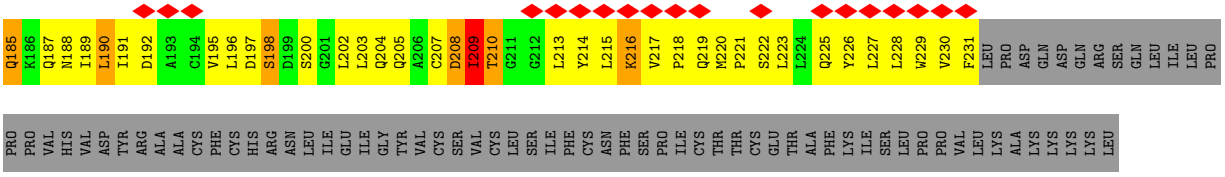
• Molecule 27: General transcription factor IIH subunit 3

Chain 3:



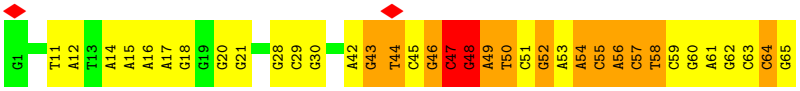






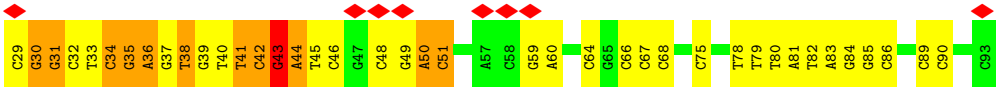
• Molecule 28: SCP-X

Chain X:



• Molecule 29: SCP-Y

Chain Y:



4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	34728	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	42	Depositor
Minimum defocus (nm)	2000	Depositor
Maximum defocus (nm)	4000	Depositor
Magnification	27500	Depositor
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.218	Depositor
Minimum map value	-0.111	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.007	Depositor
Recommended contour level	0.045	Depositor
Map size (Å)	506.88, 506.88, 506.88	wwPDB
Map dimensions	192, 192, 192	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	2.64, 2.64, 2.64	Depositor

5 Model quality (i)

5.1 Standard geometry (i)

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.33	5/11727 (0.0%)	0.66	23/15833 (0.1%)
2	B	0.29	1/9503 (0.0%)	0.63	4/12831 (0.0%)
3	C	0.27	0/2259	0.67	2/3073 (0.1%)
4	D	0.28	0/1077	0.51	0/1446
5	E	0.27	0/1753	0.66	2/2368 (0.1%)
6	F	0.25	0/700	0.51	0/946
7	G	0.27	0/1382	0.55	0/1874
8	H	0.26	0/1227	0.64	1/1654 (0.1%)
9	I	0.25	0/1038	0.90	1/1407 (0.1%)
10	J	0.27	0/542	0.56	0/730
11	K	0.26	0/956	0.52	0/1294
12	L	0.28	0/394	0.65	1/524 (0.2%)
13	M	0.26	0/2049	0.69	2/2769 (0.1%)
14	N	0.31	0/945	0.58	1/1274 (0.1%)
15	O	0.26	0/816	0.54	0/1105
16	P	0.26	0/1489	0.60	2/2005 (0.1%)
17	Q	0.28	0/1507	0.59	2/2023 (0.1%)
18	R	0.44	0/1380	0.87	2/1854 (0.1%)
19	S	0.29	0/1167	0.53	1/1576 (0.1%)
20	T	0.27	0/1817	0.57	0/2445
21	U	0.33	0/1358	0.66	2/1820 (0.1%)
22	V	1.40	13/3931 (0.3%)	1.87	96/5298 (1.8%)
23	W	1.50	22/5460 (0.4%)	2.00	154/7390 (2.1%)
24	0	1.49	5/1506 (0.3%)	1.95	43/2038 (2.1%)
25	1	0.83	0/496	1.15	1/669 (0.1%)
26	2	0.88	0/2243	1.18	8/3024 (0.3%)
27	3	0.85	0/1548	1.22	6/2090 (0.3%)
28	X	1.32	18/1510 (1.2%)	1.75	58/2332 (2.5%)
29	Y	1.26	15/1472 (1.0%)	1.71	52/2267 (2.3%)
All	All	0.75	79/63252 (0.1%)	1.09	464/85959 (0.5%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
17	Q	0	1
18	R	0	8
20	T	0	1
22	V	0	8
23	W	0	11
24	0	0	1
25	1	0	1
26	2	0	8
28	X	0	8
29	Y	0	6
All	All	0	54

All (79) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y	51	DC	O3'-P	-14.92	1.43	1.61
28	X	53	DA	P-O5'	-9.87	1.49	1.59
28	X	61	DA	C5'-C4'	8.65	1.60	1.51
29	Y	38	DT	P-O5'	8.07	1.67	1.59
23	W	158	TYR	CE1-CZ	8.04	1.49	1.38
29	Y	33	DT	C4'-C3'	7.92	1.61	1.53
22	V	672	TYR	CE1-CZ	7.85	1.48	1.38
28	X	59	DC	C5'-C4'	7.79	1.59	1.51
29	Y	36	DA	O4'-C1'	-7.78	1.32	1.42
28	X	51	DC	O3'-P	-7.64	1.51	1.61
1	A	1117	VAL	N-CA	-7.51	1.31	1.46
2	B	1090	GLU	CD-OE1	7.42	1.33	1.25
28	X	63	DC	C5'-C4'	7.21	1.59	1.51
29	Y	35	DG	P-O5'	-7.07	1.52	1.59
29	Y	36	DA	C1'-N9	7.00	1.58	1.49
22	V	391	ARG	CZ-NH2	-6.96	1.24	1.33
29	Y	32	DC	C2'-C1'	6.79	1.59	1.52
28	X	62	DG	C4'-C3'	6.78	1.60	1.53
23	W	110	SER	CA-CB	6.75	1.63	1.52
28	X	54	DA	C1'-N9	6.67	1.57	1.49
22	V	633	ARG	CZ-NH1	-6.66	1.24	1.33
28	X	57	DC	C5'-C4'	6.66	1.58	1.51
1	A	1116	ASN	CA-C	-6.64	1.35	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y	30	DG	C4'-O4'	-6.61	1.38	1.45
22	V	325	ARG	CZ-NH1	-6.59	1.24	1.33
23	W	521	GLY	N-CA	6.52	1.55	1.46
23	W	208	SER	CB-OG	-6.43	1.33	1.42
24	0	122	GLY	N-CA	6.41	1.55	1.46
22	V	606	PHE	CG-CD1	6.37	1.48	1.38
22	V	554	ARG	NE-CZ	6.30	1.41	1.33
1	A	620	HIS	N-CA	-6.27	1.33	1.46
23	W	683	ARG	CZ-NH2	-6.25	1.25	1.33
28	X	53	DA	C3'-C2'	6.23	1.59	1.52
29	Y	35	DG	O4'-C1'	-6.23	1.34	1.42
28	X	57	DC	C4'-O4'	-6.19	1.38	1.45
22	V	453	ARG	CZ-NH2	-6.08	1.25	1.33
28	X	53	DA	C4'-O4'	-5.98	1.39	1.45
29	Y	36	DA	C5'-C4'	5.88	1.57	1.51
28	X	63	DC	P-O5'	5.88	1.65	1.59
22	V	319	TYR	CE1-CZ	5.85	1.46	1.38
23	W	321	GLY	N-CA	5.85	1.54	1.46
28	X	54	DA	C2'-C1'	5.82	1.58	1.52
24	0	195	ARG	CZ-NH1	-5.79	1.25	1.33
28	X	65	DG	P-O5'	5.74	1.65	1.59
29	Y	40	DT	C1'-N1	5.74	1.56	1.49
29	Y	36	DA	C4'-O4'	-5.72	1.39	1.45
22	V	252	TYR	CE1-CZ	5.72	1.46	1.38
23	W	286	ARG	CZ-NH1	-5.71	1.25	1.33
23	W	47	GLY	N-CA	5.58	1.54	1.46
1	A	1115	LYS	N-CA	5.48	1.57	1.46
23	W	610	PHE	CG-CD1	5.47	1.47	1.38
1	A	1115	LYS	CA-C	-5.47	1.38	1.52
28	X	58	DT	C1'-N1	5.44	1.56	1.49
28	X	46	DG	O3'-P	-5.42	1.54	1.61
22	V	452	ARG	CZ-NH2	-5.42	1.26	1.33
22	V	332	ARG	CZ-NH2	-5.41	1.26	1.33
28	X	58	DT	O3'-P	5.39	1.67	1.61
23	W	334	ARG	CZ-NH2	-5.38	1.26	1.33
23	W	606	GLU	CA-CB	5.35	1.65	1.53
23	W	286	ARG	CZ-NH2	-5.31	1.26	1.33
23	W	448	PHE	CE1-CZ	5.30	1.47	1.37
23	W	253	ARG	CZ-NH1	-5.28	1.26	1.33
23	W	674	TYR	CE1-CZ	5.28	1.45	1.38
29	Y	31	DG	C1'-N9	-5.24	1.40	1.47
28	X	48	DG	C2-N2	-5.23	1.29	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	V	659	PHE	CG-CD2	5.20	1.46	1.38
29	Y	30	DG	C5'-C4'	5.13	1.56	1.51
23	W	518	ARG	CZ-NH2	-5.13	1.26	1.33
24	0	112	LYS	N-CA	5.13	1.56	1.46
23	W	511	ARG	NE-CZ	-5.12	1.26	1.33
23	W	345	ARG	CZ-NH1	-5.12	1.26	1.33
24	0	95	TYR	CG-CD1	5.11	1.45	1.39
22	V	451	PHE	CG-CD2	5.08	1.46	1.38
24	0	146	TYR	CD2-CE2	5.08	1.47	1.39
23	W	654	PHE	CG-CD1	5.07	1.46	1.38
23	W	520	TYR	CZ-OH	-5.06	1.29	1.37
23	W	254	ARG	CZ-NH1	-5.05	1.26	1.33
23	W	639	TYR	CZ-OH	-5.03	1.29	1.37
29	Y	34	DC	C4'-C3'	5.00	1.58	1.53

All (464) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
9	I	84	HIS	C-N-CD	-24.67	66.32	120.60
24	0	77	LYS	C-N-CD	-21.82	72.60	120.60
3	C	6	GLN	C-N-CD	-21.15	74.06	120.60
13	M	10	LEU	C-N-CD	-20.90	74.63	120.60
27	3	71	TYR	C-N-CD	-20.67	75.13	120.60
2	B	497	LYS	C-N-CD	-19.91	76.80	120.60
23	W	335	ARG	NE-CZ-NH1	-19.54	110.53	120.30
29	Y	32	DC	O4'-C1'-N1	19.15	121.41	108.00
23	W	26	ARG	NE-CZ-NH2	18.88	129.74	120.30
28	X	65	DG	O4'-C1'-N9	17.76	120.43	108.00
22	V	358	ARG	NE-CZ-NH2	17.71	129.16	120.30
24	0	195	ARG	NE-CZ-NH1	17.03	128.81	120.30
23	W	186	ARG	NE-CZ-NH1	16.35	128.47	120.30
18	R	194	ARG	C-N-CD	-16.13	85.11	120.60
23	W	287	ARG	NE-CZ-NH2	15.59	128.09	120.30
1	A	619	LYS	CA-C-N	-15.28	83.59	117.20
23	W	299	ARG	NE-CZ-NH1	15.16	127.88	120.30
22	V	634	ARG	NE-CZ-NH2	14.93	127.77	120.30
23	W	419	GLU	C-N-CD	-14.91	87.79	120.60
24	0	206	ARG	NE-CZ-NH1	14.67	127.63	120.30
27	3	209	ILE	N-CA-CB	14.36	143.84	110.80
23	W	592	ARG	NE-CZ-NH1	14.30	127.45	120.30
23	W	335	ARG	NE-CZ-NH2	14.12	127.36	120.30
22	V	332	ARG	NE-CZ-NH1	13.96	127.28	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	112	ARG	NE-CZ-NH1	13.90	127.25	120.30
29	Y	33	DT	O4'-C1'-N1	13.85	117.69	108.00
23	W	669	ARG	NE-CZ-NH1	13.78	127.19	120.30
23	W	272	ARG	NE-CZ-NH1	13.76	127.18	120.30
23	W	75	ARG	NE-CZ-NH1	13.22	126.91	120.30
1	A	622	SER	N-CA-C	-13.21	75.33	111.00
28	X	47	DC	O4'-C1'-N1	13.18	117.22	108.00
23	W	343	ARG	NE-CZ-NH2	12.94	126.77	120.30
22	V	633	ARG	NE-CZ-NH2	-12.84	113.88	120.30
5	E	52	ARG	C-N-CD	-12.83	92.37	120.60
29	Y	42	DC	O4'-C1'-N1	12.76	116.93	108.00
23	W	467	TYR	CB-CG-CD1	-12.22	113.67	121.00
23	W	601	ARG	NE-CZ-NH2	-12.18	114.21	120.30
23	W	627	TYR	CB-CG-CD2	-12.12	113.73	121.00
23	W	631	ARG	NE-CZ-NH1	11.94	126.27	120.30
23	W	26	ARG	NH1-CZ-NH2	-11.76	106.46	119.40
22	V	452	ARG	NE-CZ-NH1	11.61	126.11	120.30
23	W	487	ARG	NE-CZ-NH1	11.55	126.08	120.30
29	Y	50	DA	N1-C6-N6	-11.49	111.71	118.60
22	V	283	ARG	NE-CZ-NH2	-11.44	114.58	120.30
23	W	636	ARG	NE-CZ-NH1	11.41	126.01	120.30
23	W	88	ARG	NE-CZ-NH1	11.38	125.99	120.30
28	X	42	DA	O3'-P-O5'	-11.34	82.46	104.00
23	W	421	PHE	N-CA-C	11.22	141.29	111.00
23	W	343	ARG	NE-CZ-NH1	-11.20	114.70	120.30
23	W	647	ARG	NE-CZ-NH1	11.16	125.88	120.30
28	X	61	DA	O4'-C4'-C3'	10.95	112.57	106.00
23	W	683	ARG	NE-CZ-NH2	10.84	125.72	120.30
28	X	61	DA	O4'-C1'-N9	10.79	115.55	108.00
23	W	690	ARG	NE-CZ-NH2	10.69	125.65	120.30
28	X	49	DA	N1-C6-N6	-10.54	112.28	118.60
27	3	208	ASP	N-CA-C	-10.38	82.98	111.00
22	V	391	ARG	NE-CZ-NH1	-10.34	115.13	120.30
23	W	88	ARG	NE-CZ-NH2	-10.32	115.14	120.30
1	A	619	LYS	O-C-N	10.30	139.18	122.70
28	X	57	DC	O4'-C1'-N1	10.05	115.04	108.00
22	V	520	ARG	CA-C-N	-10.05	95.09	117.20
22	V	687	PHE	CB-CG-CD2	-10.04	113.77	120.80
29	Y	29	DC	O4'-C1'-N1	9.94	114.96	108.00
22	V	452	ARG	NE-CZ-NH2	-9.85	115.37	120.30
22	V	553	ARG	NE-CZ-NH2	9.82	125.21	120.30
28	X	55	DC	O4'-C1'-C2'	9.72	113.68	105.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
28	X	46	DG	O3'-P-O5'	-9.72	85.53	104.00
22	V	283	ARG	NE-CZ-NH1	9.71	125.16	120.30
29	Y	44	DA	N1-C6-N6	-9.67	112.80	118.60
24	0	59	ARG	NE-CZ-NH2	9.63	125.11	120.30
23	W	658	ARG	NE-CZ-NH2	-9.50	115.55	120.30
22	V	334	ARG	CD-NE-CZ	9.48	136.87	123.60
23	W	227	ARG	NE-CZ-NH1	9.41	125.00	120.30
29	Y	39	DG	O4'-C4'-C3'	9.28	111.57	106.00
23	W	511	ARG	NE-CZ-NH2	9.27	124.93	120.30
23	W	686	ARG	NE-CZ-NH1	9.26	124.93	120.30
29	Y	35	DG	O4'-C1'-N9	-9.23	101.54	108.00
24	0	219	TYR	CB-CG-CD1	-9.21	115.47	121.00
22	V	645	ARG	NE-CZ-NH1	9.17	124.89	120.30
8	H	74	GLU	N-CA-C	-9.14	86.31	111.00
22	V	264	GLU	OE1-CD-OE2	-9.11	112.37	123.30
23	W	627	TYR	CG-CD2-CE2	-9.10	114.02	121.30
23	W	286	ARG	NE-CZ-NH2	9.04	124.82	120.30
23	W	666	ARG	NE-CZ-NH1	9.01	124.80	120.30
16	P	161	ILE	N-CA-C	-8.95	86.85	111.00
23	W	703	ASP	CB-CG-OD2	8.94	126.34	118.30
24	0	206	ARG	NH1-CZ-NH2	-8.91	109.59	119.40
27	3	208	ASP	CB-CA-C	-8.80	92.80	110.40
28	X	46	DG	O4'-C4'-C3'	8.79	111.27	106.00
1	A	49	GLY	N-CA-C	-8.72	91.29	113.10
22	V	520	ARG	O-C-N	8.66	136.55	122.70
22	V	520	ARG	C-N-CA	-8.65	100.08	121.70
28	X	61	DA	C4'-C3'-C2'	-8.60	95.36	103.10
28	X	48	DG	O4'-C1'-C2'	-8.58	99.04	105.90
28	X	63	DC	C2-N1-C1'	-8.55	109.39	118.80
28	X	52	DG	O4'-C1'-N9	8.52	113.96	108.00
28	X	48	DG	O4'-C1'-N9	8.49	113.94	108.00
23	W	654	PHE	CB-CG-CD2	-8.48	114.86	120.80
1	A	1117	VAL	N-CA-CB	8.47	130.13	111.50
24	0	213	ARG	NE-CZ-NH1	8.43	124.51	120.30
28	X	61	DA	C1'-O4'-C4'	-8.40	101.69	110.10
28	X	47	DC	C6-N1-C2	-8.40	116.94	120.30
1	A	1116	ASN	N-CA-C	8.31	133.44	111.00
22	V	685	TYR	CB-CG-CD2	8.31	125.99	121.00
22	V	581	TYR	CG-CD1-CE1	-8.28	114.68	121.30
29	Y	39	DG	C1'-O4'-C4'	-8.27	101.83	110.10
23	W	450	ARG	NE-CZ-NH1	8.27	124.43	120.30
22	V	419	ARG	NE-CZ-NH1	8.22	124.41	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	332	PHE	CB-CG-CD2	-8.18	115.07	120.80
1	A	1311	LEU	CB-CG-CD1	-8.11	97.21	111.00
22	V	634	ARG	NE-CZ-NH1	-8.10	116.25	120.30
22	V	520	ARG	NE-CZ-NH2	8.08	124.34	120.30
28	X	47	DC	N3-C2-O2	-8.07	116.25	121.90
1	A	621	ILE	CA-C-N	-7.98	99.64	117.20
29	Y	50	DA	C4-C5-C6	-7.98	113.01	117.00
22	V	410	TYR	CB-CG-CD1	-7.96	116.22	121.00
28	X	63	DC	C6-N1-C1'	7.95	130.34	120.80
23	W	126	PHE	CB-CG-CD2	7.90	126.33	120.80
22	V	358	ARG	NH1-CZ-NH2	-7.88	110.73	119.40
29	Y	38	DT	O4'-C4'-C3'	-7.87	101.28	106.00
23	W	75	ARG	NE-CZ-NH2	-7.86	116.37	120.30
22	V	386	ASP	CB-CG-OD2	-7.84	111.24	118.30
29	Y	45	DT	C6-C5-C7	-7.84	118.19	122.90
23	W	125	ARG	NE-CZ-NH1	7.82	124.21	120.30
23	W	601	ARG	NE-CZ-NH1	7.80	124.20	120.30
23	W	644	PHE	CB-CG-CD1	7.75	126.23	120.80
23	W	448	PHE	CB-CG-CD2	7.75	126.23	120.80
29	Y	39	DG	O4'-C1'-C2'	7.72	112.08	105.90
29	Y	36	DA	O4'-C4'-C3'	7.70	110.62	106.00
23	W	467	TYR	CB-CG-CD2	7.68	125.61	121.00
26	2	402	ARG	NE-CZ-NH1	7.63	124.11	120.30
23	W	232	VAL	CA-CB-CG1	7.62	122.33	110.90
23	W	582	GLU	OE1-CD-OE2	-7.59	114.19	123.30
23	W	520	TYR	CG-CD1-CE1	-7.54	115.26	121.30
24	0	90	TYR	CB-CG-CD2	-7.54	116.48	121.00
1	A	1116	ASN	O-C-N	7.53	134.74	122.70
22	V	522	TYR	CB-CG-CD2	-7.53	116.48	121.00
29	Y	36	DA	C4'-C3'-C2'	-7.52	96.34	103.10
28	X	51	DC	N3-C2-O2	-7.51	116.64	121.90
29	Y	46	DC	N3-C2-O2	-7.50	116.65	121.90
22	V	474	ASP	CB-CG-OD2	7.50	125.05	118.30
24	0	95	TYR	CB-CG-CD1	-7.48	116.51	121.00
29	Y	44	DA	C5-C6-N1	7.47	121.43	117.70
23	W	592	ARG	NH1-CZ-NH2	-7.45	111.21	119.40
23	W	193	PHE	CB-CG-CD1	-7.43	115.60	120.80
22	V	542	ARG	NE-CZ-NH2	7.42	124.01	120.30
29	Y	42	DC	C2-N1-C1'	-7.42	110.64	118.80
29	Y	50	DA	C5-C6-N1	7.42	121.41	117.70
22	V	685	TYR	CB-CG-CD1	-7.39	116.57	121.00
23	W	272	ARG	NH1-CZ-NH2	-7.38	111.28	119.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	73	ASP	CB-CG-OD2	-7.33	111.71	118.30
24	0	236	VAL	CA-CB-CG1	7.30	121.85	110.90
29	Y	44	DA	C4-C5-C6	-7.27	113.37	117.00
22	V	249	PHE	CB-CG-CD2	7.26	125.88	120.80
23	W	186	ARG	NE-CZ-NH2	-7.26	116.67	120.30
22	V	554	ARG	NE-CZ-NH1	7.25	123.93	120.30
29	Y	32	DC	C2-N1-C1'	-7.24	110.83	118.80
29	Y	33	DT	O4'-C1'-C2'	-7.20	100.14	105.90
28	X	49	DA	C4-C5-C6	-7.19	113.41	117.00
28	X	45	DC	N3-C2-O2	-7.16	116.89	121.90
24	0	89	GLU	OE1-CD-OE2	-7.12	114.76	123.30
28	X	46	DG	P-O3'-C3'	7.10	128.22	119.70
23	W	317	GLU	OE1-CD-OE2	-7.06	114.83	123.30
23	W	166	ARG	CD-NE-CZ	7.00	133.39	123.60
1	A	266	MET	N-CA-C	-6.96	92.22	111.00
29	Y	39	DG	C8-N9-C1'	6.96	136.04	127.00
23	W	280	ARG	NE-CZ-NH1	-6.95	116.83	120.30
23	W	627	TYR	CD1-CG-CD2	6.93	125.53	117.90
28	X	61	DA	P-O3'-C3'	6.93	128.01	119.70
28	X	49	DA	C5-C6-N1	6.92	121.16	117.70
1	A	1117	VAL	N-CA-C	-6.92	92.32	111.00
29	Y	51	DC	O3'-P-O5'	6.91	117.13	104.00
22	V	643	VAL	CA-CB-CG1	6.91	121.26	110.90
28	X	55	DC	O4'-C1'-N1	6.90	112.83	108.00
24	0	195	ARG	NE-CZ-NH2	-6.90	116.85	120.30
22	V	639	ARG	NE-CZ-NH2	6.89	123.75	120.30
24	0	136	ASP	CB-CG-OD1	6.89	124.50	118.30
29	Y	39	DG	C4-N9-C1'	-6.88	117.55	126.50
23	W	253	ARG	NE-CZ-NH1	6.88	123.74	120.30
22	V	385	ASP	CB-CG-OD1	-6.87	112.12	118.30
23	W	219	ASP	CB-CG-OD1	6.83	124.44	118.30
26	2	35	TYR	CA-CB-CG	-6.83	100.43	113.40
23	W	654	PHE	CB-CG-CD1	6.81	125.57	120.80
22	V	530	ARG	NE-CZ-NH2	-6.79	116.91	120.30
22	V	334	ARG	NE-CZ-NH1	6.79	123.69	120.30
23	W	644	PHE	CB-CG-CD2	-6.78	116.05	120.80
29	Y	41	DT	O4'-C1'-N1	-6.78	103.25	108.00
24	0	95	TYR	CD1-CE1-CZ	-6.77	113.71	119.80
23	W	196	ARG	NE-CZ-NH1	6.76	123.68	120.30
23	W	332	PHE	CB-CG-CD1	6.75	125.53	120.80
23	W	566	LEU	CB-CG-CD1	6.75	122.47	111.00
23	W	125	ARG	CD-NE-CZ	6.74	133.03	123.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	345	ARG	CD-NE-CZ	6.73	133.02	123.60
22	V	655	TYR	CB-CG-CD2	-6.72	116.97	121.00
23	W	26	ARG	NE-CZ-NH1	6.72	123.66	120.30
23	W	50	VAL	CA-CB-CG1	6.70	120.95	110.90
22	V	581	TYR	CD1-CE1-CZ	6.69	125.82	119.80
26	2	61	PHE	CB-CA-C	-6.68	97.04	110.40
23	W	30	ARG	CD-NE-CZ	6.65	132.91	123.60
29	Y	32	DC	C6-N1-C1'	6.63	128.75	120.80
29	Y	48	DC	N3-C2-O2	-6.60	117.28	121.90
23	W	302	ASP	CB-CG-OD1	6.58	124.22	118.30
23	W	125	ARG	NE-CZ-NH2	-6.56	117.02	120.30
23	W	674	TYR	CB-CG-CD1	6.55	124.93	121.00
24	0	219	TYR	CG-CD1-CE1	-6.55	116.06	121.30
26	2	193	PRO	CA-N-CD	-6.52	102.37	111.50
1	A	619	LYS	C-N-CA	6.51	137.99	121.70
23	W	76	THR	CA-CB-OG1	6.51	122.66	109.00
23	W	315	LEU	CB-CG-CD1	6.50	122.05	111.00
22	V	404	SER	CB-CA-C	6.49	122.43	110.10
23	W	487	ARG	NH1-CZ-NH2	-6.49	112.26	119.40
23	W	299	ARG	NE-CZ-NH2	-6.48	117.06	120.30
23	W	616	ARG	NE-CZ-NH1	-6.47	117.06	120.30
23	W	722	ARG	CD-NE-CZ	6.45	132.62	123.60
29	Y	40	DT	C4'-C3'-C2'	-6.45	97.30	103.10
29	Y	51	DC	N3-C2-O2	-6.43	117.40	121.90
22	V	682	ASP	CB-CG-OD1	6.41	124.07	118.30
21	U	232	GLU	N-CA-C	6.40	128.28	111.00
22	V	522	TYR	CB-CG-CD1	6.39	124.84	121.00
24	0	113	ARG	NE-CZ-NH1	6.39	123.50	120.30
29	Y	38	DT	O4'-C1'-C2'	-6.38	100.79	105.90
23	W	641	ARG	NE-CZ-NH1	6.36	123.48	120.30
23	W	683	ARG	CD-NE-CZ	6.36	132.50	123.60
23	W	131	ASP	CB-CG-OD1	-6.35	112.59	118.30
28	X	45	DC	O3'-P-O5'	-6.34	91.95	104.00
1	A	924	TYR	N-CA-C	-6.34	93.88	111.00
23	W	263	LEU	N-CA-CB	-6.34	97.72	110.40
23	W	669	ARG	NH1-CZ-NH2	-6.33	112.43	119.40
28	X	65	DG	C4'-C3'-C2'	-6.33	97.40	103.10
22	V	369	VAL	CA-CB-CG1	6.33	120.39	110.90
22	V	521	GLU	OE1-CD-OE2	-6.32	115.72	123.30
22	V	332	ARG	NH1-CZ-NH2	-6.30	112.47	119.40
24	0	59	ARG	NH1-CZ-NH2	-6.30	112.47	119.40
22	V	298	ARG	NE-CZ-NH1	6.29	123.45	120.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	923	ASP	N-CA-C	6.29	127.98	111.00
16	P	160	GLY	N-CA-C	6.28	128.81	113.10
29	Y	51	DC	OP1-P-O3'	-6.27	91.41	105.20
1	A	603	ILE	N-CA-C	6.27	127.92	111.00
23	W	206	VAL	CA-CB-CG1	6.26	120.29	110.90
13	M	43	ASP	N-CA-C	6.25	127.88	111.00
23	W	639	TYR	CB-CG-CD2	-6.25	117.25	121.00
22	V	344	ALA	N-CA-CB	-6.24	101.36	110.10
23	W	175	TYR	N-CA-C	6.22	127.79	111.00
24	0	137	MET	CG-SD-CE	6.19	110.11	100.20
23	W	30	ARG	NE-CZ-NH1	6.18	123.39	120.30
23	W	420	PRO	C-N-CA	6.17	137.13	121.70
23	W	77	VAL	CG1-CB-CG2	-6.14	101.08	110.90
29	Y	42	DC	O3'-P-O5'	-6.14	92.34	104.00
28	X	45	DC	N1-C2-O2	6.12	122.57	118.90
1	A	619	LYS	CB-CA-C	6.11	122.62	110.40
24	0	183	TYR	CB-CG-CD1	-6.09	117.34	121.00
29	Y	39	DG	O4'-C1'-N9	-6.07	103.75	108.00
22	V	410	TYR	CZ-CE2-CD2	-6.05	114.35	119.80
28	X	65	DG	O4'-C1'-C2'	-6.04	101.07	105.90
23	W	552	TRP	CD1-NE1-CE2	6.00	114.40	109.00
23	W	673	ASP	CB-CG-OD1	5.99	123.69	118.30
22	V	360	ARG	CD-NE-CZ	5.96	131.95	123.60
23	W	131	ASP	CB-CG-OD2	5.96	123.66	118.30
22	V	321	GLU	OE1-CD-OE2	-5.95	116.16	123.30
24	0	218	THR	CA-CB-CG2	-5.95	104.07	112.40
23	W	472	ASP	CB-CG-OD2	5.94	123.65	118.30
14	N	319	ASP	N-CA-C	5.94	127.03	111.00
22	V	663	VAL	CG1-CB-CG2	-5.94	101.40	110.90
29	Y	29	DC	P-O3'-C3'	5.94	126.83	119.70
28	X	48	DG	P-O3'-C3'	5.93	126.82	119.70
1	A	619	LYS	CA-C-O	5.93	132.55	120.10
22	V	566	PHE	CB-CG-CD1	5.93	124.95	120.80
23	W	156	ARG	CD-NE-CZ	5.92	131.89	123.60
28	X	44	DT	O4'-C4'-C3'	5.92	109.55	106.00
28	X	60	DG	N9-C1'-C2'	5.88	123.77	112.60
28	X	50	DT	C6-C5-C7	-5.86	119.39	122.90
29	Y	34	DC	O4'-C1'-C2'	5.83	110.56	105.90
28	X	53	DA	O4'-C1'-N9	5.82	112.07	108.00
23	W	472	ASP	CB-CG-OD1	-5.81	113.07	118.30
22	V	381	TRP	CZ3-CH2-CZ2	-5.80	114.64	121.60
22	V	410	TYR	CB-CG-CD2	5.80	124.48	121.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
29	Y	50	DA	C6-C5-N7	5.80	136.36	132.30
23	W	563	ARG	NE-CZ-NH1	5.78	123.19	120.30
18	R	205	ASP	C-N-CA	5.77	136.12	121.70
2	B	1090	GLU	OE1-CD-OE2	5.77	130.22	123.30
23	W	112	ARG	NH1-CZ-NH2	-5.76	113.06	119.40
28	X	44	DT	C6-C5-C7	-5.76	119.44	122.90
22	V	472	ARG	NE-CZ-NH1	5.76	123.18	120.30
24	0	183	TYR	CD1-CE1-CZ	5.76	124.98	119.80
23	W	345	ARG	NE-CZ-NH2	-5.75	117.43	120.30
23	W	722	ARG	NE-CZ-NH1	-5.74	117.43	120.30
24	0	171	PHE	CB-CG-CD1	-5.74	116.78	120.80
29	Y	48	DC	O4'-C4'-C3'	5.73	109.44	106.00
24	0	91	PHE	CG-CD2-CE2	-5.73	114.50	120.80
22	V	542	ARG	NH1-CZ-NH2	-5.72	113.11	119.40
24	0	90	TYR	CG-CD2-CE2	-5.72	116.73	121.30
22	V	419	ARG	CD-NE-CZ	5.71	131.59	123.60
23	W	650	ASP	CB-CG-OD1	5.71	123.44	118.30
1	A	610	PRO	CA-C-O	5.70	133.89	120.20
23	W	641	ARG	CD-NE-CZ	5.70	131.57	123.60
24	0	177	CYS	CA-CB-SG	-5.69	103.75	114.00
1	A	923	ASP	CA-C-N	-5.69	104.69	117.20
24	0	80	ARG	CD-NE-CZ	5.68	131.56	123.60
28	X	48	DG	N1-C6-O6	-5.68	116.49	119.90
29	Y	32	DC	C3'-C2'-C1'	-5.68	95.69	102.50
12	L	17	TYR	N-CA-C	5.68	126.33	111.00
23	W	41	GLU	O-C-N	5.66	131.76	122.70
22	V	284	CYS	CA-CB-SG	-5.66	103.81	114.00
24	0	96	PHE	CB-CG-CD1	-5.66	116.84	120.80
29	Y	42	DC	C6-N1-C1'	5.66	127.59	120.80
22	V	482	PHE	CB-CG-CD1	-5.66	116.84	120.80
22	V	425	ARG	NE-CZ-NH1	5.66	123.13	120.30
23	W	129	ASP	CB-CG-OD1	5.65	123.39	118.30
22	V	325	ARG	NE-CZ-NH1	5.64	123.12	120.30
28	X	56	DA	C3'-C2'-C1'	-5.64	95.73	102.50
23	W	708	LEU	CB-CG-CD2	-5.64	101.41	111.00
22	V	391	ARG	NE-CZ-NH2	5.64	123.12	120.30
23	W	544	TYR	CG-CD2-CE2	-5.62	116.80	121.30
23	W	711	ASP	CB-CG-OD1	5.62	123.36	118.30
23	W	334	ARG	NE-CZ-NH2	-5.61	117.49	120.30
24	0	201	LEU	CB-CG-CD1	5.61	120.54	111.00
22	V	655	TYR	CB-CG-CD1	5.61	124.36	121.00
22	V	328	PHE	C-N-CA	5.60	134.07	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	0	226	SER	N-CA-CB	-5.60	102.10	110.50
23	W	270	VAL	CA-C-O	5.60	131.86	120.10
22	V	640	LEU	CB-CG-CD2	5.60	120.52	111.00
22	V	430	LEU	CB-CG-CD1	5.59	120.51	111.00
23	W	207	TYR	CA-CB-CG	5.59	124.02	113.40
17	Q	102	VAL	C-N-CA	-5.58	107.75	121.70
22	V	662	LEU	CB-CG-CD2	-5.57	101.53	111.00
28	X	47	DC	N1-C2-O2	5.57	122.24	118.90
29	Y	46	DC	N1-C2-O2	5.57	122.24	118.90
23	W	141	TYR	CG-CD2-CE2	5.55	125.74	121.30
23	W	684	PHE	CB-CG-CD1	-5.55	116.92	120.80
28	X	62	DG	O4'-C4'-C3'	-5.55	102.28	104.50
22	V	419	ARG	NH1-CZ-NH2	-5.54	113.30	119.40
22	V	571	TYR	CG-CD2-CE2	-5.54	116.87	121.30
28	X	56	DA	O4'-C1'-N9	5.54	111.88	108.00
29	Y	41	DT	N1-C1'-C2'	5.54	123.12	112.60
24	0	183	TYR	CG-CD1-CE1	-5.54	116.87	121.30
1	A	603	ILE	CA-C-N	-5.52	105.06	117.20
22	V	393	THR	O-C-N	-5.52	113.88	122.70
24	0	65	VAL	CA-CB-CG1	5.51	119.17	110.90
19	S	166	ARG	NE-CZ-NH1	5.51	123.05	120.30
22	V	608	SER	O-C-N	-5.50	113.91	122.70
22	V	634	ARG	CD-NE-CZ	5.50	131.29	123.60
23	W	258	ARG	NE-CZ-NH1	5.49	123.05	120.30
22	V	362	LEU	CB-CG-CD1	-5.49	101.67	111.00
29	Y	35	DG	P-O3'-C3'	5.48	126.27	119.70
22	V	289	TYR	CG-CD2-CE2	-5.47	116.92	121.30
28	X	64	DC	O4'-C1'-N1	-5.47	104.17	108.00
23	W	177	LEU	CB-CG-CD1	5.47	120.30	111.00
22	V	571	TYR	CB-CG-CD1	-5.47	117.72	121.00
28	X	47	DC	C3'-C2'-C1'	5.46	109.05	102.50
28	X	47	DC	P-O3'-C3'	5.46	126.25	119.70
29	Y	46	DC	O4'-C1'-N1	5.45	111.82	108.00
23	W	224	GLU	OE1-CD-OE2	-5.45	116.76	123.30
22	V	702	ALA	N-CA-CB	-5.45	102.47	110.10
22	V	272	VAL	CA-CB-CG2	-5.44	102.74	110.90
21	U	232	GLU	C-N-CA	-5.44	108.10	121.70
23	W	690	ARG	CD-NE-CZ	5.44	131.21	123.60
23	W	253	ARG	NH1-CZ-NH2	-5.43	113.43	119.40
23	W	285	TYR	CB-CG-CD1	-5.42	117.75	121.00
22	V	319	TYR	CB-CG-CD1	-5.42	117.75	121.00
1	A	622	SER	C-N-CD	-5.41	108.69	120.60

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	280	ARG	NE-CZ-NH2	5.41	123.01	120.30
22	V	382	SER	N-CA-CB	-5.41	102.39	110.50
23	W	625	TYR	CZ-CE2-CD2	-5.41	114.93	119.80
23	W	686	ARG	NE-CZ-NH2	-5.41	117.60	120.30
23	W	595	ILE	CB-CA-C	5.40	122.41	111.60
23	W	205	VAL	CA-CB-CG1	5.40	119.00	110.90
28	X	44	DT	N3-C2-O2	-5.40	119.06	122.30
17	Q	73	LYS	N-CA-C	-5.39	96.44	111.00
23	W	631	ARG	NH1-CZ-NH2	-5.39	113.47	119.40
29	Y	51	DC	O4'-C4'-C3'	5.39	109.23	106.00
27	3	209	ILE	N-CA-C	-5.39	96.46	111.00
1	A	514	GLU	OE1-CD-OE2	-5.38	116.84	123.30
2	B	880	LEU	N-CA-C	5.37	125.51	111.00
28	X	51	DC	O4'-C1'-N1	5.37	111.76	108.00
23	W	196	ARG	CD-NE-CZ	5.37	131.11	123.60
26	2	61	PHE	CB-CG-CD2	-5.36	117.05	120.80
23	W	287	ARG	NH1-CZ-NH2	-5.35	113.51	119.40
23	W	616	ARG	NE-CZ-NH2	5.35	122.98	120.30
23	W	33	ASP	CB-CG-OD2	5.34	123.11	118.30
23	W	663	CYS	CA-CB-SG	-5.34	104.39	114.00
2	B	546	GLU	CA-CB-CG	5.33	125.13	113.40
22	V	479	ASP	CB-CG-OD2	5.33	123.10	118.30
23	W	207	TYR	CB-CG-CD2	-5.33	117.81	121.00
29	Y	45	DT	N3-C2-O2	-5.32	119.11	122.30
23	W	540	THR	O-C-N	-5.32	114.19	122.70
28	X	48	DG	C5'-C4'-O4'	5.32	119.41	109.30
24	0	90	TYR	CB-CG-CD1	5.32	124.19	121.00
26	2	35	TYR	CB-CA-C	5.32	121.03	110.40
23	W	286	ARG	NH1-CZ-NH2	-5.30	113.57	119.40
24	0	58	MET	O-C-N	5.30	131.17	122.70
24	0	207	VAL	CA-CB-CG1	5.29	118.83	110.90
24	0	213	ARG	NH1-CZ-NH2	-5.29	113.58	119.40
24	0	125	ARG	NE-CZ-NH2	-5.28	117.66	120.30
28	X	63	DC	C4'-C3'-C2'	-5.28	98.35	103.10
23	W	162	ASP	CB-CG-OD2	5.28	123.05	118.30
23	W	623	VAL	CG1-CB-CG2	-5.28	102.46	110.90
22	V	666	ASP	CB-CG-OD1	-5.27	113.56	118.30
29	Y	43	DG	N1-C6-O6	-5.26	116.75	119.90
26	2	389	ASP	CB-CG-OD1	-5.26	113.57	118.30
29	Y	29	DC	O4'-C4'-C3'	5.25	109.15	106.00
22	V	560	VAL	CA-CB-CG2	5.25	118.78	110.90
28	X	46	DG	N1-C6-O6	-5.23	116.76	119.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
22	V	478	VAL	CA-CB-CG2	-5.23	103.05	110.90
5	E	65	ASN	N-CA-C	-5.23	96.89	111.00
22	V	250	ASP	CB-CG-OD1	5.23	123.00	118.30
24	0	64	VAL	CA-CB-CG1	5.21	118.72	110.90
23	W	449	GLU	OE1-CD-OE2	-5.21	117.05	123.30
28	X	42	DA	OP1-P-O3'	5.21	116.65	105.20
28	X	51	DC	O3'-P-O5'	5.20	113.88	104.00
29	Y	37	DG	P-O5'-C5'	5.19	129.21	120.90
28	X	51	DC	N1-C2-O2	5.17	122.00	118.90
24	0	62	TYR	CB-CG-CD1	5.16	124.10	121.00
24	0	131	LEU	CB-CG-CD1	5.16	119.77	111.00
22	V	644	LEU	CB-CG-CD2	-5.16	102.23	111.00
22	V	325	ARG	CD-NE-CZ	5.16	130.82	123.60
23	W	283	ASP	CB-CG-OD2	5.16	122.94	118.30
22	V	332	ARG	CA-CB-CG	5.15	124.73	113.40
22	V	415	HIS	CG-CD2-NE2	-5.15	99.41	109.20
1	A	621	ILE	CA-C-O	5.15	130.91	120.10
23	W	468	PRO	CA-N-CD	-5.14	104.30	111.50
23	W	461	LEU	CA-CB-CG	5.14	127.11	115.30
23	W	617	ALA	N-CA-CB	5.14	117.29	110.10
28	X	43	DG	O4'-C4'-C3'	5.13	109.08	106.00
28	X	59	DC	O4'-C1'-N1	-5.13	104.41	108.00
23	W	288	LEU	O-C-N	-5.13	114.50	122.70
26	2	457	ARG	NE-CZ-NH1	5.12	122.86	120.30
29	Y	50	DA	O4'-C4'-C3'	5.12	109.07	106.00
23	W	636	ARG	CD-NE-CZ	5.11	130.75	123.60
23	W	439	ASP	CB-CG-OD2	5.11	122.90	118.30
28	X	45	DC	O4'-C4'-C3'	5.11	109.06	106.00
22	V	434	GLU	OE1-CD-OE2	5.09	129.41	123.30
28	X	43	DG	N1-C6-O6	-5.09	116.84	119.90
23	W	714	VAL	CA-CB-CG2	5.09	118.53	110.90
23	W	695	ARG	NE-CZ-NH2	5.08	122.84	120.30
22	V	362	LEU	CB-CG-CD2	5.08	119.64	111.00
22	V	398	ASP	CB-CG-OD1	5.07	122.86	118.30
29	Y	49	DG	N1-C6-O6	-5.07	116.86	119.90
23	W	61	ARG	NE-CZ-NH1	5.07	122.83	120.30
23	W	94	TYR	CB-CG-CD2	5.07	124.04	121.00
24	0	228	TYR	CB-CG-CD2	-5.07	117.96	121.00
22	V	289	TYR	CZ-CE2-CD2	5.07	124.36	119.80
23	W	676	LEU	CB-CG-CD2	5.06	119.61	111.00
28	X	55	DC	C1'-O4'-C4'	-5.06	105.04	110.10
24	0	90	TYR	CZ-CE2-CD2	5.06	124.36	119.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
23	W	600	ALA	N-CA-CB	-5.06	103.02	110.10
23	W	126	PHE	CB-CG-CD1	-5.06	117.26	120.80
23	W	253	ARG	NE-CZ-NH2	5.06	122.83	120.30
24	0	224	ASP	N-CA-CB	-5.05	101.51	110.60
23	W	157	PHE	CB-CG-CD2	-5.05	117.27	120.80
23	W	566	LEU	CB-CG-CD2	-5.04	102.43	111.00
22	V	678	ARG	NE-CZ-NH2	5.04	122.82	120.30
22	V	344	ALA	CB-CA-C	5.03	117.65	110.10
23	W	450	ARG	CD-NE-CZ	5.03	130.64	123.60
22	V	361	CYS	N-CA-CB	-5.03	101.55	110.60
23	W	87	LEU	CB-CA-C	5.03	119.75	110.20
27	3	210	THR	CA-CB-CG2	-5.03	105.36	112.40
28	X	48	DG	O4'-C4'-C3'	5.02	109.01	106.00
22	V	607	ILE	CA-CB-CG1	5.02	120.53	111.00
25	1	16	MET	CG-SD-CE	5.01	108.22	100.20
29	Y	44	DA	C6-C5-N7	5.01	135.81	132.30
3	C	137	ASN	N-CA-C	-5.01	97.47	111.00
22	V	289	TYR	CB-CG-CD2	-5.01	118.00	121.00
23	W	599	VAL	CA-CB-CG1	5.01	118.41	110.90
23	W	346	VAL	CA-CB-CG2	5.00	118.40	110.90

There are no chirality outliers.

All (54) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
24	0	143	PRO	Mainchain
25	1	17	LYS	Mainchain
26	2	389	ASP	Mainchain,Sidechain
26	2	399	ASP	Sidechain
26	2	403	PHE	Mainchain,Peptide
26	2	406	GLY	Peptide
26	2	409	TYR	Sidechain
26	2	425	ALA	Mainchain
1	A	85	PHE	Peptide
17	Q	100	VAL	Mainchain
18	R	204	ASN	Mainchain
18	R	205	ASP	Mainchain,Peptide
18	R	206	LYS	Mainchain
18	R	213	ASP	Sidechain
18	R	219	LEU	Mainchain
18	R	230	GLU	Mainchain
18	R	235	GLU	Sidechain

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Mol	Chain	Res	Type	Group
20	T	86	GLN	Sidechain
22	V	247	ASP	Mainchain
22	V	319	TYR	Sidechain
22	V	378	PHE	Sidechain
22	V	489	TYR	Sidechain
22	V	503	ALA	Peptide
22	V	519	TYR	Sidechain
22	V	530	ARG	Sidechain
22	V	674	THR	Mainchain
23	W	197	TYR	Sidechain
23	W	206	VAL	Mainchain
23	W	208	SER	Mainchain
23	W	211	TYR	Sidechain
23	W	282	ARG	Sidechain
23	W	286	ARG	Sidechain
23	W	616	ARG	Sidechain
23	W	641	ARG	Sidechain
23	W	669	ARG	Sidechain
23	W	674	TYR	Sidechain
23	W	719	TYR	Sidechain
28	X	43	DG	Sidechain
28	X	44	DT	Sidechain
28	X	46	DG	Sidechain
28	X	47	DC	Sidechain
28	X	48	DG	Sidechain
28	X	49	DA	Sidechain
28	X	50	DT	Sidechain
28	X	54	DA	Sidechain
29	Y	41	DT	Sidechain
29	Y	42	DC	Sidechain
29	Y	43	DG	Sidechain
29	Y	44	DA	Sidechain
29	Y	50	DA	Sidechain
29	Y	51	DC	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	11515	0	11609	697	0
2	B	9317	0	9305	579	0
3	C	2213	0	2153	156	0
4	D	1062	0	1042	24	0
5	E	1723	0	1744	117	0
6	F	689	0	715	46	0
7	G	1351	0	1358	53	0
8	H	1205	0	1167	91	0
9	I	1013	0	932	93	0
10	J	533	0	553	51	0
11	K	937	0	959	47	0
12	L	388	0	393	70	0
13	M	2018	0	2059	132	0
14	N	930	0	888	68	0
15	O	806	0	818	50	0
16	P	1462	0	1549	112	0
17	Q	1484	0	1496	230	0
18	R	1357	0	1377	299	0
19	S	1138	0	1103	39	0
20	T	1788	0	1819	171	0
21	U	1343	0	1338	100	0
22	V	3855	0	3872	221	0
23	W	5348	0	5372	179	0
24	0	1479	0	1524	39	0
25	1	491	0	507	239	0
26	2	2196	0	2206	595	0
27	3	1526	0	1561	471	0
28	X	1343	0	725	35	0
29	Y	1316	0	730	36	0
30	A	1	0	0	0	0
30	B	1	0	0	0	0
31	A	2	0	0	0	0
31	B	1	0	0	0	0
31	C	1	0	0	0	0
31	I	2	0	0	0	0
31	J	1	0	0	0	0
31	L	1	0	0	0	0
31	M	1	0	0	0	0
31	Q	1	0	0	0	0
31	U	1	0	0	0	0
All	All	61839	0	60874	4132	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 34.

All (4132) 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)
23:W:421:PHE:CD1	23:W:431:PRO:HG3	1.15	1.65
5:E:27:LEU:HD12	5:E:64:HIS:CD2	1.29	1.64
27:3:59:VAL:HG12	27:3:71:TYR:CD1	1.24	1.64
5:E:27:LEU:HB2	5:E:64:HIS:CD2	1.33	1.63
22:V:315:VAL:HG13	23:W:500:ASP:CB	1.21	1.63
23:W:250:ASN:HB3	23:W:434:HIS:CD2	1.34	1.60
5:E:27:LEU:CB	5:E:64:HIS:CD2	1.85	1.59
1:A:621:ILE:CG2	1:A:623:PRO:HG3	1.13	1.57
22:V:531:ILE:HA	22:V:534:TYR:CE2	1.39	1.56
5:E:27:LEU:CB	5:E:64:HIS:HD2	0.95	1.56
17:Q:110:MET:HB2	18:R:218:LYS:CG	1.11	1.56
18:R:195:PRO:CG	18:R:199:LYS:HB2	1.32	1.56
22:V:516:PRO:CG	25:1:15:ALA:HB3	1.16	1.55
5:E:27:LEU:CD1	5:E:64:HIS:CD2	1.79	1.53
27:3:59:VAL:CG1	27:3:71:TYR:HD1	1.15	1.53
23:W:421:PHE:CD1	23:W:431:PRO:CG	1.87	1.53
24:0:54:ARG:HG3	27:3:182:PHE:CE1	1.42	1.53
17:Q:113:ARG:HD2	18:R:221:ARG:CD	1.37	1.53
5:E:27:LEU:CG	5:E:64:HIS:CD2	1.84	1.52
26:2:31:LEU:HD11	27:3:33:THR:CB	1.39	1.52
26:2:31:LEU:HD11	27:3:33:THR:CG2	1.42	1.49
22:V:516:PRO:HG3	25:1:15:ALA:CB	1.04	1.49
22:V:315:VAL:CG1	23:W:500:ASP:HB2	1.01	1.48
26:2:28:PRO:N	27:3:25:GLN:CA	1.70	1.48
1:A:621:ILE:C	1:A:623:PRO:HD3	1.10	1.48
18:R:195:PRO:CB	18:R:199:LYS:HB2	1.39	1.48
2:B:239:MET:SD	2:B:256:ILE:HG23	1.55	1.47
26:2:117:ASN:HD21	27:3:108:ASN:CB	1.27	1.45
2:B:93:LEU:N	20:T:145:LEU:HD23	1.29	1.45
26:2:117:ASN:ND2	27:3:108:ASN:CB	1.76	1.44
17:Q:109:HIS:O	18:R:221:ARG:CZ	1.64	1.43
16:P:206:GLU:HB3	16:P:207:PRO:CD	1.41	1.43
17:Q:105:TYR:CD1	18:R:234:GLU:HG2	1.52	1.43
1:A:621:ILE:HG23	1:A:623:PRO:CG	1.49	1.42
17:Q:110:MET:CE	18:R:213:ASP:HB3	1.47	1.42
1:A:1310:HIS:CB	21:U:252:LYS:HE3	1.50	1.42
22:V:321:GLU:HB3	23:W:499:ASN:ND2	1.25	1.42
18:R:155:LEU:CG	18:R:204:ASN:ND2	1.79	1.41
1:A:731:ASN:OD1	21:U:253:THR:CG2	1.69	1.41
22:V:321:GLU:HB3	23:W:499:ASN:CG	1.38	1.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:117:ASN:CG	27:3:108:ASN:HB2	1.39	1.40
12:L:16:ILE:HG13	12:L:28:ILE:N	1.33	1.40
17:Q:23:ARG:NH1	18:R:207:SER:HB3	1.32	1.40
17:Q:110:MET:CB	18:R:218:LYS:CG	2.00	1.40
1:A:621:ILE:CG2	1:A:623:PRO:CG	2.01	1.39
17:Q:187:ILE:HG23	18:R:212:VAL:CA	1.49	1.39
3:C:200:PRO:HG2	3:C:217:GLN:CG	1.51	1.38
13:M:178:LYS:O	20:T:154:LYS:CB	1.69	1.38
23:W:421:PHE:CE1	23:W:431:PRO:HG2	1.57	1.38
26:2:31:LEU:HD21	27:3:33:THR:N	1.34	1.37
17:Q:113:ARG:CD	18:R:221:ARG:HD2	1.56	1.36
24:0:54:ARG:CG	27:3:182:PHE:HE1	1.35	1.36
26:2:30:VAL:HG12	27:3:25:GLN:C	1.44	1.34
26:2:117:ASN:OD1	27:3:108:ASN:ND2	1.57	1.34
26:2:118:LEU:CD2	27:3:39:ASP:OD1	1.75	1.34
22:V:325:ARG:NH2	23:W:499:ASN:HB3	1.02	1.33
17:Q:110:MET:CB	18:R:218:LYS:HG3	1.55	1.33
22:V:523:VAL:HG11	25:1:20:LEU:CD2	1.56	1.33
17:Q:113:ARG:HB2	18:R:221:ARG:CD	1.58	1.31
9:I:99:SER:OG	9:I:105:GLU:HB2	1.26	1.31
17:Q:109:HIS:O	18:R:221:ARG:NH1	1.62	1.31
2:B:242:ARG:O	2:B:252:ILE:CG2	1.77	1.31
5:E:65:ASN:O	5:E:67:ASP:N	1.59	1.31
26:2:118:LEU:HD22	27:3:39:ASP:OD1	1.16	1.30
1:A:621:ILE:C	1:A:623:PRO:CD	1.97	1.30
9:I:105:GLU:O	9:I:107:ALA:N	1.62	1.30
17:Q:110:MET:CG	18:R:218:LYS:HB2	1.59	1.30
17:Q:113:ARG:CD	18:R:221:ARG:CD	2.08	1.30
25:1:1:MET:O	26:2:413:LEU:HG	1.25	1.28
24:0:97:ASP:O	27:3:208:ASP:HB3	1.12	1.28
22:V:325:ARG:NH2	23:W:499:ASN:CB	1.97	1.28
17:Q:110:MET:HB2	18:R:218:LYS:CB	1.63	1.27
20:T:177:ARG:CG	20:T:208:GLN:OE1	1.80	1.27
1:A:731:ASN:CG	21:U:253:THR:HG22	1.53	1.27
20:T:177:ARG:HG2	20:T:208:GLN:CD	1.54	1.27
22:V:321:GLU:CB	23:W:499:ASN:HD21	1.45	1.27
2:B:242:ARG:O	2:B:252:ILE:HG23	1.23	1.26
22:V:321:GLU:HB3	23:W:499:ASN:OD1	1.30	1.26
2:B:160:TYR:CZ	20:T:144:GLN:HG2	1.69	1.26
8:H:74:GLU:O	8:H:76:ASN:N	1.64	1.26
26:2:118:LEU:HD21	27:3:39:ASP:O	1.23	1.26

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ILE:HG12	13:M:38:GLY:O	1.14	1.26
18:R:225:VAL:HG13	18:R:226:ASP:OD1	1.13	1.25
13:M:179:GLU:CA	20:T:154:LYS:HG2	1.65	1.25
22:V:516:PRO:CG	25:1:15:ALA:CB	1.84	1.25
22:V:674:THR:HG23	26:2:392:ARG:NH2	1.50	1.25
1:A:926:ASN:OD1	1:A:931:ARG:NE	1.70	1.25
22:V:321:GLU:OE2	23:W:500:ASP:CB	1.85	1.24
27:3:59:VAL:CG1	27:3:71:TYR:CD1	1.98	1.24
1:A:1310:HIS:HB3	21:U:252:LYS:CE	1.66	1.24
3:C:200:PRO:HB2	3:C:217:GLN:OE1	1.33	1.24
5:E:27:LEU:CD1	5:E:64:HIS:NE2	1.80	1.24
17:Q:110:MET:HE3	18:R:213:ASP:CB	1.66	1.24
18:R:155:LEU:HG	18:R:204:ASN:ND2	0.93	1.24
1:A:612:ASP:O	1:A:614:ASP:N	1.69	1.24
22:V:366:ASN:HD21	22:V:613:THR:CG2	1.49	1.24
23:W:59:TYR:CZ	23:W:62:ALA:CB	2.21	1.24
24:0:165:ARG:NH1	24:0:192:ALA:O	1.68	1.24
12:L:16:ILE:HD12	12:L:28:ILE:O	1.32	1.23
23:W:209:TYR:OH	23:W:233:PHE:HA	1.37	1.23
23:W:410:TYR:O	23:W:412:LYS:N	1.71	1.23
26:2:30:VAL:HG12	27:3:25:GLN:O	1.36	1.23
18:R:212:VAL:CG2	18:R:213:ASP:H	1.46	1.22
22:V:321:GLU:CB	23:W:499:ASN:OD1	1.88	1.22
18:R:195:PRO:CG	18:R:199:LYS:CB	2.15	1.22
17:Q:105:TYR:CD1	18:R:234:GLU:CG	2.21	1.22
27:3:205:GLN:O	27:3:208:ASP:O	1.53	1.22
1:A:551:ARG:HD3	1:A:625:ASP:OD1	1.37	1.22
26:2:31:LEU:CD1	27:3:33:THR:HB	1.69	1.21
5:E:27:LEU:HD12	5:E:64:HIS:NE2	0.90	1.21
9:I:99:SER:OG	9:I:105:GLU:CB	1.88	1.21
22:V:531:ILE:CG2	22:V:534:TYR:OH	1.88	1.21
17:Q:102:VAL:O	17:Q:103:VAL:C	1.78	1.20
25:1:59:GLU:OE2	26:2:402:ARG:NH2	1.73	1.20
23:W:72:TYR:CE2	23:W:232:VAL:HG11	1.75	1.20
22:V:428:GLU:O	22:V:433:GLN:HA	1.42	1.19
2:B:160:TYR:HE1	20:T:144:GLN:CD	1.44	1.19
3:C:212:ASP:O	3:C:213:GLU:O	1.59	1.19
23:W:59:TYR:CZ	23:W:62:ALA:HB1	1.77	1.19
17:Q:113:ARG:HD2	18:R:221:ARG:CG	1.70	1.19
22:V:611:GLY:HA2	22:V:615:PHE:CD2	1.76	1.19
2:B:881:GLU:C	2:B:883:THR:H	1.41	1.19

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:250:ASN:CB	23:W:434:HIS:CD2	2.24	1.18
25:1:1:MET:CG	26:2:413:LEU:HB3	1.73	1.18
22:V:531:ILE:CA	22:V:534:TYR:CE2	2.25	1.18
17:Q:110:MET:CE	18:R:213:ASP:CB	2.13	1.18
26:2:30:VAL:CG1	27:3:24:LYS:O	1.91	1.18
27:3:58:ALA:N	27:3:71:TYR:OH	1.76	1.18
18:R:202:PHE:O	18:R:203:PHE:CD1	1.96	1.18
23:W:250:ASN:HB3	23:W:434:HIS:NE2	1.56	1.18
26:2:30:VAL:HG11	27:3:24:LYS:O	1.01	1.18
13:M:179:GLU:HA	20:T:154:LYS:CG	1.72	1.17
22:V:366:ASN:ND2	22:V:613:THR:CG2	2.05	1.17
17:Q:187:ILE:HG23	18:R:212:VAL:N	1.57	1.17
26:2:31:LEU:CD1	27:3:33:THR:CG2	2.21	1.17
26:2:117:ASN:ND2	27:3:108:ASN:HB2	0.85	1.17
1:A:610:PRO:O	1:A:611:ASP:HB2	1.41	1.17
27:3:66:GLU:HA	27:3:132:LEU:HD12	1.22	1.17
2:B:497:LYS:N	2:B:498:PRO:CD	2.07	1.16
22:V:531:ILE:HG23	22:V:534:TYR:CZ	1.79	1.16
22:V:516:PRO:HB3	25:1:15:ALA:HB1	1.24	1.16
22:V:321:GLU:CB	23:W:499:ASN:ND2	2.05	1.16
3:C:200:PRO:CB	3:C:217:GLN:OE1	1.94	1.16
17:Q:105:TYR:CG	18:R:234:GLU:HG2	1.79	1.16
17:Q:107:LEU:CA	18:R:218:LYS:HE3	1.76	1.16
26:2:171:VAL:HG22	26:2:213:TRP:HA	1.27	1.16
25:1:28:ALA:HB1	25:1:31:LYS:HD2	1.27	1.16
5:E:27:LEU:H	5:E:64:HIS:CB	1.57	1.15
26:2:160:LEU:HD23	26:2:206:LEU:HD21	1.25	1.15
2:B:873:LEU:CB	2:B:874:PRO:HD3	1.76	1.15
25:1:2:VAL:CG1	26:2:456:LYS:HG2	1.75	1.15
27:3:59:VAL:HG13	27:3:70:LEU:HB2	1.27	1.15
2:B:93:LEU:N	20:T:145:LEU:CD2	2.09	1.15
3:C:200:PRO:CG	3:C:217:GLN:HG3	1.75	1.15
5:E:27:LEU:H	5:E:64:HIS:HB2	1.09	1.15
12:L:25:GLU:HG3	12:L:27:GLU:OE2	1.47	1.15
26:2:28:PRO:N	27:3:25:GLN:HA	0.83	1.15
1:A:731:ASN:OD1	21:U:253:THR:HG22	0.99	1.14
5:E:27:LEU:CG	5:E:64:HIS:HD2	1.38	1.14
1:A:427:ILE:CG1	13:M:38:GLY:O	1.95	1.14
17:Q:113:ARG:CG	18:R:221:ARG:HD2	1.77	1.14
3:C:136:ASP:HB2	3:C:145:GLN:OE1	1.46	1.14
17:Q:23:ARG:HH11	18:R:207:SER:CB	1.61	1.14

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:30:VAL:CG1	27:3:25:GLN:O	1.96	1.13
27:3:59:VAL:N	27:3:71:TYR:CE1	2.16	1.13
2:B:497:LYS:N	2:B:498:PRO:HD3	1.47	1.13
22:V:325:ARG:HH22	23:W:499:ASN:CB	1.55	1.13
22:V:516:PRO:CB	25:1:15:ALA:HB1	1.77	1.13
18:R:127:ASN:HD21	18:R:140:LYS:HE2	1.14	1.13
1:A:621:ILE:CA	1:A:623:PRO:HD3	1.79	1.13
2:B:160:TYR:OH	20:T:144:GLN:HG2	1.47	1.13
23:W:250:ASN:CB	23:W:434:HIS:NE2	2.12	1.13
25:1:5:LEU:CD2	26:2:408:LEU:HD13	1.79	1.13
2:B:160:TYR:OH	20:T:144:GLN:CG	1.97	1.13
18:R:129:LYS:O	18:R:140:LYS:HB3	1.43	1.13
2:B:873:LEU:HB2	2:B:874:PRO:HD3	1.22	1.12
18:R:212:VAL:HG23	18:R:213:ASP:H	1.06	1.12
16:P:297:LYS:HB3	16:P:298:PRO:HD3	1.20	1.12
17:Q:25:PHE:CD2	18:R:215:GLU:CD	2.23	1.12
5:E:27:LEU:HD12	5:E:64:HIS:CE1	1.84	1.12
1:A:927:GLU:O	1:A:931:ARG:HG3	1.50	1.12
17:Q:187:ILE:HG13	18:R:212:VAL:H	1.01	1.12
23:W:59:TYR:CE2	23:W:62:ALA:CB	2.32	1.12
25:1:2:VAL:HG13	26:2:422:LEU:HD11	1.18	1.11
26:2:31:LEU:HD11	27:3:33:THR:HB	1.15	1.11
18:R:140:LYS:H	18:R:141:PRO:HD2	1.06	1.11
22:V:611:GLY:HA2	22:V:615:PHE:HD2	0.95	1.11
27:3:57:LEU:O	27:3:71:TYR:HE2	1.29	1.11
22:V:531:ILE:HG23	22:V:534:TYR:OH	0.93	1.11
25:1:5:LEU:HD11	26:2:408:LEU:HB3	1.15	1.11
22:V:516:PRO:HA	25:1:15:ALA:O	1.50	1.10
26:2:31:LEU:CD1	27:3:33:THR:CB	2.27	1.10
1:A:425:ASP:HB3	13:M:39:LEU:HD21	1.19	1.10
2:B:133:ILE:HA	2:B:139:GLN:HA	1.25	1.10
27:3:137:LEU:HB3	27:3:180:VAL:HG11	1.34	1.10
23:W:424:ARG:O	23:W:425:THR:HG23	1.52	1.10
24:0:54:ARG:CG	27:3:182:PHE:CE1	2.17	1.10
3:C:154:ARG:CD	10:J:65:LEU:HD12	1.82	1.10
17:Q:107:LEU:HA	18:R:218:LYS:HE3	1.15	1.09
21:U:256:THR:O	21:U:257:GLN:O	1.69	1.09
18:R:195:PRO:CB	18:R:199:LYS:CB	2.29	1.09
23:W:421:PHE:CE1	23:W:431:PRO:CG	2.20	1.09
17:Q:23:ARG:NH1	18:R:207:SER:CB	2.14	1.09
22:V:315:VAL:CG1	23:W:500:ASP:CB	1.94	1.09

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:2:VAL:HG11	26:2:456:LYS:CG	1.81	1.09
25:1:9:LEU:HD13	25:1:48:GLU:HA	1.32	1.09
1:A:926:ASN:OD1	1:A:931:ARG:CD	2.01	1.09
18:R:129:LYS:HB3	18:R:140:LYS:HB2	1.26	1.09
22:V:674:THR:HG23	26:2:392:ARG:CZ	1.83	1.09
25:1:5:LEU:HD21	26:2:408:LEU:CD1	1.81	1.09
9:I:99:SER:OG	9:I:105:GLU:CG	2.00	1.09
26:2:30:VAL:H	27:3:25:GLN:CB	1.66	1.09
26:2:42:LEU:HD21	26:2:55:TRP:HB2	1.20	1.08
3:C:154:ARG:CD	10:J:65:LEU:CD1	2.31	1.08
25:1:18:GLN:HB2	25:1:44:PHE:CE2	1.87	1.08
3:C:200:PRO:CG	3:C:217:GLN:CG	2.30	1.08
12:L:17:TYR:CA	12:L:46:LYS:HA	1.81	1.08
27:3:49:LEU:HB3	27:3:101:TYR:HB3	1.15	1.08
12:L:16:ILE:CD1	12:L:28:ILE:O	2.02	1.08
17:Q:110:MET:SD	18:R:218:LYS:HD2	1.93	1.08
22:V:519:TYR:CE2	25:1:20:LEU:HG	1.87	1.07
26:2:211:GLN:HG3	26:2:257:SER:HB3	1.29	1.07
2:B:876:ASN:O	2:B:879:GLU:CG	2.02	1.07
18:R:212:VAL:HG23	18:R:213:ASP:N	1.59	1.07
25:1:2:VAL:HG11	26:2:456:LYS:HG2	1.09	1.07
16:P:206:GLU:CB	16:P:207:PRO:CD	2.26	1.07
17:Q:187:ILE:HG13	18:R:212:VAL:N	1.54	1.07
18:R:194:ARG:N	18:R:195:PRO:HD3	1.64	1.07
18:R:195:PRO:HG3	18:R:199:LYS:CB	1.82	1.07
22:V:321:GLU:OE2	23:W:500:ASP:HB3	0.91	1.07
2:B:876:ASN:O	2:B:879:GLU:HG3	1.55	1.07
8:H:65:TYR:CE2	8:H:70:LEU:HB3	1.89	1.07
25:1:1:MET:CB	26:2:413:LEU:HB3	1.83	1.07
27:3:33:THR:HG23	27:3:36:LYS:H	1.13	1.07
1:A:425:ASP:CB	13:M:39:LEU:HD21	1.82	1.07
1:A:621:ILE:HG23	1:A:623:PRO:CB	1.84	1.06
1:A:926:ASN:ND2	1:A:931:ARG:HD2	1.67	1.06
3:C:136:ASP:C	3:C:138:ASP:H	1.51	1.06
5:E:62:VAL:HG23	5:E:72:MET:HB3	1.36	1.06
20:T:146:ASP:O	20:T:147:LYS:HG2	1.54	1.06
21:U:252:LYS:HE2	21:U:252:LYS:HA	1.35	1.06
26:2:30:VAL:H	27:3:25:GLN:HB3	0.89	1.06
25:1:5:LEU:HD12	26:2:409:TYR:O	1.55	1.06
26:2:30:VAL:CG1	27:3:25:GLN:C	2.23	1.06
26:2:30:VAL:N	27:3:25:GLN:HB3	1.71	1.06

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:159:VAL:HG13	26:2:161:HIS:H	1.16	1.06
1:A:926:ASN:CG	1:A:931:ARG:HD2	1.75	1.06
27:3:59:VAL:HB	27:3:71:TYR:CE1	1.88	1.06
1:A:932:ARG:HB3	1:A:939:VAL:HG11	1.10	1.06
18:R:140:LYS:H	18:R:141:PRO:CD	1.68	1.06
1:A:622:SER:N	1:A:623:PRO:HD3	1.59	1.05
18:R:129:LYS:CB	18:R:140:LYS:HB2	1.85	1.05
22:V:516:PRO:HG2	22:V:706:LYS:NZ	1.70	1.05
24:0:97:ASP:O	27:3:208:ASP:CB	2.02	1.05
26:2:192:GLU:HG3	26:2:193:PRO:HD2	1.33	1.05
2:B:79:GLU:O	2:B:80:GLU:HG2	1.52	1.05
12:L:25:GLU:HG3	12:L:27:GLU:CD	1.76	1.05
22:V:516:PRO:CG	22:V:706:LYS:NZ	2.20	1.05
17:Q:110:MET:HG3	18:R:218:LYS:HB2	1.15	1.05
12:L:15:MET:O	12:L:16:ILE:CD1	2.05	1.05
23:W:421:PHE:HD1	23:W:431:PRO:CG	1.38	1.05
17:Q:187:ILE:CG2	18:R:212:VAL:N	2.18	1.05
25:1:34:ILE:HG12	25:1:50:VAL:HG11	1.39	1.05
26:2:31:LEU:HD11	27:3:33:THR:HG22	1.37	1.05
27:3:57:LEU:C	27:3:71:TYR:OH	1.93	1.05
3:C:6:GLN:O	11:K:104:ARG:NH1	1.90	1.04
25:1:4:VAL:HG12	26:2:411:GLN:O	1.56	1.04
20:T:177:ARG:HG2	20:T:208:GLN:OE1	1.48	1.04
23:W:70:LEU:HD21	23:W:72:TYR:CE1	1.92	1.04
2:B:880:LEU:O	2:B:881:GLU:CB	2.03	1.04
22:V:426:VAL:O	22:V:427:MET:O	1.76	1.04
26:2:234:LEU:HD21	26:2:237:LEU:HD12	1.36	1.04
12:L:17:TYR:HA	12:L:46:LYS:HA	1.08	1.04
17:Q:102:VAL:HB	17:Q:105:TYR:HB3	1.09	1.04
26:2:30:VAL:HG12	27:3:25:GLN:CA	1.86	1.04
1:A:1309:MET:SD	21:U:252:LYS:CD	2.46	1.03
1:A:330:GLN:HB3	13:M:107:MET:SD	1.98	1.03
18:R:224:THR:HG21	18:R:230:GLU:HB2	1.40	1.03
2:B:160:TYR:CE1	20:T:144:GLN:CD	2.30	1.03
17:Q:113:ARG:CB	18:R:221:ARG:HD2	1.89	1.03
24:0:54:ARG:NE	27:3:182:PHE:CE1	2.26	1.03
1:A:932:ARG:CB	1:A:939:VAL:HG11	1.88	1.03
13:M:178:LYS:O	20:T:154:LYS:HB3	0.85	1.03
16:P:297:LYS:CB	16:P:298:PRO:CD	2.37	1.03
22:V:516:PRO:CB	25:1:15:ALA:CB	2.34	1.03
26:2:81:LYS:HE3	26:2:93:LEU:HD21	1.40	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:239:MET:SD	2:B:256:ILE:CG2	2.46	1.02
20:T:177:ARG:CD	20:T:208:GLN:OE1	2.06	1.02
22:V:516:PRO:HG2	22:V:706:LYS:HZ3	1.20	1.02
23:W:72:TYR:CD2	23:W:232:VAL:CG1	2.41	1.02
27:3:57:LEU:O	27:3:71:TYR:CE2	2.11	1.02
1:A:266:MET:O	1:A:267:GLN:CB	2.03	1.02
17:Q:113:ARG:HB2	18:R:221:ARG:NE	1.72	1.02
2:B:499:ARG:O	2:B:500:GLN:O	1.75	1.02
16:P:206:GLU:HB3	16:P:207:PRO:HD2	1.42	1.02
17:Q:113:ARG:HD2	18:R:221:ARG:HD2	1.04	1.02
22:V:366:ASN:HD21	22:V:613:THR:HG22	1.19	1.02
24:0:54:ARG:HB2	27:3:209:ILE:HG23	1.36	1.02
3:C:200:PRO:HG2	3:C:217:GLN:CD	1.79	1.02
24:0:77:LYS:O	24:0:79:ASN:N	1.93	1.02
17:Q:113:ARG:CB	18:R:221:ARG:CD	2.36	1.01
23:W:59:TYR:CE2	23:W:62:ALA:HB3	1.94	1.01
23:W:209:TYR:HH	23:W:233:PHE:HA	1.11	1.01
23:W:70:LEU:CD2	23:W:72:TYR:HE1	1.73	1.01
16:P:297:LYS:HB3	16:P:298:PRO:CD	1.90	1.01
17:Q:113:ARG:HB2	18:R:221:ARG:HD2	1.40	1.01
20:T:145:LEU:CD1	20:T:148:VAL:HG22	1.89	1.01
22:V:523:VAL:HG11	25:1:20:LEU:HD21	1.01	1.01
1:A:621:ILE:HG22	1:A:623:PRO:HG3	1.07	1.01
21:U:232:GLU:O	21:U:233:LEU:HB2	1.58	1.01
27:3:59:VAL:CB	27:3:71:TYR:CE1	2.44	1.01
24:0:54:ARG:CD	27:3:182:PHE:HE1	1.72	1.00
17:Q:110:MET:CB	18:R:218:LYS:CD	2.38	1.00
18:R:224:THR:CG2	18:R:230:GLU:HB2	1.91	1.00
18:R:225:VAL:CG1	18:R:226:ASP:OD1	2.07	1.00
17:Q:110:MET:HE1	18:R:213:ASP:HA	1.42	1.00
27:3:196:LEU:HD21	27:3:223:LEU:HD23	1.42	1.00
16:P:161:ILE:HG21	16:P:263:ASP:O	1.62	1.00
23:W:209:TYR:OH	23:W:233:PHE:CA	2.09	1.00
26:2:199:ALA:HB3	26:2:202:GLN:HE22	1.22	1.00
3:C:154:ARG:HD2	10:J:65:LEU:CD1	1.91	1.00
5:E:27:LEU:HG	5:E:64:HIS:CD2	1.96	1.00
3:C:5:ASN:C	3:C:7:PRO:HD3	1.81	1.00
21:U:175:ALA:HB1	21:U:222:ARG:NH2	1.76	1.00
26:2:28:PRO:CA	27:3:25:GLN:C	2.30	1.00
1:A:266:MET:O	1:A:267:GLN:HB2	1.19	0.99
1:A:1309:MET:SD	21:U:252:LYS:HD3	2.00	0.99

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:102:VAL:O	17:Q:104:LYS:N	1.95	0.99
22:V:516:PRO:CG	25:1:15:ALA:HB1	1.89	0.99
1:A:927:GLU:O	1:A:931:ARG:CG	2.10	0.99
17:Q:25:PHE:HD2	18:R:215:GLU:CD	1.61	0.99
3:C:200:PRO:HG2	3:C:217:GLN:HG3	1.02	0.99
2:B:92:TYR:HB3	20:T:145:LEU:HB3	1.44	0.99
17:Q:187:ILE:CG1	18:R:212:VAL:H	1.71	0.99
2:B:239:MET:CE	2:B:256:ILE:HD13	1.92	0.99
9:I:86:CYS:O	9:I:88:LYS:N	1.95	0.99
22:V:516:PRO:CG	22:V:706:LYS:HZ3	1.74	0.99
12:L:17:TYR:HA	12:L:46:LYS:CA	1.93	0.99
13:M:43:ASP:O	13:M:44:ARG:C	1.96	0.99
2:B:160:TYR:CE1	20:T:144:GLN:HG2	1.96	0.99
2:B:881:GLU:C	2:B:883:THR:N	2.15	0.99
1:A:1310:HIS:N	21:U:252:LYS:HD2	1.78	0.99
27:3:58:ALA:CA	27:3:71:TYR:CZ	2.45	0.99
9:I:105:GLU:C	9:I:107:ALA:H	1.65	0.98
5:E:27:LEU:HD12	5:E:64:HIS:HE2	1.28	0.98
16:P:289:PRO:HB3	29:Y:84:DG:H5'	1.44	0.98
23:W:293:ARG:O	23:W:421:PHE:HZ	1.46	0.98
16:P:307:SER:OG	29:Y:83:DA:OP1	1.80	0.98
16:P:206:GLU:HB3	16:P:207:PRO:HD3	1.01	0.98
17:Q:110:MET:CB	18:R:218:LYS:CB	2.35	0.98
26:2:118:LEU:CD2	27:3:39:ASP:O	2.12	0.98
27:3:173:GLN:HA	27:3:176:ASN:HD21	1.28	0.98
22:V:325:ARG:HH21	23:W:499:ASN:HB3	1.20	0.97
1:A:1310:HIS:H	21:U:252:LYS:CD	1.76	0.97
1:A:1310:HIS:H	21:U:252:LYS:HD2	1.23	0.97
2:B:880:LEU:O	2:B:881:GLU:HB2	1.14	0.97
9:I:99:SER:CB	9:I:105:GLU:HG3	1.94	0.97
22:V:515:SER:HB3	22:V:539:ASN:HD21	1.25	0.97
23:W:584:TYR:CD1	23:W:594:ALA:HB2	1.99	0.97
3:C:217:GLN:O	3:C:218:ALA:CB	2.12	0.97
18:R:140:LYS:N	18:R:141:PRO:HD2	1.78	0.97
26:2:118:LEU:HD11	27:3:43:VAL:CG2	1.94	0.97
9:I:64:GLU:OE1	9:I:103:ARG:NH2	1.97	0.97
18:R:195:PRO:HG3	18:R:199:LYS:HB2	1.36	0.97
27:3:165:LYS:HD2	27:3:195:VAL:HG22	1.44	0.97
17:Q:25:PHE:CE2	18:R:215:GLU:HG3	2.00	0.97
22:V:523:VAL:CG1	25:1:20:LEU:CD2	2.43	0.97
22:V:315:VAL:HG11	23:W:500:ASP:HB2	1.42	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:1:MET:HB3	26:2:413:LEU:CG	1.94	0.97
3:C:6:GLN:CG	3:C:25:ASN:ND2	2.28	0.97
26:2:176:ALA:HB1	26:2:178:LEU:HD13	1.47	0.96
2:B:499:ARG:HB3	2:B:499:ARG:NH1	1.79	0.96
17:Q:187:ILE:HG23	18:R:212:VAL:HA	1.44	0.96
22:V:523:VAL:CG1	25:1:20:LEU:HD21	1.94	0.96
27:3:59:VAL:CB	27:3:71:TYR:CD1	2.48	0.96
8:H:100:GLU:HB2	8:H:113:SER:HB2	1.48	0.96
26:2:196:ILE:HD11	26:2:210:ALA:HB2	1.45	0.96
23:W:59:TYR:CE1	23:W:62:ALA:HB1	2.01	0.96
2:B:497:LYS:H	2:B:498:PRO:HD3	1.03	0.96
17:Q:107:LEU:HA	18:R:218:LYS:CE	1.96	0.96
22:V:516:PRO:CB	22:V:706:LYS:HZ1	1.79	0.96
1:A:1112:VAL:O	21:U:252:LYS:HB3	1.66	0.96
2:B:78:VAL:O	2:B:79:GLU:HB2	1.64	0.95
17:Q:187:ILE:HG23	18:R:212:VAL:C	1.86	0.95
26:2:30:VAL:HG12	27:3:25:GLN:CB	1.94	0.95
27:3:133:LEU:HD23	27:3:177:PHE:CD1	2.01	0.95
1:A:621:ILE:HD12	1:A:623:PRO:HB3	1.47	0.95
26:2:100:LEU:HD11	26:2:119:ARG:HG3	1.46	0.95
2:B:75:SER:OG	2:B:78:VAL:HG22	1.67	0.95
1:A:425:ASP:HB3	13:M:39:LEU:CD2	1.94	0.95
22:V:531:ILE:HA	22:V:534:TYR:CD2	2.02	0.95
8:H:74:GLU:C	8:H:76:ASN:H	1.70	0.95
17:Q:32:LEU:HD11	18:R:203:PHE:CD2	2.00	0.95
17:Q:110:MET:CB	18:R:218:LYS:HD2	1.94	0.95
17:Q:110:MET:CB	18:R:218:LYS:HB2	1.93	0.95
17:Q:187:ILE:CG2	18:R:212:VAL:CA	2.45	0.95
25:1:2:VAL:CG1	26:2:422:LEU:HD11	1.96	0.95
26:2:35:TYR:CE1	26:2:62:LEU:HG	2.02	0.95
26:2:211:GLN:HA	26:2:261:PHE:CZ	2.02	0.95
27:3:148:ASN:HB2	27:3:157:MET:HE2	1.46	0.95
12:L:15:MET:O	12:L:16:ILE:CG1	2.15	0.95
2:B:92:TYR:CB	20:T:145:LEU:HD22	1.97	0.95
1:A:1314:THR:OG1	1:A:1332:GLN:NE2	2.00	0.95
23:W:72:TYR:CE2	23:W:232:VAL:CG1	2.50	0.95
18:R:212:VAL:CG2	18:R:213:ASP:N	2.15	0.95
22:V:516:PRO:HB2	22:V:706:LYS:HZ1	1.32	0.95
26:2:30:VAL:HB	27:3:25:GLN:HB2	1.48	0.94
26:2:117:ASN:CG	27:3:108:ASN:CB	2.20	0.94
22:V:321:GLU:CA	23:W:499:ASN:HD21	1.78	0.94

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:515:SER:CB	22:V:539:ASN:HD21	1.80	0.94
1:A:932:ARG:HB3	1:A:939:VAL:CG1	1.96	0.94
12:L:15:MET:O	12:L:16:ILE:HG12	1.67	0.94
20:T:177:ARG:HD3	20:T:208:GLN:OE1	1.66	0.94
18:R:140:LYS:NZ	20:T:238:GLU:OE2	2.00	0.94
26:2:31:LEU:CD2	27:3:33:THR:N	2.29	0.94
1:A:612:ASP:HB3	1:A:617:PRO:HD3	1.46	0.94
1:A:1309:MET:SD	21:U:252:LYS:HD2	2.08	0.94
8:H:64:LEU:H	8:H:70:LEU:HD21	1.30	0.94
25:1:1:MET:HB3	26:2:413:LEU:HB3	1.50	0.94
1:A:621:ILE:HG23	1:A:623:PRO:HG3	0.95	0.94
18:R:195:PRO:HB3	18:R:199:LYS:HB2	1.49	0.93
18:R:202:PHE:O	18:R:203:PHE:CG	2.21	0.93
12:L:15:MET:O	12:L:16:ILE:HD13	1.68	0.93
2:B:712:PRO:HB3	2:B:999:ALA:HB1	1.51	0.93
26:2:118:LEU:HD23	27:3:42:MET:HB2	1.50	0.93
27:3:190:LEU:HA	27:3:210:THR:HG22	1.50	0.93
22:V:531:ILE:HG23	22:V:534:TYR:HH	1.32	0.93
23:W:696:TRP:CD1	23:W:697:ILE:HG12	2.03	0.93
26:2:117:ASN:N	27:3:104:LEU:HD21	1.83	0.93
23:W:421:PHE:HE1	23:W:431:PRO:HG2	1.25	0.93
22:V:392:PHE:O	22:V:418:LYS:HD2	1.69	0.93
25:1:18:GLN:HB2	25:1:44:PHE:HE2	1.28	0.93
3:C:154:ARG:HD3	10:J:65:LEU:CD1	1.98	0.93
25:1:8:VAL:HG11	25:1:45:VAL:CG1	1.99	0.93
25:1:9:LEU:HD22	25:1:51:ASN:HD22	1.33	0.93
22:V:631:GLY:O	22:V:632:SER:CB	2.14	0.93
25:1:13:ASP:OD2	25:1:17:LYS:HB3	1.69	0.93
26:2:159:VAL:HG22	26:2:160:LEU:HD12	1.51	0.93
27:3:187:GLN:HG3	27:3:189:ILE:HG12	1.51	0.93
12:L:16:ILE:HG13	12:L:28:ILE:H	1.32	0.92
17:Q:102:VAL:CB	17:Q:105:TYR:HB3	1.98	0.92
27:3:165:LYS:HE3	27:3:200:SER:CB	2.00	0.92
2:B:160:TYR:CE1	20:T:144:GLN:CG	2.52	0.92
18:R:195:PRO:HG2	18:R:199:LYS:HB2	1.52	0.92
1:A:625:ASP:O	1:A:638:GLY:HA2	1.68	0.92
23:W:59:TYR:CE1	23:W:62:ALA:CB	2.52	0.92
22:V:366:ASN:HD21	22:V:613:THR:HG23	1.33	0.92
24:0:54:ARG:HG3	27:3:182:PHE:CZ	2.05	0.92
13:M:178:LYS:C	20:T:154:LYS:CB	2.37	0.92
17:Q:110:MET:CG	18:R:218:LYS:CB	2.47	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:155:LEU:CG	18:R:204:ASN:HD21	1.55	0.92
24:0:97:ASP:OD1	27:3:208:ASP:OD1	1.87	0.92
23:W:432:ILE:HG12	23:W:434:HIS:CE1	2.04	0.92
20:T:154:LYS:HD2	20:T:154:LYS:H	1.33	0.92
23:W:72:TYR:CD2	23:W:232:VAL:HG13	2.05	0.92
1:A:1308:TYR:HB3	1:A:1336:LEU:HD13	1.52	0.92
2:B:93:LEU:H	20:T:145:LEU:HD23	1.24	0.92
26:2:177:GLN:HA	26:2:220:LEU:CD2	1.99	0.92
1:A:551:ARG:HH22	8:H:121:LEU:HA	1.34	0.91
17:Q:112:ARG:HB3	18:R:221:ARG:HH22	1.33	0.91
26:2:81:LYS:CE	26:2:93:LEU:HD21	2.00	0.91
2:B:160:TYR:CZ	20:T:144:GLN:CG	2.51	0.91
13:M:179:GLU:HA	20:T:154:LYS:HG2	0.92	0.91
16:P:206:GLU:CB	16:P:207:PRO:HD3	1.96	0.91
27:3:165:LYS:HG3	27:3:203:LEU:HD12	1.52	0.91
12:L:25:GLU:HB2	12:L:27:GLU:HG3	1.50	0.91
17:Q:25:PHE:CD2	18:R:215:GLU:CG	2.53	0.91
3:C:212:ASP:O	3:C:213:GLU:C	2.07	0.91
12:L:16:ILE:CG1	12:L:28:ILE:N	2.30	0.91
27:3:133:LEU:HD13	27:3:133:LEU:H	1.33	0.91
27:3:137:LEU:CB	27:3:180:VAL:HG11	2.01	0.91
26:2:117:ASN:ND2	27:3:42:MET:HE1	1.86	0.91
27:3:11:LEU:HD22	27:3:160:ARG:HG2	1.51	0.91
27:3:59:VAL:HB	27:3:71:TYR:HE1	1.24	0.91
16:P:297:LYS:CB	16:P:298:PRO:HD3	1.98	0.91
25:1:1:MET:O	26:2:413:LEU:CG	2.19	0.91
25:1:1:MET:HB3	26:2:413:LEU:CB	2.01	0.91
17:Q:110:MET:HB2	18:R:218:LYS:CD	2.00	0.91
13:M:178:LYS:C	20:T:154:LYS:HB3	1.89	0.90
25:1:2:VAL:HG13	26:2:422:LEU:CD1	2.01	0.90
17:Q:23:ARG:HH11	18:R:207:SER:HB3	0.75	0.90
1:A:1287:CYS:HA	2:B:250:SER:HB2	1.52	0.90
18:R:162:GLY:C	18:R:164:GLY:H	1.66	0.90
1:A:1308:TYR:O	1:A:1336:LEU:HD22	1.70	0.90
17:Q:107:LEU:N	18:R:218:LYS:HE3	1.87	0.90
1:A:426:ARG:HB3	13:M:40:VAL:CG2	2.01	0.90
1:A:1310:HIS:H	21:U:252:LYS:CE	1.83	0.90
9:I:105:GLU:C	9:I:107:ALA:N	2.14	0.90
23:W:430:ASN:HB3	23:W:431:PRO:HD2	1.54	0.90
22:V:531:ILE:HA	22:V:534:TYR:HE2	1.09	0.90
17:Q:110:MET:HE1	18:R:213:ASP:CA	2.00	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:22:TRP:O	27:3:25:GLN:HG2	1.71	0.90
2:B:93:LEU:CA	20:T:145:LEU:HD23	2.01	0.90
2:B:133:ILE:O	2:B:134:LYS:HG2	1.70	0.90
13:M:10:LEU:O	13:M:12:ARG:N	2.05	0.90
1:A:1310:HIS:CA	21:U:252:LYS:HE3	2.01	0.90
18:R:155:LEU:HG	18:R:204:ASN:HD21	1.12	0.90
23:W:432:ILE:HG12	23:W:434:HIS:HE1	1.37	0.89
8:H:65:TYR:CE2	8:H:70:LEU:CB	2.55	0.89
17:Q:113:ARG:NE	18:R:217:GLN:O	2.06	0.89
5:E:6:GLU:OE2	5:E:54:ARG:NH2	2.05	0.89
14:N:343:HIS:HB3	14:N:350:LYS:HB2	1.51	0.89
17:Q:187:ILE:CG2	18:R:212:VAL:O	2.20	0.89
1:A:621:ILE:HG22	1:A:623:PRO:CG	1.82	0.89
26:2:81:LYS:HD2	26:2:89:LEU:HD21	1.52	0.89
3:C:45:ILE:HG12	3:C:79:VAL:HB	1.55	0.89
3:C:200:PRO:CG	3:C:217:GLN:OE1	2.20	0.89
23:W:70:LEU:HD21	23:W:72:TYR:HE1	1.30	0.89
26:2:218:GLN:HB3	26:2:264:HIS:HD2	1.38	0.89
2:B:92:TYR:HB3	20:T:145:LEU:HD22	1.54	0.89
17:Q:25:PHE:CD2	18:R:215:GLU:HG3	2.07	0.89
17:Q:113:ARG:HB2	18:R:221:ARG:CZ	1.74	0.89
25:1:4:VAL:HG11	26:2:412:PHE:HD2	1.36	0.89
20:T:231:ASN:HB2	29:Y:68:DC:H5"	1.53	0.89
26:2:117:ASN:CB	27:3:42:MET:CE	2.51	0.89
27:3:71:TYR:CD2	27:3:72:PRO:HD2	2.08	0.89
27:3:59:VAL:CG1	27:3:70:LEU:HB2	2.03	0.89
1:A:1310:HIS:CB	21:U:252:LYS:CE	2.39	0.88
26:2:30:VAL:CB	27:3:25:GLN:HB2	2.01	0.88
13:M:11:PRO:O	13:M:12:ARG:HB3	1.71	0.88
16:P:166:GLN:HG3	29:Y:81:DA:H5"	1.55	0.88
17:Q:110:MET:HB3	18:R:218:LYS:HD2	1.55	0.88
18:R:129:LYS:C	18:R:140:LYS:HB3	1.92	0.88
22:V:315:VAL:HG13	23:W:500:ASP:CA	2.03	0.88
23:W:250:ASN:HB2	23:W:434:HIS:CE1	2.08	0.88
27:3:177:PHE:CD2	27:3:181:ILE:HD11	2.08	0.88
3:C:154:ARG:HD2	10:J:65:LEU:HD12	1.52	0.88
9:I:99:SER:HB3	9:I:105:GLU:HG3	1.55	0.88
1:A:551:ARG:CD	1:A:625:ASP:OD1	2.22	0.88
2:B:876:ASN:O	2:B:879:GLU:HG2	1.74	0.88
9:I:102:ALA:C	9:I:104:ALA:H	1.69	0.88
20:T:145:LEU:O	20:T:147:LYS:N	2.07	0.88

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:393:THR:HA	22:V:418:LYS:CE	2.03	0.88
25:1:47:ALA:CB	25:1:50:VAL:HB	2.03	0.88
27:3:165:LYS:HE3	27:3:200:SER:HB2	1.56	0.88
12:L:17:TYR:O	12:L:18:ILE:HB	1.70	0.88
26:2:160:LEU:CB	26:2:206:LEU:HD11	2.04	0.88
18:R:129:LYS:O	18:R:140:LYS:CB	2.22	0.88
2:B:873:LEU:HB2	2:B:874:PRO:CD	2.03	0.88
17:Q:23:ARG:NH2	18:R:206:LYS:HB3	1.89	0.88
22:V:611:GLY:CA	22:V:615:PHE:HD2	1.83	0.88
27:3:177:PHE:CE2	27:3:181:ILE:HD11	2.08	0.88
8:H:110:THR:O	8:H:111:ARG:HB2	1.71	0.88
26:2:160:LEU:CD2	26:2:206:LEU:HD21	2.04	0.88
26:2:224:GLN:HB2	26:2:268:PHE:CZ	2.09	0.88
3:C:136:ASP:C	3:C:138:ASP:N	2.23	0.88
21:U:175:ALA:HB1	21:U:222:ARG:HH21	1.35	0.88
25:1:8:VAL:HG11	25:1:45:VAL:HG13	1.55	0.88
26:2:243:SER:CB	26:2:258:LEU:HD22	2.04	0.88
23:W:696:TRP:CD1	23:W:697:ILE:CG1	2.57	0.87
26:2:28:PRO:HA	27:3:25:GLN:C	1.92	0.87
26:2:218:GLN:HB3	26:2:264:HIS:CD2	2.09	0.87
17:Q:106:LYS:HG2	18:R:218:LYS:HE2	1.54	0.87
26:2:118:LEU:HD11	27:3:43:VAL:HG22	1.56	0.87
23:W:37:HIS:CE1	23:W:454:VAL:HG13	2.09	0.87
26:2:28:PRO:CD	27:3:25:GLN:HA	2.03	0.87
26:2:163:MET:SD	26:2:196:ILE:HG21	2.14	0.87
26:2:177:GLN:HA	26:2:220:LEU:HD21	1.56	0.87
27:3:59:VAL:HG12	27:3:71:TYR:CG	2.08	0.87
1:A:614:ASP:O	1:A:616:GLY:N	2.06	0.87
21:U:134:PRO:O	21:U:145:ARG:NH1	2.07	0.87
17:Q:102:VAL:HB	17:Q:105:TYR:CB	2.03	0.87
17:Q:113:ARG:CD	18:R:221:ARG:HD3	2.03	0.87
26:2:160:LEU:CA	26:2:206:LEU:HD11	2.04	0.87
27:3:64:ILE:HG13	27:3:123:ASP:HB3	1.57	0.87
26:2:160:LEU:HB3	26:2:206:LEU:HD11	1.52	0.87
26:2:211:GLN:HG3	26:2:257:SER:CB	2.05	0.87
1:A:624:GLY:HA3	8:H:122:LEU:HD11	1.55	0.87
2:B:881:GLU:O	2:B:883:THR:N	2.07	0.87
22:V:413:LEU:HD12	28:X:56:DA:H5'	1.56	0.87
23:W:584:TYR:CE2	23:W:614:TYR:HB2	2.10	0.87
27:3:58:ALA:HA	27:3:71:TYR:CE2	2.09	0.87
3:C:217:GLN:O	3:C:218:ALA:HB3	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:48:LEU:HB3	26:2:49:PRO:HD3	1.57	0.87
20:T:146:ASP:O	20:T:147:LYS:CG	2.23	0.87
26:2:118:LEU:HD22	27:3:39:ASP:CG	1.93	0.87
27:3:69:PHE:CZ	27:3:139:LYS:HB3	2.10	0.86
1:A:926:ASN:CG	1:A:931:ARG:CD	2.41	0.86
23:W:59:TYR:CG	23:W:62:ALA:HB2	2.10	0.86
25:1:28:ALA:CB	25:1:31:LYS:HD2	2.04	0.86
26:2:221:GLN:HG2	26:2:268:PHE:CZ	2.11	0.86
3:C:6:GLN:HG3	3:C:25:ASN:ND2	1.88	0.86
5:E:27:LEU:N	5:E:64:HIS:HB2	1.89	0.86
23:W:293:ARG:O	23:W:421:PHE:CZ	2.28	0.86
26:2:167:PRO:O	26:2:171:VAL:HG23	1.76	0.86
17:Q:113:ARG:HD2	18:R:221:ARG:HG3	1.55	0.86
26:2:159:VAL:HG22	26:2:160:LEU:H	1.41	0.86
27:3:70:LEU:HD13	27:3:115:ILE:HD11	1.55	0.86
18:R:162:GLY:O	18:R:164:GLY:N	2.08	0.86
22:V:516:PRO:CD	25:1:15:ALA:HB3	2.06	0.86
26:2:138:PRO:HG3	26:2:189:GLU:HG3	1.57	0.86
27:3:14:VAL:HG21	27:3:163:VAL:HG22	1.57	0.86
1:A:426:ARG:O	13:M:39:LEU:HA	1.74	0.85
25:1:2:VAL:CG1	26:2:422:LEU:CD1	2.54	0.85
26:2:29:GLY:N	27:3:25:GLN:OE1	2.09	0.85
26:2:45:PHE:HB2	26:2:51:LEU:HD13	1.56	0.85
26:2:81:LYS:CD	26:2:89:LEU:HD21	2.06	0.85
27:3:184:ALA:HA	27:3:187:GLN:HG2	1.58	0.85
27:3:124:ILE:HD13	27:3:125:LYS:N	1.91	0.85
26:2:28:PRO:N	27:3:25:GLN:C	2.28	0.85
27:3:190:LEU:HA	27:3:210:THR:CG2	2.05	0.85
14:N:327:GLU:HB2	16:P:188:ARG:HH12	1.40	0.85
26:2:171:VAL:HG22	26:2:213:TRP:CA	2.06	0.85
2:B:92:TYR:HB3	20:T:145:LEU:CB	2.06	0.85
27:3:100:LYS:HB3	27:3:103:LEU:HD13	1.58	0.85
18:R:224:THR:HG21	18:R:230:GLU:CB	2.05	0.85
19:S:102:VAL:HB	19:S:108:ARG:HB3	1.59	0.85
23:W:70:LEU:CD2	23:W:72:TYR:CE1	2.55	0.85
23:W:696:TRP:NE1	23:W:697:ILE:HG12	1.91	0.85
22:V:315:VAL:HG12	23:W:500:ASP:HB2	1.54	0.85
2:B:646:ARG:HD3	2:B:651:TYR:H	1.40	0.85
3:C:200:PRO:HG3	3:C:217:GLN:HB3	1.58	0.85
5:E:62:VAL:CG2	5:E:72:MET:HB3	2.07	0.85
23:W:59:TYR:CD2	23:W:62:ALA:HB2	2.12	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:78:GLU:O	26:2:81:LYS:HG2	1.77	0.85
26:2:117:ASN:OD1	27:3:108:ASN:CB	2.23	0.85
21:U:252:LYS:CE	21:U:252:LYS:HA	2.01	0.84
22:V:631:GLY:O	22:V:632:SER:HB2	1.76	0.84
2:B:133:ILE:HA	2:B:139:GLN:CA	2.08	0.84
26:2:30:VAL:CG1	27:3:25:GLN:HB2	2.07	0.84
2:B:239:MET:HE1	2:B:256:ILE:HD13	1.58	0.84
17:Q:191:LEU:HD21	18:R:212:VAL:HG11	1.59	0.84
26:2:118:LEU:HD12	26:2:119:ARG:N	1.92	0.84
2:B:133:ILE:O	2:B:134:LYS:CG	2.25	0.84
3:C:136:ASP:CB	3:C:145:GLN:OE1	2.26	0.84
26:2:118:LEU:CD2	27:3:39:ASP:HA	2.08	0.84
26:2:118:LEU:CD2	27:3:42:MET:HB2	2.06	0.84
27:3:160:ARG:HB3	27:3:190:LEU:HD21	1.57	0.84
12:L:15:MET:C	12:L:16:ILE:HG12	1.98	0.84
1:A:731:ASN:ND2	21:U:253:THR:HG22	1.92	0.84
3:C:154:ARG:CD	10:J:65:LEU:HD13	2.05	0.84
27:3:216:LYS:H	27:3:216:LYS:HD2	1.43	0.84
1:A:643:LYS:NZ	21:U:301:CYS:O	2.11	0.84
22:V:674:THR:CG2	26:2:392:ARG:CZ	2.55	0.84
1:A:426:ARG:HB3	13:M:40:VAL:HG22	1.59	0.84
2:B:718:GLN:HG2	2:B:720:PRO:HD2	1.57	0.84
27:3:58:ALA:C	27:3:71:TYR:CZ	2.51	0.84
22:V:523:VAL:HG11	25:1:20:LEU:HD23	1.60	0.83
27:3:49:LEU:CB	27:3:101:TYR:HB3	2.05	0.83
22:V:674:THR:CG2	26:2:392:ARG:NH2	2.39	0.83
26:2:176:ALA:CB	26:2:178:LEU:HD13	2.07	0.83
10:J:63:ALA:HB3	10:J:64:PRO:HD3	1.59	0.83
2:B:24:GLU:OE1	2:B:762:ARG:NH1	2.11	0.83
26:2:31:LEU:CD1	27:3:33:THR:HG22	1.96	0.83
26:2:86:SER:HB3	26:2:140:LYS:HE2	1.60	0.83
26:2:229:ASP:O	26:2:233:ILE:HG12	1.78	0.83
2:B:490:GLY:O	2:B:491:ARG:C	2.14	0.83
3:C:49:TRP:HB3	3:C:164:TYR:HB2	1.59	0.83
17:Q:110:MET:SD	18:R:218:LYS:CD	2.66	0.83
18:R:212:VAL:HG22	18:R:213:ASP:H	1.38	0.83
22:V:516:PRO:CA	25:1:15:ALA:O	2.27	0.83
26:2:81:LYS:CD	26:2:93:LEU:HD21	2.07	0.83
27:3:196:LEU:HD21	27:3:223:LEU:CD2	2.09	0.83
20:T:228:ILE:HA	28:X:30:DG:H5"	1.59	0.83
25:1:9:LEU:CD1	25:1:48:GLU:HA	2.09	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
12:L:19:CYS:HB3	12:L:22:CYS:SG	2.19	0.83
22:V:516:PRO:HA	25:1:15:ALA:C	1.98	0.83
25:1:52:VAL:CG2	25:1:53:LEU:HD12	2.09	0.83
26:2:160:LEU:O	26:2:164:VAL:HG23	1.79	0.83
26:2:259:LEU:HD12	26:2:260:ASN:N	1.94	0.83
27:3:57:LEU:HD23	27:3:58:ALA:N	1.91	0.83
26:2:221:GLN:NE2	26:2:230:LEU:HB2	1.93	0.82
17:Q:105:TYR:CD1	18:R:234:GLU:HG3	2.14	0.82
26:2:37:HIS:HB3	26:2:38:PRO:HD3	1.61	0.82
5:E:147:GLU:HB3	5:E:194:ILE:HB	1.62	0.82
25:1:1:MET:HE2	26:2:440:LEU:HD13	1.62	0.82
25:1:47:ALA:HB2	25:1:50:VAL:HB	1.61	0.82
20:T:177:ARG:CG	20:T:208:GLN:CD	2.34	0.82
23:W:293:ARG:HG2	23:W:421:PHE:CE1	2.14	0.82
26:2:174:ASP:O	26:2:220:LEU:HD23	1.79	0.82
12:L:16:ILE:CD1	12:L:28:ILE:C	2.48	0.82
22:V:316:LEU:HB2	22:V:321:GLU:HG3	1.59	0.82
22:V:415:HIS:CD2	22:V:416:THR:HG23	2.15	0.82
26:2:159:VAL:HG22	26:2:160:LEU:CD1	2.08	0.82
27:3:12:VAL:HG21	27:3:161:ILE:HG12	1.61	0.82
1:A:731:ASN:OD1	21:U:253:THR:HG21	1.80	0.82
26:2:160:LEU:HD23	26:2:206:LEU:CD2	2.07	0.82
5:E:15:LYS:NZ	5:E:35:GLN:OE1	2.12	0.82
22:V:366:ASN:ND2	22:V:613:THR:HG22	1.84	0.82
23:W:52:LEU:HD23	23:W:72:TYR:OH	1.80	0.82
26:2:57:MET:HA	26:2:60:LEU:CD1	2.09	0.82
25:1:9:LEU:HB2	25:1:51:ASN:HD21	1.43	0.82
27:3:49:LEU:HB3	27:3:101:TYR:CB	2.05	0.82
27:3:59:VAL:HG11	27:3:71:TYR:HD1	1.39	0.82
22:V:516:PRO:HG3	25:1:15:ALA:HB2	1.53	0.82
1:A:549:THR:O	1:A:589:LYS:NZ	2.13	0.82
1:A:1274:GLU:O	1:A:1276:VAL:HG23	1.80	0.82
2:B:133:ILE:CA	2:B:139:GLN:HA	2.05	0.82
5:E:21:CYS:SG	5:E:62:VAL:HG11	2.19	0.82
16:P:297:LYS:HA	16:P:297:LYS:CE	2.08	0.82
17:Q:110:MET:HB2	18:R:218:LYS:HG3	0.82	0.82
18:R:155:LEU:CD2	18:R:204:ASN:ND2	2.43	0.82
18:R:191:PHE:HB3	18:R:202:PHE:CE1	2.15	0.82
22:V:703:PHE:HZ	22:V:712:LEU:HD22	1.44	0.82
25:1:52:VAL:HG23	25:1:53:LEU:HD12	1.60	0.82
25:1:59:GLU:OE1	26:2:402:ARG:NH1	2.11	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:499:ARG:O	2:B:500:GLN:C	2.16	0.81
3:C:200:PRO:HG2	3:C:217:GLN:OE1	1.79	0.81
23:W:408:SER:O	23:W:409:THR:HB	1.77	0.81
25:1:1:MET:SD	26:2:415:GLN:O	2.38	0.81
26:2:174:ASP:OD1	26:2:179:LEU:HD12	1.80	0.81
1:A:723:ASN:HB2	9:I:109:ARG:HB2	1.61	0.81
18:R:127:ASN:HD21	18:R:140:LYS:CE	1.90	0.81
20:T:175:ARG:HD2	20:T:207:LYS:HB3	1.60	0.81
26:2:175:LEU:HB3	26:2:216:MET:SD	2.20	0.81
27:3:12:VAL:CG2	27:3:161:ILE:HG12	2.11	0.81
2:B:873:LEU:CB	2:B:874:PRO:CD	2.59	0.81
22:V:528:LYS:HE2	29:Y:36:DA:O3'	1.80	0.81
24:0:54:ARG:NE	27:3:182:PHE:HE1	1.73	0.81
26:2:117:ASN:OD1	27:3:108:ASN:CG	2.18	0.81
22:V:321:GLU:HB2	23:W:499:ASN:OD1	1.77	0.81
1:A:1209:PRO:HB3	9:I:33:ARG:HH12	1.44	0.81
5:E:27:LEU:CD1	5:E:64:HIS:HE2	1.86	0.81
17:Q:106:LYS:NZ	18:R:219:LEU:HD13	1.94	0.81
26:2:221:GLN:OE1	26:2:224:GLN:HA	1.80	0.81
1:A:653:VAL:HG23	1:A:669:TYR:HE2	1.46	0.81
2:B:227:ASN:O	2:B:405:ARG:NH2	2.14	0.81
9:I:102:ALA:C	9:I:104:ALA:N	2.31	0.81
26:2:100:LEU:HG	26:2:119:ARG:HE	1.45	0.81
27:3:165:LYS:HE2	27:3:167:ALA:O	1.81	0.81
2:B:92:TYR:C	20:T:145:LEU:CD2	2.49	0.81
2:B:488:PRO:O	2:B:489:ILE:CG1	2.29	0.81
25:1:1:MET:HB3	26:2:413:LEU:HD23	1.63	0.81
2:B:289:ILE:HG13	2:B:291:ASP:H	1.43	0.81
22:V:427:MET:O	22:V:432:THR:O	1.98	0.81
23:W:59:TYR:CD1	23:W:62:ALA:HB2	2.16	0.81
25:1:1:MET:CB	26:2:413:LEU:CB	2.56	0.81
25:1:34:ILE:HG22	25:1:46:ILE:HD11	1.63	0.81
25:1:50:VAL:HG12	25:1:54:GLN:HG2	1.62	0.81
2:B:488:PRO:O	2:B:489:ILE:HG12	1.80	0.80
26:2:52:ALA:O	26:2:56:VAL:HG13	1.81	0.80
2:B:160:TYR:OH	20:T:144:GLN:HG3	1.79	0.80
10:J:67:LYS:HB2	12:L:23:HIS:HD2	1.47	0.80
17:Q:25:PHE:HD2	18:R:215:GLU:CG	1.90	0.80
8:H:40:ILE:HD12	8:H:124:ARG:HD3	1.61	0.80
17:Q:187:ILE:C	18:R:212:VAL:HA	2.01	0.80
22:V:523:VAL:HG21	25:1:20:LEU:HG	1.64	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:0:55:LEU:HD12	27:3:178:MET:HE3	1.63	0.80
22:V:366:ASN:ND2	22:V:613:THR:HG23	1.88	0.80
26:2:42:LEU:HD12	26:2:59:MET:CE	2.11	0.80
10:J:67:LYS:HG3	12:L:23:HIS:HB3	1.63	0.80
23:W:250:ASN:CB	23:W:434:HIS:CE1	2.65	0.80
26:2:35:TYR:CD1	26:2:62:LEU:HG	2.16	0.80
26:2:205:LEU:O	26:2:209:PRO:HD2	1.81	0.80
26:2:224:GLN:HB2	26:2:268:PHE:CE2	2.17	0.80
26:2:93:LEU:HA	26:2:96:TRP:CD1	2.17	0.80
18:R:195:PRO:HB2	18:R:199:LYS:HB2	1.61	0.80
27:3:214:TYR:O	27:3:215:LEU:HD23	1.82	0.80
8:H:106:THR:O	8:H:108:ALA:N	2.12	0.79
17:Q:110:MET:HB3	18:R:218:LYS:CD	2.09	0.79
18:R:196:ASP:O	18:R:197:LYS:HB2	1.81	0.79
26:2:190:PRO:O	26:2:194:PRO:HD2	1.83	0.79
27:3:64:ILE:HG23	27:3:128:HIS:CD2	2.17	0.79
1:A:621:ILE:HG23	1:A:623:PRO:HB3	1.62	0.79
1:A:637:MET:SD	8:H:120:GLY:O	2.40	0.79
1:A:1313:GLN:CB	1:A:1333:GLU:HG2	2.12	0.79
5:E:27:LEU:CG	5:E:64:HIS:CG	2.64	0.79
25:1:38:ILE:HA	25:1:44:PHE:HD1	1.48	0.79
26:2:77:LYS:HD3	26:2:78:GLU:N	1.97	0.79
26:2:234:LEU:O	26:2:234:LEU:HD23	1.83	0.79
27:3:11:LEU:CD2	27:3:160:ARG:HG2	2.12	0.79
2:B:238:SER:O	2:B:256:ILE:O	1.99	0.79
17:Q:110:MET:CE	18:R:213:ASP:CA	2.58	0.79
18:R:163:LEU:O	18:R:164:GLY:O	2.00	0.79
25:1:1:MET:HB3	26:2:413:LEU:CD2	2.12	0.79
25:1:1:MET:HA	26:2:414:SER:H	1.47	0.79
26:2:256:ASP:O	26:2:259:LEU:HG	1.81	0.79
2:B:79:GLU:O	2:B:80:GLU:CG	2.29	0.79
2:B:623:ARG:NH2	2:B:697:GLU:OE2	2.15	0.79
27:3:121:LYS:O	27:3:124:ILE:HB	1.81	0.79
5:E:27:LEU:HB2	5:E:64:HIS:CG	2.14	0.79
13:M:178:LYS:HG2	20:T:156:VAL:HG12	1.64	0.79
17:Q:71:PHE:HA	17:Q:100:VAL:HG22	1.65	0.79
22:V:523:VAL:CB	25:1:20:LEU:HD23	2.12	0.79
25:1:1:MET:CE	26:2:440:LEU:HD13	2.12	0.79
26:2:118:LEU:HD22	27:3:39:ASP:HA	1.65	0.79
27:3:185:GLN:HA	27:3:185:GLN:HE21	1.47	0.79
10:J:17:LYS:HB3	10:J:38:LEU:HD22	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:104:LYS:HZ2	18:R:238:LYS:HD2	1.48	0.78
26:2:118:LEU:CD1	27:3:39:ASP:OD1	2.31	0.78
27:3:222:SER:O	27:3:225:GLN:HG2	1.83	0.78
5:E:65:ASN:C	5:E:67:ASP:N	2.30	0.78
16:P:206:GLU:CB	16:P:207:PRO:HD2	2.02	0.78
17:Q:187:ILE:CG2	18:R:212:VAL:C	2.52	0.78
9:I:99:SER:CB	9:I:105:GLU:CG	2.58	0.78
25:1:38:ILE:HG22	25:1:44:PHE:CD1	2.19	0.78
26:2:42:LEU:HD12	26:2:59:MET:HE3	1.63	0.78
26:2:203:PHE:CD2	26:2:205:LEU:HD23	2.18	0.78
13:M:43:ASP:O	13:M:45:VAL:N	2.15	0.78
25:1:34:ILE:CG2	25:1:46:ILE:HD11	2.13	0.78
26:2:30:VAL:HG22	26:2:34:LEU:HD23	1.65	0.78
26:2:208:THR:HG23	26:2:209:PRO:HD3	1.66	0.78
9:I:105:GLU:O	9:I:106:ASP:C	2.19	0.78
26:2:34:LEU:O	26:2:38:PRO:HD2	1.84	0.78
26:2:196:ILE:CD1	26:2:210:ALA:HB2	2.13	0.78
1:A:604:ARG:HA	1:A:628:VAL:O	1.83	0.78
24:0:54:ARG:HB2	27:3:209:ILE:CG2	2.14	0.78
1:A:30:GLU:HA	1:A:33:ARG:HB2	1.65	0.78
26:2:207:ASP:O	26:2:211:GLN:HG2	1.84	0.78
27:3:14:VAL:CG2	27:3:163:VAL:HG22	2.13	0.78
1:A:1112:VAL:O	21:U:252:LYS:HG3	1.83	0.78
26:2:163:MET:CE	26:2:206:LEU:HD12	2.14	0.78
12:L:16:ILE:HG13	12:L:27:GLU:C	2.03	0.77
27:3:58:ALA:HA	27:3:71:TYR:CZ	2.19	0.77
27:3:58:ALA:C	27:3:71:TYR:CE1	2.58	0.77
27:3:147:MET:O	27:3:151:VAL:HG23	1.84	0.77
25:1:1:MET:HG3	26:2:415:GLN:O	1.84	0.77
26:2:42:LEU:HD21	26:2:55:TRP:CB	2.10	0.77
26:2:179:LEU:HB3	26:2:184:LEU:HD11	1.65	0.77
1:A:921:ARG:O	1:A:1052:ARG:NH1	2.17	0.77
18:R:155:LEU:CG	18:R:204:ASN:HD22	1.72	0.77
20:T:174:LYS:HB3	28:X:20:DG:H4'	1.65	0.77
18:R:155:LEU:CB	18:R:204:ASN:HD21	1.97	0.77
20:T:221:GLY:HA2	20:T:236:LYS:HG3	1.67	0.77
23:W:408:SER:O	23:W:409:THR:CB	2.31	0.77
27:3:58:ALA:N	27:3:71:TYR:CZ	2.53	0.77
22:V:703:PHE:CZ	22:V:712:LEU:HD22	2.18	0.77
26:2:181:GLN:OE1	26:2:229:ASP:HB2	1.84	0.77
27:3:185:GLN:NE2	27:3:210:THR:HA	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:187:ILE:CG1	18:R:212:VAL:N	2.13	0.77
27:3:133:LEU:HD23	27:3:177:PHE:HD1	1.49	0.77
26:2:189:GLU:HB2	26:2:190:PRO:HD3	1.66	0.77
1:A:537:ILE:HB	1:A:645:LEU:HD21	1.67	0.77
1:A:611:ASP:OD2	1:A:617:PRO:HB3	1.84	0.77
1:A:731:ASN:HD21	21:U:253:THR:HA	1.47	0.77
3:C:154:ARG:HD2	10:J:65:LEU:HD13	1.64	0.77
26:2:29:GLY:N	27:3:25:GLN:HB3	1.99	0.77
26:2:53:LYS:O	26:2:56:VAL:HG22	1.84	0.77
26:2:118:LEU:CG	27:3:39:ASP:OD1	2.32	0.77
26:2:221:GLN:HE22	26:2:230:LEU:HB2	1.47	0.77
18:R:195:PRO:HB3	18:R:199:LYS:CB	2.08	0.77
22:V:689:VAL:HB	26:2:391:ILE:HD11	1.67	0.77
27:3:151:VAL:HG12	27:3:155:GLN:O	1.84	0.77
1:A:1310:HIS:N	21:U:252:LYS:CD	2.40	0.77
17:Q:102:VAL:C	17:Q:104:LYS:N	2.38	0.77
21:U:250:MET:O	21:U:251:ALA:HB2	1.83	0.77
17:Q:32:LEU:CD1	18:R:203:PHE:CD2	2.67	0.76
23:W:424:ARG:O	23:W:425:THR:CG2	2.32	0.76
18:R:191:PHE:HB3	18:R:202:PHE:CD1	2.19	0.76
26:2:218:GLN:NE2	26:2:265:LEU:HA	2.00	0.76
2:B:1072:ARG:HH21	2:B:1113:PRO:HG2	1.50	0.76
5:E:27:LEU:N	5:E:64:HIS:CB	2.42	0.76
1:A:1169:VAL:HG21	1:A:1298:LEU:HD22	1.66	0.76
3:C:154:ARG:NH1	10:J:65:LEU:HB2	2.01	0.76
17:Q:191:LEU:CD2	18:R:212:VAL:HG11	2.15	0.76
20:T:174:LYS:HG2	28:X:20:DG:O3'	1.86	0.76
23:W:432:ILE:CG1	23:W:434:HIS:HE1	1.99	0.76
25:1:1:MET:SD	26:2:413:LEU:HB3	2.25	0.76
26:2:251:VAL:HG11	26:2:254:MET:CG	2.16	0.76
18:R:162:GLY:C	18:R:164:GLY:N	2.39	0.76
25:1:13:ASP:OD2	25:1:17:LYS:CB	2.33	0.76
3:C:130:VAL:O	3:C:134:ASN:ND2	2.19	0.76
25:1:24:ASP:OD2	25:1:57:VAL:HG11	1.85	0.76
1:A:137:PRO:HB3	1:A:237:GLY:HA3	1.68	0.76
22:V:444:HIS:O	22:V:447:PRO:HD2	1.85	0.76
1:A:884:ASN:ND2	6:F:111:PRO:O	2.18	0.76
2:B:92:TYR:HB3	20:T:145:LEU:CD2	2.15	0.76
9:I:73:SER:O	9:I:80:ARG:NH2	2.17	0.76
26:2:127:LYS:N	26:2:178:LEU:HD23	2.01	0.76
26:2:159:VAL:HG13	26:2:161:HIS:N	1.96	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1274:GLU:O	1:A:1276:VAL:N	2.19	0.76
19:S:50:ASP:HB3	19:S:97:PRO:HG2	1.66	0.76
22:V:516:PRO:CD	22:V:706:LYS:HZ3	1.98	0.76
27:3:172:LEU:HD13	27:3:172:LEU:O	1.86	0.76
12:L:18:ILE:O	12:L:45:TYR:N	2.18	0.76
21:U:250:MET:O	21:U:251:ALA:CB	2.33	0.76
12:L:16:ILE:HG13	12:L:28:ILE:CA	2.17	0.75
17:Q:107:LEU:N	18:R:218:LYS:CE	2.50	0.75
21:U:173:GLU:OE2	21:U:187:TYR:OH	2.04	0.75
27:3:190:LEU:HD23	27:3:190:LEU:H	1.51	0.75
12:L:40:GLY:O	12:L:42:ARG:NH1	2.19	0.75
20:T:177:ARG:NH1	28:X:20:DG:OP1	2.20	0.75
26:2:86:SER:HB3	26:2:140:LYS:CE	2.16	0.75
2:B:160:TYR:HE1	20:T:144:GLN:NE2	1.84	0.75
17:Q:106:LYS:C	18:R:218:LYS:HE3	2.07	0.75
1:A:1206:ARG:HD3	1:A:1265:ASP:HA	1.69	0.75
26:2:35:TYR:CD2	26:2:62:LEU:HB3	2.22	0.75
26:2:44:VAL:HG13	26:2:45:PHE:CD1	2.20	0.75
26:2:251:VAL:HG12	26:2:254:MET:H	1.51	0.75
3:C:5:ASN:O	3:C:7:PRO:HD3	1.85	0.75
18:R:129:LYS:HB3	18:R:140:LYS:CB	2.12	0.75
27:3:14:VAL:CG2	27:3:163:VAL:HA	2.16	0.75
2:B:754:PRO:HB2	2:B:773:PRO:HG2	1.69	0.75
5:E:65:ASN:O	5:E:66:ASP:C	2.24	0.75
25:1:38:ILE:H	25:1:38:ILE:HD13	1.51	0.75
1:A:1208:SER:HB2	1:A:1261:ILE:HG12	1.69	0.75
25:1:10:ILE:CG2	26:2:407:VAL:HG21	2.16	0.75
26:2:51:LEU:HD23	26:2:51:LEU:O	1.87	0.75
1:A:1112:VAL:O	21:U:252:LYS:CB	2.34	0.75
26:2:53:LYS:HE3	26:2:95:ILE:HD11	1.67	0.75
1:A:1310:HIS:N	21:U:252:LYS:CE	2.49	0.75
2:B:160:TYR:CE1	20:T:144:GLN:NE2	2.54	0.75
17:Q:106:LYS:C	18:R:218:LYS:CE	2.55	0.75
23:W:608:ILE:HG23	23:W:614:TYR:CE2	2.22	0.75
26:2:100:LEU:CD1	26:2:119:ARG:HG3	2.16	0.75
26:2:117:ASN:CG	27:3:42:MET:CE	2.55	0.75
13:M:179:GLU:N	20:T:154:LYS:HG2	2.02	0.74
18:R:127:ASN:ND2	18:R:140:LYS:HE2	1.98	0.74
18:R:154:LEU:HD23	18:R:162:GLY:O	1.86	0.74
23:W:52:LEU:HD23	23:W:72:TYR:CE2	2.22	0.74
26:2:208:THR:HG23	26:2:209:PRO:CD	2.16	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:425:ASP:CG	13:M:39:LEU:HD21	2.06	0.74
1:A:539:GLN:HE21	2:B:970:HIS:HB2	1.52	0.74
2:B:134:LYS:HD3	2:B:138:GLU:HB2	1.68	0.74
2:B:817:GLN:HE21	2:B:916:TYR:HB2	1.52	0.74
2:B:924:ARG:NH1	3:C:62:GLU:OE1	2.19	0.74
3:C:100:GLU:OE2	3:C:162:ARG:NH2	2.20	0.74
26:2:28:PRO:CA	27:3:25:GLN:CA	2.61	0.74
1:A:612:ASP:OD2	1:A:614:ASP:O	2.05	0.74
1:A:700:GLN:OE1	1:A:703:GLN:NE2	2.20	0.74
22:V:415:HIS:HA	22:V:421:TRP:CD1	2.22	0.74
26:2:196:ILE:HD11	26:2:210:ALA:CB	2.17	0.74
27:3:8:LEU:HD23	27:3:54:SER:HB3	1.68	0.74
1:A:1310:HIS:HB3	21:U:252:LYS:HE3	0.78	0.74
18:R:140:LYS:O	18:R:143:TYR:CE1	2.41	0.74
23:W:430:ASN:HB3	23:W:431:PRO:CD	2.17	0.74
26:2:30:VAL:CG1	27:3:25:GLN:CB	2.65	0.74
27:3:38:ILE:O	27:3:41:VAL:HG12	1.87	0.74
27:3:59:VAL:CA	27:3:71:TYR:CE1	2.70	0.74
1:A:374:SER:OG	1:A:666:ARG:NH2	2.20	0.74
1:A:1310:HIS:CE1	1:A:1334:TRP:HE3	2.06	0.74
2:B:894:THR:HA	13:M:52:TRP:CH2	2.23	0.74
3:C:12:THR:H	3:C:21:PHE:HA	1.52	0.74
17:Q:107:LEU:CA	18:R:218:LYS:CE	2.62	0.74
18:R:224:THR:CG2	18:R:230:GLU:CB	2.64	0.74
20:T:47:LYS:HG2	20:T:52:THR:HG23	1.69	0.74
21:U:232:GLU:O	21:U:233:LEU:CB	2.28	0.74
26:2:177:GLN:CD	26:2:220:LEU:HD22	2.06	0.74
1:A:958:ARG:NH1	1:A:962:ASP:OD1	2.21	0.74
2:B:79:GLU:HA	2:B:79:GLU:OE2	1.85	0.74
17:Q:187:ILE:CB	18:R:212:VAL:N	2.49	0.74
22:V:519:TYR:HE2	25:1:20:LEU:HG	1.52	0.74
26:2:132:ASP:O	26:2:135:GLN:HG2	1.88	0.74
27:3:11:LEU:HD22	27:3:160:ARG:CG	2.16	0.74
2:B:806:PHE:O	2:B:1050:ARG:NH1	2.21	0.74
5:E:27:LEU:HG	5:E:64:HIS:CG	2.21	0.74
18:R:195:PRO:CG	18:R:199:LYS:CA	2.65	0.74
22:V:412:MET:CA	22:V:417:THR:HG21	2.17	0.74
22:V:534:TYR:CE1	22:V:535:THR:OG1	2.40	0.74
26:2:234:LEU:CD2	26:2:237:LEU:HD12	2.14	0.74
1:A:621:ILE:O	1:A:623:PRO:HD3	1.84	0.74
26:2:180:SER:O	26:2:184:LEU:HG	1.87	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:321:GLU:OE1	23:W:499:ASN:OD1	2.06	0.74
26:2:211:GLN:CG	26:2:257:SER:HB3	2.13	0.74
17:Q:113:ARG:HB2	18:R:221:ARG:HD3	1.68	0.74
18:R:195:PRO:HG2	18:R:199:LYS:H	1.53	0.74
22:V:674:THR:OG1	26:2:392:ARG:NE	2.21	0.74
25:1:1:MET:HG2	26:2:413:LEU:HB3	1.68	0.74
27:3:12:VAL:HG23	27:3:161:ILE:HG23	1.70	0.74
1:A:631:GLU:HG3	1:A:636:ILE:HD11	1.70	0.73
1:A:1307:VAL:CG1	1:A:1339:ASP:H	2.01	0.73
2:B:74:ALA:O	2:B:76:GLY:N	2.21	0.73
12:L:18:ILE:HA	12:L:25:GLU:HA	1.70	0.73
17:Q:112:ARG:HB3	18:R:221:ARG:NH2	2.03	0.73
23:W:73:CYS:HB2	23:W:209:TYR:CZ	2.22	0.73
27:3:111:ILE:HG13	27:3:112:VAL:N	2.03	0.73
25:1:1:MET:C	26:2:413:LEU:HG	2.09	0.73
27:3:144:ILE:HG12	27:3:147:MET:HE2	1.68	0.73
5:E:52:ARG:HG3	5:E:53:PRO:N	2.03	0.73
26:2:237:LEU:O	26:2:240:LEU:HD13	1.88	0.73
26:2:243:SER:HB3	26:2:258:LEU:HD22	1.69	0.73
20:T:146:ASP:O	20:T:147:LYS:CB	2.37	0.73
22:V:523:VAL:HG21	25:1:20:LEU:CD2	2.17	0.73
26:2:41:CYS:O	26:2:44:VAL:HG12	1.88	0.73
26:2:243:SER:HB2	26:2:258:LEU:HD22	1.71	0.73
25:1:34:ILE:HD13	25:1:54:GLN:OE1	1.88	0.73
27:3:226:TYR:HA	27:3:230:VAL:HG23	1.71	0.73
2:B:242:ARG:O	2:B:252:ILE:HG22	1.82	0.73
3:C:101:PHE:HB2	3:C:163:ALA:HB3	1.71	0.73
18:R:195:PRO:HG3	18:R:199:LYS:C	2.09	0.73
25:1:28:ALA:HB3	25:1:31:LYS:HB2	1.71	0.73
27:3:214:TYR:HE2	27:3:216:LYS:HE2	1.53	0.73
2:B:759:VAL:HG12	2:B:999:ALA:HB2	1.71	0.73
3:C:200:PRO:HG3	3:C:217:GLN:CB	2.19	0.73
20:T:139:VAL:O	20:T:140:ARG:CB	2.37	0.73
22:V:516:PRO:HB3	25:1:15:ALA:CB	2.05	0.73
25:1:25:GLU:CD	25:1:35:ILE:HG12	2.09	0.73
26:2:117:ASN:HB3	27:3:42:MET:CE	2.18	0.73
27:3:141:LEU:O	27:3:144:ILE:HG22	1.89	0.73
8:H:65:TYR:HE2	8:H:70:LEU:HB3	1.53	0.73
26:2:175:LEU:HD22	26:2:216:MET:SD	2.29	0.73
20:T:146:ASP:C	20:T:147:LYS:HG2	2.09	0.72
2:B:1119:CYS:HB2	2:B:1137:CYS:SG	2.28	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:66:GLU:O	8:H:67:ASP:CB	2.35	0.72
12:L:17:TYR:O	12:L:18:ILE:CB	2.33	0.72
17:Q:110:MET:HE3	18:R:213:ASP:HB3	0.75	0.72
22:V:667:THR:HA	25:1:62:ASP:OD1	1.89	0.72
23:W:59:TYR:CD2	23:W:62:ALA:CB	2.71	0.72
26:2:172:SER:HA	26:2:175:LEU:CD2	2.19	0.72
1:A:831:LEU:HB2	2:B:715:ASP:HB2	1.70	0.72
12:L:37:ARG:O	12:L:39:CYS:N	2.22	0.72
16:P:297:LYS:HB2	16:P:298:PRO:HD2	1.71	0.72
27:3:57:LEU:C	27:3:71:TYR:CE2	2.63	0.72
9:I:99:SER:HG	9:I:105:GLU:HB2	1.51	0.72
14:N:26:ARG:NE	14:N:36:GLU:OE1	2.21	0.72
17:Q:32:LEU:HD13	18:R:203:PHE:CE2	2.24	0.72
17:Q:144:LEU:O	17:Q:153:ARG:N	2.23	0.72
2:B:100:GLU:OE2	2:B:116:ARG:NH1	2.22	0.72
19:S:126:ILE:HB	19:S:138:PHE:HB2	1.70	0.72
22:V:394:SER:HB3	22:V:416:THR:O	1.88	0.72
26:2:117:ASN:HB2	27:3:104:LEU:HD11	1.71	0.72
26:2:160:LEU:HA	26:2:206:LEU:HD11	1.70	0.72
27:3:57:LEU:C	27:3:71:TYR:CZ	2.62	0.72
27:3:165:LYS:HG3	27:3:203:LEU:CD1	2.20	0.72
1:A:625:ASP:N	1:A:637:MET:HB3	2.03	0.72
22:V:516:PRO:HG2	22:V:706:LYS:CE	2.19	0.72
24:0:76:LEU:O	24:0:77:LYS:O	2.07	0.72
26:2:60:LEU:HD11	26:2:95:ILE:HB	1.71	0.72
2:B:57:ARG:NH1	2:B:60:GLU:OE1	2.23	0.72
14:N:318:ASP:CB	16:P:239:ARG:HH21	2.03	0.72
22:V:523:VAL:CG1	25:1:20:LEU:HD23	2.15	0.72
26:2:118:LEU:CD2	27:3:39:ASP:CA	2.68	0.72
26:2:134:SER:O	26:2:138:PRO:HD2	1.89	0.72
26:2:211:GLN:HA	26:2:261:PHE:HZ	1.49	0.72
1:A:257:PRO:HD2	1:A:260:VAL:HB	1.71	0.72
1:A:621:ILE:O	1:A:623:PRO:CD	2.36	0.72
9:I:94:ALA:HA	9:I:114:CYS:HA	1.72	0.72
23:W:209:TYR:OH	23:W:234:ASP:N	2.23	0.72
23:W:584:TYR:HD1	23:W:594:ALA:HB2	1.51	0.72
26:2:35:TYR:CG	26:2:62:LEU:HD12	2.25	0.72
26:2:117:ASN:HB3	27:3:42:MET:HE3	1.71	0.72
2:B:205:VAL:O	2:B:371:ARG:NH1	2.23	0.72
9:I:101:SER:H	9:I:104:ALA:HA	1.55	0.72
20:T:145:LEU:HD11	20:T:148:VAL:HG22	1.72	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:2:VAL:HG12	26:2:422:LEU:HD13	1.71	0.72
1:A:1163:HIS:HA	1:A:1300:GLY:HA3	1.70	0.72
1:A:1314:THR:HG1	1:A:1332:GLN:NE2	1.85	0.72
2:B:878:ASP:O	2:B:879:GLU:O	2.07	0.72
2:B:1129:ASN:HA	2:B:1135:TYR:HA	1.71	0.72
26:2:118:LEU:HD22	27:3:39:ASP:CA	2.19	0.72
26:2:251:VAL:CG1	26:2:254:MET:HB2	2.20	0.72
27:3:217:VAL:HG13	27:3:226:TYR:CZ	2.25	0.72
1:A:546:ARG:HG3	1:A:639:ILE:HD11	1.72	0.71
1:A:621:ILE:CG2	1:A:623:PRO:CD	2.68	0.71
1:A:611:ASP:OD2	1:A:617:PRO:HG3	1.91	0.71
1:A:790:GLN:NE2	1:A:820:ARG:O	2.22	0.71
1:A:1211:LEU:HD11	1:A:1258:ARG:HB2	1.71	0.71
14:N:311:GLU:HB3	16:P:251:LEU:HD23	1.72	0.71
17:Q:191:LEU:CD2	18:R:212:VAL:CG1	2.67	0.71
20:T:176:ALA:C	20:T:177:ARG:HG3	2.10	0.71
1:A:1308:TYR:CD1	1:A:1338:THR:CG2	2.73	0.71
1:A:1457:ASN:OD1	1:A:1462:GLN:NE2	2.22	0.71
27:3:222:SER:HB2	27:3:226:TYR:HE2	1.54	0.71
1:A:1303:GLN:HE22	1:A:1342:SER:HB3	1.55	0.71
23:W:410:TYR:C	23:W:412:LYS:H	1.94	0.71
27:3:33:THR:HG23	27:3:36:LYS:N	1.98	0.71
27:3:33:THR:HG22	27:3:36:LYS:HB2	1.73	0.71
1:A:610:PRO:O	1:A:611:ASP:CB	2.28	0.71
1:A:621:ILE:HA	1:A:623:PRO:HD3	1.68	0.71
26:2:218:GLN:HE22	26:2:265:LEU:HA	1.55	0.71
1:A:1308:TYR:CD1	1:A:1338:THR:HG21	2.25	0.71
2:B:849:ASP:OD2	12:L:29:LYS:NZ	2.23	0.71
7:G:110:ARG:NH2	7:G:118:GLU:OE2	2.24	0.71
20:T:139:VAL:O	20:T:140:ARG:HB3	1.90	0.71
23:W:209:TYR:HE1	23:W:233:PHE:CD1	2.08	0.71
25:1:9:LEU:HD22	25:1:51:ASN:ND2	2.04	0.71
26:2:163:MET:O	26:2:167:PRO:HD2	1.91	0.71
26:2:189:GLU:HA	26:2:192:GLU:HG2	1.72	0.71
27:3:69:PHE:CE1	27:3:139:LYS:HD2	2.25	0.71
17:Q:191:LEU:HD22	18:R:212:VAL:CG1	2.21	0.71
25:1:1:MET:HG2	26:2:413:LEU:C	2.11	0.71
25:1:29:LEU:HD23	25:1:30:GLY:N	2.06	0.71
26:2:81:LYS:HD2	26:2:89:LEU:CD2	2.20	0.71
26:2:86:SER:CB	26:2:140:LYS:HE2	2.20	0.71
26:2:171:VAL:HG12	26:2:216:MET:SD	2.31	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:582:PRO:HD2	8:H:47:ILE:HD12	1.72	0.71
14:N:326:GLN:O	15:O:92:LYS:NZ	2.22	0.71
20:T:176:ALA:O	20:T:208:GLN:NE2	2.24	0.71
26:2:31:LEU:N	27:3:25:GLN:O	2.23	0.71
27:3:133:LEU:HD22	27:3:134:ALA:H	1.56	0.71
27:3:144:ILE:CD1	27:3:147:MET:HE3	2.21	0.71
1:A:611:ASP:CG	1:A:617:PRO:HG3	2.11	0.70
1:A:790:GLN:HA	1:A:822:PHE:HA	1.71	0.70
2:B:743:ARG:O	2:B:922:ARG:NH1	2.24	0.70
2:B:803:ARG:NH1	10:J:8:PHE:O	2.24	0.70
3:C:47:ILE:HA	3:C:165:ALA:HA	1.72	0.70
17:Q:106:LYS:HG2	18:R:218:LYS:HG2	1.73	0.70
18:R:154:LEU:CD2	18:R:162:GLY:O	2.39	0.70
22:V:504:LYS:HB3	22:V:654:GLU:O	1.91	0.70
25:1:55:GLU:OE2	26:2:402:ARG:HG3	1.90	0.70
2:B:1067:ILE:HG22	2:B:1068:GLN:H	1.55	0.70
6:F:56:TYR:O	6:F:108:ARG:NH2	2.22	0.70
17:Q:67:LYS:HG3	17:Q:72:ILE:HD11	1.73	0.70
21:U:286:THR:HG21	21:U:299:LYS:HB3	1.72	0.70
2:B:93:LEU:C	20:T:145:LEU:CD2	2.60	0.70
26:2:185:MET:SD	26:2:232:GLU:HB2	2.32	0.70
3:C:154:ARG:HD3	10:J:65:LEU:CB	2.21	0.70
15:O:79:VAL:HG21	15:O:93:VAL:HG12	1.73	0.70
20:T:177:ARG:HG3	20:T:208:GLN:OE1	1.88	0.70
25:1:2:VAL:HG12	26:2:456:LYS:HE2	1.72	0.70
26:2:199:ALA:CB	26:2:202:GLN:HE22	2.02	0.70
27:3:177:PHE:CZ	27:3:203:LEU:HD23	2.27	0.70
13:M:297:PRO:HB3	13:M:310:VAL:HG21	1.73	0.70
16:P:271:GLU:OE1	16:P:271:GLU:N	2.23	0.70
26:2:117:ASN:HD21	27:3:108:ASN:CA	2.05	0.70
26:2:192:GLU:HG3	26:2:193:PRO:CD	2.18	0.70
1:A:611:ASP:OD2	1:A:617:PRO:CG	2.38	0.70
2:B:216:ALA:N	2:B:239:MET:O	2.25	0.70
25:1:2:VAL:CG1	26:2:456:LYS:CG	2.53	0.70
3:C:6:GLN:HG2	3:C:25:ASN:ND2	2.04	0.70
22:V:393:THR:HA	22:V:418:LYS:CD	2.21	0.70
25:1:34:ILE:HG12	25:1:50:VAL:CG1	2.18	0.70
26:2:30:VAL:HG13	27:3:25:GLN:O	1.88	0.70
1:A:625:ASP:OD1	1:A:637:MET:CE	2.39	0.70
22:V:531:ILE:CG2	22:V:534:TYR:CZ	2.64	0.70
26:2:117:ASN:HD21	27:3:108:ASN:HB3	1.47	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:497:LYS:N	2:B:498:PRO:HD2	2.04	0.70
3:C:10:ARG:NH2	3:C:24:GLU:OE2	2.23	0.70
17:Q:112:ARG:CB	18:R:221:ARG:HH22	2.03	0.70
23:W:696:TRP:CD1	23:W:697:ILE:HG13	2.26	0.70
25:1:18:GLN:CB	25:1:44:PHE:HE2	2.02	0.70
26:2:48:LEU:CB	26:2:49:PRO:HD3	2.19	0.70
10:J:63:ALA:N	10:J:64:PRO:CD	2.55	0.70
2:B:92:TYR:C	20:T:145:LEU:HD22	2.13	0.69
3:C:211:LEU:C	3:C:213:GLU:H	1.95	0.69
8:H:110:THR:O	8:H:111:ARG:CB	2.40	0.69
13:M:286:ARG:HG3	13:M:316:LEU:HG	1.74	0.69
22:V:648:LYS:O	22:V:650:MET:N	2.24	0.69
23:W:589:GLU:O	23:W:594:ALA:HB1	1.91	0.69
24:0:54:ARG:NE	27:3:182:PHE:CD1	2.60	0.69
25:1:1:MET:HB2	26:2:418:PHE:CB	2.21	0.69
26:2:117:ASN:CB	27:3:42:MET:HE3	2.21	0.69
1:A:121:SER:HA	1:A:126:ILE:HG21	1.73	0.69
1:A:1313:GLN:HB2	1:A:1333:GLU:HG2	1.74	0.69
14:N:353:LEU:HB2	14:N:370:ALA:HB3	1.74	0.69
18:R:90:GLN:NE2	18:R:172:GLU:OE2	2.25	0.69
25:1:8:VAL:HG11	25:1:45:VAL:HG12	1.74	0.69
26:2:218:GLN:OE1	26:2:265:LEU:HA	1.92	0.69
8:H:65:TYR:CD2	8:H:70:LEU:HD23	2.28	0.69
18:R:195:PRO:HG2	18:R:199:LYS:CA	2.22	0.69
17:Q:25:PHE:HA	18:R:215:GLU:OE1	1.93	0.69
25:1:1:MET:HG3	26:2:418:PHE:HB2	1.73	0.69
2:B:499:ARG:HB3	2:B:499:ARG:HH11	1.57	0.69
2:B:983:GLU:OE2	2:B:1047:TYR:N	2.19	0.69
22:V:609:LYS:HZ2	29:Y:38:DT:P	2.15	0.69
25:1:53:LEU:HD12	25:1:53:LEU:H	1.57	0.69
27:3:69:PHE:CZ	27:3:139:LYS:HD2	2.27	0.69
2:B:777:ASN:O	10:J:47:ARG:NH1	2.25	0.69
5:E:80:PRO:HA	5:E:107:GLN:HB2	1.73	0.69
18:R:195:PRO:CG	18:R:199:LYS:O	2.40	0.69
2:B:499:ARG:HB3	2:B:499:ARG:CZ	2.20	0.69
8:H:113:SER:OG	8:H:126:GLN:NE2	2.26	0.69
17:Q:109:HIS:O	18:R:221:ARG:NH2	2.25	0.69
26:2:130:SER:O	26:2:133:THR:HG22	1.92	0.69
1:A:625:ASP:OD1	1:A:637:MET:HE3	1.92	0.69
1:A:625:ASP:H	1:A:637:MET:HB3	1.56	0.69
22:V:370:SER:OG	22:V:614:SER:OG	2.10	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:70:LEU:HD21	23:W:72:TYR:CZ	2.27	0.69
25:1:19:PHE:O	25:1:23:LEU:HG	1.92	0.69
27:3:34:LEU:O	27:3:34:LEU:HD13	1.92	0.69
5:E:27:LEU:H	5:E:64:HIS:HB3	1.51	0.69
26:2:31:LEU:CD1	27:3:33:THR:HG21	2.22	0.69
27:3:162:LEU:HA	27:3:192:ASP:OD1	1.92	0.69
27:3:178:MET:HE2	27:3:202:LEU:CD1	2.23	0.69
1:A:529:GLN:HE22	1:A:1097:GLU:HB3	1.55	0.69
2:B:360:LYS:HG3	2:B:553:LEU:HD23	1.74	0.69
2:B:427:LYS:HE3	20:T:164:GLU:HG2	1.74	0.69
2:B:634:LEU:HD23	2:B:661:VAL:HA	1.75	0.69
17:Q:113:ARG:CD	18:R:217:GLN:O	2.41	0.69
19:S:157:ALA:HA	19:S:161:GLU:HB2	1.75	0.69
23:W:189:TRP:HE1	23:W:194:LEU:HB2	1.56	0.69
26:2:211:GLN:HA	26:2:261:PHE:CE1	2.28	0.69
8:H:2:ALA:N	8:H:66:GLU:O	2.25	0.68
20:T:228:ILE:CA	28:X:30:DG:H5”	2.22	0.68
26:2:118:LEU:HD21	27:3:39:ASP:C	2.12	0.68
26:2:140:LYS:HD3	26:2:162:PHE:HE1	1.58	0.68
27:3:215:LEU:HD12	27:3:230:VAL:CG1	2.23	0.68
2:B:245:GLN:HE21	2:B:252:ILE:HD12	1.58	0.68
3:C:136:ASP:O	3:C:138:ASP:N	2.22	0.68
5:E:15:LYS:NZ	5:E:33:LEU:O	2.27	0.68
26:2:176:ALA:HB1	26:2:178:LEU:CD1	2.23	0.68
20:T:8:ASP:HB3	20:T:105:SER:HA	1.75	0.68
22:V:523:VAL:HG21	25:1:20:LEU:CG	2.22	0.68
1:A:1310:HIS:H	21:U:252:LYS:NZ	1.90	0.68
2:B:36:GLU:OE1	2:B:652:SER:OG	2.11	0.68
12:L:22:CYS:HB3	12:L:39:CYS:HB2	1.75	0.68
13:M:106:THR:HG22	13:M:109:SER:OG	1.92	0.68
22:V:451:PHE:CZ	28:X:57:DC:H5”	2.27	0.68
1:A:926:ASN:HD21	1:A:931:ARG:HD2	1.58	0.68
6:F:47:ALA:HB1	6:F:51:ARG:HE	1.58	0.68
26:2:163:MET:CE	26:2:206:LEU:HB3	2.23	0.68
27:3:114:GLU:O	27:3:118:LEU:HD23	1.92	0.68
1:A:844:ARG:NH2	2:B:500:GLN:O	2.26	0.68
10:J:3:ILE:HG21	10:J:18:TRP:HB2	1.74	0.68
14:N:375:GLU:OE1	15:O:59:ARG:NH2	2.26	0.68
17:Q:32:LEU:CD1	18:R:203:PHE:CE2	2.76	0.68
26:2:118:LEU:HD13	27:3:39:ASP:OD1	1.93	0.68
1:A:71:CYS:H	1:A:75:ALA:HA	1.59	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:420:ILE:N	1:A:445:LYS:O	2.24	0.68
1:A:601:ASN:HD21	1:A:632:ASN:H	1.42	0.68
17:Q:110:MET:CG	18:R:218:LYS:HD2	2.24	0.68
1:A:67:ARG:HH22	13:M:48:VAL:HG23	1.59	0.68
1:A:653:VAL:HG23	1:A:669:TYR:CE2	2.27	0.68
1:A:1287:CYS:HA	2:B:250:SER:CB	2.23	0.68
2:B:201:ALA:O	2:B:222:ARG:NH2	2.26	0.68
2:B:830:GLU:OE2	2:B:870:THR:OG1	2.11	0.68
8:H:111:ARG:NE	8:H:126:GLN:OE1	2.26	0.68
25:1:39:ASP:OD1	25:1:43:VAL:HB	1.94	0.68
25:1:59:GLU:OE2	26:2:402:ARG:CZ	2.42	0.68
26:2:199:ALA:HB3	26:2:202:GLN:NE2	2.02	0.68
2:B:87:LYS:HB3	2:B:129:THR:HB	1.76	0.68
2:B:93:LEU:CA	20:T:145:LEU:CD2	2.67	0.68
2:B:894:THR:HA	13:M:52:TRP:HH2	1.56	0.68
3:C:253:LYS:NZ	11:K:102:GLU:OE1	2.27	0.68
11:K:44:ASN:OD1	11:K:45:ILE:N	2.27	0.68
13:M:134:ILE:HG12	13:M:171:GLU:HG3	1.76	0.68
21:U:206:LEU:HD11	21:U:228:MET:HB3	1.76	0.68
27:3:130:GLU:HB2	27:3:173:GLN:NE2	2.09	0.68
27:3:159:SER:OG	27:3:189:ILE:HD12	1.94	0.68
1:A:826:SER:H	1:A:829:ALA:HB3	1.59	0.68
2:B:1106:ARG:HA	2:B:1110:ALA:HB3	1.76	0.68
12:L:17:TYR:CA	12:L:46:LYS:CA	2.64	0.68
26:2:56:VAL:O	26:2:60:LEU:HG	1.94	0.68
26:2:117:ASN:ND2	27:3:108:ASN:CA	2.57	0.68
27:3:66:GLU:CA	27:3:132:LEU:HD12	2.13	0.68
1:A:625:ASP:O	1:A:638:GLY:CA	2.41	0.67
5:E:170:LEU:HD23	5:E:208:LEU:HB2	1.76	0.67
16:P:163:PRO:HA	16:P:262:CYS:HB3	1.75	0.67
1:A:552:ASP:HB3	8:H:24:ARG:HD3	1.76	0.67
1:A:1310:HIS:CA	21:U:252:LYS:CE	2.70	0.67
7:G:93:ASN:OD1	7:G:94:LYS:N	2.26	0.67
7:G:99:THR:HG21	7:G:143:ILE:HD11	1.76	0.67
17:Q:113:ARG:HD3	18:R:221:ARG:HD3	1.75	0.67
2:B:483:ARG:NH2	2:B:527:ALA:O	2.27	0.67
7:G:153:ASP:O	7:G:155:ASN:N	2.27	0.67
9:I:105:GLU:O	9:I:107:ALA:CA	2.42	0.67
17:Q:106:LYS:CG	18:R:218:LYS:HE2	2.23	0.67
19:S:49:ARG:NH1	19:S:96:GLN:O	2.25	0.67
23:W:73:CYS:C	23:W:209:TYR:CE2	2.67	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:1:MET:CG	26:2:415:GLN:O	2.42	0.67
26:2:163:MET:HE2	26:2:206:LEU:HD12	1.76	0.67
27:3:111:ILE:O	27:3:115:ILE:HD13	1.94	0.67
1:A:22:GLN:HB3	2:B:1170:ARG:HG3	1.77	0.67
1:A:65:ILE:HD12	1:A:263:ALA:HB3	1.76	0.67
17:Q:106:LYS:HZ3	18:R:219:LEU:HD13	1.58	0.67
19:S:166:ARG:HH11	19:S:166:ARG:HG3	1.59	0.67
26:2:160:LEU:HD12	26:2:160:LEU:H	1.60	0.67
27:3:59:VAL:N	27:3:71:TYR:CD1	2.63	0.67
3:C:53:ASP:HB3	3:C:160:ARG:HB3	1.76	0.67
21:U:180:ILE:HG21	21:U:187:TYR:HB2	1.76	0.67
22:V:393:THR:HA	22:V:418:LYS:HE3	1.76	0.67
22:V:515:SER:HB3	22:V:539:ASN:ND2	2.04	0.67
10:J:63:ALA:H	10:J:64:PRO:HD2	1.60	0.67
26:2:118:LEU:HD11	27:3:43:VAL:HG23	1.75	0.67
26:2:211:GLN:HB3	26:2:261:PHE:HE1	1.59	0.67
1:A:874:LYS:HG3	1:A:880:ARG:HD2	1.77	0.67
9:I:99:SER:OG	9:I:105:GLU:HG3	1.84	0.67
14:N:353:LEU:N	14:N:370:ALA:O	2.17	0.67
18:R:195:PRO:HG2	18:R:199:LYS:N	2.08	0.67
21:U:218:ASP:O	21:U:222:ARG:HB2	1.95	0.67
25:1:1:MET:SD	26:2:419:GLU:HB2	2.34	0.67
27:3:137:LEU:HB3	27:3:180:VAL:CG1	2.20	0.67
1:A:1196:TYR:CD2	1:A:1246:ILE:HD11	2.29	0.67
2:B:63:PRO:HB3	2:B:408:PHE:HZ	1.59	0.67
8:H:17:PRO:HG3	8:H:27:ARG:H	1.58	0.67
25:1:34:ILE:CG1	25:1:50:VAL:HG11	2.21	0.67
26:2:198:SER:HG	26:2:238:PHE:HE2	1.42	0.67
13:M:10:LEU:C	13:M:12:ARG:H	1.99	0.67
18:R:224:THR:HG23	18:R:230:GLU:HB2	1.75	0.67
26:2:170:ALA:HB1	26:2:213:TRP:CZ3	2.29	0.67
26:2:251:VAL:HG11	26:2:254:MET:HG3	1.77	0.67
2:B:892:CYS:HA	13:M:52:TRP:HE1	1.58	0.67
26:2:44:VAL:HG13	26:2:45:PHE:HD1	1.59	0.67
27:3:148:ASN:CB	27:3:157:MET:HE2	2.24	0.67
27:3:217:VAL:HG13	27:3:226:TYR:CE2	2.30	0.67
2:B:501:LEU:HD11	2:B:505:LEU:HD22	1.77	0.66
20:T:145:LEU:HD13	20:T:148:VAL:HG22	1.75	0.66
1:A:43:TYR:HD1	1:A:45:GLU:HG2	1.59	0.66
1:A:418:TYR:O	1:A:447:GLU:N	2.28	0.66
20:T:154:LYS:HD2	20:T:154:LYS:N	2.08	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:516:PRO:CB	22:V:706:LYS:NZ	2.51	0.66
22:V:516:PRO:CD	22:V:706:LYS:NZ	2.55	0.66
22:V:519:TYR:CE2	25:1:20:LEU:CG	2.73	0.66
23:W:52:LEU:HD23	23:W:72:TYR:CZ	2.29	0.66
1:A:642:LYS:HD3	21:U:284:PRO:HD3	1.77	0.66
1:A:1323:THR:HG23	1:A:1325:ASP:H	1.59	0.66
3:C:50:VAL:HB	12:L:55:PHE:HB2	1.77	0.66
10:J:21:TYR:HB2	10:J:38:LEU:HD11	1.77	0.66
12:L:25:GLU:CG	12:L:27:GLU:CD	2.61	0.66
14:N:46:TRP:HZ2	15:O:11:LEU:HD12	1.60	0.66
14:N:318:ASP:HB2	16:P:239:ARG:HH21	1.59	0.66
16:P:309:LYS:HD2	29:Y:82:DT:H3'	1.78	0.66
27:3:18:ASN:CG	27:3:20:ILE:HD13	2.15	0.66
27:3:187:GLN:CG	27:3:189:ILE:HG12	2.24	0.66
2:B:842:HIS:HE1	13:M:27:TYR:HB3	1.61	0.66
27:3:130:GLU:HB2	27:3:173:GLN:HE22	1.61	0.66
27:3:184:ALA:CA	27:3:187:GLN:HG2	2.25	0.66
1:A:885:GLN:NE2	5:E:168:ASN:OD1	2.22	0.66
11:K:18:LYS:O	11:K:36:ASN:N	2.23	0.66
26:2:189:GLU:HA	26:2:192:GLU:CG	2.26	0.66
2:B:1029:TYR:OH	3:C:185:GLU:OE1	2.13	0.66
5:E:52:ARG:CB	5:E:53:PRO:CD	2.73	0.66
12:L:34:ILE:HG13	12:L:42:ARG:HD2	1.78	0.66
23:W:209:TYR:HH	23:W:233:PHE:CA	1.94	0.66
23:W:293:ARG:HG2	23:W:421:PHE:CZ	2.30	0.66
26:2:126:GLY:C	26:2:178:LEU:HD23	2.16	0.66
2:B:848:LEU:HD21	2:B:868:GLY:HA3	1.77	0.66
3:C:67:ARG:NH1	3:C:150:ILE:O	2.28	0.66
16:P:179:ASP:OD1	16:P:181:LYS:NZ	2.29	0.66
16:P:293:TYR:HD2	16:P:302:LEU:HD13	1.61	0.66
26:2:56:VAL:HG11	26:2:91:SER:HB2	1.77	0.66
27:3:45:GLY:O	27:3:49:LEU:HD23	1.96	0.66
18:R:191:PHE:CB	18:R:202:PHE:CD1	2.78	0.66
27:3:207:CYS:SG	27:3:214:TYR:HB2	2.34	0.66
28:X:52:DG:N2	29:Y:43:DG:C2	2.64	0.66
1:A:361:PHE:H	2:B:1063:ALA:HA	1.61	0.66
9:I:84:HIS:H	9:I:84:HIS:CD2	2.13	0.66
13:M:124:MET:HA	13:M:127:ARG:NH2	2.11	0.66
23:W:432:ILE:CD1	23:W:434:HIS:HE1	2.09	0.66
27:3:178:MET:HE2	27:3:202:LEU:HD12	1.78	0.66
1:A:782:SER:O	1:A:787:VAL:N	2.29	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:99:VAL:HG13	3:C:124:SER:HB2	1.77	0.66
9:I:86:CYS:C	9:I:88:LYS:N	2.48	0.66
20:T:174:LYS:CB	28:X:20:DG:H4'	2.26	0.66
27:3:144:ILE:O	27:3:147:MET:HG3	1.96	0.66
3:C:200:PRO:CG	3:C:217:GLN:CB	2.74	0.65
18:R:191:PHE:CB	18:R:202:PHE:CE1	2.79	0.65
1:A:1112:VAL:O	21:U:252:LYS:CG	2.44	0.65
2:B:935:PHE:HE2	2:B:945:CYS:HB2	1.62	0.65
20:T:164:GLU:OE2	20:T:167:ARG:NH2	2.29	0.65
26:2:218:GLN:CG	26:2:268:PHE:HB3	2.26	0.65
1:A:784:VAL:HG23	1:A:785:ILE:HG13	1.78	0.65
17:Q:105:TYR:CE1	18:R:234:GLU:CG	2.78	0.65
22:V:631:GLY:O	22:V:632:SER:HB3	1.95	0.65
25:1:8:VAL:HG12	25:1:9:LEU:N	2.10	0.65
26:2:172:SER:O	26:2:175:LEU:HD23	1.95	0.65
26:2:236:PHE:CZ	26:2:262:LEU:HD22	2.32	0.65
27:3:14:VAL:HG22	27:3:163:VAL:HA	1.78	0.65
1:A:73:THR:OG1	2:B:1130:THR:OG1	2.15	0.65
17:Q:187:ILE:O	18:R:212:VAL:HA	1.97	0.65
22:V:531:ILE:CA	22:V:534:TYR:HE2	1.89	0.65
25:1:10:ILE:HG21	26:2:407:VAL:HG21	1.77	0.65
25:1:35:ILE:HG22	25:1:46:ILE:HD12	1.78	0.65
1:A:1172:ASN:O	1:A:1215:GLU:N	2.19	0.65
2:B:93:LEU:C	20:T:145:LEU:HD23	2.17	0.65
26:2:57:MET:HA	26:2:60:LEU:HD11	1.76	0.65
26:2:171:VAL:HG13	26:2:216:MET:CB	2.26	0.65
26:2:218:GLN:CD	26:2:265:LEU:HA	2.17	0.65
1:A:434:LYS:HB2	1:A:437:ASP:HB3	1.79	0.65
1:A:604:ARG:O	1:A:606:HIS:N	2.28	0.65
1:A:1146:GLN:O	1:A:1150:ASP:N	2.27	0.65
5:E:65:ASN:O	5:E:67:ASP:CA	2.43	0.65
23:W:584:TYR:CZ	23:W:614:TYR:HB2	2.32	0.65
24:0:98:GLN:OE1	27:3:209:ILE:HA	1.96	0.65
1:A:113:PHE:CE1	18:R:229:ASP:N	2.62	0.65
1:A:611:ASP:OD2	1:A:617:PRO:CB	2.45	0.65
3:C:214:ASP:OD2	3:C:216:SER:OG	2.12	0.65
22:V:412:MET:HA	22:V:417:THR:HG21	1.77	0.65
24:0:54:ARG:CD	27:3:182:PHE:CE1	2.60	0.65
27:3:131:THR:O	27:3:133:LEU:HD13	1.97	0.65
27:3:146:ARG:O	27:3:149:LYS:HG2	1.95	0.65
1:A:275:ASP:HB2	1:A:342:ARG:NH2	2.10	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:65:ILE:HG21	2:B:412:LEU:HD11	1.76	0.65
22:V:520:ARG:HG3	25:1:23:LEU:HD11	1.79	0.65
26:2:159:VAL:HG11	26:2:161:HIS:HD2	1.62	0.65
26:2:163:MET:HE3	26:2:206:LEU:HD12	1.78	0.65
26:2:181:GLN:HG3	26:2:229:ASP:CG	2.18	0.65
26:2:266:ARG:O	26:2:270:LEU:HB2	1.97	0.65
27:3:70:LEU:CD1	27:3:115:ILE:HD11	2.27	0.65
2:B:93:LEU:HD12	2:B:123:PRO:O	1.97	0.65
5:E:62:VAL:HG23	5:E:72:MET:CB	2.22	0.65
26:2:45:PHE:HB2	26:2:51:LEU:CD1	2.26	0.65
1:A:1290:SER:HB3	2:B:250:SER:O	1.97	0.64
2:B:102:ASP:O	13:M:217:ARG:NE	2.27	0.64
22:V:522:TYR:HE2	25:1:62:ASP:CG	1.96	0.64
26:2:81:LYS:HE3	26:2:93:LEU:CD2	2.20	0.64
27:3:106:SER:O	27:3:110:VAL:HG23	1.97	0.64
7:G:91:GLN:HB2	7:G:98:PHE:HD2	1.62	0.64
11:K:77:THR:OG1	11:K:81:TYR:O	2.14	0.64
27:3:33:THR:CG2	27:3:36:LYS:HB2	2.26	0.64
27:3:187:GLN:HG3	27:3:189:ILE:CG1	2.24	0.64
1:A:612:ASP:O	1:A:613:GLU:C	2.33	0.64
1:A:1310:HIS:HE1	1:A:1334:TRP:HA	1.61	0.64
23:W:581:LEU:HD21	23:W:608:ILE:HG21	1.78	0.64
26:2:270:LEU:HD23	26:2:273:GLN:HE21	1.62	0.64
1:A:370:ASP:HB2	1:A:483:ARG:HB3	1.80	0.64
1:A:1244:ASN:HB3	1:A:1260:ARG:HB2	1.79	0.64
2:B:874:PRO:O	2:B:876:ASN:N	2.27	0.64
25:1:35:ILE:HG22	25:1:46:ILE:CD1	2.27	0.64
26:2:270:LEU:HD23	26:2:270:LEU:O	1.97	0.64
27:3:192:ASP:HB2	27:3:231:PHE:CE1	2.32	0.64
1:A:425:ASP:HB3	13:M:39:LEU:CG	2.28	0.64
2:B:714:PRO:HD2	2:B:1001:PRO:HB3	1.77	0.64
3:C:13:GLU:O	3:C:20:LYS:N	2.30	0.64
26:2:202:GLN:HE21	26:2:202:GLN:H	1.44	0.64
11:K:29:ASN:ND2	11:K:78:THR:O	2.30	0.64
18:R:140:LYS:HG2	18:R:141:PRO:HD3	1.78	0.64
23:W:696:TRP:HD1	23:W:697:ILE:HG13	1.62	0.64
27:3:17:ALA:CB	27:3:63:HIS:HD2	2.10	0.64
1:A:621:ILE:HG22	1:A:623:PRO:CD	2.28	0.64
1:A:1250:ASP:HA	1:A:1255:LEU:HD21	1.78	0.64
3:C:258:ASP:OD2	11:K:18:LYS:NZ	2.31	0.64
18:R:195:PRO:HB3	18:R:199:LYS:CD	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:59:TYR:CE1	23:W:62:ALA:HB2	2.26	0.64
1:A:1253:GLU:HG2	1:A:1254:LYS:HG2	1.79	0.64
17:Q:102:VAL:O	17:Q:105:TYR:N	2.31	0.64
18:R:161:ARG:NE	18:R:203:PHE:CE1	2.60	0.64
19:S:126:ILE:N	19:S:138:PHE:O	2.23	0.64
22:V:516:PRO:HD2	22:V:706:LYS:HZ3	1.61	0.64
27:3:160:ARG:NH2	27:3:190:LEU:HD12	2.13	0.64
2:B:92:TYR:CB	20:T:145:LEU:HB3	2.26	0.64
2:B:1107:LEU:O	2:B:1111:SER:OG	2.15	0.64
18:R:129:LYS:CB	18:R:140:LYS:CB	2.69	0.64
22:V:426:VAL:HG13	22:V:427:MET:H	1.63	0.64
26:2:117:ASN:CG	27:3:108:ASN:ND2	2.50	0.64
26:2:140:LYS:HG2	26:2:162:PHE:CE1	2.33	0.64
27:3:165:LYS:O	27:3:165:LYS:HD3	1.98	0.64
1:A:1036:ASN:HB2	5:E:202:ARG:HB3	1.78	0.64
1:A:1288:ILE:O	1:A:1292:MET:N	2.27	0.64
2:B:646:ARG:HD3	2:B:651:TYR:N	2.13	0.64
9:I:64:GLU:CD	9:I:103:ARG:HH21	2.01	0.64
20:T:158:ASN:HB3	20:T:161:TYR:HB3	1.80	0.64
26:2:258:LEU:HG	26:2:262:LEU:CD2	2.28	0.64
27:3:214:TYR:CE2	27:3:216:LYS:HE2	2.32	0.64
8:H:10:PHE:N	8:H:56:PHE:O	2.28	0.63
12:L:16:ILE:HD11	12:L:28:ILE:C	2.17	0.63
17:Q:187:ILE:CB	18:R:212:VAL:H	2.09	0.63
1:A:629:VAL:HG13	1:A:636:ILE:HB	1.81	0.63
17:Q:17:LEU:HD13	17:Q:194:THR:HB	1.80	0.63
17:Q:106:LYS:HG2	18:R:218:LYS:CE	2.27	0.63
27:3:59:VAL:HB	27:3:71:TYR:CD1	2.25	0.63
27:3:64:ILE:HB	27:3:123:ASP:OD2	1.98	0.63
12:L:25:GLU:HB2	12:L:27:GLU:CG	2.25	0.63
12:L:26:ASN:HA	12:L:37:ARG:HH12	1.63	0.63
18:R:155:LEU:CB	18:R:204:ASN:ND2	2.59	0.63
20:T:174:LYS:HE3	28:X:20:DG:H1'	1.80	0.63
25:1:38:ILE:HB	25:1:44:PHE:HE1	1.63	0.63
27:3:133:LEU:HD22	27:3:134:ALA:N	2.14	0.63
2:B:692:THR:HB	9:I:76:PRO:HB2	1.79	0.63
2:B:829:PHE:HE1	2:B:869:LYS:HD3	1.63	0.63
26:2:30:VAL:CG1	27:3:25:GLN:CA	2.72	0.63
27:3:59:VAL:CB	27:3:71:TYR:HE1	1.94	0.63
1:A:514:GLU:OE2	2:B:1101:GLN:HB2	1.99	0.63
2:B:840:MET:O	2:B:842:HIS:N	2.31	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:956:PHE:O	2:B:1029:TYR:N	2.23	0.63
23:W:419:GLU:HB3	23:W:420:PRO:CD	2.29	0.63
25:1:5:LEU:HD21	26:2:408:LEU:HD13	0.85	0.63
26:2:123:LEU:O	26:2:123:LEU:HD23	1.99	0.63
26:2:220:LEU:O	26:2:220:LEU:HD13	1.98	0.63
27:3:18:ASN:CG	27:3:64:ILE:HD11	2.19	0.63
2:B:1087:GLY:N	2:B:1090:GLU:OE1	2.28	0.63
14:N:333:ASN:HB3	14:N:359:ASN:O	1.99	0.63
26:2:173:GLN:HG2	26:2:179:LEU:HG	1.81	0.63
26:2:177:GLN:OE1	26:2:220:LEU:HD22	1.98	0.63
26:2:211:GLN:CB	26:2:261:PHE:HE1	2.11	0.63
27:3:190:LEU:H	27:3:190:LEU:CD2	2.11	0.63
22:V:516:PRO:HB2	22:V:706:LYS:NZ	2.10	0.63
1:A:485:ASN:HB3	1:A:488:VAL:HG23	1.79	0.63
1:A:497:ASP:HB2	2:B:942:LYS:HE3	1.80	0.63
17:Q:21:VAL:HA	18:R:210:PHE:HE2	1.64	0.63
17:Q:25:PHE:HD2	18:R:215:GLU:OE2	1.80	0.63
22:V:315:VAL:HG12	23:W:500:ASP:CB	2.17	0.63
26:2:31:LEU:CG	27:3:33:THR:HB	2.28	0.63
26:2:89:LEU:HD23	26:2:89:LEU:O	1.99	0.63
26:2:117:ASN:HD22	27:3:42:MET:HE1	1.61	0.63
27:3:147:MET:HE3	27:3:157:MET:SD	2.39	0.63
27:3:149:LYS:HG3	27:3:150:GLU:N	2.12	0.63
27:3:196:LEU:CD2	27:3:223:LEU:HD23	2.25	0.63
1:A:1208:SER:O	1:A:1260:ARG:NH1	2.31	0.63
2:B:242:ARG:O	2:B:244:GLY:N	2.31	0.63
2:B:765:GLU:O	2:B:768:ARG:NH1	2.31	0.63
13:M:297:PRO:HA	13:M:310:VAL:HG11	1.81	0.63
14:N:368:SER:N	15:O:54:ASN:O	2.25	0.63
21:U:256:THR:O	21:U:257:GLN:C	2.38	0.63
26:2:60:LEU:HD11	26:2:95:ILE:CB	2.29	0.63
1:A:191:ILE:HD12	1:A:216:LEU:HD11	1.81	0.62
9:I:92:LYS:NZ	9:I:93:GLU:OE2	2.32	0.62
25:1:18:GLN:NE2	25:1:44:PHE:HZ	1.96	0.62
25:1:47:ALA:HB1	25:1:50:VAL:HB	1.81	0.62
27:3:58:ALA:CA	27:3:71:TYR:OH	2.41	0.62
2:B:513:GLU:O	2:B:525:ASN:ND2	2.32	0.62
3:C:129:PRO:HG2	3:C:134:ASN:HD22	1.63	0.62
10:J:40:LEU:O	10:J:46:ARG:NE	2.32	0.62
22:V:316:LEU:HB2	22:V:321:GLU:CG	2.29	0.62
27:3:184:ALA:HA	27:3:187:GLN:CG	2.29	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:427:ILE:CD1	13:M:38:GLY:O	2.46	0.62
2:B:79:GLU:C	2:B:80:GLU:HG2	2.20	0.62
2:B:779:ILE:HA	2:B:1045:PRO:HA	1.80	0.62
22:V:451:PHE:CE2	28:X:57:DC:H5"	2.34	0.62
26:2:46:ARG:CD	26:2:85:GLU:HB2	2.30	0.62
3:C:35:ARG:HA	3:C:38:PHE:CD2	2.35	0.62
10:J:63:ALA:H	10:J:64:PRO:CD	2.12	0.62
18:R:210:PHE:HD1	18:R:210:PHE:O	1.82	0.62
25:1:1:MET:HB3	26:2:413:LEU:HG	1.81	0.62
25:1:38:ILE:HB	25:1:44:PHE:CE1	2.35	0.62
26:2:35:TYR:CZ	26:2:62:LEU:HG	2.34	0.62
1:A:43:TYR:CD1	1:A:45:GLU:HG2	2.34	0.62
1:A:1451:MET:HE1	1:A:1460:LEU:HD22	1.81	0.62
2:B:831:LYS:NZ	2:B:845:TYR:O	2.27	0.62
3:C:47:ILE:HG21	3:C:68:LEU:HD23	1.80	0.62
13:M:173:VAL:HB	13:M:175:ARG:HH12	1.63	0.62
17:Q:113:ARG:HE	18:R:217:GLN:HB3	1.64	0.62
25:1:4:VAL:CG1	26:2:411:GLN:O	2.40	0.62
25:1:35:ILE:HA	25:1:46:ILE:HG13	1.80	0.62
1:A:934:LEU:O	1:A:936:GLU:N	2.30	0.62
1:A:1313:GLN:OE1	1:A:1335:ILE:HD13	1.99	0.62
2:B:838:GLN:OE1	2:B:886:ARG:NH1	2.33	0.62
12:L:25:GLU:CB	12:L:27:GLU:HG3	2.26	0.62
22:V:517:GLU:HB2	22:V:713:LEU:HD22	1.79	0.62
23:W:584:TYR:CG	23:W:594:ALA:HB2	2.34	0.62
27:3:17:ALA:HB1	27:3:63:HIS:HD2	1.63	0.62
1:A:1080:ILE:HD13	6:F:54:THR:HG21	1.82	0.62
1:A:1290:SER:CB	2:B:250:SER:O	2.48	0.62
1:A:1307:VAL:O	1:A:1308:TYR:CD2	2.52	0.62
2:B:87:LYS:O	2:B:129:THR:N	2.23	0.62
2:B:322:GLY:HA3	2:B:335:ARG:HB3	1.81	0.62
3:C:110:ASP:HA	3:C:155:LYS:HD2	1.82	0.62
17:Q:22:ILE:HG22	17:Q:34:LEU:HD13	1.81	0.62
22:V:667:THR:HA	25:1:62:ASP:CG	2.19	0.62
26:2:117:ASN:ND2	27:3:42:MET:CE	2.60	0.62
1:A:939:VAL:HA	1:A:942:VAL:HG22	1.81	0.62
18:R:195:PRO:HB3	18:R:199:LYS:HD2	1.82	0.62
25:1:17:LYS:O	25:1:20:LEU:HB3	1.99	0.62
27:3:70:LEU:HD13	27:3:115:ILE:CD1	2.28	0.62
2:B:808:SER:OG	2:B:1050:ARG:NH1	2.33	0.62
5:E:107:GLN:HG2	5:E:132:GLN:NE2	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:9:ILE:O	8:H:33:GLU:HG2	1.99	0.62
9:I:95:VAL:N	9:I:113:VAL:O	2.24	0.62
13:M:107:MET:HB2	13:M:112:ARG:HH12	1.65	0.62
20:T:31:TRP:HD1	20:T:62:LEU:HD21	1.64	0.62
25:1:1:MET:HA	26:2:413:LEU:HA	1.80	0.62
25:1:13:ASP:OD1	25:1:14:PRO:HD2	2.00	0.62
1:A:948:ILE:HG13	1:A:1007:ILE:HD11	1.81	0.62
1:A:1204:VAL:HA	1:A:1207:ILE:HG23	1.81	0.62
2:B:194:LEU:HD11	2:B:466:VAL:HG12	1.81	0.62
2:B:226:GLU:OE1	2:B:227:ASN:ND2	2.33	0.62
2:B:801:VAL:HA	2:B:805:PHE:HB3	1.81	0.62
3:C:56:SER:OG	3:C:158:GLU:N	2.33	0.62
3:C:154:ARG:NE	10:J:65:LEU:HD12	2.15	0.62
5:E:149:VAL:HB	5:E:192:LYS:HB3	1.80	0.62
6:F:78:PRO:HD3	7:G:16:ARG:HA	1.82	0.62
14:N:344:ARG:NH2	29:Y:78:DT:OP1	2.23	0.62
25:1:10:ILE:HG22	26:2:407:VAL:HG21	1.80	0.62
26:2:163:MET:HE1	26:2:206:LEU:HB3	1.80	0.62
1:A:931:ARG:O	1:A:933:THR:N	2.32	0.61
1:A:1307:VAL:HG13	1:A:1338:THR:HA	1.82	0.61
14:N:34:VAL:HG11	15:O:28:ILE:HG22	1.82	0.61
17:Q:23:ARG:CZ	18:R:207:SER:H	2.13	0.61
17:Q:110:MET:CA	18:R:218:LYS:HG3	2.29	0.61
27:3:9:ASN:O	27:3:56:LYS:HD3	1.99	0.61
23:W:250:ASN:CB	23:W:434:HIS:CG	2.82	0.61
26:2:189:GLU:O	26:2:193:PRO:HD2	2.00	0.61
26:2:218:GLN:HG2	26:2:268:PHE:HB3	1.82	0.61
1:A:85:PHE:CD1	1:A:257:PRO:HD3	2.35	0.61
2:B:50:PHE:HA	2:B:54:SER:HB2	1.82	0.61
2:B:131:THR:O	2:B:132:VAL:HG12	1.99	0.61
3:C:1:MET:HG3	3:C:2:PRO:HD2	1.82	0.61
26:2:117:ASN:CG	27:3:42:MET:HE2	2.20	0.61
26:2:160:LEU:HB3	26:2:206:LEU:CD1	2.27	0.61
7:G:58:VAL:HB	7:G:67:LEU:HB3	1.82	0.61
9:I:87:GLN:HE21	9:I:121:HIS:HB3	1.65	0.61
14:N:314:LEU:HD11	16:P:238:ALA:HB1	1.82	0.61
17:Q:187:ILE:O	18:R:212:VAL:CA	2.47	0.61
1:A:208:ASP:OD2	1:A:212:LYS:NZ	2.33	0.61
1:A:1147:SER:OG	1:A:1351:ASP:OD2	2.15	0.61
2:B:788:TYR:HB2	2:B:795:ILE:HD11	1.81	0.61
6:F:100:ARG:HB2	6:F:120:VAL:HG12	1.83	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:96:VAL:HB	8:H:136:GLU:HA	1.83	0.61
15:O:59:ARG:O	15:O:80:GLU:N	2.32	0.61
25:1:1:MET:HG2	26:2:414:SER:N	2.16	0.61
26:2:31:LEU:HG	27:3:25:GLN:O	2.00	0.61
26:2:83:GLN:OE1	26:2:83:GLN:HA	2.01	0.61
27:3:16:ASP:O	27:3:21:TRP:NE1	2.27	0.61
27:3:134:ALA:HB2	27:3:176:ASN:OD1	1.99	0.61
1:A:551:ARG:NH1	1:A:637:MET:HE1	2.15	0.61
1:A:784:VAL:HA	1:A:827:TYR:HB2	1.83	0.61
10:J:63:ALA:N	10:J:64:PRO:HD2	2.15	0.61
16:P:161:ILE:O	16:P:161:ILE:HG22	1.99	0.61
16:P:192:TYR:HB2	16:P:200:VAL:HG22	1.83	0.61
27:3:8:LEU:HA	27:3:54:SER:HB3	1.83	0.61
27:3:18:ASN:O	27:3:21:TRP:HD1	1.83	0.61
1:A:475:ARG:NH2	11:K:68:GLU:OE2	2.26	0.61
1:A:637:MET:HG3	8:H:122:LEU:HD21	1.83	0.61
9:I:86:CYS:O	9:I:87:GLN:C	2.39	0.61
20:T:20:LEU:O	20:T:114:ALA:N	2.34	0.61
22:V:611:GLY:O	22:V:615:PHE:HB3	2.01	0.61
1:A:275:ASP:HA	1:A:278:HIS:ND1	2.16	0.61
1:A:1290:SER:OG	2:B:250:SER:O	2.19	0.61
2:B:713:PHE:HB3	2:B:716:HIS:ND1	2.15	0.61
8:H:65:TYR:CD2	8:H:70:LEU:CD2	2.84	0.61
16:P:167:ASN:HB2	29:Y:80:DT:C4'	2.30	0.61
18:R:142:LYS:HE2	18:R:144:ASN:HB3	1.83	0.61
26:2:60:LEU:CD1	26:2:95:ILE:HB	2.31	0.61
26:2:93:LEU:HA	26:2:96:TRP:HD1	1.64	0.61
27:3:64:ILE:CG1	27:3:123:ASP:HB3	2.29	0.61
1:A:72:GLN:HE22	1:A:84:HIS:CD2	2.19	0.61
1:A:935:GLN:HA	1:A:1001:PRO:HA	1.81	0.61
5:E:104:ILE:O	5:E:129:GLN:NE2	2.33	0.61
8:H:66:GLU:O	8:H:67:ASP:HB2	1.99	0.61
23:W:37:HIS:ND1	23:W:454:VAL:HG13	2.15	0.61
1:A:693:ILE:HG13	2:B:1023:ARG:HE	1.63	0.61
1:A:1347:LEU:HB3	5:E:137:ILE:HG12	1.83	0.61
2:B:67:LEU:HD22	2:B:419:ALA:HB1	1.83	0.61
8:H:105:SER:O	8:H:106:THR:CB	2.48	0.61
12:L:15:MET:HG3	12:L:47:LYS:HB2	1.83	0.61
13:M:279:GLY:HA2	20:T:153:TYR:CE1	2.35	0.61
18:R:195:PRO:HG3	18:R:199:LYS:CA	2.28	0.61
26:2:173:GLN:CD	26:2:179:LEU:HD21	2.22	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:181:GLN:CD	26:2:229:ASP:HB2	2.19	0.61
2:B:242:ARG:HB3	2:B:252:ILE:CG2	2.30	0.60
2:B:405:ARG:O	2:B:409:LYS:HG3	2.01	0.60
14:N:341:LYS:HB3	14:N:352:HIS:HB2	1.80	0.60
23:W:209:TYR:CE1	23:W:233:PHE:CD1	2.89	0.60
27:3:24:LYS:HE2	27:3:220:MET:SD	2.41	0.60
28:X:17:DA:H2"	28:X:18:DG:C8	2.36	0.60
1:A:18:ILE:HG21	2:B:1171:MET:HG3	1.83	0.60
1:A:731:ASN:CG	21:U:253:THR:CG2	2.41	0.60
2:B:37:LYS:HE2	2:B:653:TRP:CD1	2.36	0.60
17:Q:25:PHE:HE2	18:R:215:GLU:HG3	1.61	0.60
25:1:50:VAL:HA	25:1:53:LEU:HD13	1.82	0.60
26:2:100:LEU:HG	26:2:119:ARG:NE	2.13	0.60
27:3:58:ALA:CA	27:3:71:TYR:CE2	2.80	0.60
27:3:100:LYS:HG3	27:3:101:TYR:N	2.16	0.60
1:A:1143:LEU:HB3	1:A:1147:SER:HB2	1.83	0.60
2:B:85:LEU:H	2:B:132:VAL:HG12	1.64	0.60
17:Q:106:LYS:C	18:R:218:LYS:HE2	2.20	0.60
23:W:423:ASP:O	23:W:425:THR:N	2.34	0.60
24:0:55:LEU:HD12	27:3:178:MET:CE	2.31	0.60
26:2:164:VAL:HG13	26:2:209:PRO:HG2	1.83	0.60
26:2:202:GLN:NE2	26:2:202:GLN:H	2.00	0.60
1:A:426:ARG:O	13:M:40:VAL:N	2.34	0.60
2:B:225:LEU:HD13	2:B:228:SER:HB2	1.83	0.60
2:B:568:PHE:O	2:B:614:ILE:N	2.34	0.60
8:H:31:GLU:HA	8:H:38:ASP:HA	1.82	0.60
18:R:195:PRO:HG3	18:R:199:LYS:O	2.00	0.60
20:T:138:PRO:O	20:T:140:ARG:N	2.34	0.60
20:T:224:ASN:HB3	20:T:226:LYS:HG2	1.82	0.60
23:W:37:HIS:CE1	23:W:454:VAL:CG1	2.82	0.60
23:W:423:ASP:C	23:W:425:THR:H	2.04	0.60
23:W:584:TYR:HB2	23:W:594:ALA:HB2	1.81	0.60
26:2:30:VAL:HG22	26:2:34:LEU:CD2	2.31	0.60
2:B:737:ILE:HD11	2:B:743:ARG:HG3	1.83	0.60
4:D:103:LEU:HD22	7:G:144:ARG:HH12	1.65	0.60
26:2:171:VAL:HG13	26:2:216:MET:HB2	1.83	0.60
1:A:1248:ASN:ND2	1:A:1254:LYS:O	2.28	0.60
2:B:75:SER:O	2:B:78:VAL:HG22	2.00	0.60
2:B:257:VAL:HG23	2:B:257:VAL:O	2.00	0.60
2:B:873:LEU:HB3	2:B:874:PRO:HD3	1.79	0.60
6:F:96:GLU:O	6:F:100:ARG:N	2.34	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
9:I:22:ASN:OD1	9:I:41:ASN:ND2	2.35	0.60
13:M:106:THR:CG2	13:M:109:SER:OG	2.49	0.60
16:P:297:LYS:CB	16:P:298:PRO:HD2	2.22	0.60
20:T:228:ILE:HD12	20:T:230:LYS:HD3	1.83	0.60
22:V:368:ALA:O	22:V:371:VAL:HG22	2.00	0.60
23:W:59:TYR:OH	23:W:63:TYR:CE2	2.52	0.60
25:1:8:VAL:O	26:2:407:VAL:HG12	2.00	0.60
26:2:236:PHE:CE2	26:2:262:LEU:HD13	2.36	0.60
4:D:108:ALA:N	4:D:128:GLN:OE1	2.32	0.60
7:G:11:ILE:O	7:G:68:TYR:N	2.25	0.60
8:H:98:ARG:HD3	8:H:115:TYR:HD2	1.66	0.60
12:L:22:CYS:SG	12:L:24:THR:OG1	2.56	0.60
15:O:86:GLU:HG3	15:O:88:ILE:HD11	1.82	0.60
18:R:195:PRO:CB	18:R:199:LYS:HD2	2.31	0.60
19:S:47:LEU:HD22	20:T:7:LEU:HD22	1.84	0.60
1:A:628:VAL:HA	1:A:638:GLY:HA3	1.84	0.60
1:A:1274:GLU:O	1:A:1275:VAL:C	2.40	0.60
1:A:1313:GLN:HB2	1:A:1333:GLU:CG	2.31	0.60
2:B:117:ASN:HA	2:B:189:GLY:HA3	1.84	0.60
2:B:655:ASP:O	2:B:659:SER:N	2.35	0.60
3:C:154:ARG:HD3	10:J:65:LEU:HD13	1.71	0.60
13:M:178:LYS:C	20:T:154:LYS:HB2	2.21	0.60
14:N:308:GLN:NE2	14:N:310:GLU:O	2.28	0.60
18:R:155:LEU:HG	18:R:204:ASN:HD22	0.77	0.60
20:T:155:PRO:O	20:T:157:ALA:N	2.27	0.60
23:W:410:TYR:HE2	23:W:413:GLY:HA3	1.65	0.60
25:1:1:MET:HB2	26:2:418:PHE:HB3	1.84	0.60
26:2:44:VAL:HG13	26:2:45:PHE:N	2.17	0.60
1:A:611:ASP:CB	1:A:617:PRO:HG3	2.32	0.60
2:B:600:GLU:O	2:B:620:ARG:NH2	2.30	0.60
20:T:138:PRO:C	20:T:140:ARG:H	2.05	0.60
23:W:73:CYS:CB	23:W:209:TYR:CZ	2.84	0.60
1:A:1028:PRO:O	1:A:1032:GLN:N	2.34	0.59
2:B:242:ARG:C	2:B:244:GLY:H	2.06	0.59
5:E:63:ALA:O	5:E:64:HIS:CG	2.54	0.59
1:A:1212:LEU:HD23	1:A:1259:ILE:HD11	1.83	0.59
2:B:56:GLN:O	2:B:60:GLU:N	2.30	0.59
3:C:183:ALA:HB3	3:C:232:ASN:HB3	1.84	0.59
11:K:20:THR:N	11:K:34:THR:O	2.28	0.59
25:1:1:MET:HA	26:2:414:SER:N	2.14	0.59
26:2:217:LEU:HD23	26:2:233:ILE:CD1	2.32	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1394:ASN:HB3	1:A:1397:HIS:ND1	2.17	0.59
3:C:146:ASP:O	3:C:148:ILE:N	2.36	0.59
3:C:154:ARG:HD3	10:J:65:LEU:HB2	1.82	0.59
4:D:26:PHE:HZ	7:G:42:TYR:HA	1.66	0.59
8:H:14:ASP:HB3	8:H:29:HIS:HB2	1.85	0.59
18:R:129:LYS:HB2	18:R:140:LYS:HB2	1.75	0.59
20:T:20:LEU:N	20:T:112:GLN:O	2.28	0.59
26:2:203:PHE:HD2	26:2:205:LEU:HD23	1.64	0.59
9:I:86:CYS:SG	9:I:119:CYS:SG	3.00	0.59
19:S:102:VAL:O	19:S:108:ARG:N	2.35	0.59
25:1:59:GLU:CD	26:2:402:ARG:NH1	2.56	0.59
27:3:143:TYR:O	27:3:146:ARG:HG2	2.01	0.59
1:A:612:ASP:O	1:A:614:ASP:CA	2.50	0.59
3:C:106:ARG:NE	3:C:108:ASN:OD1	2.35	0.59
3:C:211:LEU:C	3:C:213:GLU:N	2.52	0.59
6:F:51:ARG:NH1	6:F:122:GLU:OE1	2.34	0.59
20:T:222:VAL:HG22	20:T:223:GLN:H	1.67	0.59
26:2:42:LEU:CD2	26:2:55:TRP:HB2	2.13	0.59
26:2:196:ILE:HA	26:2:202:GLN:OE1	2.02	0.59
26:2:215:PHE:CD2	26:2:264:HIS:HB2	2.38	0.59
27:3:131:THR:HG23	27:3:133:LEU:CD1	2.33	0.59
27:3:213:LEU:HD23	27:3:230:VAL:HG12	1.84	0.59
27:3:216:LYS:H	27:3:216:LYS:CD	2.13	0.59
1:A:544:ALA:HB2	1:A:680:LEU:HD13	1.83	0.59
1:A:593:SER:HB3	1:A:634:GLU:HA	1.84	0.59
1:A:816:GLY:O	1:A:819:SER:OG	2.14	0.59
2:B:131:THR:O	2:B:132:VAL:CG1	2.50	0.59
6:F:44:ARG:H	6:F:45:PRO:HD2	1.66	0.59
9:I:112:TYR:N	9:I:123:TRP:O	2.34	0.59
20:T:177:ARG:HG2	20:T:208:GLN:CG	2.29	0.59
22:V:520:ARG:NE	22:V:521:GLU:OE2	2.28	0.59
1:A:880:ARG:NH1	1:A:884:ASN:O	2.35	0.59
8:H:3:GLY:N	8:H:67:ASP:OD1	2.34	0.59
9:I:119:CYS:SG	9:I:120:GLY:N	2.76	0.59
11:K:21:ILE:HG23	11:K:33:PHE:CE1	2.38	0.59
12:L:16:ILE:HG22	12:L:16:ILE:O	2.03	0.59
14:N:318:ASP:CA	16:P:239:ARG:HE	2.16	0.59
20:T:145:LEU:C	20:T:147:LYS:H	2.03	0.59
24:0:77:LYS:C	24:0:79:ASN:H	2.03	0.59
26:2:35:TYR:CB	26:2:62:LEU:HD12	2.33	0.59
26:2:206:LEU:HD22	26:2:206:LEU:N	2.17	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:110:VAL:O	27:3:114:GLU:HG2	2.02	0.59
1:A:479:TRP:N	11:K:2:ASN:O	2.35	0.59
14:N:21:VAL:HG11	15:O:40:PHE:HD1	1.68	0.59
16:P:205:ARG:O	16:P:206:GLU:C	2.40	0.59
16:P:261:SER:HB3	29:Y:81:DA:H4'	1.85	0.59
17:Q:105:TYR:OH	18:R:222:SER:HA	2.03	0.59
26:2:159:VAL:HG22	26:2:160:LEU:N	2.16	0.59
1:A:686:THR:HG21	2:B:1041:ILE:HG13	1.84	0.59
1:A:1168:LYS:HG3	1:A:1220:HIS:CE1	2.37	0.59
22:V:609:LYS:NZ	29:Y:38:DT:OP1	2.34	0.59
22:V:703:PHE:CZ	22:V:712:LEU:CD2	2.86	0.59
24:0:77:LYS:H	24:0:77:LYS:HD2	1.68	0.59
25:1:38:ILE:H	25:1:38:ILE:CD1	2.16	0.59
26:2:177:GLN:HE22	26:2:220:LEU:HA	1.68	0.59
2:B:175:ASN:O	2:B:739:ASN:ND2	2.32	0.59
2:B:556:ILE:HD12	2:B:561:ILE:HG21	1.84	0.59
2:B:897:ARG:NH1	2:B:1079:SER:OG	2.35	0.59
5:E:13:ILE:HG22	5:E:136:LEU:HA	1.85	0.59
13:M:182:ALA:HB2	20:T:154:LYS:HA	1.84	0.59
17:Q:131:VAL:HG21	17:Q:159:THR:HG21	1.85	0.59
23:W:175:TYR:HD1	23:W:175:TYR:H	1.46	0.59
23:W:584:TYR:HB2	23:W:594:ALA:CB	2.32	0.59
25:1:34:ILE:O	25:1:46:ILE:HG13	2.03	0.59
26:2:56:VAL:HG11	26:2:91:SER:CB	2.32	0.59
1:A:622:SER:N	1:A:623:PRO:CD	2.21	0.58
1:A:1264:SER:O	1:A:1266:GLU:N	2.33	0.58
2:B:88:PHE:CD2	2:B:128:ILE:HG12	2.37	0.58
2:B:542:LEU:HA	2:B:545:LEU:HD12	1.85	0.58
3:C:217:GLN:O	3:C:218:ALA:HB2	1.99	0.58
22:V:321:GLU:HA	23:W:499:ASN:HD21	1.65	0.58
26:2:203:PHE:CE2	26:2:205:LEU:HD23	2.38	0.58
27:3:169:ASP:CB	27:3:202:LEU:HD23	2.33	0.58
28:X:64:DC:O2	29:Y:31:DG:N2	2.36	0.58
1:A:1307:VAL:O	1:A:1308:TYR:CG	2.56	0.58
17:Q:113:ARG:CD	18:R:221:ARG:HG3	2.29	0.58
24:0:109:THR:HB	24:0:144:SER:H	1.67	0.58
26:2:160:LEU:HD12	26:2:160:LEU:N	2.18	0.58
27:3:215:LEU:HD12	27:3:230:VAL:HG13	1.85	0.58
1:A:426:ARG:HB3	13:M:40:VAL:HG21	1.84	0.58
2:B:63:PRO:HB3	2:B:408:PHE:CZ	2.38	0.58
2:B:430:ASN:HB2	20:T:159:HIS:HE1	1.67	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1022:LEU:HD12	2:B:1023:ARG:HG2	1.85	0.58
8:H:110:THR:O	8:H:110:THR:HG22	2.02	0.58
17:Q:104:LYS:NZ	18:R:238:LYS:HD2	2.18	0.58
28:X:47:DC:H2"	28:X:48:DG:C8	2.39	0.58
1:A:565:MET:HG2	11:K:61:TYR:C	2.24	0.58
1:A:625:ASP:H	1:A:637:MET:CB	2.17	0.58
2:B:109:MET:HE1	2:B:174:LEU:HB3	1.85	0.58
2:B:171:LEU:HD22	2:B:176:GLU:HG2	1.83	0.58
2:B:866:ILE:H	2:B:895:PHE:HA	1.67	0.58
14:N:49:LYS:NZ	15:O:17:GLU:OE1	2.25	0.58
16:P:207:PRO:HB2	16:P:229:GLN:OE1	2.03	0.58
25:1:34:ILE:HG22	25:1:46:ILE:CD1	2.32	0.58
26:2:159:VAL:HG13	26:2:160:LEU:N	2.17	0.58
27:3:131:THR:CG2	27:3:133:LEU:HD12	2.33	0.58
27:3:215:LEU:CD1	27:3:230:VAL:HG13	2.32	0.58
27:3:222:SER:HB2	27:3:226:TYR:CE2	2.36	0.58
29:Y:30:DG:C2	29:Y:31:DG:C4	2.92	0.58
1:A:555:LEU:HD22	1:A:591:ILE:HG13	1.84	0.58
2:B:1115:GLN:HB2	2:B:1148:LEU:HD11	1.84	0.58
18:R:196:ASP:O	18:R:197:LYS:CB	2.50	0.58
25:1:53:LEU:HD12	25:1:53:LEU:N	2.18	0.58
2:B:548:TRP:CD1	2:B:583:LEU:HD13	2.38	0.58
2:B:573:TRP:CZ2	2:B:576:ILE:HG23	2.38	0.58
2:B:1036:LYS:HB2	3:C:194:HIS:HB3	1.85	0.58
7:G:6:SER:HA	7:G:73:LYS:HA	1.85	0.58
10:J:12:LYS:HE2	10:J:40:LEU:HA	1.86	0.58
14:N:318:ASP:HA	16:P:239:ARG:NE	2.18	0.58
21:U:143:LYS:NZ	21:U:147:MET:SD	2.75	0.58
24:0:77:LYS:C	24:0:79:ASN:N	2.56	0.58
26:2:118:LEU:CD2	27:3:39:ASP:C	2.72	0.58
1:A:47:THR:HG23	1:A:53:LYS:HA	1.86	0.58
1:A:286:ILE:HD13	1:A:313:HIS:CD2	2.38	0.58
1:A:1164:THR:N	1:A:1299:GLN:O	2.34	0.58
7:G:98:PHE:HZ	17:Q:152:PHE:CE1	2.22	0.58
17:Q:25:PHE:HB3	18:R:215:GLU:OE2	2.04	0.58
21:U:200:ASP:OD2	21:U:203:ASN:ND2	2.30	0.58
27:3:14:VAL:HG23	27:3:163:VAL:HG13	1.86	0.58
27:3:144:ILE:HG12	27:3:147:MET:CE	2.34	0.58
1:A:381:PRO:HB3	11:K:2:ASN:HD21	1.68	0.58
1:A:423:ASN:ND2	1:A:425:ASP:OD2	2.30	0.58
1:A:611:ASP:HB3	1:A:617:PRO:HG3	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:734:ARG:HH21	9:I:105:GLU:C	2.07	0.58
1:A:734:ARG:NH2	9:I:105:GLU:O	2.36	0.58
2:B:936:ALA:HB2	2:B:1051:LEU:HD11	1.86	0.58
22:V:534:TYR:CD1	22:V:535:THR:N	2.71	0.58
25:1:2:VAL:CG1	26:2:456:LYS:CD	2.81	0.58
1:A:1223:ASP:OD2	1:A:1224:ARG:NE	2.36	0.58
1:A:1308:TYR:CD1	1:A:1338:THR:HG22	2.37	0.58
4:D:23:PRO:O	4:D:27:GLU:N	2.35	0.58
5:E:52:ARG:HB2	5:E:53:PRO:CD	2.33	0.58
11:K:11:LEU:O	11:K:37:LYS:NZ	2.36	0.58
17:Q:106:LYS:HZ1	18:R:219:LEU:HD13	1.67	0.58
17:Q:113:ARG:HE	18:R:217:GLN:C	2.06	0.58
18:R:140:LYS:HA	18:R:143:TYR:CZ	2.39	0.58
27:3:21:TRP:CD2	27:3:34:LEU:HD23	2.39	0.58
1:A:607:SER:HB2	1:A:641:CYS:SG	2.44	0.58
2:B:755:GLN:HB2	2:B:776:ILE:HA	1.85	0.58
5:E:52:ARG:CG	5:E:53:PRO:N	2.60	0.58
7:G:55:GLY:N	7:G:69:PRO:O	2.35	0.58
7:G:78:ARG:NH1	7:G:79:PRO:O	2.37	0.58
19:S:112:GLY:HA2	19:S:145:ASN:O	2.04	0.58
23:W:584:TYR:CB	23:W:594:ALA:HB2	2.33	0.58
25:1:2:VAL:HB	26:2:456:LYS:HD3	1.86	0.58
26:2:236:PHE:CZ	26:2:258:LEU:HD11	2.39	0.58
1:A:66:GLU:HB2	1:A:265:VAL:HG21	1.86	0.57
1:A:612:ASP:C	1:A:614:ASP:N	2.55	0.57
2:B:133:ILE:C	2:B:134:LYS:HG2	2.25	0.57
2:B:224:CYS:HB2	2:B:230:ARG:HA	1.86	0.57
2:B:718:GLN:NE2	2:B:975:ARG:O	2.32	0.57
9:I:98:GLN:NE2	9:I:108:MET:HG3	2.17	0.57
25:1:13:ASP:CG	25:1:14:PRO:HD2	2.24	0.57
1:A:44:PRO:HG3	1:A:284:VAL:HB	1.85	0.57
1:A:1187:ALA:HA	1:A:1190:GLN:HB2	1.84	0.57
2:B:552:ASN:OD1	2:B:553:LEU:N	2.37	0.57
2:B:897:ARG:HD2	2:B:1079:SER:HA	1.85	0.57
2:B:1072:ARG:HE	2:B:1113:PRO:HD2	1.68	0.57
3:C:77:ASP:HB2	3:C:128:ILE:HG22	1.85	0.57
9:I:105:GLU:HB3	9:I:107:ALA:HB3	1.86	0.57
12:L:16:ILE:O	12:L:17:TYR:CD2	2.57	0.57
18:R:140:LYS:CG	18:R:141:PRO:HD3	2.34	0.57
26:2:423:ALA:HA	26:2:426:ARG:HE	1.70	0.57
27:3:46:ASN:CG	27:3:104:LEU:HD22	2.25	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:797:ARG:HB3	1:A:820:ARG:HB3	1.85	0.57
5:E:44:SER:OG	5:E:46:ASP:HB2	2.04	0.57
8:H:65:TYR:CD2	8:H:70:LEU:HB3	2.39	0.57
9:I:86:CYS:C	9:I:88:LYS:H	2.08	0.57
14:N:318:ASP:HB3	16:P:239:ARG:HE	1.68	0.57
16:P:180:LEU:HB3	16:P:200:VAL:HG23	1.86	0.57
17:Q:25:PHE:CD2	18:R:215:GLU:OE2	2.56	0.57
17:Q:32:LEU:HD13	18:R:161:ARG:NH2	2.19	0.57
2:B:411:LEU:HD12	2:B:440:ILE:HD11	1.86	0.57
5:E:27:LEU:HD12	5:E:64:HIS:CG	2.20	0.57
11:K:7:PHE:HA	11:K:10:PHE:CE2	2.39	0.57
13:M:295:ARG:HG2	13:M:299:LEU:HG	1.86	0.57
14:N:354:LYS:HA	14:N:369:LYS:HA	1.86	0.57
19:S:31:PHE:HB2	20:T:92:THR:HB	1.86	0.57
23:W:70:LEU:CG	23:W:72:TYR:CE1	2.87	0.57
1:A:1037:ALA:HA	5:E:200:ALA:HB1	1.86	0.57
1:A:1308:TYR:CE1	1:A:1338:THR:HG21	2.40	0.57
5:E:63:ALA:O	5:E:64:HIS:CB	2.53	0.57
10:J:43:TYR:HA	10:J:46:ARG:HB2	1.86	0.57
16:P:296:ILE:O	16:P:297:LYS:C	2.42	0.57
16:P:297:LYS:HB2	16:P:298:PRO:CD	2.24	0.57
22:V:415:HIS:CD2	22:V:416:THR:CG2	2.88	0.57
25:1:4:VAL:HG11	26:2:412:PHE:CD2	2.28	0.57
27:3:19:PRO:HG2	27:3:123:ASP:O	2.05	0.57
1:A:642:LYS:HZ3	21:U:283:GLU:HA	1.69	0.57
5:E:110:MET:HB2	5:E:115:LYS:HE3	1.87	0.57
17:Q:23:ARG:CZ	18:R:207:SER:CB	2.76	0.57
17:Q:129:CYS:SG	17:Q:159:THR:OG1	2.62	0.57
20:T:12:ALA:HA	20:T:109:ILE:HD11	1.85	0.57
20:T:174:LYS:HE3	28:X:21:DG:H5'	1.87	0.57
22:V:523:VAL:HG21	25:1:20:LEU:HD23	1.86	0.57
27:3:14:VAL:HG23	27:3:163:VAL:HA	1.84	0.57
3:C:193:ARG:NH2	3:C:218:ALA:O	2.38	0.57
17:Q:187:ILE:O	18:R:212:VAL:N	2.38	0.57
22:V:520:ARG:HD3	25:1:19:PHE:HB3	1.85	0.57
26:2:192:GLU:CG	26:2:193:PRO:HD2	2.23	0.57
27:3:195:VAL:HG21	27:3:214:TYR:OH	2.05	0.57
2:B:1114:TYR:CE1	2:B:1153:TYR:HD2	2.22	0.57
8:H:17:PRO:HB3	8:H:27:ARG:HB3	1.87	0.57
17:Q:202:GLU:O	17:Q:203:ILE:HB	2.05	0.57
26:2:30:VAL:N	27:3:25:GLN:CB	2.48	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:181:GLN:HA	26:2:181:GLN:HE21	1.70	0.57
27:3:223:LEU:HD11	27:3:227:LEU:HD11	1.87	0.57
1:A:21:VAL:HB	1:A:1449:ASP:HB3	1.87	0.57
1:A:66:GLU:O	1:A:68:THR:N	2.38	0.57
3:C:6:GLN:CG	3:C:25:ASN:HD22	2.17	0.57
3:C:115:VAL:O	3:C:150:ILE:N	2.36	0.57
8:H:74:GLU:C	8:H:76:ASN:N	2.39	0.57
16:P:293:TYR:HB3	16:P:302:LEU:HB2	1.87	0.57
19:S:8:SER:HB3	20:T:49:GLN:HA	1.86	0.57
26:2:60:LEU:HD11	26:2:95:ILE:CG2	2.35	0.57
1:A:1307:VAL:HG12	1:A:1339:ASP:H	1.70	0.57
1:A:1309:MET:CG	21:U:252:LYS:HD2	2.34	0.57
15:O:66:ARG:NE	16:P:185:LEU:O	2.37	0.57
2:B:851:ASP:OD2	12:L:17:TYR:OH	2.11	0.56
5:E:148:HIS:HB2	5:E:183:PHE:CZ	2.40	0.56
13:M:169:ARG:NH1	13:M:207:ASP:O	2.37	0.56
18:R:140:LYS:N	18:R:141:PRO:CD	2.39	0.56
18:R:195:PRO:CG	18:R:199:LYS:C	2.73	0.56
22:V:413:LEU:HD11	28:X:55:DC:C4'	2.35	0.56
23:W:209:TYR:OH	23:W:233:PHE:C	2.42	0.56
23:W:410:TYR:CE2	23:W:413:GLY:HA3	2.40	0.56
25:1:9:LEU:CB	25:1:51:ASN:HD21	2.14	0.56
26:2:211:GLN:HB3	26:2:261:PHE:CE1	2.40	0.56
1:A:202:TRP:HB2	1:A:212:LYS:HE2	1.87	0.56
1:A:1246:ILE:HG23	1:A:1258:ARG:HG3	1.86	0.56
2:B:490:GLY:O	2:B:491:ARG:O	2.23	0.56
2:B:823:PHE:HD1	13:M:140:ASN:HB3	1.69	0.56
3:C:205:LYS:HB3	3:C:209:SER:OG	2.05	0.56
8:H:66:GLU:O	8:H:67:ASP:CG	2.44	0.56
13:M:173:VAL:O	13:M:175:ARG:NH1	2.38	0.56
15:O:66:ARG:HD3	16:P:185:LEU:HA	1.87	0.56
17:Q:113:ARG:CB	18:R:221:ARG:HD3	2.31	0.56
22:V:550:PHE:CZ	22:V:554:ARG:CZ	2.88	0.56
26:2:197:THR:HG21	26:2:239:GLN:CD	2.24	0.56
1:A:275:ASP:HB2	1:A:342:ARG:HH22	1.70	0.56
1:A:621:ILE:CD1	1:A:623:PRO:HB3	2.27	0.56
1:A:891:TYR:CZ	1:A:1087:VAL:HG21	2.40	0.56
1:A:1305:SER:O	1:A:1306:LYS:HB3	2.05	0.56
2:B:488:PRO:O	2:B:489:ILE:HG13	2.04	0.56
2:B:544:PHE:O	2:B:548:TRP:N	2.39	0.56
2:B:803:ARG:HD3	10:J:8:PHE:HA	1.88	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:C:48:ASP:HB3	3:C:166:LYS:HD2	1.86	0.56
3:C:136:ASP:HB2	3:C:145:GLN:CD	2.22	0.56
3:C:154:ARG:HH11	10:J:65:LEU:HB2	1.68	0.56
13:M:214:PHE:HB3	13:M:218:PHE:CE2	2.40	0.56
17:Q:128:LYS:NZ	17:Q:133:SER:O	2.37	0.56
25:1:3:ASN:CB	26:2:412:PHE:O	2.52	0.56
26:2:82:ALA:HA	26:2:89:LEU:HD11	1.85	0.56
26:2:185:MET:HB2	26:2:229:ASP:OD1	2.05	0.56
27:3:210:THR:HG22	27:3:210:THR:O	2.04	0.56
1:A:47:THR:HG22	1:A:49:GLY:H	1.70	0.56
8:H:7:GLU:HG3	8:H:59:VAL:HG22	1.87	0.56
12:L:33:PRO:HG2	12:L:35:ARG:HG2	1.87	0.56
23:W:143:ARG:HG2	23:W:143:ARG:NH1	2.19	0.56
26:2:47:GLU:HG3	26:2:48:LEU:N	2.20	0.56
4:D:15:GLU:HG2	4:D:23:PRO:HD3	1.87	0.56
17:Q:113:ARG:HE	18:R:217:GLN:CA	2.18	0.56
18:R:155:LEU:CD2	18:R:204:ASN:HD21	2.11	0.56
23:W:209:TYR:CZ	23:W:233:PHE:HA	2.38	0.56
25:1:8:VAL:HG12	25:1:9:LEU:H	1.69	0.56
25:1:52:VAL:HG22	25:1:53:LEU:HD12	1.87	0.56
26:2:130:SER:HB2	26:2:173:GLN:OE1	2.06	0.56
28:X:57:DC:H2"	28:X:58:DT:H72	1.86	0.56
1:A:357:LYS:O	2:B:1086:PHE:N	2.36	0.56
1:A:740:GLN:O	1:A:743:ARG:HG2	2.05	0.56
13:M:11:PRO:O	13:M:12:ARG:CB	2.47	0.56
27:3:173:GLN:CA	27:3:176:ASN:HD21	2.10	0.56
27:3:187:GLN:NE2	27:3:189:ILE:HG13	2.20	0.56
1:A:1196:TYR:HD2	1:A:1246:ILE:HD11	1.68	0.56
2:B:626:LEU:HD22	2:B:633:LEU:HD11	1.87	0.56
8:H:65:TYR:CZ	8:H:70:LEU:HD22	2.41	0.56
25:1:10:ILE:C	25:1:10:ILE:HD13	2.26	0.56
27:3:44:LEU:HD13	27:3:44:LEU:O	2.06	0.56
27:3:178:MET:SD	27:3:181:ILE:HD12	2.46	0.56
1:A:329:MET:HE1	1:A:335:PRO:HA	1.87	0.56
1:A:375:ILE:HD11	1:A:666:ARG:HE	1.69	0.56
7:G:63:ARG:NH2	7:G:65:PHE:O	2.38	0.56
26:2:117:ASN:HB2	27:3:104:LEU:CD1	2.35	0.56
1:A:181:HIS:ND1	1:A:181:HIS:O	2.38	0.56
2:B:225:LEU:H	2:B:231:PRO:HD2	1.71	0.56
6:F:79:VAL:HG12	6:F:81:VAL:H	1.71	0.56
8:H:107:GLU:O	8:H:108:ALA:C	2.44	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:126:ILE:O	19:S:138:PHE:N	2.35	0.56
20:T:229:HIS:CD2	28:X:28:DG:H21	2.24	0.56
1:A:85:PHE:HD1	1:A:257:PRO:HD3	1.70	0.56
1:A:924:TYR:N	1:A:924:TYR:CD1	2.74	0.56
3:C:63:PHE:O	3:C:67:ARG:HG3	2.06	0.56
13:M:214:PHE:O	13:M:218:PHE:HD2	1.89	0.56
17:Q:104:LYS:HZ1	18:R:238:LYS:HE3	1.70	0.56
17:Q:141:ALA:HB1	17:Q:152:PHE:CE1	2.40	0.56
19:S:166:ARG:HH11	19:S:166:ARG:CG	2.19	0.56
24:0:54:ARG:CB	27:3:209:ILE:HG23	2.25	0.56
27:3:71:TYR:CG	27:3:72:PRO:HD2	2.18	0.56
1:A:47:THR:HA	1:A:54:LEU:HG	1.87	0.55
1:A:686:THR:HG21	2:B:1041:ILE:HA	1.88	0.55
2:B:156:LEU:HB2	2:B:183:GLY:H	1.71	0.55
2:B:591:ARG:HA	2:B:596:ILE:HB	1.88	0.55
2:B:676:ALA:N	2:B:695:HIS:O	2.33	0.55
14:N:318:ASP:HB3	16:P:239:ARG:HH21	1.71	0.55
22:V:519:TYR:CD2	25:1:20:LEU:HB2	2.42	0.55
26:2:117:ASN:CG	27:3:108:ASN:CG	2.65	0.55
26:2:160:LEU:H	26:2:160:LEU:CD1	2.18	0.55
27:3:165:LYS:HZ1	27:3:200:SER:H	1.54	0.55
1:A:1209:PRO:HB3	9:I:33:ARG:NH1	2.19	0.55
2:B:93:LEU:C	20:T:145:LEU:HD21	2.27	0.55
2:B:268:PRO:HB2	2:B:271:ILE:HG12	1.88	0.55
2:B:485:LEU:HB2	2:B:524:LYS:HB2	1.88	0.55
2:B:633:LEU:HG	2:B:635:LEU:H	1.71	0.55
2:B:829:PHE:CE1	2:B:869:LYS:HD3	2.40	0.55
2:B:876:ASN:OD1	2:B:879:GLU:CD	2.44	0.55
5:E:30:GLN:O	5:E:34:ASP:N	2.34	0.55
13:M:17:ASN:OD1	13:M:18:HIS:ND1	2.39	0.55
13:M:107:MET:HA	13:M:107:MET:CE	2.32	0.55
25:1:18:GLN:HB2	25:1:44:PHE:CZ	2.38	0.55
25:1:36:GLN:HB3	25:1:45:VAL:HG12	1.88	0.55
26:2:81:LYS:HG3	26:2:82:ALA:N	2.21	0.55
2:B:837:CYS:HB2	2:B:889:LYS:HD2	1.89	0.55
3:C:200:PRO:CG	3:C:217:GLN:CD	2.57	0.55
9:I:68:ILE:HG23	9:I:122:ARG:HD2	1.88	0.55
16:P:288:PHE:CD1	16:P:289:PRO:HD2	2.41	0.55
22:V:531:ILE:CB	22:V:534:TYR:CE2	2.89	0.55
25:1:31:LYS:O	25:1:32:LYS:HB2	2.06	0.55
27:3:160:ARG:HB3	27:3:190:LEU:CD2	2.32	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:223:LEU:HD13	27:3:227:LEU:HG	1.89	0.55
1:A:46:THR:HA	1:A:57:LEU:HD13	1.89	0.55
1:A:364:ARG:NH1	1:A:461:GLN:OE1	2.39	0.55
1:A:408:ARG:NH1	1:A:414:PRO:HB2	2.21	0.55
2:B:248:LYS:C	2:B:249:LYS:HG2	2.27	0.55
4:D:79:THR:HG23	4:D:137:LYS:HG2	1.89	0.55
19:S:119:THR:HG22	19:S:123:SER:HA	1.89	0.55
19:S:127:PHE:HB2	20:T:19:TRP:HB2	1.87	0.55
20:T:217:LEU:HB3	20:T:233:TRP:CE3	2.40	0.55
27:3:22:TRP:O	27:3:25:GLN:NE2	2.38	0.55
1:A:372:ASN:O	1:A:372:ASN:ND2	2.38	0.55
3:C:205:LYS:NZ	3:C:213:GLU:OE2	2.34	0.55
5:E:54:ARG:O	5:E:58:LEU:N	2.35	0.55
15:O:67:PHE:HB2	15:O:72:TRP:CE3	2.41	0.55
22:V:519:TYR:HD2	25:1:20:LEU:HB2	1.72	0.55
26:2:222:THR:HG23	26:2:222:THR:O	2.07	0.55
27:3:223:LEU:HD13	27:3:223:LEU:O	2.06	0.55
1:A:43:TYR:CD2	1:A:44:PRO:HD2	2.42	0.55
1:A:516:GLN:HA	1:A:520:MET:HG2	1.89	0.55
1:A:621:ILE:C	1:A:623:PRO:HD2	2.18	0.55
1:A:1280:ASP:HB3	1:A:1283:VAL:HG22	1.87	0.55
2:B:566:LYS:HA	2:B:576:ILE:HG22	1.89	0.55
2:B:814:TYR:N	2:B:921:ILE:O	2.32	0.55
3:C:101:PHE:O	3:C:163:ALA:N	2.28	0.55
14:N:360:LEU:HD11	15:O:81:PHE:CD2	2.41	0.55
23:W:408:SER:O	23:W:409:THR:CG2	2.54	0.55
26:2:259:LEU:HD12	26:2:259:LEU:C	2.27	0.55
27:3:190:LEU:HD23	27:3:190:LEU:N	2.18	0.55
1:A:65:ILE:HG22	1:A:66:GLU:H	1.72	0.55
1:A:489:THR:O	1:A:493:ASN:N	2.39	0.55
1:A:625:ASP:N	1:A:637:MET:HE2	2.22	0.55
1:A:1027:ASP:OD2	5:E:162:ARG:NE	2.25	0.55
1:A:1150:ASP:OD2	1:A:1153:ARG:N	2.39	0.55
16:P:270:LEU:HD22	16:P:291:LEU:HD13	1.89	0.55
18:R:88:ARG:NH1	18:R:97:LEU:HD23	2.22	0.55
23:W:143:ARG:HG2	23:W:143:ARG:HH11	1.71	0.55
26:2:251:VAL:HG12	26:2:254:MET:HB2	1.85	0.55
1:A:43:TYR:CG	1:A:44:PRO:HD2	2.41	0.55
1:A:426:ARG:NE	1:A:447:GLU:OE2	2.33	0.55
1:A:910:LYS:HD2	1:A:911:PRO:HD2	1.88	0.55
1:A:1162:GLU:HA	1:A:1308:TYR:HE2	1.71	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1304:ILE:O	1:A:1306:LYS:N	2.40	0.55
2:B:109:MET:HE3	2:B:111:ASN:HB2	1.89	0.55
2:B:829:PHE:HD1	2:B:869:LYS:HB3	1.72	0.55
2:B:934:LYS:HG2	2:B:1051:LEU:HD12	1.88	0.55
16:P:167:ASN:ND2	29:Y:79:DT:H1'	2.21	0.55
16:P:171:THR:HG23	16:P:256:GLN:HG3	1.89	0.55
16:P:205:ARG:O	16:P:206:GLU:O	2.25	0.55
21:U:205:ASN:HB3	21:U:231:ASP:OD2	2.06	0.55
26:2:214:TYR:CD2	26:2:261:PHE:CD2	2.95	0.55
27:3:42:MET:SD	27:3:111:ILE:HD13	2.46	0.55
1:A:551:ARG:HD3	1:A:637:MET:CE	2.37	0.55
9:I:105:GLU:O	9:I:107:ALA:C	2.45	0.55
17:Q:113:ARG:NE	18:R:217:GLN:HB3	2.21	0.55
20:T:31:TRP:CD1	20:T:62:LEU:HD21	2.41	0.55
25:1:25:GLU:HG2	25:1:32:LYS:HA	1.89	0.55
26:2:53:LYS:CE	26:2:95:ILE:HD11	2.36	0.55
26:2:123:LEU:CD2	26:2:178:LEU:HD11	2.37	0.55
26:2:208:THR:O	26:2:212:LEU:HG	2.07	0.55
1:A:21:VAL:HG21	1:A:1427:LEU:HD11	1.88	0.55
1:A:515:ILE:HG23	1:A:519:ALA:HB3	1.89	0.55
1:A:621:ILE:CA	1:A:623:PRO:CD	2.71	0.55
1:A:926:ASN:OD1	1:A:931:ARG:CG	2.55	0.55
1:A:928:ARG:O	1:A:930:LEU:N	2.40	0.55
1:A:935:GLN:O	1:A:1002:SER:N	2.40	0.55
2:B:751:LEU:HD11	2:B:806:PHE:HA	1.89	0.55
2:B:810:PHE:HB2	2:B:927:ARG:HG2	1.89	0.55
12:L:17:TYR:OH	12:L:46:LYS:NZ	2.39	0.55
13:M:179:GLU:HG2	20:T:154:LYS:HE3	1.89	0.55
14:N:332:GLU:HB2	15:O:93:VAL:HA	1.88	0.55
21:U:221:ALA:C	21:U:223:MET:H	2.10	0.55
21:U:230:SER:O	21:U:231:ASP:HB3	2.07	0.55
21:U:266:CYS:O	21:U:268:LYS:N	2.32	0.55
1:A:1121:VAL:HA	1:A:1124:LEU:HB3	1.89	0.54
1:A:1146:GLN:HG2	1:A:1150:ASP:HB2	1.88	0.54
1:A:1463:LEU:HD21	6:F:64:ARG:HH22	1.71	0.54
2:B:552:ASN:HB3	2:B:555:GLU:HB3	1.89	0.54
2:B:1040:GLN:NE2	3:C:195:THR:OG1	2.40	0.54
8:H:65:TYR:CE2	8:H:70:LEU:HB2	2.41	0.54
22:V:251:PHE:O	22:V:257:LYS:HA	2.06	0.54
2:B:953:ASP:HA	3:C:36:ARG:HH12	1.72	0.54
10:J:14:VAL:HG23	10:J:17:LYS:HB2	1.90	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:69:ASP:HA	18:R:225:VAL:CG2	2.37	0.54
22:V:514:MET:SD	22:V:537:ASN:ND2	2.80	0.54
1:A:880:ARG:HG2	1:A:886:VAL:HA	1.88	0.54
2:B:778:SER:O	2:B:1046:THR:N	2.37	0.54
5:E:10:LEU:HB3	5:E:58:LEU:HD11	1.89	0.54
7:G:98:PHE:HE2	17:Q:145:PHE:CG	2.25	0.54
16:P:214:PHE:HD2	16:P:218:LYS:HB2	1.73	0.54
22:V:667:THR:HA	25:1:62:ASP:OD2	2.07	0.54
23:W:408:SER:O	23:W:409:THR:HG22	2.08	0.54
27:3:71:TYR:HD2	27:3:72:PRO:HD2	1.70	0.54
1:A:320:ASN:HB2	1:A:336:LEU:HD23	1.90	0.54
3:C:68:LEU:HD12	3:C:71:ILE:HD12	1.90	0.54
6:F:81:VAL:HG12	6:F:101:LYS:HD3	1.88	0.54
10:J:67:LYS:HB2	12:L:23:HIS:CD2	2.35	0.54
14:N:360:LEU:HB2	14:N:365:TYR:HE2	1.72	0.54
22:V:609:LYS:CE	29:Y:38:DT:OP1	2.55	0.54
23:W:52:LEU:CD2	23:W:72:TYR:OH	2.55	0.54
25:1:29:LEU:HD23	25:1:29:LEU:C	2.27	0.54
26:2:123:LEU:HD21	26:2:178:LEU:CD1	2.38	0.54
26:2:138:PRO:O	26:2:139:ASP:HB2	2.08	0.54
1:A:608:THR:HG21	1:A:639:ILE:HG23	1.89	0.54
2:B:512:ALA:HA	2:B:723:THR:HG22	1.89	0.54
2:B:1094:GLN:HA	2:B:1097:HIS:HB2	1.88	0.54
3:C:44:ILE:N	3:C:168:GLY:O	2.31	0.54
5:E:105:VAL:HG12	5:E:132:GLN:HG3	1.88	0.54
9:I:59:THR:O	9:I:59:THR:HG22	2.08	0.54
16:P:165:LEU:HA	16:P:260:GLY:HA2	1.89	0.54
20:T:139:VAL:O	20:T:139:VAL:HG12	2.06	0.54
25:1:13:ASP:OD1	25:1:14:PRO:CD	2.56	0.54
26:2:138:PRO:HG3	26:2:189:GLU:CG	2.35	0.54
1:A:1309:MET:O	1:A:1336:LEU:HA	2.07	0.54
2:B:440:ILE:H	2:B:440:ILE:HD12	1.71	0.54
2:B:836:THR:HG22	2:B:885:ARG:HB3	1.90	0.54
3:C:125:PRO:O	3:C:127:VAL:N	2.40	0.54
5:E:149:VAL:O	5:E:192:LYS:N	2.23	0.54
11:K:35:ILE:HB	11:K:71:ILE:HG13	1.89	0.54
15:O:28:ILE:HB	15:O:32:LEU:HD23	1.88	0.54
18:R:103:LEU:HB3	18:R:109:LEU:HA	1.90	0.54
19:S:110:PHE:CD1	19:S:148:PRO:HA	2.42	0.54
22:V:321:GLU:CA	23:W:499:ASN:ND2	2.58	0.54
1:A:526:VAL:HA	1:A:533:PRO:HA	1.88	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:573:TRP:CZ3	2:B:575:GLY:HA2	2.43	0.54
9:I:110:LEU:O	9:I:124:THR:OG1	2.26	0.54
13:M:267:GLU:OE1	13:M:269:ARG:NH2	2.41	0.54
20:T:30:GLN:HG2	20:T:62:LEU:HG	1.89	0.54
25:1:34:ILE:HG23	25:1:50:VAL:HG11	1.89	0.54
26:2:177:GLN:NE2	26:2:220:LEU:HA	2.22	0.54
1:A:43:TYR:OH	1:A:285:LYS:HE2	2.06	0.54
1:A:378:VAL:O	1:A:475:ARG:N	2.41	0.54
2:B:248:LYS:O	2:B:249:LYS:HG2	2.08	0.54
2:B:1117:HIS:HA	2:B:1147:SER:O	2.07	0.54
2:B:1135:TYR:HB2	2:B:1146:ILE:HG13	1.90	0.54
3:C:23:ILE:HB	3:C:231:TYR:HE2	1.72	0.54
5:E:166:ARG:HB2	5:E:169:GLN:HG3	1.90	0.54
8:H:8:ASP:OD1	8:H:9:ILE:N	2.41	0.54
9:I:17:CYS:N	9:I:22:ASN:O	2.35	0.54
22:V:325:ARG:HH22	23:W:499:ASN:HB3	0.72	0.54
25:1:52:VAL:HG23	25:1:53:LEU:N	2.21	0.54
27:3:64:ILE:HG23	27:3:128:HIS:CG	2.42	0.54
27:3:160:ARG:NH2	27:3:192:ASP:HB3	2.23	0.54
1:A:910:LYS:O	1:A:963:ARG:NH2	2.37	0.54
1:A:927:GLU:O	1:A:931:ARG:CB	2.56	0.54
1:A:936:GLU:HB2	1:A:939:VAL:HG23	1.89	0.54
2:B:131:THR:C	2:B:132:VAL:CG1	2.76	0.54
2:B:568:PHE:N	2:B:612:ILE:O	2.33	0.54
3:C:46:ALA:HB3	3:C:176:TRP:NE1	2.23	0.54
25:1:1:MET:HA	26:2:413:LEU:CA	2.38	0.54
27:3:105:THR:HG23	27:3:106:SER:N	2.23	0.54
1:A:1305:SER:O	1:A:1306:LYS:CB	2.55	0.54
2:B:670:GLU:HA	2:B:673:VAL:HG22	1.90	0.54
2:B:813:SER:HA	2:B:922:ARG:HA	1.89	0.54
5:E:73:PHE:O	5:E:103:LEU:N	2.28	0.54
14:N:38:VAL:HG13	15:O:22:LEU:HD22	1.89	0.54
19:S:48:GLU:O	19:S:99:LEU:N	2.38	0.54
26:2:62:LEU:HD13	26:2:62:LEU:C	2.28	0.54
26:2:118:LEU:HD12	26:2:118:LEU:C	2.29	0.54
1:A:871:VAL:HG23	1:A:1088:GLY:HA3	1.90	0.53
3:C:177:ASN:ND2	3:C:179:THR:O	2.41	0.53
8:H:6:PHE:HB3	8:H:60:ILE:HB	1.90	0.53
12:L:25:GLU:O	12:L:37:ARG:NH2	2.39	0.53
15:O:71:VAL:HG22	15:O:98:CYS:HA	1.90	0.53
18:R:191:PHE:CB	18:R:202:PHE:HD1	2.21	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
22:V:504:LYS:HD2	22:V:654:GLU:O	2.08	0.53
22:V:516:PRO:HD2	22:V:706:LYS:NZ	2.22	0.53
24:0:54:ARG:C	27:3:209:ILE:HD11	2.26	0.53
25:1:1:MET:HE1	26:2:440:LEU:HD13	1.90	0.53
26:2:28:PRO:HB3	27:3:33:THR:OG1	2.08	0.53
27:3:15:VAL:HG23	27:3:15:VAL:O	2.08	0.53
1:A:1005:HIS:CE1	1:A:1007:ILE:HB	2.43	0.53
2:B:752:TYR:HE1	2:B:809:VAL:HG23	1.72	0.53
5:E:65:ASN:O	5:E:67:ASP:C	2.47	0.53
5:E:172:ARG:O	5:E:207:ARG:NE	2.36	0.53
12:L:17:TYR:CB	12:L:46:LYS:HA	2.38	0.53
14:N:32:ASP:OD1	15:O:29:THR:OG1	2.23	0.53
14:N:318:ASP:CB	16:P:239:ARG:HE	2.20	0.53
22:V:638:GLN:O	22:V:642:ARG:HG2	2.08	0.53
25:1:1:MET:CB	26:2:418:PHE:HB2	2.38	0.53
26:2:31:LEU:HD13	27:3:33:THR:HG22	1.86	0.53
26:2:211:GLN:HE21	26:2:257:SER:CB	2.21	0.53
27:3:169:ASP:CG	27:3:202:LEU:HD23	2.28	0.53
1:A:46:THR:HG23	1:A:57:LEU:HD22	1.88	0.53
1:A:875:TYR:HA	1:A:1083:PRO:HB2	1.91	0.53
2:B:242:ARG:HB3	2:B:252:ILE:HG21	1.90	0.53
2:B:868:GLY:HA2	2:B:893:SER:HB2	1.89	0.53
8:H:88:PHE:HD1	8:H:146:LYS:HD2	1.73	0.53
17:Q:34:LEU:HA	17:Q:37:LEU:HD12	1.90	0.53
20:T:177:ARG:HD3	20:T:209:PRO:HD2	1.90	0.53
21:U:132:ARG:N	21:U:167:GLU:OE2	2.41	0.53
22:V:523:VAL:CG2	25:1:20:LEU:HD23	2.37	0.53
23:W:419:GLU:CB	23:W:420:PRO:CD	2.81	0.53
25:1:2:VAL:HG12	26:2:422:LEU:CD1	2.27	0.53
26:2:37:HIS:HB3	26:2:38:PRO:CD	2.35	0.53
1:A:551:ARG:HD3	1:A:637:MET:HE1	1.89	0.53
1:A:625:ASP:H	1:A:637:MET:HE2	1.73	0.53
2:B:51:ILE:HD12	2:B:160:TYR:CE2	2.44	0.53
2:B:935:PHE:CE2	2:B:945:CYS:HB2	2.42	0.53
4:D:112:LYS:HE2	4:D:124:ASP:OD2	2.09	0.53
17:Q:20:TYR:O	18:R:210:PHE:CE2	2.61	0.53
20:T:30:GLN:NE2	20:T:62:LEU:O	2.28	0.53
27:3:106:SER:O	27:3:109:GLU:HG3	2.08	0.53
1:A:1123:ARG:NH1	1:A:1126:GLU:OE1	2.40	0.53
3:C:74:ILE:HG13	3:C:76:ASP:H	1.74	0.53
13:M:225:PRO:HG2	13:M:228:VAL:HG23	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:187:ILE:O	18:R:212:VAL:HG12	2.08	0.53
25:1:1:MET:HB2	26:2:418:PHE:HB2	1.90	0.53
27:3:191:ILE:N	27:3:210:THR:HG21	2.23	0.53
1:A:225:PHE:HA	1:A:228:ILE:HG12	1.91	0.53
1:A:579:ILE:O	1:A:584:PRO:HA	2.09	0.53
2:B:309:PHE:HE2	9:I:25:TYR:HE2	1.57	0.53
2:B:591:ARG:NH2	2:B:669:GLU:OE1	2.42	0.53
4:D:73:ARG:NH1	4:D:103:LEU:O	2.41	0.53
16:P:325:PHE:CZ	16:P:329:TYR:HD2	2.26	0.53
22:V:366:ASN:ND2	22:V:613:THR:HG21	2.16	0.53
23:W:189:TRP:NE1	23:W:194:LEU:HB2	2.22	0.53
25:1:21:LEU:O	25:1:24:ASP:HB3	2.09	0.53
26:2:241:SER:O	26:2:245:LEU:HD23	2.09	0.53
27:3:172:LEU:HD13	27:3:172:LEU:C	2.29	0.53
1:A:124:PRO:HA	1:A:127:LYS:HB2	1.91	0.53
1:A:272:ASN:ND2	1:A:278:HIS:HD2	2.07	0.53
1:A:602:CYS:HB2	1:A:655:ILE:HD11	1.91	0.53
2:B:471:ASN:OD1	2:B:473:LEU:HG	2.09	0.53
16:P:297:LYS:HA	16:P:297:LYS:NZ	2.23	0.53
20:T:229:HIS:HA	28:X:29:DC:H4'	1.90	0.53
26:2:141:HIS:HA	26:2:162:PHE:CE2	2.44	0.53
26:2:208:THR:HG23	26:2:209:PRO:HD2	1.91	0.53
1:A:734:ARG:NH2	9:I:105:GLU:C	2.62	0.53
1:A:1308:TYR:HA	1:A:1338:THR:HG22	1.90	0.53
2:B:956:PHE:HB2	2:B:960:GLY:HA2	1.90	0.53
4:D:26:PHE:CZ	7:G:42:TYR:HA	2.44	0.53
24:0:54:ARG:CB	27:3:209:ILE:CG2	2.87	0.53
25:1:35:ILE:O	25:1:35:ILE:HG13	2.08	0.53
1:A:579:ILE:HB	1:A:585:LEU:HB2	1.91	0.53
2:B:152:ILE:HG23	2:B:154:ILE:HD11	1.90	0.53
2:B:182:GLY:HA2	2:B:184:TYR:CE1	2.44	0.53
2:B:792:ASP:OD1	2:B:975:ARG:NH2	2.42	0.53
5:E:62:VAL:HG21	5:E:72:MET:HE2	1.91	0.53
18:R:89:HIS:ND1	18:R:139:PHE:HE1	2.06	0.53
18:R:202:PHE:C	18:R:203:PHE:CG	2.82	0.53
23:W:70:LEU:HD21	23:W:72:TYR:OH	2.08	0.53
26:2:159:VAL:CG1	26:2:161:HIS:H	2.06	0.53
27:3:10:LEU:HD21	27:3:143:TYR:CE2	2.44	0.53
27:3:14:VAL:HG23	27:3:14:VAL:O	2.09	0.53
27:3:100:LYS:O	27:3:103:LEU:HB2	2.08	0.53
1:A:568:SER:N	1:A:671:ASN:OD1	2.29	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:623:ARG:O	2:B:665:ILE:N	2.37	0.53
2:B:753:TYR:CZ	10:J:4:PRO:HB3	2.44	0.53
17:Q:71:PHE:HD1	17:Q:72:ILE:HG23	1.74	0.53
17:Q:77:ARG:N	17:Q:93:PHE:O	2.35	0.53
22:V:413:LEU:HD11	28:X:55:DC:H4'	1.91	0.53
26:2:28:PRO:C	27:3:25:GLN:O	2.47	0.53
2:B:71:ALA:HA	2:B:81:PRO:HB3	1.90	0.52
3:C:14:LEU:HD23	11:K:112:LYS:HE2	1.91	0.52
3:C:19:VAL:HG12	3:C:233:VAL:HB	1.90	0.52
3:C:63:PHE:HE2	10:J:2:ILE:HG21	1.73	0.52
5:E:27:LEU:CB	5:E:64:HIS:CG	2.74	0.52
7:G:119:PHE:HB2	7:G:128:TYR:CE1	2.44	0.52
7:G:119:PHE:HB2	7:G:128:TYR:HE1	1.74	0.52
8:H:24:ARG:HG2	8:H:46:GLN:HE22	1.73	0.52
17:Q:105:TYR:CE2	18:R:222:SER:HB2	2.44	0.52
19:S:46:ARG:HB2	19:S:101:ARG:HB2	1.91	0.52
26:2:206:LEU:HD22	26:2:206:LEU:H	1.71	0.52
1:A:152:ASN:O	1:A:152:ASN:ND2	2.41	0.52
1:A:403:GLN:HG3	1:A:440:LEU:HD21	1.92	0.52
1:A:621:ILE:O	1:A:623:PRO:HD2	2.07	0.52
2:B:83:ARG:O	2:B:134:LYS:HA	2.08	0.52
7:G:22:LEU:HD21	7:G:68:TYR:CE2	2.44	0.52
8:H:74:GLU:O	8:H:76:ASN:CA	2.54	0.52
15:O:9:THR:O	15:O:13:ASN:N	2.30	0.52
17:Q:113:ARG:CD	18:R:221:ARG:CG	2.62	0.52
26:2:42:LEU:HD12	26:2:59:MET:HE1	1.92	0.52
26:2:160:LEU:CG	26:2:206:LEU:HD21	2.39	0.52
26:2:171:VAL:CG2	26:2:213:TRP:HA	2.20	0.52
26:2:220:LEU:HD13	26:2:220:LEU:C	2.28	0.52
27:3:10:LEU:HD21	27:3:143:TYR:CD2	2.45	0.52
27:3:21:TRP:O	27:3:24:LYS:HB2	2.09	0.52
27:3:70:LEU:HD22	27:3:114:GLU:HB3	1.91	0.52
2:B:1068:GLN:N	2:B:1073:GLN:O	2.43	0.52
3:C:212:ASP:C	3:C:213:GLU:O	2.43	0.52
20:T:94:THR:HG22	20:T:109:ILE:HG23	1.91	0.52
21:U:194:ARG:HD2	21:U:220:PHE:CE2	2.44	0.52
23:W:52:LEU:HD23	23:W:72:TYR:HE2	1.71	0.52
26:2:30:VAL:O	26:2:34:LEU:HD23	2.09	0.52
1:A:457:ILE:HG21	2:B:1102:PHE:CZ	2.44	0.52
1:A:914:LYS:O	1:A:918:LYS:N	2.38	0.52
1:A:998:PRO:HA	1:A:1059:ARG:NE	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1021:HIS:CE1	2:B:1023:ARG:HB2	2.44	0.52
8:H:28:LEU:HD11	8:H:50:VAL:HG21	1.91	0.52
8:H:40:ILE:HB	8:H:124:ARG:HG2	1.91	0.52
9:I:66:THR:HA	9:I:122:ARG:NH2	2.25	0.52
13:M:127:ARG:HG3	13:M:127:ARG:HH21	1.74	0.52
14:N:360:LEU:HD11	15:O:81:PHE:HD2	1.73	0.52
21:U:230:SER:O	21:U:231:ASP:CB	2.56	0.52
23:W:584:TYR:HB2	23:W:591:GLY:HA3	1.92	0.52
25:1:1:MET:CG	26:2:418:PHE:HB2	2.38	0.52
1:A:1219:LYS:O	1:A:1222:THR:OG1	2.22	0.52
2:B:24:GLU:HA	2:B:27:TRP:HD1	1.74	0.52
2:B:131:THR:C	2:B:132:VAL:HG13	2.28	0.52
2:B:242:ARG:C	2:B:244:GLY:N	2.62	0.52
2:B:455:ASP:O	2:B:457:LYS:N	2.37	0.52
6:F:56:TYR:HE1	6:F:124:ILE:HD12	1.74	0.52
13:M:214:PHE:HB3	13:M:218:PHE:HE2	1.75	0.52
16:P:297:LYS:HA	16:P:297:LYS:HE2	1.87	0.52
24:0:77:LYS:HG2	24:0:225:GLU:OE2	2.09	0.52
25:1:59:GLU:CD	26:2:402:ARG:HH12	2.12	0.52
1:A:641:CYS:SG	1:A:644:SER:OG	2.52	0.52
1:A:876:ASP:HA	6:F:52:ILE:HD13	1.92	0.52
1:A:1243:LEU:HD11	1:A:1259:ILE:HD12	1.91	0.52
2:B:21:LEU:HD21	2:B:635:LEU:HD23	1.90	0.52
2:B:1026:GLU:N	2:B:1041:ILE:O	2.39	0.52
14:N:25:VAL:HB	15:O:36:VAL:HG22	1.91	0.52
17:Q:18:ALA:HA	17:Q:21:VAL:HG22	1.90	0.52
18:R:195:PRO:CB	18:R:199:LYS:CG	2.88	0.52
26:2:86:SER:O	26:2:90:LEU:HD13	2.08	0.52
1:A:410:ASN:OD1	1:A:417:LYS:NZ	2.35	0.52
1:A:817:PRO:HB2	1:A:822:PHE:HB3	1.92	0.52
2:B:75:SER:OG	2:B:78:VAL:CG2	2.50	0.52
2:B:239:MET:SD	2:B:256:ILE:HD13	2.49	0.52
2:B:613:ARG:HD3	2:B:615:TYR:HE2	1.74	0.52
8:H:65:TYR:CE2	8:H:70:LEU:CD2	2.92	0.52
14:N:15:ARG:HA	14:N:18:ILE:HD12	1.91	0.52
17:Q:72:ILE:HD12	17:Q:96:TYR:CD1	2.45	0.52
17:Q:110:MET:SD	18:R:218:LYS:HB2	2.49	0.52
25:1:3:ASN:HB2	26:2:412:PHE:O	2.10	0.52
13:M:23:LEU:HD21	13:M:41:VAL:HG21	1.92	0.52
22:V:520:ARG:CG	25:1:23:LEU:HD11	2.39	0.52
24:0:77:LYS:HD2	24:0:77:LYS:N	2.23	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:199:ALA:HB1	26:2:201:PHE:CD2	2.43	0.52
2:B:40:VAL:HA	2:B:42:GLN:HE22	1.75	0.52
2:B:345:LYS:O	2:B:349:PRO:HG3	2.10	0.52
2:B:711:ILE:HD12	2:B:939:HIS:HA	1.90	0.52
2:B:780:VAL:HG13	2:B:965:ILE:HB	1.90	0.52
3:C:100:GLU:N	3:C:124:SER:OG	2.43	0.52
23:W:428:ILE:HA	23:W:430:ASN:ND2	2.23	0.52
27:3:57:LEU:HD23	27:3:58:ALA:C	2.31	0.52
27:3:100:LYS:HG3	27:3:101:TYR:H	1.74	0.52
27:3:165:LYS:HE3	27:3:200:SER:OG	2.09	0.52
1:A:138:LYS:HE3	1:A:1441:GLU:HG3	1.91	0.52
1:A:405:LEU:HD23	1:A:448:ARG:HB2	1.92	0.52
1:A:600:ILE:HD12	1:A:659:GLU:HB2	1.92	0.52
1:A:1416:ARG:NH2	1:A:1434:GLU:OE2	2.43	0.52
2:B:249:LYS:O	2:B:251:ALA:N	2.42	0.52
2:B:867:ILE:O	2:B:894:THR:N	2.43	0.52
3:C:101:PHE:N	3:C:163:ALA:O	2.27	0.52
14:N:317:GLU:OE2	16:P:235:ARG:HD2	2.10	0.52
17:Q:187:ILE:HG22	18:R:212:VAL:O	2.08	0.52
27:3:42:MET:CG	27:3:111:ILE:HD11	2.40	0.52
1:A:433:PRO:HD3	13:M:35:PRO:O	2.10	0.51
1:A:529:GLN:NE2	1:A:1098:PRO:HD3	2.25	0.51
3:C:151:VAL:HG22	3:C:152:LYS:H	1.75	0.51
8:H:75:TYR:CZ	8:H:77:PRO:HG3	2.44	0.51
8:H:103:GLU:HG2	8:H:109:ALA:HB2	1.92	0.51
14:N:42:LEU:HD11	15:O:15:LEU:HD12	1.91	0.51
14:N:312:GLU:O	14:N:314:LEU:N	2.37	0.51
16:P:167:ASN:HD21	29:Y:79:DT:H1'	1.75	0.51
22:V:531:ILE:O	22:V:534:TYR:CZ	2.63	0.51
22:V:689:VAL:CB	26:2:391:ILE:HD11	2.36	0.51
27:3:204:GLN:HG2	27:3:214:TYR:CZ	2.44	0.51
1:A:432:HIS:HD2	13:M:38:GLY:HA3	1.76	0.51
1:A:674:THR:O	1:A:678:ASN:ND2	2.41	0.51
1:A:879:VAL:O	1:A:887:VAL:N	2.29	0.51
1:A:1139:LEU:N	1:A:1338:THR:O	2.42	0.51
1:A:1162:GLU:OE2	1:A:1224:ARG:NH1	2.42	0.51
2:B:92:TYR:HB2	20:T:145:LEU:HD22	1.90	0.51
2:B:273:PHE:HA	2:B:276:LEU:HD12	1.92	0.51
2:B:331:THR:HG21	2:B:334:LYS:HE2	1.92	0.51
7:G:12:LEU:HG	7:G:63:ARG:NH1	2.26	0.51
13:M:124:MET:HA	13:M:127:ARG:HH22	1.75	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:218:PHE:HD1	13:M:277:ILE:HG22	1.74	0.51
16:P:199:ALA:HB2	16:P:214:PHE:HD1	1.74	0.51
17:Q:113:ARG:HE	18:R:217:GLN:CB	2.23	0.51
17:Q:146:ASP:HB3	17:Q:149:THR:HG22	1.90	0.51
22:V:412:MET:N	22:V:417:THR:HG21	2.25	0.51
23:W:116:CYS:SG	23:W:191:PRO:HD2	2.51	0.51
25:1:18:GLN:CD	25:1:44:PHE:HZ	2.13	0.51
26:2:257:SER:O	26:2:261:PHE:HD1	1.93	0.51
27:3:165:LYS:HD3	27:3:165:LYS:C	2.31	0.51
1:A:381:PRO:HB3	11:K:2:ASN:ND2	2.25	0.51
1:A:604:ARG:HD3	1:A:604:ARG:N	2.25	0.51
1:A:1453:GLY:O	1:A:1457:ASN:ND2	2.44	0.51
2:B:222:ARG:HB3	2:B:232:THR:O	2.09	0.51
2:B:258:ALA:HB2	2:B:269:ILE:HG22	1.93	0.51
2:B:551:GLU:OE1	2:B:551:GLU:N	2.42	0.51
9:I:88:LYS:HD2	9:I:121:HIS:CE1	2.46	0.51
11:K:19:ILE:HA	11:K:35:ILE:HA	1.93	0.51
13:M:263:GLN:HA	13:M:268:LYS:HG2	1.91	0.51
14:N:358:MET:HB2	14:N:365:TYR:HB2	1.92	0.51
20:T:146:ASP:O	20:T:147:LYS:HB3	2.09	0.51
20:T:206:THR:HG21	20:T:213:LEU:HD13	1.92	0.51
22:V:428:GLU:OE1	22:V:460:ALA:HA	2.11	0.51
25:1:8:VAL:CG1	25:1:45:VAL:HG13	2.35	0.51
27:3:10:LEU:HD22	27:3:147:MET:HG2	1.92	0.51
27:3:44:LEU:HD13	27:3:44:LEU:C	2.29	0.51
27:3:133:LEU:HD13	27:3:133:LEU:N	2.14	0.51
27:3:222:SER:HB3	27:3:225:GLN:HG2	1.92	0.51
1:A:696:SER:O	1:A:700:GLN:N	2.36	0.51
1:A:1175:ILE:HB	9:I:54:TYR:HB3	1.93	0.51
2:B:125:TYR:HE1	2:B:148:PHE:HB2	1.76	0.51
2:B:842:HIS:ND1	13:M:25:GLU:O	2.43	0.51
2:B:1137:CYS:HB3	2:B:1142:ASN:HB3	1.91	0.51
5:E:99:ILE:HD11	5:E:102:ALA:HB2	1.93	0.51
13:M:231:ALA:HA	13:M:301:PRO:HG3	1.93	0.51
18:R:89:HIS:CG	18:R:139:PHE:CZ	2.98	0.51
20:T:184:LEU:HA	20:T:187:LEU:HD12	1.92	0.51
22:V:523:VAL:CG2	25:1:20:LEU:CD2	2.86	0.51
22:V:531:ILE:O	22:V:534:TYR:CE2	2.63	0.51
22:V:612:ASP:OD2	22:V:635:GLN:OE1	2.27	0.51
23:W:419:GLU:HB3	23:W:420:PRO:HD2	1.92	0.51
26:2:215:PHE:CE2	26:2:264:HIS:HB2	2.46	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:64:ILE:HG21	27:3:128:HIS:CB	2.40	0.51
1:A:21:VAL:HG23	1:A:1451:MET:SD	2.51	0.51
1:A:551:ARG:HH12	8:H:120:GLY:C	2.14	0.51
2:B:108:MET:SD	2:B:120:TYR:HA	2.51	0.51
8:H:10:PHE:CE1	8:H:32:SER:HB2	2.46	0.51
8:H:65:TYR:CD1	8:H:65:TYR:N	2.79	0.51
14:N:312:GLU:HB2	14:N:313:PRO:HD3	1.93	0.51
14:N:356:GLY:HA3	14:N:367:PHE:CZ	2.46	0.51
15:O:3:TYR:OH	15:O:99:ASP:O	2.24	0.51
26:2:28:PRO:HG3	27:3:33:THR:OG1	2.11	0.51
1:A:583:ARG:NH2	3:C:223:ASN:OD1	2.34	0.51
1:A:926:ASN:ND2	1:A:931:ARG:CD	2.57	0.51
1:A:1204:VAL:O	1:A:1207:ILE:HG12	2.11	0.51
2:B:934:LYS:HE3	2:B:1053:HIS:CG	2.44	0.51
16:P:167:ASN:HB3	16:P:259:VAL:HB	1.92	0.51
17:Q:105:TYR:CZ	18:R:234:GLU:OE2	2.63	0.51
26:2:160:LEU:HB3	26:2:206:LEU:HD21	1.93	0.51
1:A:1127:LEU:HD21	1:A:1378:LEU:HD11	1.93	0.51
2:B:85:LEU:HB3	2:B:131:THR:O	2.10	0.51
2:B:1062:ARG:NH1	2:B:1066:PRO:O	2.43	0.51
4:D:72:SER:O	4:D:142:TYR:OH	2.23	0.51
8:H:65:TYR:HE2	8:H:70:LEU:CB	2.17	0.51
16:P:167:ASN:HB2	29:Y:80:DT:H4'	1.92	0.51
18:R:103:LEU:HD12	18:R:116:LYS:HE3	1.92	0.51
23:W:423:ASP:C	23:W:425:THR:N	2.63	0.51
26:2:57:MET:HA	26:2:60:LEU:CG	2.41	0.51
26:2:77:LYS:CD	26:2:78:GLU:HG3	2.41	0.51
26:2:193:PRO:HB2	26:2:194:PRO:HD3	1.92	0.51
27:3:141:LEU:HG	27:3:187:GLN:HE22	1.75	0.51
1:A:426:ARG:NH1	13:M:40:VAL:HG11	2.26	0.51
1:A:478:PRO:HB3	11:K:4:PRO:CD	2.40	0.51
2:B:566:LYS:NZ	2:B:609:GLU:O	2.43	0.51
2:B:1079:SER:O	13:M:53:ARG:NH2	2.44	0.51
26:2:231:VAL:O	26:2:234:LEU:HB3	2.11	0.51
27:3:12:VAL:HG12	27:3:58:ALA:HB3	1.92	0.51
1:A:909:LEU:HB2	1:A:975:SER:OG	2.11	0.51
1:A:987:ILE:HG12	1:A:1068:LEU:HD21	1.91	0.51
1:A:1435:THR:OG1	1:A:1436:VAL:N	2.42	0.51
2:B:519:ALA:HB1	2:B:523:VAL:HG23	1.93	0.51
3:C:43:PRO:HA	3:C:169:PHE:HB3	1.91	0.51
3:C:101:PHE:HB3	3:C:120:LEU:HD11	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:65:TYR:CE2	8:H:70:LEU:HD22	2.45	0.51
12:L:38:GLU:O	13:M:226:LYS:NZ	2.43	0.51
16:P:277:HIS:O	16:P:281:SER:N	2.42	0.51
17:Q:183:GLN:O	17:Q:186:PRO:HD2	2.11	0.51
22:V:315:VAL:CG1	23:W:500:ASP:HB3	2.26	0.51
26:2:251:VAL:CG1	26:2:254:MET:CB	2.89	0.51
27:3:131:THR:HG23	27:3:133:LEU:HD12	1.92	0.51
1:A:564:LEU:HD22	1:A:570:TRP:CE2	2.45	0.51
1:A:722:ASN:HB2	1:A:724:GLU:HG2	1.93	0.51
2:B:92:TYR:HB3	20:T:145:LEU:CG	2.40	0.51
2:B:425:ARG:HH11	2:B:425:ARG:HG3	1.75	0.51
3:C:20:LYS:HE2	3:C:232:ASN:ND2	2.25	0.51
3:C:58:VAL:CG1	10:J:65:LEU:HD22	2.41	0.51
4:D:86:LEU:O	4:D:89:GLN:HG2	2.10	0.51
5:E:59:THR:HG23	5:E:75:PHE:HA	1.92	0.51
5:E:103:LEU:HA	5:E:128:GLU:HB2	1.93	0.51
16:P:167:ASN:O	16:P:259:VAL:N	2.41	0.51
16:P:291:LEU:N	16:P:304:ILE:O	2.31	0.51
19:S:31:PHE:O	20:T:92:THR:N	2.44	0.51
22:V:393:THR:CA	22:V:418:LYS:HE3	2.41	0.51
26:2:81:LYS:CE	26:2:89:LEU:HD21	2.42	0.51
26:2:236:PHE:CE1	26:2:261:PHE:CB	2.94	0.51
1:A:456:VAL:HG21	1:A:503:LEU:HD11	1.92	0.50
1:A:613:GLU:HG3	21:U:261:PHE:HD1	1.76	0.50
1:A:721:HIS:HA	9:I:108:MET:O	2.11	0.50
2:B:278:PHE:HZ	2:B:359:THR:HG23	1.77	0.50
5:E:27:LEU:N	5:E:64:HIS:HB3	2.18	0.50
12:L:26:ASN:HA	12:L:37:ARG:NH1	2.26	0.50
17:Q:106:LYS:O	18:R:218:LYS:HE3	2.11	0.50
20:T:27:LEU:HD11	20:T:58:LEU:HD21	1.93	0.50
21:U:276:VAL:HG22	21:U:277:GLN:H	1.76	0.50
22:V:516:PRO:CB	25:1:15:ALA:O	2.59	0.50
22:V:689:VAL:CG2	26:2:391:ILE:CD1	2.88	0.50
27:3:121:LYS:HD3	27:3:121:LYS:N	2.25	0.50
1:A:371:PRO:HD2	2:B:788:TYR:CE1	2.46	0.50
2:B:264:LYS:HE3	2:B:326:ALA:HA	1.93	0.50
6:F:70:ALA:HB1	6:F:89:PRO:HB2	1.93	0.50
17:Q:105:TYR:CE1	18:R:234:GLU:HG3	2.45	0.50
1:A:595:ILE:HG22	1:A:668:PHE:CE1	2.46	0.50
2:B:797:ASN:ND2	2:B:954:MET:SD	2.85	0.50
2:B:1028:LEU:HD13	2:B:1041:ILE:HB	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:11:ILE:HB	7:G:68:TYR:HB2	1.93	0.50
20:T:159:HIS:CG	20:T:160:GLN:N	2.79	0.50
22:V:504:LYS:CB	22:V:654:GLU:O	2.59	0.50
23:W:73:CYS:O	23:W:209:TYR:CE2	2.64	0.50
26:2:35:TYR:CD1	26:2:35:TYR:N	2.79	0.50
26:2:199:ALA:HB1	26:2:201:PHE:CE2	2.47	0.50
27:3:64:ILE:CG2	27:3:128:HIS:HB3	2.41	0.50
27:3:107:ALA:O	27:3:111:ILE:HG23	2.11	0.50
27:3:226:TYR:O	27:3:230:VAL:HB	2.10	0.50
1:A:489:THR:HG23	1:A:494:ALA:HB3	1.92	0.50
1:A:500:GLU:OE2	2:B:1058:LYS:HB3	2.12	0.50
2:B:1123:GLY:HA3	2:B:1170:ARG:HB2	1.93	0.50
5:E:150:VAL:HG12	5:E:185:ILE:HD13	1.93	0.50
20:T:93:LEU:HB2	20:T:110:VAL:HB	1.93	0.50
25:1:2:VAL:HG23	25:1:2:VAL:O	2.11	0.50
26:2:28:PRO:HA	27:3:33:THR:HB	1.92	0.50
26:2:51:LEU:CD2	26:2:55:TRP:CD1	2.94	0.50
26:2:236:PHE:CZ	26:2:262:LEU:CD2	2.94	0.50
26:2:245:LEU:HD22	26:2:245:LEU:N	2.27	0.50
27:3:12:VAL:HG23	27:3:12:VAL:O	2.10	0.50
1:A:66:GLU:HB2	1:A:265:VAL:CG2	2.40	0.50
1:A:292:ARG:NH1	1:A:295:GLN:OE1	2.45	0.50
2:B:36:GLU:OE1	2:B:654:GLN:N	2.34	0.50
2:B:568:PHE:CZ	2:B:573:TRP:HD1	2.28	0.50
2:B:884:ASN:OD1	2:B:885:ARG:N	2.44	0.50
2:B:1094:GLN:HG2	2:B:1103:LEU:HB2	1.93	0.50
3:C:172:GLU:HG2	12:L:58:ARG:HH22	1.77	0.50
6:F:44:ARG:HD3	6:F:113:GLY:O	2.12	0.50
8:H:98:ARG:HB3	8:H:115:TYR:HB2	1.93	0.50
11:K:12:LEU:HD21	11:K:18:LYS:HA	1.92	0.50
12:L:25:GLU:CG	12:L:27:GLU:OE2	2.40	0.50
22:V:393:THR:HA	22:V:418:LYS:CG	2.41	0.50
25:1:34:ILE:HG21	25:1:54:GLN:CD	2.31	0.50
27:3:12:VAL:CG2	27:3:161:ILE:HA	2.42	0.50
27:3:144:ILE:HD11	27:3:147:MET:HE3	1.91	0.50
1:A:1317:LYS:HB2	21:U:295:GLY:HA3	1.93	0.50
2:B:205:VAL:HG21	2:B:368:MET:HG3	1.92	0.50
2:B:713:PHE:CD1	2:B:1001:PRO:HA	2.46	0.50
3:C:11:ILE:HG12	11:K:108:ALA:HB1	1.93	0.50
5:E:54:ARG:HA	5:E:57:ASP:HB2	1.93	0.50
13:M:105:ARG:NH1	29:Y:64:DC:O5'	2.43	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:25:PHE:CD1	18:R:210:PHE:HZ	2.30	0.50
17:Q:187:ILE:CG2	18:R:211:SER:C	2.79	0.50
21:U:175:ALA:CB	21:U:222:ARG:NH2	2.63	0.50
26:2:78:GLU:HB3	26:2:81:LYS:HZ1	1.76	0.50
26:2:140:LYS:CG	26:2:162:PHE:CE1	2.94	0.50
27:3:202:LEU:HD22	27:3:202:LEU:N	2.27	0.50
1:A:267:GLN:NE2	1:A:267:GLN:HA	2.27	0.50
1:A:551:ARG:NH1	1:A:637:MET:SD	2.84	0.50
1:A:731:ASN:ND2	21:U:253:THR:CG2	2.70	0.50
2:B:988:LYS:O	2:B:992:ASN:ND2	2.43	0.50
4:D:76:ASN:HB3	4:D:79:THR:HB	1.92	0.50
13:M:222:LEU:HD22	13:M:269:ARG:HG3	1.94	0.50
14:N:333:ASN:HB3	14:N:360:LEU:HA	1.93	0.50
16:P:289:PRO:HB3	29:Y:84:DG:C5'	2.29	0.50
17:Q:106:LYS:HG2	18:R:218:LYS:CG	2.41	0.50
17:Q:113:ARG:HD3	18:R:217:GLN:O	2.10	0.50
17:Q:120:ASP:HB3	17:Q:174:ARG:HG3	1.94	0.50
21:U:188:LYS:O	21:U:192:ARG:HG3	2.11	0.50
23:W:494:ILE:HD11	23:W:680:ALA:HB2	1.93	0.50
25:1:4:VAL:HG12	26:2:411:GLN:C	2.30	0.50
26:2:199:ALA:CB	26:2:201:PHE:CE2	2.95	0.50
27:3:216:LYS:O	27:3:216:LYS:HG2	2.12	0.50
1:A:233:CYS:O	1:A:238:MET:N	2.45	0.50
2:B:157:ARG:HB2	2:B:181:PRO:O	2.12	0.50
2:B:761:THR:H	2:B:764:MET:HE3	1.76	0.50
2:B:1072:ARG:HD3	2:B:1112:ASP:OD1	2.12	0.50
13:M:289:TYR:OH	13:M:314:PRO:O	2.17	0.50
18:R:163:LEU:C	18:R:164:GLY:O	2.49	0.50
23:W:325:THR:HG22	23:W:329:PHE:CE2	2.47	0.50
26:2:211:GLN:CA	26:2:261:PHE:CE1	2.95	0.50
27:3:215:LEU:HD12	27:3:230:VAL:CG2	2.42	0.50
1:A:432:HIS:CE1	1:A:438:LEU:HB2	2.47	0.50
1:A:618:TYR:O	1:A:620:HIS:N	2.44	0.50
2:B:1030:ASN:ND2	2:B:1033:THR:OG1	2.45	0.50
2:B:1075:MET:HB2	2:B:1082:GLY:HA2	1.94	0.50
7:G:12:LEU:HG	7:G:63:ARG:HH11	1.77	0.50
20:T:229:HIS:ND1	28:X:29:DC:O4'	2.45	0.50
26:2:118:LEU:HD21	27:3:39:ASP:OD1	1.95	0.50
26:2:214:TYR:CB	26:2:261:PHE:CE2	2.95	0.50
27:3:10:LEU:CD2	27:3:143:TYR:HE2	2.25	0.50
27:3:18:ASN:O	27:3:21:TRP:CD1	2.63	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:ARG:HD2	2:B:1147:SER:HB3	1.93	0.49
1:A:510:GLU:HA	6:F:67:GLY:HA3	1.94	0.49
1:A:922:PHE:CD1	1:A:1052:ARG:HB2	2.47	0.49
2:B:10:TYR:CE2	2:B:12:GLU:HB3	2.47	0.49
2:B:591:ARG:HG2	2:B:598:VAL:HG12	1.93	0.49
5:E:14:ARG:O	5:E:18:MET:HG2	2.11	0.49
7:G:93:ASN:HD21	17:Q:151:THR:HA	1.76	0.49
13:M:118:PHE:HE1	13:M:142:PHE:HB3	1.77	0.49
17:Q:105:TYR:CB	18:R:234:GLU:HG2	2.41	0.49
18:R:191:PHE:CB	18:R:202:PHE:HE1	2.23	0.49
18:R:195:PRO:HG3	18:R:199:LYS:HB3	1.87	0.49
23:W:624:PRO:O	23:W:656:ALA:HB1	2.12	0.49
25:1:43:VAL:HG12	25:1:44:PHE:N	2.27	0.49
26:2:35:TYR:CD1	26:2:62:LEU:CD1	2.95	0.49
26:2:170:ALA:CB	26:2:213:TRP:CZ3	2.95	0.49
26:2:181:GLN:HE21	26:2:181:GLN:CA	2.23	0.49
26:2:236:PHE:CZ	26:2:258:LEU:CD1	2.95	0.49
27:3:137:LEU:CD1	27:3:177:PHE:CE1	2.95	0.49
27:3:190:LEU:HA	27:3:210:THR:HG21	1.91	0.49
1:A:380:VAL:N	1:A:475:ARG:O	2.37	0.49
1:A:389:THR:HG22	1:A:449:HIS:HA	1.94	0.49
1:A:926:ASN:OD1	1:A:927:GLU:N	2.45	0.49
9:I:88:LYS:HD2	9:I:121:HIS:HE1	1.77	0.49
10:J:7:CYS:HB3	10:J:10:CYS:SG	2.52	0.49
12:L:19:CYS:HB2	12:L:36:CYS:SG	2.53	0.49
18:R:88:ARG:NH2	18:R:93:ASP:HB3	2.27	0.49
22:V:516:PRO:HG2	22:V:706:LYS:HE2	1.92	0.49
26:2:223:ALA:O	26:2:224:GLN:HB3	2.12	0.49
26:2:236:PHE:CE2	26:2:262:LEU:CD1	2.94	0.49
1:A:33:ARG:O	2:B:1138:ARG:HG2	2.11	0.49
1:A:286:ILE:HD13	1:A:313:HIS:HD2	1.77	0.49
1:A:525:ILE:O	1:A:534:VAL:N	2.36	0.49
2:B:166:LEU:HB3	2:B:170:ASP:HB2	1.94	0.49
2:B:1066:PRO:HD3	13:M:30:GLY:HA3	1.94	0.49
3:C:94:CYS:O	3:C:98:SER:N	2.46	0.49
13:M:279:GLY:CA	20:T:153:TYR:HE1	2.25	0.49
14:N:310:GLU:HB3	14:N:313:PRO:HD2	1.93	0.49
14:N:345:SER:N	14:N:348:LYS:O	2.43	0.49
15:O:11:LEU:HG	15:O:40:PHE:HZ	1.77	0.49
18:R:194:ARG:N	18:R:195:PRO:CD	2.54	0.49
20:T:135:SER:O	20:T:137:LYS:HG3	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:35:TYR:CD1	26:2:62:LEU:CG	2.92	0.49
26:2:90:LEU:CD2	26:2:140:LYS:HD3	2.42	0.49
26:2:189:GLU:CA	26:2:192:GLU:HG2	2.41	0.49
26:2:251:VAL:HG11	26:2:254:MET:HB2	1.94	0.49
27:3:177:PHE:CZ	27:3:203:LEU:CD2	2.95	0.49
2:B:89:GLU:OE2	20:T:140:ARG:NH1	2.46	0.49
2:B:936:ALA:O	2:B:1049:GLN:N	2.29	0.49
4:D:19:GLN:HB2	4:D:21:ILE:HG12	1.94	0.49
11:K:109:ILE:HA	11:K:112:LYS:NZ	2.27	0.49
16:P:293:TYR:CD2	16:P:302:LEU:HD13	2.44	0.49
17:Q:105:TYR:CE1	18:R:234:GLU:OE2	2.65	0.49
22:V:667:THR:CA	25:1:62:ASP:OD1	2.59	0.49
23:W:596:LEU:HG	23:W:597:LEU:N	2.27	0.49
23:W:608:ILE:O	23:W:614:TYR:OH	2.21	0.49
27:3:223:LEU:HD13	27:3:223:LEU:C	2.32	0.49
1:A:97:VAL:HG21	1:A:322:LEU:HD11	1.94	0.49
1:A:1223:ASP:OD2	1:A:1224:ARG:NH2	2.44	0.49
1:A:1313:GLN:C	1:A:1315:ASP:N	2.66	0.49
2:B:342:VAL:HG13	2:B:346:GLU:HB2	1.94	0.49
6:F:45:PRO:HD3	6:F:115:TYR:CZ	2.48	0.49
17:Q:188:TYR:N	18:R:212:VAL:HA	2.27	0.49
18:R:177:ASN:HD21	18:R:202:PHE:HE2	1.61	0.49
20:T:162:ASN:O	20:T:165:TYR:HB3	2.13	0.49
26:2:46:ARG:HD3	26:2:85:GLU:HB2	1.93	0.49
26:2:57:MET:HA	26:2:60:LEU:HG	1.94	0.49
27:3:33:THR:CG2	27:3:36:LYS:H	2.04	0.49
1:A:456:VAL:O	1:A:472:HIS:N	2.35	0.49
1:A:581:LYS:HB2	8:H:91:VAL:H	1.77	0.49
1:A:1143:LEU:HB3	1:A:1147:SER:CB	2.42	0.49
1:A:1372:GLU:CD	5:E:195:ARG:HH21	2.15	0.49
2:B:133:ILE:O	2:B:134:LYS:HG3	2.09	0.49
2:B:1142:ASN:ND2	2:B:1145:GLN:HG2	2.28	0.49
8:H:70:LEU:O	8:H:72:ASP:N	2.39	0.49
9:I:28:GLU:OE2	9:I:33:ARG:NH1	2.46	0.49
13:M:169:ARG:HD3	13:M:207:ASP:H	1.77	0.49
18:R:210:PHE:CD1	18:R:210:PHE:C	2.86	0.49
22:V:531:ILE:C	22:V:534:TYR:CE2	2.85	0.49
23:W:419:GLU:HG3	23:W:432:ILE:CG2	2.42	0.49
26:2:118:LEU:HD23	27:3:42:MET:CB	2.35	0.49
26:2:176:ALA:O	26:2:177:GLN:HB2	2.12	0.49
27:3:21:TRP:CG	27:3:34:LEU:HD23	2.48	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:108:ASN:O	27:3:111:ILE:HG12	2.12	0.49
1:A:364:ARG:HG3	1:A:501:MET:O	2.12	0.49
1:A:764:ASN:OD1	1:A:766:PHE:N	2.36	0.49
1:A:1169:VAL:HG22	1:A:1220:HIS:NE2	2.28	0.49
1:A:1319:LYS:HE3	1:A:1331:LEU:HD23	1.95	0.49
2:B:89:GLU:HG3	2:B:90:GLN:H	1.77	0.49
3:C:27:ASP:HB3	3:C:30:VAL:HG23	1.95	0.49
7:G:95:VAL:HG11	17:Q:127:PHE:CZ	2.48	0.49
11:K:56:VAL:HA	11:K:77:THR:HG22	1.95	0.49
11:K:81:TYR:HE2	11:K:86:ALA:HB2	1.78	0.49
24:0:55:LEU:N	27:3:209:ILE:HD11	2.28	0.49
26:2:93:LEU:CD2	26:2:96:TRP:HE1	2.25	0.49
26:2:181:GLN:HE22	26:2:220:LEU:HD12	1.76	0.49
26:2:188:THR:HG23	26:2:189:GLU:N	2.27	0.49
1:A:903:PHE:HA	1:A:978:VAL:HA	1.95	0.49
2:B:418:TYR:OH	2:B:433:LEU:HD23	2.12	0.49
8:H:105:SER:HB2	8:H:108:ALA:HB2	1.93	0.49
22:V:534:TYR:CD1	22:V:534:TYR:C	2.86	0.49
25:1:38:ILE:HG22	25:1:44:PHE:CE1	2.48	0.49
26:2:30:VAL:CB	27:3:25:GLN:CB	2.83	0.49
27:3:12:VAL:HG22	27:3:161:ILE:HA	1.94	0.49
27:3:34:LEU:HD13	27:3:34:LEU:C	2.33	0.49
27:3:187:GLN:O	27:3:188:ASN:HB2	2.12	0.49
27:3:220:MET:N	27:3:221:PRO:HD2	2.28	0.49
1:A:781:ILE:HA	1:A:784:VAL:HG22	1.95	0.49
1:A:802:PHE:HZ	2:B:670:GLU:O	1.96	0.49
1:A:821:GLY:HA2	1:A:838:PHE:CD2	2.48	0.49
1:A:1189:ASP:HA	1:A:1192:TRP:HD1	1.77	0.49
1:A:1310:HIS:CE1	1:A:1334:TRP:HA	2.46	0.49
2:B:763:SER:HA	2:B:766:TYR:CD2	2.47	0.49
2:B:798:ARG:O	2:B:801:VAL:HB	2.13	0.49
2:B:915:GLY:HA3	13:M:133:ASN:OD1	2.13	0.49
3:C:45:ILE:CG1	3:C:79:VAL:HB	2.37	0.49
18:R:196:ASP:OD2	18:R:198:LYS:NZ	2.46	0.49
22:V:370:SER:O	22:V:374:TRP:HD1	1.96	0.49
22:V:634:ARG:HG2	22:V:679:PHE:CZ	2.48	0.49
24:0:209:THR:HA	24:0:219:TYR:CD1	2.48	0.49
26:2:159:VAL:N	26:2:162:PHE:HB3	2.28	0.49
26:2:211:GLN:HE21	26:2:257:SER:HB3	1.78	0.49
26:2:426:ARG:HD2	26:2:444:THR:CG2	2.43	0.49
27:3:166:ALA:O	27:3:198:SER:HB2	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:527:THR:N	1:A:532:ARG:O	2.36	0.49
1:A:540:ASP:HB3	1:A:680:LEU:HD21	1.94	0.49
1:A:922:PHE:HB3	1:A:1052:ARG:HD2	1.95	0.49
2:B:835:GLU:OE1	2:B:835:GLU:N	2.45	0.49
3:C:210:GLU:O	3:C:213:GLU:HB2	2.13	0.49
4:D:44:ARG:HD2	4:D:47:GLN:OE1	2.12	0.49
8:H:62:SER:HA	8:H:141:VAL:HA	1.93	0.49
13:M:279:GLY:CA	20:T:153:TYR:CE1	2.96	0.49
18:R:192:VAL:HG12	18:R:201:LEU:O	2.13	0.49
18:R:195:PRO:CB	18:R:199:LYS:CD	2.89	0.49
22:V:516:PRO:HB3	25:1:15:ALA:O	2.13	0.49
22:V:523:VAL:HB	25:1:20:LEU:HD23	1.92	0.49
23:W:608:ILE:HG23	23:W:614:TYR:CZ	2.48	0.49
26:2:77:LYS:HD3	26:2:78:GLU:HG3	1.94	0.49
27:3:12:VAL:CG2	27:3:161:ILE:HG23	2.43	0.49
1:A:432:HIS:HE2	1:A:438:LEU:HD13	1.77	0.48
1:A:597:PRO:HB2	1:A:660:MET:HE3	1.94	0.48
1:A:642:LYS:NZ	21:U:283:GLU:HA	2.28	0.48
2:B:249:LYS:HE3	2:B:249:LYS:HB3	1.46	0.48
2:B:956:PHE:HD2	2:B:960:GLY:HA2	1.77	0.48
8:H:105:SER:O	8:H:106:THR:HB	2.12	0.48
13:M:107:MET:HB2	13:M:112:ARG:NH1	2.28	0.48
17:Q:124:ARG:HG2	17:Q:126:SER:H	1.76	0.48
20:T:155:PRO:C	20:T:157:ALA:H	2.14	0.48
23:W:285:TYR:CE1	23:W:403:PHE:CZ	3.01	0.48
27:3:10:LEU:CD2	27:3:143:TYR:CE2	2.95	0.48
1:A:65:ILE:HD11	1:A:258:LEU:HB2	1.95	0.48
1:A:987:ILE:HG23	1:A:1060:LEU:HD11	1.95	0.48
1:A:1162:GLU:HA	1:A:1308:TYR:CE2	2.47	0.48
1:A:1304:ILE:HG22	1:A:1340:GLY:HA3	1.95	0.48
1:A:1372:GLU:OE1	5:E:193:ILE:HG21	2.13	0.48
2:B:57:ARG:O	2:B:61:ASP:N	2.46	0.48
2:B:867:ILE:HB	2:B:894:THR:HB	1.94	0.48
2:B:1003:ASN:ND2	2:B:1007:ASN:OD1	2.42	0.48
12:L:17:TYR:CB	12:L:46:LYS:CA	2.90	0.48
23:W:37:HIS:NE2	23:W:454:VAL:CG1	2.76	0.48
25:1:38:ILE:CG2	25:1:44:PHE:CE1	2.96	0.48
26:2:89:LEU:HD23	26:2:93:LEU:HG	1.94	0.48
26:2:159:VAL:HG22	26:2:160:LEU:HD13	1.95	0.48
26:2:179:LEU:CB	26:2:184:LEU:HD11	2.40	0.48
26:2:234:LEU:HD23	26:2:234:LEU:C	2.34	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:3:60:ILE:HG22	27:3:61:ALA:N	2.26	0.48
27:3:217:VAL:CG1	27:3:226:TYR:CE2	2.95	0.48
1:A:1031:ARG:HA	1:A:1034:GLN:HB3	1.94	0.48
2:B:573:TRP:HZ2	2:B:576:ILE:HG23	1.78	0.48
2:B:848:LEU:HD23	2:B:852:GLY:HA2	1.95	0.48
2:B:1163:MET:HA	2:B:1167:ILE:O	2.13	0.48
3:C:105:VAL:HG12	3:C:159:LEU:HB3	1.95	0.48
3:C:266:GLU:O	3:C:270:ASP:HB2	2.14	0.48
5:E:149:VAL:HB	5:E:192:LYS:HE2	1.95	0.48
9:I:57:LYS:HE2	9:I:60:HIS:CE1	2.48	0.48
11:K:40:HIS:CE1	11:K:63:VAL:H	2.31	0.48
13:M:40:VAL:C	13:M:42:GLY:H	2.17	0.48
13:M:117:ALA:O	13:M:121:ILE:N	2.46	0.48
13:M:295:ARG:NH2	13:M:298:ASP:OD2	2.45	0.48
17:Q:123:ASN:O	17:Q:123:ASN:ND2	2.45	0.48
18:R:210:PHE:HD1	18:R:210:PHE:C	2.16	0.48
26:2:178:LEU:HD12	26:2:178:LEU:N	2.28	0.48
26:2:218:GLN:HG2	26:2:268:PHE:CB	2.44	0.48
27:3:59:VAL:HG13	27:3:59:VAL:O	2.12	0.48
27:3:160:ARG:HE	27:3:190:LEU:HG	1.78	0.48
27:3:174:TYR:HD1	27:3:202:LEU:HD11	1.78	0.48
1:A:14:PRO:HG2	1:A:16:ARG:NH1	2.29	0.48
1:A:613:GLU:CG	21:U:261:PHE:HD1	2.26	0.48
1:A:798:ILE:O	1:A:820:ARG:NE	2.46	0.48
1:A:1220:HIS:HA	1:A:1223:ASP:HB3	1.94	0.48
2:B:209:ALA:HB1	2:B:211:LYS:HG3	1.96	0.48
2:B:294:ASP:OD2	2:B:379:ARG:NH2	2.44	0.48
2:B:837:CYS:HB3	2:B:840:MET:HE3	1.95	0.48
3:C:134:ASN:OD1	3:C:135:ARG:N	2.46	0.48
5:E:28:VAL:HG13	5:E:32:GLU:OE1	2.13	0.48
17:Q:187:ILE:C	18:R:212:VAL:CA	2.80	0.48
19:S:49:ARG:HB3	19:S:96:GLN:HB3	1.95	0.48
21:U:225:ALA:HB3	21:U:228:MET:HG2	1.95	0.48
23:W:73:CYS:HB2	23:W:209:TYR:CE1	2.48	0.48
26:2:166:SER:HB3	26:2:167:PRO:CD	2.43	0.48
2:B:26:CYS:O	2:B:29:VAL:HB	2.13	0.48
3:C:262:GLN:O	3:C:266:GLU:HG2	2.14	0.48
13:M:178:LYS:O	20:T:154:LYS:HB2	1.94	0.48
16:P:206:GLU:OE2	16:P:206:GLU:HA	2.12	0.48
17:Q:106:LYS:CB	18:R:218:LYS:HE2	2.43	0.48
18:R:129:LYS:C	18:R:140:LYS:CB	2.72	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:170:ASP:OD1	18:R:180:LYS:NZ	2.34	0.48
1:A:345:GLY:O	1:A:351:ARG:HB3	2.13	0.48
1:A:1191:GLU:HG2	9:I:1:MET:SD	2.54	0.48
2:B:75:SER:O	2:B:78:VAL:N	2.47	0.48
2:B:675:LEU:HD21	2:B:697:GLU:OE2	2.13	0.48
2:B:1068:GLN:O	2:B:1072:ARG:N	2.45	0.48
6:F:108:ARG:HB2	6:F:116:GLU:HG3	1.96	0.48
17:Q:25:PHE:CD1	18:R:210:PHE:CZ	3.01	0.48
17:Q:71:PHE:HA	17:Q:100:VAL:CG2	2.40	0.48
19:S:127:PHE:HB2	20:T:19:TRP:CB	2.43	0.48
21:U:145:ARG:NE	21:U:173:GLU:OE1	2.34	0.48
25:1:38:ILE:CG2	25:1:44:PHE:CD1	2.94	0.48
26:2:35:TYR:CE2	26:2:62:LEU:CB	2.96	0.48
26:2:89:LEU:CD2	26:2:93:LEU:HG	2.44	0.48
26:2:203:PHE:CE2	26:2:205:LEU:CD2	2.96	0.48
1:A:140:ARG:NH1	1:A:234:PHE:O	2.47	0.48
1:A:156:GLY:HA2	1:A:181:HIS:CE1	2.49	0.48
2:B:562:ALA:O	2:B:610:ARG:NH2	2.38	0.48
6:F:86:GLU:N	6:F:86:GLU:OE1	2.47	0.48
7:G:97:LEU:HD13	7:G:128:TYR:CD2	2.48	0.48
12:L:38:GLU:HG2	12:L:39:CYS:N	2.27	0.48
15:O:76:LEU:HD13	15:O:95:ILE:HD12	1.95	0.48
17:Q:166:SER:OG	17:Q:170:LYS:HB3	2.14	0.48
18:R:89:HIS:ND1	18:R:139:PHE:CE1	2.81	0.48
25:1:38:ILE:HA	25:1:44:PHE:CD1	2.37	0.48
1:A:330:GLN:CB	13:M:107:MET:SD	2.88	0.48
1:A:927:GLU:O	1:A:931:ARG:HB2	2.14	0.48
1:A:981:CYS:SG	1:A:1075:LYS:HB3	2.54	0.48
2:B:97:THR:HG22	2:B:107:PRO:HA	1.95	0.48
4:D:124:ASP:HA	4:D:127:LEU:HB3	1.96	0.48
5:E:106:VAL:HG23	5:E:129:GLN:HE22	1.78	0.48
24:0:77:LYS:HA	24:0:77:LYS:HE3	1.94	0.48
25:1:5:LEU:HD11	26:2:408:LEU:CB	2.11	0.48
25:1:34:ILE:HG22	25:1:46:ILE:CG1	2.44	0.48
25:1:38:ILE:HD13	25:1:38:ILE:N	2.26	0.48
1:A:71:CYS:O	1:A:75:ALA:N	2.47	0.48
1:A:253:LEU:HD12	1:A:254:PRO:HD2	1.96	0.48
1:A:660:MET:HB3	1:A:664:ILE:HB	1.94	0.48
1:A:817:PRO:HB2	1:A:822:PHE:CB	2.42	0.48
2:B:932:GLY:N	2:B:945:CYS:O	2.37	0.48
5:E:41:LYS:O	5:E:46:ASP:N	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:107:GLU:OE1	8:H:107:GLU:HA	2.13	0.48
8:H:108:ALA:O	8:H:109:ALA:C	2.52	0.48
10:J:30:THR:HG22	10:J:33:ASP:H	1.78	0.48
12:L:22:CYS:HB3	12:L:39:CYS:CB	2.40	0.48
16:P:169:VAL:HB	16:P:257:ASN:HB3	1.96	0.48
16:P:261:SER:CB	29:Y:81:DA:H4'	2.43	0.48
24:0:98:GLN:OE1	27:3:209:ILE:CA	2.60	0.48
26:2:60:LEU:CD1	26:2:95:ILE:CG2	2.91	0.48
26:2:133:THR:HG23	26:2:134:SER:N	2.28	0.48
26:2:221:GLN:CD	26:2:230:LEU:HB2	2.34	0.48
26:2:251:VAL:HG11	26:2:254:MET:CB	2.43	0.48
1:A:198:LEU:HB3	1:A:216:LEU:HD12	1.95	0.48
1:A:921:ARG:HB2	1:A:956:PHE:CZ	2.48	0.48
1:A:1310:HIS:N	21:U:252:LYS:NZ	2.59	0.48
1:A:1430:CYS:HB2	1:A:1435:THR:HA	1.96	0.48
2:B:10:TYR:HE2	2:B:12:GLU:HB3	1.79	0.48
2:B:198:GLU:O	2:B:488:PRO:HD3	2.14	0.48
2:B:438:ARG:HA	2:B:441:SER:HB2	1.96	0.48
2:B:1029:TYR:CE1	2:B:1036:LYS:HG2	2.48	0.48
3:C:33:SER:O	3:C:37:VAL:HG23	2.14	0.48
7:G:14:HIS:HB3	7:G:17:TYR:CD2	2.49	0.48
7:G:97:LEU:HD13	7:G:128:TYR:HD2	1.79	0.48
14:N:345:SER:O	14:N:347:ASN:N	2.43	0.48
22:V:519:TYR:HE2	25:1:20:LEU:CG	2.19	0.48
23:W:70:LEU:HG	23:W:72:TYR:CE1	2.49	0.48
23:W:73:CYS:HB3	23:W:209:TYR:CG	2.48	0.48
23:W:430:ASN:CB	23:W:431:PRO:CD	2.85	0.48
24:0:165:ARG:HB2	24:0:193:LYS:O	2.14	0.48
27:3:216:LYS:O	27:3:218:PRO:HD3	2.14	0.48
1:A:913:ASN:OD1	1:A:967:ARG:NH2	2.47	0.47
1:A:959:MET:HE1	1:A:1047:SER:HA	1.95	0.47
2:B:956:PHE:CD2	2:B:960:GLY:HA2	2.49	0.47
2:B:1130:THR:HB	2:B:1134:THR:N	2.29	0.47
3:C:16:ASP:HA	3:C:240:ARG:HG3	1.96	0.47
6:F:45:PRO:HA	6:F:115:TYR:O	2.14	0.47
13:M:244:LEU:HD11	13:M:295:ARG:HD3	1.95	0.47
17:Q:55:ASP:HB3	17:Q:58:GLN:HB2	1.96	0.47
20:T:138:PRO:O	20:T:141:LEU:HG	2.13	0.47
22:V:394:SER:CB	22:V:416:THR:O	2.59	0.47
26:2:30:VAL:CG2	26:2:34:LEU:HD23	2.41	0.47
27:3:195:VAL:HG23	27:3:214:TYR:CE1	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:101:VAL:O	1:A:105:LYS:HG3	2.14	0.47
1:A:702:ILE:HG23	1:A:752:THR:HB	1.96	0.47
5:E:39:GLU:O	5:E:43:GLN:N	2.40	0.47
17:Q:126:SER:HB2	17:Q:136:PHE:O	2.14	0.47
18:R:224:THR:HG23	18:R:230:GLU:CB	2.41	0.47
22:V:361:CYS:HB3	22:V:405:VAL:HG21	1.96	0.47
22:V:428:GLU:OE1	22:V:428:GLU:HA	2.13	0.47
23:W:73:CYS:HB3	23:W:209:TYR:CD1	2.50	0.47
25:1:9:LEU:N	25:1:9:LEU:HD12	2.29	0.47
27:3:34:LEU:HD13	27:3:38:ILE:HG12	1.96	0.47
27:3:131:THR:HG23	27:3:133:LEU:HD13	1.95	0.47
1:A:376:ASP:OD2	1:A:473:ARG:NE	2.47	0.47
1:A:465:HIS:CE1	1:A:467:MET:HB2	2.50	0.47
1:A:551:ARG:CG	1:A:625:ASP:OD1	2.62	0.47
1:A:637:MET:CG	8:H:122:LEU:HD21	2.44	0.47
1:A:1313:GLN:HB3	1:A:1333:GLU:HG2	1.95	0.47
2:B:780:VAL:HG21	2:B:1048:TYR:CE2	2.50	0.47
2:B:1040:GLN:HG2	3:C:203:TRP:CZ2	2.48	0.47
5:E:52:ARG:HA	5:E:53:PRO:HD3	1.69	0.47
9:I:25:TYR:N	9:I:38:ALA:O	2.40	0.47
12:L:18:ILE:HB	12:L:45:TYR:HB3	1.96	0.47
16:P:180:LEU:HA	16:P:183:ILE:HD12	1.96	0.47
16:P:299:ARG:HA	16:P:299:ARG:HD2	1.49	0.47
20:T:138:PRO:C	20:T:140:ARG:N	2.68	0.47
21:U:218:ASP:O	21:U:222:ARG:NE	2.35	0.47
22:V:413:LEU:HA	28:X:56:DA:C5'	2.44	0.47
22:V:528:LYS:HD3	29:Y:36:DA:H4'	1.96	0.47
23:W:419:GLU:HG3	23:W:432:ILE:HG23	1.96	0.47
26:2:30:VAL:CG2	26:2:34:LEU:CD2	2.91	0.47
26:2:42:LEU:HD22	26:2:52:ALA:HA	1.95	0.47
27:3:226:TYR:CA	27:3:230:VAL:HG23	2.42	0.47
28:X:15:DA:H2"	28:X:16:DA:C8	2.49	0.47
1:A:775:LYS:HB3	2:B:974:SER:HB3	1.95	0.47
2:B:309:PHE:HE2	9:I:25:TYR:CE2	2.32	0.47
5:E:20:LEU:HD12	5:E:182:TYR:CE1	2.49	0.47
7:G:52:ASP:H	7:G:72:TYR:HA	1.79	0.47
15:O:64:THR:OG1	15:O:75:VAL:HB	2.14	0.47
16:P:207:PRO:CB	16:P:229:GLN:OE1	2.62	0.47
21:U:174:GLU:O	21:U:178:GLN:N	2.42	0.47
26:2:203:PHE:CD2	26:2:204:LEU:N	2.82	0.47
29:Y:59:DG:H2"	29:Y:60:DA:C8	2.50	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:HIS:CD2	1:A:207:GLU:HG2	2.50	0.47
1:A:592:PHE:CE2	1:A:596:ILE:HD11	2.49	0.47
2:B:273:PHE:CD1	2:B:284:ILE:HG23	2.49	0.47
2:B:388:TYR:HE1	2:B:502:HIS:HB3	1.80	0.47
5:E:173:ILE:N	5:E:208:LEU:O	2.41	0.47
11:K:35:ILE:HB	11:K:71:ILE:CG1	2.44	0.47
17:Q:109:HIS:O	18:R:221:ARG:NE	2.35	0.47
17:Q:154:CYS:SG	17:Q:155:THR:N	2.88	0.47
25:1:53:LEU:H	25:1:53:LEU:CD1	2.26	0.47
26:2:85:GLU:O	26:2:89:LEU:HB2	2.14	0.47
27:3:10:LEU:HA	27:3:56:LYS:HG2	1.96	0.47
27:3:160:ARG:HB2	27:3:190:LEU:HG	1.96	0.47
29:Y:30:DG:N2	29:Y:31:DG:N3	2.62	0.47
1:A:111:CYS:HA	1:A:188:GLN:NE2	2.29	0.47
1:A:478:PRO:HB3	11:K:4:PRO:HD2	1.96	0.47
1:A:621:ILE:HA	1:A:623:PRO:CD	2.41	0.47
2:B:497:LYS:H	2:B:498:PRO:CD	1.85	0.47
2:B:1028:LEU:HB2	2:B:1041:ILE:HD13	1.95	0.47
6:F:52:ILE:HG21	6:F:110:LEU:HD21	1.97	0.47
8:H:112:LEU:HB3	8:H:131:ASN:HD21	1.80	0.47
27:3:70:LEU:HD22	27:3:114:GLU:CB	2.44	0.47
29:Y:34:DC:H2'	29:Y:35:DG:C8	2.50	0.47
1:A:616:GLY:O	1:A:619:LYS:HB2	2.15	0.47
1:A:625:ASP:CA	1:A:637:MET:HE2	2.44	0.47
1:A:662:HIS:NE2	6:F:127:ASP:OD2	2.28	0.47
1:A:868:MET:HB2	1:A:1092:ALA:HB2	1.95	0.47
2:B:274:ARG:NH2	2:B:312:GLN:OE1	2.45	0.47
2:B:626:LEU:HG	2:B:698:ILE:HD13	1.95	0.47
2:B:936:ALA:HA	2:B:942:LYS:HA	1.95	0.47
3:C:169:PHE:HZ	11:K:10:PHE:CZ	2.32	0.47
5:E:188:GLY:HA2	5:E:208:LEU:HD21	1.97	0.47
6:F:80:MET:HG3	6:F:103:PRO:HD3	1.97	0.47
6:F:99:ALA:O	6:F:100:ARG:HG2	2.15	0.47
12:L:25:GLU:O	12:L:37:ARG:NH1	2.47	0.47
17:Q:69:ASP:CA	18:R:225:VAL:CG2	2.92	0.47
23:W:73:CYS:CB	23:W:209:TYR:CE1	2.97	0.47
24:0:54:ARG:CG	27:3:182:PHE:CZ	2.80	0.47
25:1:45:VAL:HG21	26:2:409:TYR:CE2	2.50	0.47
26:2:46:ARG:CD	26:2:85:GLU:CB	2.93	0.47
26:2:84:GLU:OE1	26:2:84:GLU:HA	2.15	0.47
26:2:163:MET:HE2	26:2:206:LEU:CD1	2.42	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:236:PHE:HE2	26:2:262:LEU:CD1	2.27	0.47
27:3:8:LEU:HD23	27:3:54:SER:CB	2.42	0.47
27:3:34:LEU:HD22	27:3:37:CYS:SG	2.54	0.47
27:3:53:ARG:HA	27:3:101:TYR:HE1	1.78	0.47
27:3:56:LYS:HD3	27:3:56:LYS:N	2.30	0.47
1:A:391:ALA:HB2	1:A:447:GLU:HG2	1.97	0.47
2:B:551:GLU:HB3	2:B:556:ILE:HD13	1.96	0.47
2:B:604:ILE:O	2:B:613:ARG:N	2.44	0.47
9:I:96:PHE:HD2	9:I:110:LEU:HD22	1.79	0.47
14:N:332:GLU:HB3	15:O:92:LYS:HE2	1.97	0.47
17:Q:191:LEU:HD21	18:R:212:VAL:CG1	2.32	0.47
19:S:42:TRP:CD1	19:S:102:VAL:HG11	2.50	0.47
23:W:37:HIS:CG	23:W:454:VAL:HG13	2.50	0.47
25:1:38:ILE:O	25:1:38:ILE:HG12	2.15	0.47
26:2:35:TYR:CD2	26:2:62:LEU:CB	2.95	0.47
26:2:205:LEU:HD22	26:2:205:LEU:N	2.29	0.47
26:2:236:PHE:CD1	26:2:261:PHE:HB3	2.49	0.47
27:3:15:VAL:HG12	27:3:164:ILE:HD12	1.97	0.47
27:3:137:LEU:HD11	27:3:177:PHE:CE1	2.50	0.47
2:B:539:SER:HA	2:B:542:LEU:HB3	1.97	0.47
2:B:1036:LYS:HB2	3:C:194:HIS:CB	2.43	0.47
3:C:8:THR:H	3:C:25:ASN:HB3	1.80	0.47
5:E:71:GLN:O	5:E:100:THR:OG1	2.25	0.47
17:Q:110:MET:HB3	18:R:218:LYS:CG	2.24	0.47
17:Q:191:LEU:HD22	18:R:212:VAL:HB	1.97	0.47
19:S:10:ASN:O	20:T:47:LYS:HB2	2.15	0.47
20:T:161:TYR:O	20:T:164:GLU:HB3	2.15	0.47
21:U:184:ASP:O	21:U:188:LYS:HG3	2.14	0.47
26:2:217:LEU:CD2	26:2:233:ILE:HD11	2.45	0.47
1:A:1290:SER:OG	2:B:250:SER:C	2.53	0.47
2:B:685:LYS:HA	2:B:688:ALA:HB2	1.97	0.47
3:C:7:PRO:O	3:C:8:THR:C	2.52	0.47
3:C:24:GLU:HG2	3:C:228:ARG:HA	1.97	0.47
6:F:108:ARG:HB2	6:F:116:GLU:CG	2.45	0.47
17:Q:188:TYR:CD2	17:Q:192:ARG:HB2	2.49	0.47
18:R:195:PRO:HG2	18:R:199:LYS:CB	2.17	0.47
25:1:22:TYR:O	25:1:25:GLU:HB3	2.14	0.47
26:2:93:LEU:CA	26:2:96:TRP:CD1	2.94	0.47
27:3:58:ALA:C	27:3:71:TYR:OH	2.52	0.47
1:A:426:ARG:O	13:M:39:LEU:CA	2.55	0.46
1:A:427:ILE:HG23	13:M:38:GLY:CA	2.45	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:601:ASN:ND2	1:A:632:ASN:H	2.09	0.46
1:A:848:ILE:HD13	2:B:499:ARG:HG3	1.97	0.46
3:C:53:ASP:N	3:C:160:ARG:O	2.48	0.46
10:J:67:LYS:NZ	12:L:23:HIS:O	2.47	0.46
11:K:99:SER:O	11:K:103:GLU:HG3	2.15	0.46
15:O:4:GLN:OE1	15:O:4:GLN:N	2.43	0.46
16:P:297:LYS:CE	16:P:297:LYS:CA	2.88	0.46
17:Q:104:LYS:HZ2	18:R:238:LYS:CD	2.25	0.46
17:Q:104:LYS:NZ	18:R:238:LYS:CE	2.78	0.46
23:W:584:TYR:CD1	23:W:594:ALA:CB	2.87	0.46
23:W:623:VAL:HG23	23:W:681:ASP:HB2	1.98	0.46
25:1:10:ILE:HG12	25:1:43:VAL:CG1	2.45	0.46
25:1:53:LEU:O	25:1:57:VAL:HG12	2.15	0.46
26:2:51:LEU:HD21	26:2:55:TRP:CD1	2.50	0.46
27:3:24:LYS:HE2	27:3:196:LEU:HB3	1.97	0.46
1:A:74:CYS:HA	2:B:1129:ASN:O	2.15	0.46
1:A:924:TYR:CD1	1:A:949:GLN:NE2	2.81	0.46
2:B:242:ARG:HB3	2:B:252:ILE:HG23	1.96	0.46
2:B:455:ASP:C	2:B:457:LYS:H	2.18	0.46
20:T:137:LYS:HB3	20:T:138:PRO:HD2	1.97	0.46
22:V:366:ASN:HD22	22:V:613:THR:CG2	2.14	0.46
22:V:413:LEU:HD11	28:X:55:DC:O4'	2.15	0.46
23:W:408:SER:C	23:W:409:THR:HG22	2.35	0.46
25:1:11:GLU:HG2	26:2:404:THR:OG1	2.14	0.46
25:1:45:VAL:CG2	26:2:409:TYR:CE2	2.98	0.46
26:2:96:TRP:CZ2	26:2:97:HIS:NE2	2.83	0.46
26:2:189:GLU:CB	26:2:190:PRO:HD3	2.43	0.46
27:3:124:ILE:O	27:3:127:GLN:HB2	2.14	0.46
27:3:177:PHE:O	27:3:181:ILE:HG13	2.15	0.46
1:A:520:MET:HB3	1:A:522:PRO:HD2	1.97	0.46
1:A:1371:ILE:HD11	1:A:1406:THR:HG22	1.98	0.46
2:B:46:SER:HB2	2:B:395:LEU:HD23	1.96	0.46
2:B:1132:THR:HG23	2:B:1133:HIS:CD2	2.50	0.46
9:I:12:VAL:HG11	9:I:15:ARG:NH2	2.31	0.46
13:M:15:CYS:HB2	13:M:18:HIS:O	2.15	0.46
13:M:48:VAL:O	13:M:52:TRP:N	2.48	0.46
14:N:32:ASP:HB3	14:N:34:VAL:HG23	1.98	0.46
14:N:349:TRP:HH2	16:P:191:GLU:OE2	1.98	0.46
18:R:89:HIS:CG	18:R:139:PHE:HZ	2.34	0.46
25:1:38:ILE:CB	25:1:44:PHE:CE1	2.98	0.46
1:A:18:ILE:HD11	1:A:1460:LEU:CD2	2.46	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:60:PRO:HG2	1:A:62:GLN:HB3	1.97	0.46
1:A:76:GLY:HA3	2:B:1131:ARG:NH2	2.31	0.46
1:A:452:ASP:HA	1:A:474:VAL:HG23	1.97	0.46
1:A:609:HIS:N	1:A:610:PRO:HD2	2.31	0.46
2:B:239:MET:HE3	2:B:256:ILE:HD13	1.90	0.46
2:B:1061:SER:HA	2:B:1084:LEU:HD11	1.96	0.46
2:B:1114:TYR:CD1	2:B:1153:TYR:HB2	2.51	0.46
3:C:4:ALA:HB1	11:K:97:GLU:OE1	2.14	0.46
6:F:56:TYR:HD1	6:F:124:ILE:HB	1.81	0.46
8:H:50:VAL:HG13	8:H:56:PHE:CZ	2.51	0.46
10:J:35:LEU:HB3	10:J:46:ARG:HD2	1.98	0.46
17:Q:25:PHE:CB	18:R:215:GLU:OE2	2.63	0.46
20:T:174:LYS:CG	28:X:20:DG:H4'	2.45	0.46
23:W:581:LEU:C	23:W:581:LEU:HD13	2.36	0.46
25:1:1:MET:CE	26:2:415:GLN:C	2.84	0.46
25:1:54:GLN:O	25:1:57:VAL:HG12	2.16	0.46
26:2:29:GLY:N	27:3:25:GLN:CB	2.76	0.46
27:3:64:ILE:CG2	27:3:128:HIS:CG	2.99	0.46
27:3:165:LYS:HZ1	27:3:200:SER:N	2.12	0.46
1:A:384:ILE:O	1:A:388:MET:N	2.43	0.46
1:A:1468:THR:O	6:F:64:ARG:NH2	2.42	0.46
2:B:172:CYS:HB2	10:J:62:TYR:CG	2.51	0.46
2:B:386:ASP:HB3	2:B:502:HIS:HD2	1.80	0.46
2:B:1130:THR:N	2:B:1134:THR:O	2.48	0.46
7:G:95:VAL:HG11	17:Q:127:PHE:HZ	1.79	0.46
13:M:10:LEU:H	13:M:11:PRO:HD3	1.36	0.46
13:M:118:PHE:CE1	13:M:142:PHE:HB3	2.51	0.46
14:N:318:ASP:HB2	16:P:239:ARG:NH2	2.28	0.46
16:P:268:ILE:HD13	16:P:332:LEU:HG	1.98	0.46
18:R:205:ASP:HA	18:R:206:LYS:HB2	1.96	0.46
23:W:657:MET:O	23:W:660:ALA:HB3	2.15	0.46
25:1:1:MET:CG	26:2:413:LEU:CB	2.68	0.46
25:1:18:GLN:OE1	25:1:19:PHE:CD1	2.68	0.46
26:2:90:LEU:HD21	26:2:140:LYS:HD3	1.98	0.46
26:2:100:LEU:HD11	26:2:119:ARG:CG	2.31	0.46
26:2:201:PHE:CD1	26:2:202:GLN:N	2.83	0.46
26:2:214:TYR:CE1	26:2:233:ILE:HG23	2.51	0.46
27:3:10:LEU:CD1	27:3:56:LYS:HG2	2.44	0.46
1:A:408:ARG:HH11	1:A:414:PRO:HB2	1.79	0.46
2:B:75:SER:HG	2:B:78:VAL:HG22	1.76	0.46
2:B:752:TYR:HE1	2:B:809:VAL:CG2	2.29	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:910:THR:HB	12:L:43:ILE:HD13	1.98	0.46
3:C:14:LEU:HB3	3:C:19:VAL:HG23	1.98	0.46
3:C:54:ALA:HB3	3:C:160:ARG:HB2	1.97	0.46
17:Q:185:GLU:O	17:Q:189:ALA:N	2.48	0.46
17:Q:187:ILE:HG23	18:R:212:VAL:O	1.96	0.46
22:V:615:PHE:O	22:V:642:ARG:NH2	2.48	0.46
26:2:28:PRO:C	27:3:25:GLN:C	2.74	0.46
26:2:198:SER:OG	26:2:238:PHE:HE2	1.96	0.46
27:3:165:LYS:NZ	27:3:200:SER:H	2.12	0.46
1:A:357:LYS:HE3	2:B:1073:GLN:HG2	1.98	0.46
1:A:432:HIS:NE2	1:A:438:LEU:HD13	2.31	0.46
1:A:923:ASP:C	1:A:925:THR:H	2.19	0.46
1:A:994:PHE:CZ	1:A:1064:ALA:HA	2.50	0.46
2:B:425:ARG:HD3	2:B:427:LYS:HD2	1.98	0.46
2:B:451:GLY:HA2	2:B:467:SER:HB3	1.97	0.46
2:B:1066:PRO:HB2	2:B:1075:MET:HG3	1.98	0.46
6:F:116:GLU:HG3	6:F:118:TRP:HE1	1.81	0.46
19:S:26:TYR:HB2	19:S:139:PRO:O	2.16	0.46
21:U:291:CYS:N	21:U:296:ASN:O	2.36	0.46
26:2:187:SER:OG	26:2:190:PRO:HD2	2.16	0.46
27:3:21:TRP:HA	27:3:24:LYS:CG	2.45	0.46
1:A:527:THR:HG22	1:A:532:ARG:O	2.16	0.46
1:A:788:VAL:HB	1:A:823:VAL:HB	1.98	0.46
2:B:939:HIS:CD2	2:B:980:HIS:HA	2.50	0.46
5:E:122:ALA:HB3	5:E:125:TYR:HB3	1.98	0.46
9:I:73:SER:HB2	9:I:115:THR:OG1	2.15	0.46
17:Q:110:MET:O	17:Q:113:ARG:HB3	2.16	0.46
19:S:109:LYS:HD2	19:S:149:LEU:HD23	1.97	0.46
20:T:142:SER:C	20:T:144:GLN:H	2.19	0.46
22:V:519:TYR:HA	22:V:522:TYR:HB3	1.98	0.46
27:3:121:LYS:HD3	27:3:121:LYS:H	1.81	0.46
1:A:364:ARG:HB2	1:A:502:ASN:OD1	2.16	0.46
2:B:29:VAL:HG22	2:B:643:LEU:HD11	1.98	0.46
2:B:63:PRO:HG2	2:B:64:PRO:HD3	1.97	0.46
2:B:520:VAL:C	2:B:522:LEU:H	2.19	0.46
2:B:1093:CYS:O	2:B:1097:HIS:N	2.48	0.46
3:C:6:GLN:HG2	3:C:25:ASN:HD21	1.76	0.46
3:C:117:SER:HB2	3:C:130:VAL:HG11	1.98	0.46
18:R:190:LEU:O	18:R:203:PHE:N	2.49	0.46
20:T:172:ASP:OD1	20:T:173:GLY:N	2.48	0.46
22:V:609:LYS:HD2	29:Y:38:DT:OP1	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
26:2:96:TRP:CH2	26:2:97:HIS:CE1	3.03	0.46
27:3:10:LEU:HB2	27:3:56:LYS:HE3	1.98	0.46
1:A:63:GLY:HA3	1:A:258:LEU:HD23	1.98	0.46
1:A:625:ASP:HA	1:A:637:MET:CE	2.46	0.46
2:B:26:CYS:O	2:B:30:ILE:HG13	2.16	0.46
2:B:89:GLU:HB3	2:B:127:ASP:HB3	1.98	0.46
2:B:573:TRP:CH2	2:B:575:GLY:HA2	2.51	0.46
5:E:56:THR:OG1	5:E:78:GLU:OE2	2.32	0.46
8:H:117:SER:HA	8:H:121:LEU:O	2.16	0.46
9:I:81:THR:HG22	9:I:94:ALA:O	2.16	0.46
13:M:177:PHE:O	13:M:181:CYS:N	2.38	0.46
13:M:185:ARG:HA	20:T:158:ASN:HB2	1.98	0.46
16:P:237:TYR:O	16:P:240:VAL:CG2	2.64	0.46
17:Q:69:ASP:CA	18:R:225:VAL:HG22	2.46	0.46
20:T:30:GLN:O	20:T:62:LEU:HD11	2.16	0.46
22:V:408:SER:HB3	22:V:418:LYS:HB3	1.98	0.46
25:1:2:VAL:HG12	26:2:456:LYS:CE	2.43	0.46
1:A:385:ALA:HB2	1:A:476:ILE:HD12	1.97	0.45
1:A:625:ASP:HA	1:A:637:MET:HE3	1.97	0.45
1:A:909:LEU:HD13	1:A:973:GLY:HA2	1.98	0.45
2:B:175:ASN:HA	10:J:62:TYR:CD2	2.51	0.45
2:B:1062:ARG:NH2	2:B:1074:PRO:HB3	2.31	0.45
16:P:161:ILE:O	16:P:162:VAL:C	2.55	0.45
21:U:133:ALA:HB2	21:U:167:GLU:HG3	1.98	0.45
25:1:22:TYR:HD1	25:1:23:LEU:HD23	1.80	0.45
27:3:144:ILE:HD13	27:3:147:MET:HE3	1.97	0.45
29:Y:66:DC:H2"	29:Y:67:DC:C6	2.50	0.45
1:A:51:ARG:H	1:A:52:PRO:HD2	1.81	0.45
1:A:452:ASP:CG	1:A:476:ILE:HG12	2.36	0.45
1:A:721:HIS:O	9:I:109:ARG:HA	2.16	0.45
1:A:930:LEU:HD11	8:H:107:GLU:OE2	2.16	0.45
1:A:1036:ASN:OD1	1:A:1037:ALA:N	2.49	0.45
2:B:254:GLN:NE2	2:B:300:MET:SD	2.74	0.45
2:B:834:ARG:HA	2:B:840:MET:SD	2.55	0.45
5:E:72:MET:HG3	5:E:101:ARG:HB2	1.97	0.45
7:G:165:ASP:HB2	7:G:168:LEU:HD11	1.98	0.45
9:I:25:TYR:HD2	9:I:40:ARG:HG3	1.81	0.45
9:I:56:ASN:CG	9:I:57:LYS:H	2.20	0.45
17:Q:12:ALA:O	17:Q:15:LYS:HB2	2.15	0.45
17:Q:18:ALA:O	17:Q:22:ILE:HG23	2.15	0.45
17:Q:106:LYS:CG	18:R:218:LYS:HG2	2.44	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:57:VAL:HG13	25:1:58:GLY:N	2.31	0.45
26:2:130:SER:HB2	26:2:179:LEU:HD23	1.99	0.45
27:3:10:LEU:N	27:3:56:LYS:HE3	2.31	0.45
27:3:69:PHE:HE1	27:3:139:LYS:HD2	1.77	0.45
1:A:75:ALA:C	2:B:1131:ARG:HH21	2.19	0.45
1:A:427:ILE:HG23	13:M:38:GLY:C	2.37	0.45
1:A:923:ASP:C	1:A:925:THR:N	2.68	0.45
2:B:125:TYR:HE2	20:T:148:VAL:O	1.99	0.45
2:B:128:ILE:HB	2:B:145:GLN:HB2	1.98	0.45
2:B:295:PRO:O	2:B:299:GLU:HG2	2.16	0.45
2:B:845:TYR:OH	2:B:891:ASP:OD1	2.33	0.45
6:F:44:ARG:HB3	6:F:114:SER:HA	1.97	0.45
13:M:268:LYS:O	13:M:269:ARG:NH1	2.37	0.45
14:N:343:HIS:O	14:N:350:LYS:N	2.36	0.45
20:T:197:TYR:HB2	20:T:202:LEU:HD21	1.98	0.45
20:T:198:ASN:OD1	20:T:199:LEU:N	2.50	0.45
22:V:550:PHE:CZ	22:V:554:ARG:NH2	2.84	0.45
26:2:35:TYR:HB2	26:2:62:LEU:HD12	1.98	0.45
26:2:203:PHE:CD2	26:2:205:LEU:CD2	2.95	0.45
27:3:60:ILE:HG23	27:3:68:ARG:O	2.17	0.45
27:3:69:PHE:HZ	27:3:139:LYS:HB3	1.73	0.45
1:A:551:ARG:NH1	1:A:637:MET:CE	2.79	0.45
1:A:956:PHE:HA	1:A:959:MET:HB2	1.99	0.45
2:B:68:GLN:HA	2:B:83:ARG:HA	1.98	0.45
2:B:631:GLN:O	2:B:683:GLN:HG2	2.16	0.45
8:H:2:ALA:O	8:H:4:ILE:N	2.50	0.45
8:H:10:PHE:CE2	8:H:58:LEU:HD13	2.52	0.45
11:K:64:PRO:HD2	11:K:70:LYS:O	2.16	0.45
23:W:37:HIS:CD2	23:W:454:VAL:CG1	3.00	0.45
25:1:1:MET:HE3	26:2:415:GLN:N	2.32	0.45
25:1:4:VAL:CG1	26:2:412:PHE:HD2	2.19	0.45
25:1:40:ASP:HB2	25:1:43:VAL:H	1.81	0.45
26:2:117:ASN:CG	27:3:42:MET:HE1	2.25	0.45
26:2:211:GLN:CB	26:2:261:PHE:CE1	2.95	0.45
27:3:196:LEU:HB3	27:3:220:MET:SD	2.56	0.45
1:A:478:PRO:HB2	1:A:479:TRP:CE3	2.52	0.45
1:A:611:ASP:HB3	1:A:617:PRO:CG	2.47	0.45
1:A:1137:PRO:HA	1:A:1360:ASN:HD21	1.80	0.45
2:B:384:ASP:OD2	2:B:387:HIS:N	2.49	0.45
7:G:116:GLU:O	7:G:130:THR:HA	2.16	0.45
13:M:105:ARG:NH1	29:Y:64:DC:H3'	2.31	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
13:M:123:THR:O	13:M:127:ARG:NH2	2.50	0.45
14:N:25:VAL:HG11	15:O:36:VAL:HG13	1.99	0.45
14:N:318:ASP:CA	16:P:239:ARG:NE	2.79	0.45
16:P:264:VAL:HG23	16:P:266:PHE:H	1.81	0.45
20:T:23:VAL:HG21	20:T:31:TRP:CZ3	2.51	0.45
21:U:136:THR:OG1	21:U:141:ARG:NH1	2.49	0.45
22:V:321:GLU:CG	23:W:499:ASN:ND2	2.76	0.45
27:3:64:ILE:HG21	27:3:128:HIS:HB3	1.97	0.45
27:3:69:PHE:HZ	27:3:139:LYS:HD2	1.81	0.45
1:A:431:PHE:HD2	13:M:33:ILE:HG21	1.82	0.45
1:A:1030:SER:O	1:A:1034:GLN:N	2.41	0.45
1:A:1310:HIS:NE2	1:A:1334:TRP:HE3	2.14	0.45
2:B:795:ILE:HG12	2:B:947:ILE:HG22	1.99	0.45
2:B:1029:TYR:CD1	2:B:1036:LYS:HG2	2.51	0.45
19:S:172:ASN:OD1	19:S:173:HIS:N	2.50	0.45
21:U:299:LYS:HB2	21:U:301:CYS:O	2.17	0.45
26:2:100:LEU:CG	26:2:119:ARG:HE	2.22	0.45
26:2:117:ASN:HB2	27:3:104:LEU:CG	2.47	0.45
26:2:217:LEU:CD2	26:2:233:ILE:CD1	2.95	0.45
26:2:240:LEU:HD12	26:2:240:LEU:N	2.30	0.45
1:A:84:HIS:N	1:A:257:PRO:HB3	2.32	0.45
1:A:514:GLU:OE1	2:B:1099:ALA:HB1	2.17	0.45
1:A:902:GLU:O	1:A:979:LEU:N	2.34	0.45
1:A:1301:ILE:O	1:A:1304:ILE:HG12	2.17	0.45
1:A:1479:LYS:HD3	6:F:103:PRO:HA	1.99	0.45
2:B:281:ASP:CG	9:I:22:ASN:HD22	2.20	0.45
2:B:738:THR:OG1	10:J:62:TYR:OH	2.23	0.45
2:B:881:GLU:HA	2:B:883:THR:OG1	2.16	0.45
3:C:11:ILE:HA	3:C:21:PHE:CB	2.46	0.45
7:G:60:GLN:HB2	7:G:63:ARG:NE	2.32	0.45
7:G:107:PHE:O	7:G:160:ILE:HG13	2.17	0.45
8:H:57:ARG:O	8:H:145:MET:HA	2.17	0.45
8:H:98:ARG:HD3	8:H:115:TYR:CD2	2.48	0.45
10:J:3:ILE:HD13	10:J:18:TRP:CB	2.47	0.45
16:P:329:TYR:N	16:P:330:PRO:HD2	2.32	0.45
18:R:202:PHE:O	18:R:203:PHE:CE1	2.63	0.45
25:1:2:VAL:HG12	26:2:456:LYS:HG2	1.81	0.45
26:2:117:ASN:CA	27:3:104:LEU:HD21	2.47	0.45
1:A:426:ARG:CB	13:M:40:VAL:HG22	2.38	0.45
1:A:1085:GLU:OE1	6:F:60:TYR:OH	2.28	0.45
2:B:856:PRO:HD3	12:L:46:LYS:HD3	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:46:ILE:HD11	7:G:77:PHE:HB2	1.99	0.45
12:L:16:ILE:CG1	12:L:27:GLU:C	2.79	0.45
16:P:297:LYS:HE2	16:P:297:LYS:CA	2.46	0.45
17:Q:145:PHE:HA	17:Q:152:PHE:HA	1.98	0.45
18:R:156:ASP:O	18:R:158:HIS:N	2.50	0.45
20:T:95:VAL:O	20:T:106:LEU:HD12	2.17	0.45
27:3:64:ILE:CG2	27:3:128:HIS:CB	2.94	0.45
27:3:148:ASN:ND2	27:3:157:MET:HG3	2.32	0.45
2:B:66:ASP:HB3	2:B:85:LEU:HD13	1.99	0.45
2:B:75:SER:O	2:B:78:VAL:CG2	2.65	0.45
2:B:193:VAL:HG11	2:B:481:HIS:CD2	2.52	0.45
2:B:201:ALA:HA	2:B:392:ARG:HG2	1.98	0.45
2:B:626:LEU:HA	2:B:662:VAL:HG12	1.98	0.45
2:B:640:ILE:HA	2:B:643:LEU:HD12	1.98	0.45
20:T:199:LEU:HD13	20:T:233:TRP:NE1	2.31	0.45
22:V:315:VAL:CG1	23:W:500:ASP:CG	2.80	0.45
22:V:689:VAL:CG2	26:2:391:ILE:HD13	2.46	0.45
23:W:37:HIS:NE2	23:W:454:VAL:HG11	2.32	0.45
26:2:203:PHE:CG	26:2:204:LEU:N	2.84	0.45
27:3:219:GLN:OE1	27:3:219:GLN:HA	2.17	0.45
1:A:548:PHE:HE2	1:A:592:PHE:HB2	1.81	0.45
1:A:909:LEU:HD22	1:A:1328:PHE:CZ	2.51	0.45
1:A:1178:ASP:OD1	1:A:1184:THR:HA	2.16	0.45
1:A:1241:ASP:O	1:A:1262:MET:HG3	2.17	0.45
2:B:876:ASN:OD1	2:B:879:GLU:OE2	2.35	0.45
5:E:134:GLU:CD	5:E:181:ARG:HH12	2.20	0.45
21:U:229:ALA:HB1	21:U:234:LYS:HB3	1.99	0.45
26:2:94:ARG:HD2	26:2:95:ILE:CD1	2.47	0.45
26:2:117:ASN:ND2	27:3:108:ASN:N	2.65	0.45
26:2:251:VAL:HG11	26:2:254:MET:SD	2.56	0.45
26:2:258:LEU:HG	26:2:262:LEU:HD21	1.99	0.45
27:3:42:MET:CG	27:3:111:ILE:CD1	2.95	0.45
27:3:100:LYS:HB3	27:3:103:LEU:CD1	2.38	0.45
1:A:902:GLU:N	1:A:979:LEU:O	2.48	0.44
2:B:369:VAL:O	2:B:373:LEU:N	2.41	0.44
2:B:674:MET:HB2	9:I:77:THR:HG22	1.98	0.44
2:B:862:GLY:O	2:B:898:THR:HA	2.18	0.44
13:M:107:MET:CE	13:M:107:MET:CA	2.94	0.44
16:P:301:VAL:HG11	28:X:14:DA:H5”	1.98	0.44
17:Q:55:ASP:O	17:Q:59:LEU:N	2.42	0.44
19:S:29:MET:HB2	20:T:96:PHE:CD1	2.52	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
25:1:1:MET:SD	26:2:413:LEU:CB	3.03	0.44
26:2:123:LEU:CD2	26:2:178:LEU:CD1	2.95	0.44
1:A:404:GLU:OE1	1:A:407:ARG:HD2	2.17	0.44
1:A:431:PHE:HB2	13:M:33:ILE:HG21	1.99	0.44
1:A:556:GLU:HG3	1:A:559:GLU:H	1.82	0.44
1:A:1022:ILE:HG12	1:A:1034:GLN:OE1	2.17	0.44
1:A:1361:ASP:OD2	1:A:1364:GLU:HG2	2.16	0.44
2:B:84:TYR:HA	2:B:132:VAL:CG1	2.47	0.44
2:B:93:LEU:HD23	2:B:160:TYR:CE2	2.52	0.44
2:B:385:ARG:HD2	2:B:497:LYS:HE3	1.99	0.44
2:B:780:VAL:HG21	2:B:1048:TYR:HE2	1.81	0.44
2:B:939:HIS:HE2	2:B:983:GLU:HB2	1.82	0.44
2:B:1117:HIS:CE1	2:B:1148:LEU:HD13	2.51	0.44
4:D:83:VAL:HG13	4:D:134:ILE:HG12	1.99	0.44
5:E:104:ILE:HG23	5:E:129:GLN:NE2	2.32	0.44
8:H:71:ASP:OD1	8:H:71:ASP:N	2.50	0.44
10:J:63:ALA:CB	10:J:64:PRO:HD3	2.32	0.44
12:L:13:GLN:O	12:L:29:LYS:HD3	2.17	0.44
18:R:155:LEU:HD11	18:R:203:PHE:HA	1.98	0.44
20:T:165:TYR:O	20:T:169:LYS:HG2	2.17	0.44
21:U:177:TYR:CE1	21:U:181:ARG:HA	2.52	0.44
22:V:370:SER:O	22:V:374:TRP:CD1	2.71	0.44
26:2:159:VAL:HG12	26:2:161:HIS:HB2	1.99	0.44
28:X:57:DC:H2"	28:X:58:DT:C7	2.46	0.44
1:A:361:PHE:N	2:B:1062:ARG:O	2.50	0.44
1:A:894:ASP:OD1	1:A:1396:ARG:NH2	2.50	0.44
1:A:972:THR:O	1:A:1317:LYS:HD3	2.17	0.44
2:B:99:TRP:HB2	13:M:129:ASN:ND2	2.32	0.44
11:K:105:PHE:O	11:K:109:ILE:HG12	2.17	0.44
16:P:212:LEU:O	16:P:219:MET:HA	2.18	0.44
17:Q:135:THR:HG23	17:Q:164:ASP:OD1	2.18	0.44
26:2:61:PHE:CE1	26:2:99:GLN:NE2	2.85	0.44
26:2:81:LYS:CG	26:2:82:ALA:N	2.79	0.44
26:2:171:VAL:HG13	26:2:216:MET:HB3	1.98	0.44
26:2:206:LEU:CD2	26:2:206:LEU:H	2.31	0.44
26:2:236:PHE:HZ	26:2:258:LEU:HD11	1.82	0.44
1:A:283:ILE:HA	1:A:286:ILE:HG12	2.00	0.44
1:A:578:ALA:N	1:A:585:LEU:O	2.51	0.44
1:A:636:ILE:O	1:A:637:MET:SD	2.76	0.44
2:B:629:GLU:N	2:B:632:LYS:O	2.41	0.44
5:E:192:LYS:HA	5:E:206:TYR:HD1	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:G:60:GLN:HB2	7:G:63:ARG:HE	1.82	0.44
9:I:96:PHE:HA	9:I:111:TYR:O	2.18	0.44
13:M:138:THR:HG23	13:M:163:CYS:HB3	1.99	0.44
14:N:29:PHE:CE1	15:O:36:VAL:HG21	2.52	0.44
16:P:294:ARG:HH21	16:P:294:ARG:HG3	1.82	0.44
20:T:223:GLN:HB3	20:T:233:TRP:CE3	2.52	0.44
22:V:321:GLU:OE2	23:W:500:ASP:CA	2.59	0.44
26:2:28:PRO:CB	27:3:33:THR:OG1	2.65	0.44
26:2:214:TYR:OH	26:2:265:LEU:HD13	2.18	0.44
27:3:144:ILE:O	27:3:144:ILE:HD13	2.18	0.44
27:3:160:ARG:CB	27:3:190:LEU:CD2	2.95	0.44
1:A:579:ILE:HD12	1:A:585:LEU:HD12	1.99	0.44
1:A:931:ARG:C	1:A:933:THR:H	2.19	0.44
2:B:11:ASP:HB2	2:B:638:ARG:HD3	2.00	0.44
2:B:21:LEU:HD23	2:B:633:LEU:HD23	2.00	0.44
2:B:134:LYS:HG3	2:B:136:GLY:H	1.83	0.44
2:B:627:ILE:HA	2:B:695:HIS:CD2	2.53	0.44
2:B:888:THR:O	2:B:890:ARG:HG2	2.17	0.44
2:B:905:ASP:OD2	2:B:922:ARG:NE	2.44	0.44
3:C:37:VAL:HG12	3:C:248:ALA:HB1	1.99	0.44
5:E:71:GLN:NE2	5:E:97:GLU:HG3	2.32	0.44
6:F:53:THR:HB	6:F:108:ARG:HH11	1.83	0.44
8:H:76:ASN:OD1	8:H:78:THR:OG1	2.33	0.44
20:T:146:ASP:C	20:T:147:LYS:CG	2.75	0.44
22:V:519:TYR:CE2	22:V:523:VAL:HG21	2.53	0.44
23:W:73:CYS:CB	23:W:209:TYR:CE2	3.00	0.44
27:3:22:TRP:O	27:3:25:GLN:CG	2.55	0.44
27:3:33:THR:CG2	27:3:36:LYS:CB	2.95	0.44
1:A:551:ARG:CZ	1:A:637:MET:HE1	2.48	0.44
2:B:109:MET:CE	2:B:174:LEU:HB3	2.47	0.44
2:B:318:LEU:HD13	2:B:336:ILE:HG23	1.99	0.44
2:B:655:ASP:HA	2:B:658:ALA:HB3	2.00	0.44
2:B:663:GLU:OE2	2:B:695:HIS:NE2	2.51	0.44
2:B:888:THR:O	2:B:890:ARG:N	2.50	0.44
3:C:101:PHE:HA	3:C:121:ILE:O	2.18	0.44
3:C:211:LEU:O	3:C:213:GLU:N	2.51	0.44
4:D:44:ARG:HB2	4:D:61:PHE:CZ	2.53	0.44
7:G:84:VAL:HG12	7:G:144:ARG:HD3	1.98	0.44
8:H:65:TYR:CE1	8:H:70:LEU:HD22	2.53	0.44
9:I:17:CYS:O	9:I:21:ASN:N	2.46	0.44
16:P:174:LEU:O	16:P:249:LYS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
18:R:154:LEU:HD21	18:R:162:GLY:O	2.15	0.44
22:V:516:PRO:CA	25:1:15:ALA:C	2.76	0.44
22:V:534:TYR:HE1	22:V:535:THR:OG1	2.00	0.44
23:W:73:CYS:HB3	23:W:209:TYR:CD2	2.52	0.44
24:0:60:HIS:CE1	24:0:159:MET:SD	3.11	0.44
25:1:1:MET:HG2	26:2:413:LEU:CB	2.44	0.44
26:2:56:VAL:HG23	26:2:57:MET:N	2.32	0.44
26:2:127:LYS:CA	26:2:178:LEU:HD23	2.48	0.44
26:2:140:LYS:CD	26:2:162:PHE:HE1	2.29	0.44
27:3:178:MET:CE	27:3:202:LEU:CD1	2.95	0.44
1:A:607:SER:O	21:U:301:CYS:HA	2.17	0.44
1:A:1199:MET:O	1:A:1201:ASP:N	2.51	0.44
2:B:198:GLU:OE1	2:B:487:SER:OG	2.33	0.44
2:B:242:ARG:C	2:B:252:ILE:HG23	2.21	0.44
8:H:94:GLY:HA3	8:H:118:TYR:HA	1.98	0.44
21:U:225:ALA:CB	21:U:228:MET:HG2	2.48	0.44
22:V:405:VAL:HG12	22:V:406:ALA:H	1.82	0.44
23:W:143:ARG:HH11	23:W:143:ARG:CG	2.31	0.44
26:2:35:TYR:CD1	26:2:62:LEU:HD12	2.52	0.44
26:2:164:VAL:HG13	26:2:209:PRO:CG	2.45	0.44
26:2:189:GLU:HB2	26:2:190:PRO:CD	2.43	0.44
1:A:129:ILE:CD1	1:A:140:ARG:HA	2.48	0.44
1:A:367:ILE:HD13	1:A:494:ALA:HB1	1.99	0.44
1:A:395:THR:OG1	1:A:398:ASN:OD1	2.31	0.44
2:B:133:ILE:C	2:B:134:LYS:CG	2.84	0.44
2:B:1056:ASP:OD1	2:B:1056:ASP:N	2.51	0.44
3:C:74:ILE:HG22	3:C:129:PRO:O	2.17	0.44
6:F:68:THR:O	6:F:72:GLN:HG3	2.17	0.44
8:H:39:LEU:HA	8:H:124:ARG:O	2.17	0.44
9:I:97:PHE:O	9:I:111:TYR:N	2.47	0.44
9:I:99:SER:OG	9:I:105:GLU:HG2	2.08	0.44
9:I:102:ALA:O	9:I:104:ALA:N	2.50	0.44
14:N:337:CYS:O	15:O:97:ALA:HA	2.17	0.44
15:O:64:THR:HG22	16:P:188:ARG:HB3	2.00	0.44
16:P:289:PRO:CB	29:Y:84:DG:H5'	2.32	0.44
17:Q:45:GLU:OE1	17:Q:94:ILE:N	2.43	0.44
17:Q:188:TYR:HD1	18:R:212:VAL:HB	1.83	0.44
18:R:160:GLN:C	18:R:162:GLY:H	2.21	0.44
20:T:17:GLY:HA2	20:T:109:ILE:O	2.17	0.44
21:U:216:PRO:HD2	21:U:219:LEU:HD23	1.99	0.44
22:V:531:ILE:CG1	22:V:534:TYR:HE2	2.31	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:W:59:TYR:CE2	23:W:62:ALA:HB2	2.22	0.44
23:W:189:TRP:CE3	23:W:190:CYS:N	2.86	0.44
25:1:25:GLU:OE2	25:1:35:ILE:HG12	2.18	0.44
1:A:349:ARG:O	1:A:353:ASN:HB2	2.17	0.44
1:A:875:TYR:HE1	1:A:1470:CYS:SG	2.40	0.44
1:A:908:THR:C	1:A:910:LYS:H	2.21	0.44
1:A:1014:LYS:O	1:A:1018:LYS:HG3	2.18	0.44
2:B:280:SER:HB3	9:I:21:ASN:HB2	1.99	0.44
3:C:241:PRO:HA	3:C:244:ILE:HD12	2.00	0.44
20:T:223:GLN:HB3	20:T:233:TRP:CD2	2.52	0.44
21:U:150:ALA:HA	21:U:153:ARG:NH1	2.33	0.44
21:U:176:ILE:HG22	21:U:187:TYR:CD2	2.53	0.44
22:V:518:PHE:CD1	22:V:713:LEU:HD13	2.53	0.44
22:V:519:TYR:HB3	25:1:16:MET:HG3	2.00	0.44
23:W:28:LEU:HD13	23:W:28:LEU:C	2.38	0.44
26:2:34:LEU:N	26:2:34:LEU:HD22	2.33	0.44
26:2:140:LYS:HD3	26:2:162:PHE:CE1	2.47	0.44
26:2:203:PHE:HD2	26:2:205:LEU:H	1.65	0.44
1:A:30:GLU:O	1:A:34:MET:N	2.35	0.43
1:A:64:VAL:HB	1:A:70:ARG:O	2.18	0.43
1:A:636:ILE:O	1:A:637:MET:HG2	2.17	0.43
1:A:1031:ARG:O	1:A:1035:GLU:N	2.42	0.43
1:A:1310:HIS:CA	21:U:252:LYS:CD	2.95	0.43
2:B:249:LYS:C	2:B:251:ALA:H	2.21	0.43
2:B:602:SER:O	2:B:614:ILE:HG23	2.18	0.43
2:B:746:THR:O	2:B:812:ARG:HA	2.18	0.43
4:D:96:GLU:OE2	4:D:117:SER:OG	2.22	0.43
6:F:51:ARG:HD3	6:F:118:TRP:CZ2	2.53	0.43
8:H:50:VAL:HG13	8:H:56:PHE:HZ	1.83	0.43
15:O:48:LEU:HD23	15:O:52:VAL:HG21	2.00	0.43
17:Q:106:LYS:HG2	18:R:218:LYS:CD	2.48	0.43
17:Q:123:ASN:O	17:Q:125:ALA:N	2.50	0.43
17:Q:202:GLU:O	17:Q:203:ILE:CB	2.65	0.43
18:R:163:LEU:O	18:R:164:GLY:C	2.56	0.43
19:S:47:LEU:HG	19:S:98:TRP:CE3	2.53	0.43
20:T:225:VAL:HG23	20:T:227:GLY:H	1.83	0.43
22:V:409:THR:H	22:V:418:LYS:CB	2.31	0.43
22:V:446:ILE:HD12	22:V:451:PHE:HB3	1.99	0.43
22:V:647:LYS:O	22:V:648:LYS:O	2.35	0.43
26:2:215:PHE:CE2	26:2:264:HIS:ND1	2.86	0.43
27:3:71:TYR:CG	27:3:71:TYR:O	2.70	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:932:ARG:HA	1:A:932:ARG:HD2	1.61	0.43
2:B:37:LYS:HE2	2:B:653:TRP:HD1	1.80	0.43
2:B:169:ARG:HA	2:B:172:CYS:SG	2.57	0.43
2:B:654:GLN:O	2:B:658:ALA:N	2.39	0.43
2:B:979:GLY:HA2	2:B:982:ILE:HD12	2.00	0.43
2:B:1030:ASN:OD1	2:B:1031:GLY:N	2.51	0.43
5:E:192:LYS:HG3	5:E:206:TYR:CE1	2.54	0.43
7:G:49:THR:H	7:G:74:ALA:HA	1.82	0.43
9:I:84:HIS:CD2	9:I:84:HIS:N	2.84	0.43
17:Q:191:LEU:HD22	18:R:212:VAL:HG12	1.97	0.43
18:R:141:PRO:HG2	18:R:142:LYS:H	1.83	0.43
18:R:158:HIS:CE1	18:R:206:LYS:HD3	2.53	0.43
19:S:46:ARG:N	19:S:101:ARG:O	2.38	0.43
19:S:143:TRP:NE1	19:S:145:ASN:OD1	2.37	0.43
24:0:106:ILE:HD11	24:0:127:HIS:HB3	2.00	0.43
25:1:18:GLN:HG3	25:1:19:PHE:H	1.83	0.43
25:1:34:ILE:CG2	25:1:50:VAL:HG11	2.48	0.43
1:A:43:TYR:O	1:A:45:GLU:N	2.51	0.43
1:A:219:GLU:O	1:A:223:GLU:HG2	2.18	0.43
1:A:1184:THR:HG22	1:A:1190:GLN:HA	2.00	0.43
2:B:161:CYS:O	2:B:164:ASN:ND2	2.51	0.43
2:B:309:PHE:CD2	9:I:40:ARG:HD2	2.54	0.43
2:B:845:TYR:CE2	2:B:865:VAL:HG11	2.53	0.43
2:B:970:HIS:C	2:B:973:PRO:HD2	2.39	0.43
8:H:106:THR:C	8:H:108:ALA:N	2.71	0.43
9:I:97:PHE:HD1	9:I:98:GLN:O	2.00	0.43
14:N:327:GLU:OE1	16:P:188:ARG:NH1	2.51	0.43
14:N:363:ARG:NH2	15:O:86:GLU:OE2	2.51	0.43
16:P:174:LEU:HD22	16:P:248:ALA:HB1	2.00	0.43
20:T:196:TYR:HD1	20:T:232:THR:HG21	1.83	0.43
26:2:117:ASN:HD21	27:3:108:ASN:N	2.16	0.43
26:2:270:LEU:HA	26:2:273:GLN:HG3	2.00	0.43
27:3:160:ARG:HE	27:3:160:ARG:HB2	1.58	0.43
1:A:20:ARG:HE	2:B:1174:VAL:C	2.22	0.43
1:A:28:PRO:HB3	1:A:251:THR:OG1	2.18	0.43
1:A:137:PRO:HB3	1:A:237:GLY:CA	2.45	0.43
1:A:456:VAL:HG12	1:A:505:LEU:HD13	2.00	0.43
1:A:621:ILE:CG2	1:A:623:PRO:HD3	2.44	0.43
2:B:68:GLN:HG3	2:B:82:PRO:O	2.19	0.43
2:B:84:TYR:HA	2:B:132:VAL:HG12	1.99	0.43
2:B:431:LEU:O	2:B:435:ILE:HG12	2.17	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H:56:PHE:CE1	8:H:148:LEU:HA	2.54	0.43
9:I:84:HIS:CG	9:I:85:PRO:CD	2.84	0.43
13:M:279:GLY:CA	20:T:153:TYR:OH	2.67	0.43
15:O:57:ASN:OD1	15:O:58:PHE:N	2.51	0.43
17:Q:32:LEU:HD11	18:R:203:PHE:HD2	1.68	0.43
21:U:266:CYS:O	21:U:267:LYS:HG2	2.18	0.43
22:V:282:LYS:HE3	22:V:482:PHE:CD1	2.54	0.43
26:2:35:TYR:CG	26:2:62:LEU:CD1	2.99	0.43
26:2:47:GLU:HG3	26:2:48:LEU:H	1.83	0.43
26:2:117:ASN:ND2	27:3:104:LEU:O	2.52	0.43
1:A:457:ILE:CG2	1:A:504:HIS:HB2	2.48	0.43
1:A:910:LYS:HB3	1:A:963:ARG:HH12	1.83	0.43
1:A:1018:LYS:O	1:A:1021:VAL:HG23	2.17	0.43
1:A:1151:ALA:HB2	1:A:1334:TRP:CZ2	2.53	0.43
1:A:1345:ARG:O	1:A:1349:GLU:HG2	2.19	0.43
1:A:1369:LEU:HD23	5:E:139:ILE:HB	2.00	0.43
2:B:360:LYS:HA	2:B:363:TYR:HD2	1.82	0.43
2:B:454:GLY:HA3	2:B:459:ALA:O	2.18	0.43
2:B:736:TYR:CD2	2:B:737:ILE:HG12	2.54	0.43
2:B:1036:LYS:HG3	3:C:186:TYR:OH	2.18	0.43
15:O:60:GLY:O	15:O:76:LEU:HD23	2.18	0.43
16:P:303:LEU:O	16:P:310:VAL:HA	2.18	0.43
20:T:191:PHE:CD2	20:T:235:LEU:HG	2.54	0.43
20:T:198:ASN:HD21	20:T:200:LYS:HE2	1.83	0.43
22:V:615:PHE:CD1	22:V:616:ASP:N	2.86	0.43
22:V:689:VAL:CG2	26:2:391:ILE:HD11	2.48	0.43
26:2:159:VAL:CG2	26:2:160:LEU:H	2.16	0.43
26:2:221:GLN:HG2	26:2:268:PHE:HZ	1.75	0.43
1:A:367:ILE:CD1	1:A:494:ALA:HB1	2.47	0.43
1:A:391:ALA:HA	1:A:446:VAL:O	2.19	0.43
1:A:618:TYR:C	1:A:620:HIS:N	2.70	0.43
1:A:1167:ARG:HA	1:A:1293:LEU:HD22	2.01	0.43
1:A:1301:ILE:HD13	1:A:1342:SER:OG	2.19	0.43
2:B:240:LEU:HD13	2:B:242:ARG:NE	2.33	0.43
3:C:235:SER:HB2	3:C:241:PRO:HG3	1.99	0.43
5:E:76:PHE:HA	5:E:77:PRO:HD2	1.81	0.43
8:H:90:TYR:O	8:H:144:LEU:HA	2.18	0.43
10:J:21:TYR:CZ	10:J:25:LEU:HD21	2.54	0.43
11:K:109:ILE:HA	11:K:112:LYS:HZ3	1.83	0.43
14:N:46:TRP:CZ2	15:O:11:LEU:HD12	2.48	0.43
14:N:337:CYS:SG	14:N:353:LEU:HD13	2.58	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:T:21:VAL:HA	20:T:114:ALA:O	2.18	0.43
27:3:121:LYS:H	27:3:121:LYS:CD	2.32	0.43
27:3:124:ILE:O	27:3:124:ILE:HG23	2.18	0.43
27:3:178:MET:HA	27:3:181:ILE:HD12	1.99	0.43
1:A:19:LYS:N	2:B:1173:SER:HA	2.34	0.43
1:A:312:PHE:HE2	1:A:326:PRO:HB2	1.82	0.43
1:A:425:ASP:HB3	13:M:39:LEU:HD11	1.99	0.43
1:A:874:LYS:HD2	6:F:111:PRO:HB3	2.00	0.43
1:A:967:ARG:HH11	1:A:967:ARG:HG3	1.84	0.43
1:A:1013:VAL:HG22	1:A:1049:LEU:HD23	2.00	0.43
1:A:1274:GLU:OE1	1:A:1274:GLU:HA	2.16	0.43
1:A:1308:TYR:CB	1:A:1336:LEU:HD13	2.36	0.43
10:J:20:ALA:O	10:J:24:LEU:HG	2.19	0.43
15:O:20:ASP:OD1	15:O:24:GLN:NE2	2.52	0.43
16:P:165:LEU:HD13	16:P:318:ARG:HG3	2.00	0.43
17:Q:34:LEU:HD23	17:Q:37:LEU:HD12	2.00	0.43
23:W:293:ARG:HG2	23:W:421:PHE:HE1	1.76	0.43
25:1:4:VAL:HG22	25:1:5:LEU:N	2.32	0.43
25:1:22:TYR:CD1	25:1:22:TYR:C	2.92	0.43
25:1:50:VAL:HG12	25:1:50:VAL:O	2.18	0.43
26:2:202:GLN:HE21	26:2:202:GLN:N	2.15	0.43
26:2:214:TYR:HB3	26:2:261:PHE:CE2	2.53	0.43
26:2:223:ALA:H	26:2:268:PHE:HE1	1.64	0.43
27:3:137:LEU:HD12	27:3:177:PHE:CE1	2.54	0.43
27:3:184:ALA:O	27:3:187:GLN:HG2	2.19	0.43
1:A:807:LEU:HB2	1:A:810:PHE:CD2	2.54	0.43
1:A:877:ALA:O	1:A:890:ARG:HA	2.19	0.43
1:A:945:ASN:HB3	1:A:948:ILE:HG22	2.00	0.43
1:A:1027:ASP:OD1	1:A:1027:ASP:N	2.52	0.43
1:A:1310:HIS:CE1	1:A:1334:TRP:CE3	2.96	0.43
2:B:442:ASP:HA	2:B:445:LYS:HD2	1.99	0.43
3:C:173:HIS:HB3	3:C:176:TRP:CE3	2.53	0.43
3:C:211:LEU:HD12	3:C:230:TYR:OH	2.18	0.43
5:E:62:VAL:HG21	5:E:72:MET:CE	2.48	0.43
5:E:112:PRO:HA	5:E:115:LYS:HD2	2.00	0.43
13:M:169:ARG:HD3	13:M:206:VAL:HB	1.99	0.43
15:O:60:GLY:HA3	15:O:79:VAL:HA	2.01	0.43
15:O:64:THR:HG21	16:P:188:ARG:CZ	2.49	0.43
16:P:289:PRO:HB2	29:Y:83:DA:H4'	2.00	0.43
17:Q:19:LYS:O	17:Q:22:ILE:HG13	2.19	0.43
17:Q:106:LYS:HG3	18:R:222:SER:OG	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:53:ASN:HB2	19:S:96:GLN:OE1	2.19	0.43
19:S:127:PHE:CB	20:T:19:TRP:HB2	2.48	0.43
21:U:184:ASP:OD1	21:U:185:MET:N	2.52	0.43
21:U:262:THR:HA	21:U:269:LYS:HG2	2.00	0.43
21:U:276:VAL:HG13	21:U:277:GLN:HG3	2.00	0.43
24:0:165:ARG:HD3	24:0:194:ILE:HG12	2.01	0.43
25:1:3:ASN:HB3	26:2:412:PHE:O	2.18	0.43
26:2:117:ASN:CB	27:3:42:MET:HE1	2.46	0.43
26:2:409:TYR:CD2	26:2:443:VAL:HG22	2.54	0.43
1:A:18:ILE:HD13	2:B:1171:MET:HB2	2.00	0.43
1:A:805:ARG:NH2	2:B:671:GLU:O	2.52	0.43
1:A:907:ALA:H	1:A:975:SER:HB3	1.82	0.43
1:A:1209:PRO:CB	9:I:33:ARG:HH12	2.23	0.43
1:A:1309:MET:HG3	21:U:252:LYS:HD2	1.99	0.43
3:C:9:VAL:HG11	11:K:105:PHE:HA	1.99	0.43
4:D:74:PHE:CD2	4:D:80:ILE:HG12	2.54	0.43
7:G:94:LYS:O	7:G:110:ARG:HD2	2.18	0.43
13:M:14:THR:N	13:M:20:ASP:HB3	2.34	0.43
13:M:18:HIS:NE2	13:M:36:GLU:OE2	2.52	0.43
14:N:332:GLU:HB3	15:O:92:LYS:CE	2.49	0.43
17:Q:104:LYS:NZ	18:R:238:LYS:HE3	2.34	0.43
20:T:212:TYR:O	20:T:215:GLU:HB2	2.19	0.43
20:T:228:ILE:HA	28:X:30:DG:C5'	2.41	0.43
26:2:118:LEU:CD1	27:3:43:VAL:HG22	2.39	0.43
27:3:14:VAL:CG2	27:3:163:VAL:HG13	2.48	0.43
27:3:65:GLN:O	27:3:132:LEU:HD11	2.18	0.43
27:3:124:ILE:HD13	27:3:124:ILE:C	2.38	0.43
28:X:11:DT:H2"	28:X:12:DA:H8	1.83	0.43
1:A:460:ARG:HA	1:A:501:MET:SD	2.59	0.43
1:A:601:ASN:HB2	1:A:988:TRP:CZ3	2.54	0.43
1:A:826:SER:OG	1:A:829:ALA:N	2.47	0.43
1:A:1313:GLN:C	1:A:1315:ASP:H	2.22	0.43
2:B:777:ASN:O	10:J:47:ARG:HD2	2.19	0.43
2:B:838:GLN:HE21	2:B:890:ARG:HD3	1.83	0.43
2:B:874:PRO:C	2:B:876:ASN:H	2.17	0.43
3:C:151:VAL:HG22	3:C:152:LYS:N	2.34	0.43
13:M:178:LYS:O	20:T:154:LYS:CG	2.58	0.43
17:Q:22:ILE:HG21	17:Q:34:LEU:HB3	2.00	0.43
26:2:243:SER:HB3	26:2:258:LEU:CD2	2.45	0.43
27:3:105:THR:CG2	27:3:106:SER:N	2.82	0.43
28:X:18:DG:O6	29:Y:75:DC:N4	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1175:ILE:HG12	1:A:1212:LEU:HD13	1.99	0.42
1:A:1317:LYS:HE2	21:U:295:GLY:HA3	2.00	0.42
1:A:1365:ILE:O	1:A:1370:GLY:N	2.47	0.42
1:A:1372:GLU:HG3	5:E:148:HIS:HE1	1.84	0.42
1:A:1470:CYS:O	6:F:109:TYR:HD2	2.02	0.42
2:B:94:SER:O	2:B:122:ALA:HB1	2.19	0.42
2:B:805:PHE:O	2:B:929:PRO:HG2	2.19	0.42
2:B:860:VAL:HG12	2:B:902:GLY:C	2.38	0.42
8:H:9:ILE:HA	8:H:57:ARG:HA	2.01	0.42
15:O:42:LYS:HE3	15:O:42:LYS:HB3	1.75	0.42
25:1:13:ASP:CG	25:1:14:PRO:CD	2.88	0.42
25:1:18:GLN:CD	25:1:44:PHE:CZ	2.93	0.42
26:2:181:GLN:HA	26:2:181:GLN:NE2	2.34	0.42
26:2:224:GLN:N	26:2:268:PHE:HZ	2.16	0.42
27:3:9:ASN:OD1	27:3:158:LYS:HB3	2.19	0.42
27:3:141:LEU:HA	27:3:144:ILE:HG22	2.01	0.42
1:A:364:ARG:NH2	1:A:500:GLU:O	2.52	0.42
1:A:368:THR:O	1:A:483:ARG:HA	2.19	0.42
2:B:23:GLN:OE1	2:B:23:GLN:N	2.51	0.42
2:B:132:VAL:O	2:B:132:VAL:HG23	2.18	0.42
2:B:757:PRO:HD3	2:B:769:PHE:CE2	2.55	0.42
2:B:1028:LEU:HD13	2:B:1041:ILE:HD13	2.01	0.42
2:B:1030:ASN:HB3	2:B:1034:GLY:N	2.34	0.42
3:C:11:ILE:HA	3:C:21:PHE:HB2	2.01	0.42
3:C:40:ALA:HB1	3:C:171:LYS:HB2	2.00	0.42
5:E:26:TYR:HA	5:E:64:HIS:O	2.18	0.42
5:E:58:LEU:HB3	5:E:76:PHE:CD2	2.54	0.42
10:J:35:LEU:HB3	10:J:46:ARG:CD	2.49	0.42
17:Q:187:ILE:C	18:R:212:VAL:H	2.23	0.42
22:V:415:HIS:HD2	22:V:416:THR:CG2	2.31	0.42
25:1:1:MET:SD	26:2:419:GLU:N	2.92	0.42
25:1:43:VAL:CG1	25:1:44:PHE:N	2.83	0.42
27:3:137:LEU:HB2	27:3:180:VAL:HG11	1.96	0.42
27:3:165:LYS:CG	27:3:203:LEU:HD12	2.36	0.42
27:3:228:LEU:O	27:3:228:LEU:HD23	2.17	0.42
1:A:64:VAL:HG21	1:A:68:THR:HG23	2.00	0.42
1:A:88:ILE:HD13	1:A:284:VAL:HG22	2.01	0.42
1:A:875:TYR:HA	1:A:1083:PRO:CB	2.49	0.42
1:A:1166:LEU:HD12	1:A:1296:MET:SD	2.59	0.42
2:B:53:MET:O	2:B:57:ARG:N	2.49	0.42
2:B:92:TYR:CA	20:T:145:LEU:HD22	2.46	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:255:ARG:NH2	2:B:307:GLU:OE2	2.52	0.42
2:B:728:MET:HE2	2:B:942:LYS:HE2	2.01	0.42
5:E:82:VAL:HG23	5:E:106:VAL:HG13	2.00	0.42
8:H:24:ARG:HG2	8:H:46:GLN:NE2	2.33	0.42
9:I:98:GLN:HB2	9:I:100:HIS:CE1	2.55	0.42
11:K:57:LEU:H	11:K:77:THR:HA	1.84	0.42
16:P:223:GLY:CA	29:Y:79:DT:H4'	2.49	0.42
21:U:191:VAL:O	21:U:195:ILE:N	2.46	0.42
22:V:674:THR:HG23	26:2:392:ARG:HH22	1.66	0.42
26:2:236:PHE:CE1	26:2:239:GLN:NE2	2.87	0.42
1:A:540:ASP:OD2	2:B:968:ASN:ND2	2.53	0.42
1:A:880:ARG:HH12	5:E:169:GLN:CD	2.22	0.42
2:B:65:ILE:CG2	2:B:412:LEU:HD11	2.44	0.42
2:B:1102:PHE:O	2:B:1106:ARG:HG2	2.19	0.42
5:E:177:ASP:OD2	5:E:179:VAL:HB	2.19	0.42
9:I:37:TYR:N	9:I:46:GLN:O	2.35	0.42
11:K:13:PHE:HB2	11:K:16:GLU:HG3	2.00	0.42
11:K:37:LYS:HA	11:K:69:HIS:HB3	2.01	0.42
16:P:227:GLU:HG2	16:P:228:GLU:H	1.84	0.42
16:P:284:GLU:HB3	16:P:287:LEU:HB3	2.01	0.42
18:R:158:HIS:HE1	18:R:206:LYS:HD3	1.84	0.42
25:1:8:VAL:CG1	25:1:9:LEU:N	2.80	0.42
1:A:10:ASP:N	2:B:1132:THR:HA	2.34	0.42
1:A:371:PRO:HD2	2:B:788:TYR:CD1	2.53	0.42
1:A:903:PHE:CZ	1:A:976:LYS:HB3	2.55	0.42
1:A:1274:GLU:O	1:A:1276:VAL:CG2	2.62	0.42
2:B:69:ALA:N	2:B:82:PRO:O	2.46	0.42
2:B:588:ARG:O	2:B:592:ARG:N	2.41	0.42
2:B:862:GLY:N	2:B:900:GLU:O	2.53	0.42
2:B:1130:THR:HB	2:B:1134:THR:H	1.84	0.42
6:F:45:PRO:HB3	6:F:115:TYR:CE1	2.54	0.42
10:J:1:MET:SD	10:J:55:LEU:N	2.81	0.42
13:M:12:ARG:HG3	13:M:13:VAL:HG13	2.01	0.42
13:M:158:ALA:HA	13:M:186:ILE:HG13	2.01	0.42
13:M:214:PHE:HA	13:M:217:ARG:NH1	2.34	0.42
17:Q:106:LYS:O	18:R:218:LYS:CE	2.66	0.42
26:2:77:LYS:HD3	26:2:78:GLU:CG	2.49	0.42
26:2:93:LEU:HA	26:2:93:LEU:HD23	1.77	0.42
27:3:11:LEU:CD1	27:3:48:HIS:NE2	2.82	0.42
1:A:72:GLN:HG2	1:A:74:CYS:H	1.83	0.42
1:A:275:ASP:N	1:A:275:ASP:OD1	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:319:ASP:O	1:A:322:LEU:HG	2.19	0.42
1:A:606:HIS:HB3	1:A:627:LYS:HA	2.01	0.42
1:A:609:HIS:HB2	21:U:300:PHE:CZ	2.54	0.42
1:A:775:LYS:CB	2:B:974:SER:HB3	2.50	0.42
1:A:909:LEU:HD22	1:A:1328:PHE:CE2	2.55	0.42
2:B:240:LEU:HD23	2:B:257:VAL:HG13	2.01	0.42
2:B:442:ASP:OD1	2:B:445:LYS:HD2	2.19	0.42
2:B:527:ALA:HB3	2:B:530:ALA:HB2	2.01	0.42
2:B:1116:VAL:HG11	2:B:1125:MET:SD	2.59	0.42
3:C:200:PRO:C	3:C:217:GLN:OE1	2.58	0.42
4:D:32:LEU:HD11	7:G:75:ILE:HG22	2.02	0.42
5:E:130:PHE:HB3	5:E:135:LEU:HD11	2.02	0.42
7:G:55:GLY:HA3	7:G:69:PRO:HB2	2.00	0.42
10:J:20:ALA:O	10:J:24:LEU:N	2.45	0.42
12:L:16:ILE:CG1	12:L:28:ILE:O	2.63	0.42
13:M:135:VAL:HG12	13:M:139:ASN:ND2	2.34	0.42
19:S:13:GLU:HG3	20:T:44:ARG:HA	2.00	0.42
20:T:225:VAL:HG11	28:X:29:DC:H5”	2.02	0.42
21:U:175:ALA:HB1	21:U:222:ARG:HH22	1.73	0.42
22:V:315:VAL:HG13	23:W:500:ASP:HB2	0.42	0.42
22:V:524:ALA:HB2	25:1:23:LEU:HD13	2.01	0.42
26:2:51:LEU:HD23	26:2:51:LEU:C	2.37	0.42
26:2:185:MET:SD	26:2:232:GLU:CB	3.07	0.42
27:3:128:HIS:NE2	27:3:130:GLU:CG	2.82	0.42
1:A:908:THR:O	1:A:963:ARG:NH1	2.53	0.42
1:A:939:VAL:O	1:A:943:LEU:HG	2.18	0.42
2:B:972:ILE:O	2:B:976:MET:N	2.51	0.42
2:B:1015:LEU:HD21	2:B:1024:GLY:HA2	2.02	0.42
3:C:61:ASP:OD1	3:C:61:ASP:N	2.52	0.42
5:E:52:ARG:HB2	5:E:53:PRO:HD2	2.00	0.42
5:E:55:ARG:HH11	5:E:107:GLN:HE22	1.68	0.42
14:N:38:VAL:CG1	15:O:22:LEU:HD22	2.49	0.42
14:N:329:PHE:HB3	14:N:331:THR:HG23	2.01	0.42
16:P:168:ILE:HG13	16:P:226:SER:C	2.40	0.42
21:U:185:MET:HE3	21:U:192:ARG:HH22	1.84	0.42
21:U:218:ASP:C	21:U:218:ASP:OD1	2.58	0.42
22:V:514:MET:HB3	25:1:16:MET:SD	2.59	0.42
25:1:59:GLU:CD	26:2:402:ARG:CZ	2.88	0.42
26:2:221:GLN:CG	26:2:268:PHE:CZ	2.95	0.42
1:A:419:ILE:O	1:A:426:ARG:HA	2.19	0.42
1:A:484:LEU:HD21	1:A:496:PHE:HE1	1.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:931:ARG:C	1:A:933:THR:N	2.73	0.42
1:A:1151:ALA:C	1:A:1155:LYS:HZ3	2.22	0.42
2:B:109:MET:HB3	2:B:112:GLU:HB2	2.02	0.42
2:B:411:LEU:HD12	2:B:440:ILE:CD1	2.49	0.42
2:B:837:CYS:SG	2:B:838:GLN:N	2.93	0.42
2:B:849:ASP:HB3	2:B:851:ASP:OD1	2.20	0.42
2:B:896:LEU:HD21	2:B:900:GLU:HB2	2.00	0.42
3:C:81:LYS:HG3	3:C:82:LEU:HD12	2.01	0.42
5:E:26:TYR:HA	5:E:64:HIS:CB	2.50	0.42
5:E:27:LEU:HD13	5:E:64:HIS:HE2	1.77	0.42
11:K:24:ASP:H	11:K:31:CYS:HA	1.84	0.42
18:R:131:GLU:HB3	18:R:138:ALA:HB3	2.01	0.42
22:V:325:ARG:HH21	23:W:499:ASN:CB	1.95	0.42
22:V:444:HIS:O	22:V:447:PRO:CD	2.61	0.42
27:3:42:MET:SD	27:3:111:ILE:CD1	3.07	0.42
27:3:109:GLU:HG3	27:3:110:VAL:N	2.35	0.42
27:3:146:ARG:HG3	27:3:147:MET:N	2.35	0.42
27:3:178:MET:O	27:3:182:PHE:HD2	2.01	0.42
1:A:13:CYS:HB2	2:B:1135:TYR:CE2	2.55	0.42
1:A:71:CYS:N	1:A:75:ALA:HA	2.31	0.42
1:A:1454:VAL:HG11	1:A:1466:ALA:HB3	2.02	0.42
1:A:1460:LEU:O	2:B:1152:PRO:HD3	2.20	0.42
2:B:487:SER:C	2:B:489:ILE:H	2.24	0.42
2:B:800:ALA:O	2:B:805:PHE:HB2	2.20	0.42
9:I:57:LYS:HE2	9:I:60:HIS:NE2	2.35	0.42
12:L:21:GLU:OE1	12:L:21:GLU:N	2.53	0.42
21:U:215:ILE:HG22	21:U:220:PHE:HB2	2.01	0.42
21:U:286:THR:CG2	21:U:299:LYS:HB3	2.47	0.42
23:W:25:MET:SD	23:W:58:ALA:HB2	2.59	0.42
23:W:263:LEU:C	23:W:263:LEU:HD23	2.39	0.42
26:2:236:PHE:CE1	26:2:261:PHE:HB3	2.54	0.42
27:3:147:MET:CE	27:3:157:MET:SD	3.07	0.42
1:A:546:ARG:CG	1:A:639:ILE:HD11	2.47	0.42
1:A:1217:ASP:OD2	1:A:1220:HIS:N	2.53	0.42
1:A:1302:GLU:O	1:A:1303:GLN:HB3	2.20	0.42
2:B:67:LEU:CD2	2:B:419:ALA:HB1	2.48	0.42
2:B:92:TYR:O	2:B:125:TYR:N	2.30	0.42
2:B:499:ARG:C	2:B:500:GLN:O	2.53	0.42
2:B:798:ARG:N	2:B:949:TYR:O	2.48	0.42
2:B:1080:ARG:HG2	13:M:53:ARG:CZ	2.50	0.42
3:C:75:SER:N	3:C:238:SER:O	2.42	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:E:158:GLU:OE2	5:E:162:ARG:NH2	2.53	0.42
7:G:158:PHE:CZ	17:Q:139:LEU:HA	2.55	0.42
8:H:81:ARG:C	8:H:83:SER:H	2.24	0.42
9:I:7:TYR:CZ	9:I:9:PRO:HG3	2.55	0.42
11:K:1:MET:SD	11:K:3:ALA:HB3	2.59	0.42
13:M:154:ARG:HD3	13:M:154:ARG:HA	1.88	0.42
17:Q:75:ARG:N	17:Q:95:ASN:O	2.41	0.42
22:V:411:SER:O	22:V:417:THR:HB	2.19	0.42
22:V:517:GLU:CB	22:V:713:LEU:HD22	2.46	0.42
26:2:118:LEU:HD22	27:3:39:ASP:CB	2.50	0.42
26:2:176:ALA:HB3	26:2:178:LEU:HD13	1.98	0.42
26:2:211:GLN:HE21	26:2:257:SER:HB2	1.84	0.42
26:2:251:VAL:HG12	26:2:254:MET:N	2.28	0.42
27:3:160:ARG:CZ	27:3:190:LEU:CD1	2.97	0.42
27:3:217:VAL:HG12	27:3:218:PRO:O	2.20	0.42
1:A:1096:GLY:O	1:A:1100:THR:HG23	2.20	0.41
2:B:552:ASN:O	2:B:556:ILE:HG12	2.19	0.41
2:B:934:LYS:HA	2:B:944:THR:HG22	2.01	0.41
3:C:20:LYS:HA	3:C:232:ASN:HA	2.00	0.41
5:E:31:ASP:O	5:E:35:GLN:N	2.53	0.41
7:G:40:GLY:HA2	7:G:152:VAL:HG11	2.02	0.41
9:I:101:SER:N	9:I:104:ALA:HA	2.29	0.41
14:N:318:ASP:CB	16:P:239:ARG:NH2	2.76	0.41
15:O:18:SER:O	15:O:22:LEU:HG	2.20	0.41
16:P:227:GLU:HG2	16:P:228:GLU:N	2.35	0.41
16:P:231:ARG:O	16:P:235:ARG:HG3	2.20	0.41
18:R:188:GLN:HG3	18:R:189:ILE:HG13	2.02	0.41
19:S:37:VAL:HG11	19:S:42:TRP:CZ2	2.55	0.41
21:U:161:ILE:HG21	21:U:211:LEU:HB3	2.01	0.41
22:V:448:ALA:HB1	28:X:58:DT:OP1	2.19	0.41
26:2:166:SER:HB3	26:2:167:PRO:HD3	2.00	0.41
27:3:185:GLN:HE21	27:3:185:GLN:CA	2.18	0.41
27:3:197:ASP:O	27:3:198:SER:HB3	2.20	0.41
28:X:11:DT:H2"	28:X:12:DA:C8	2.55	0.41
1:A:65:ILE:HG22	1:A:66:GLU:N	2.34	0.41
1:A:202:TRP:O	1:A:211:GLU:HA	2.21	0.41
1:A:378:VAL:N	1:A:473:ARG:O	2.52	0.41
1:A:478:PRO:HB3	11:K:4:PRO:HD3	2.01	0.41
1:A:606:HIS:HB3	1:A:628:VAL:H	1.85	0.41
1:A:632:ASN:OD1	1:A:992:LYS:NZ	2.52	0.41
1:A:1171:ALA:O	9:I:57:LYS:HD3	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:192:LYS:HE3	2:B:192:LYS:HB3	1.87	0.41
2:B:505:LEU:HG	2:B:509:VAL:HB	2.02	0.41
3:C:6:GLN:HG3	3:C:25:ASN:CG	2.37	0.41
7:G:63:ARG:HH22	7:G:67:LEU:N	2.18	0.41
7:G:79:PRO:HG3	7:G:104:MET:SD	2.60	0.41
8:H:105:SER:HB2	8:H:108:ALA:CB	2.50	0.41
13:M:283:VAL:O	13:M:287:GLN:HG2	2.21	0.41
16:P:166:GLN:HG3	29:Y:81:DA:C5'	2.39	0.41
16:P:206:GLU:HB2	16:P:207:PRO:HD2	1.96	0.41
16:P:281:SER:HG	16:P:293:TYR:HD1	1.66	0.41
18:R:155:LEU:HB3	18:R:204:ASN:HD21	1.80	0.41
18:R:194:ARG:H	18:R:195:PRO:HD3	1.69	0.41
26:2:89:LEU:O	26:2:93:LEU:HG	2.21	0.41
27:3:18:ASN:ND2	27:3:64:ILE:HD11	2.35	0.41
1:A:419:ILE:HA	1:A:446:VAL:HA	2.02	0.41
1:A:504:HIS:HB3	2:B:1106:ARG:NH2	2.35	0.41
1:A:614:ASP:C	1:A:616:GLY:N	2.71	0.41
1:A:963:ARG:HG2	1:A:967:ARG:NH1	2.35	0.41
1:A:1207:ILE:HD12	1:A:1260:ARG:CB	2.51	0.41
2:B:374:LEU:O	2:B:378:GLY:N	2.51	0.41
2:B:473:LEU:HD22	2:B:1052:LYS:HD3	2.02	0.41
3:C:6:GLN:HB2	11:K:104:ARG:HH12	1.85	0.41
7:G:146:LYS:HD3	7:G:165:ASP:OD2	2.21	0.41
8:H:88:PHE:CD1	8:H:146:LYS:HD2	2.52	0.41
13:M:279:GLY:HA2	20:T:153:TYR:CZ	2.54	0.41
16:P:167:ASN:HB2	29:Y:80:DT:O4'	2.20	0.41
21:U:193:SER:OG	21:U:194:ARG:NH1	2.53	0.41
21:U:223:MET:HB2	21:U:224:THR:H	1.68	0.41
27:3:12:VAL:HG22	27:3:161:ILE:HG12	2.00	0.41
1:A:349:ARG:HB3	2:B:1158:LEU:HD12	2.02	0.41
1:A:374:SER:HB3	1:A:377:GLN:HG3	2.02	0.41
1:A:1355:VAL:HA	5:E:142:HIS:HA	2.02	0.41
2:B:75:SER:OG	2:B:75:SER:O	2.35	0.41
2:B:92:TYR:CB	20:T:145:LEU:CD2	2.79	0.41
2:B:166:LEU:HB3	2:B:170:ASP:CB	2.49	0.41
2:B:302:LYS:HB3	2:B:303:PRO:HD3	2.02	0.41
2:B:453:TRP:HB3	2:B:463:ARG:CB	2.49	0.41
2:B:531:TYR:HD2	2:B:622:CYS:SG	2.44	0.41
2:B:720:PRO:HG2	2:B:721:ARG:NH1	2.35	0.41
2:B:833:THR:O	2:B:840:MET:HE3	2.20	0.41
2:B:836:THR:C	2:B:886:ARG:HA	2.41	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:865:VAL:HA	2:B:895:PHE:HB3	2.02	0.41
4:D:52:GLU:O	4:D:54:GLU:N	2.52	0.41
5:E:41:LYS:HA	5:E:46:ASP:HB3	2.02	0.41
6:F:53:THR:HB	6:F:108:ARG:NH1	2.36	0.41
7:G:154:LYS:HG3	7:G:155:ASN:H	1.86	0.41
13:M:118:PHE:HA	13:M:121:ILE:HB	2.03	0.41
13:M:182:ALA:HB2	20:T:154:LYS:HG3	2.02	0.41
14:N:25:VAL:HG12	15:O:39:GLN:HB3	2.02	0.41
16:P:180:LEU:HD12	16:P:183:ILE:HD12	2.02	0.41
23:W:584:TYR:CB	23:W:591:GLY:HA3	2.48	0.41
25:1:52:VAL:CG2	25:1:53:LEU:N	2.83	0.41
26:2:44:VAL:CG1	26:2:45:PHE:N	2.82	0.41
26:2:133:THR:CG2	26:2:134:SER:N	2.83	0.41
26:2:211:GLN:CD	26:2:261:PHE:CE1	2.94	0.41
27:3:228:LEU:HD23	27:3:228:LEU:C	2.41	0.41
1:A:1167:ARG:HE	1:A:1293:LEU:HB3	1.86	0.41
1:A:1173:THR:HB	9:I:56:ASN:CB	2.49	0.41
1:A:1175:ILE:H	9:I:54:TYR:HB3	1.86	0.41
2:B:258:ALA:HB2	2:B:269:ILE:CG2	2.49	0.41
2:B:1126:ALA:HB3	2:B:1137:CYS:SG	2.61	0.41
2:B:1130:THR:C	2:B:1132:THR:H	2.21	0.41
4:D:23:PRO:HG2	4:D:26:PHE:HB2	2.03	0.41
6:F:93:ALA:O	6:F:97:LEU:N	2.52	0.41
7:G:142:GLU:O	7:G:170:LEU:HA	2.20	0.41
13:M:216:SER:HA	13:M:229:GLN:NE2	2.35	0.41
14:N:10:VAL:HB	14:N:11:PRO:HD3	2.02	0.41
14:N:39:LEU:HD12	14:N:42:LEU:HD23	2.01	0.41
15:O:62:LEU:HA	15:O:76:LEU:HG	2.02	0.41
16:P:207:PRO:HG2	16:P:209:THR:HG23	2.03	0.41
20:T:202:LEU:HD11	20:T:233:TRP:HB2	2.03	0.41
22:V:427:MET:HA	22:V:435:TRP:HB2	2.01	0.41
25:1:50:VAL:CG1	25:1:54:GLN:HG2	2.41	0.41
27:3:64:ILE:CB	27:3:123:ASP:HB3	2.49	0.41
27:3:125:LYS:C	27:3:127:GLN:H	2.24	0.41
27:3:144:ILE:HG13	27:3:159:SER:OG	2.20	0.41
27:3:165:LYS:HE3	27:3:200:SER:N	2.36	0.41
27:3:202:LEU:N	27:3:202:LEU:CD2	2.82	0.41
29:Y:85:DG:C2	29:Y:86:DC:C2	3.08	0.41
1:A:37:THR:OG1	1:A:86:GLY:HA3	2.20	0.41
1:A:1000:LEU:HD12	1:A:1001:PRO:HD2	2.02	0.41
1:A:1456:GLU:HG2	1:A:1457:ASN:N	2.35	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:78:VAL:O	2:B:79:GLU:CB	2.48	0.41
2:B:764:MET:HG2	2:B:767:LEU:HD12	2.01	0.41
2:B:790:GLN:HA	2:B:968:ASN:HD22	1.86	0.41
2:B:799:SER:O	2:B:802:ASP:HB2	2.21	0.41
9:I:69:ILE:O	9:I:72:VAL:HG22	2.21	0.41
20:T:23:VAL:HG13	20:T:27:LEU:HD23	2.01	0.41
23:W:175:TYR:CD1	23:W:175:TYR:N	2.76	0.41
26:2:30:VAL:HG13	26:2:31:LEU:N	2.35	0.41
1:A:120:ASP:OD1	1:A:121:SER:N	2.51	0.41
1:A:201:GLU:HA	1:A:212:LYS:O	2.21	0.41
1:A:375:ILE:HG12	1:A:666:ARG:HB2	2.03	0.41
1:A:1080:ILE:CD1	6:F:54:THR:HG21	2.50	0.41
2:B:471:ASN:HD22	2:B:730:LYS:HE3	1.85	0.41
2:B:1040:GLN:NE2	3:C:197:TYR:H	2.18	0.41
3:C:199:LYS:NZ	3:C:201:GLU:OE1	2.46	0.41
7:G:117:MET:HE1	7:G:163:LEU:HD22	2.03	0.41
8:H:39:LEU:HD12	8:H:124:ARG:O	2.21	0.41
12:L:38:GLU:HG2	12:L:39:CYS:H	1.86	0.41
13:M:108:SER:O	13:M:110:SER:OG	2.28	0.41
14:N:315:ASN:C	14:N:317:GLU:H	2.23	0.41
15:O:19:LEU:HD23	15:O:22:LEU:HD12	2.03	0.41
17:Q:21:VAL:O	17:Q:25:PHE:HD1	2.04	0.41
23:W:157:PHE:HA	23:W:189:TRP:CZ3	2.55	0.41
26:2:42:LEU:HD23	26:2:42:LEU:HA	1.78	0.41
26:2:57:MET:CA	26:2:60:LEU:HG	2.49	0.41
26:2:60:LEU:CD1	26:2:95:ILE:CB	2.95	0.41
27:3:18:ASN:OD1	27:3:19:PRO:HD2	2.21	0.41
27:3:133:LEU:CD2	27:3:134:ALA:N	2.82	0.41
27:3:187:GLN:CG	27:3:189:ILE:CG1	2.94	0.41
27:3:222:SER:HB3	27:3:225:GLN:OE1	2.21	0.41
1:A:61:ARG:O	1:A:72:GLN:HB3	2.19	0.41
1:A:516:GLN:O	1:A:523:ARG:NH1	2.41	0.41
1:A:916:PHE:CD1	1:A:963:ARG:HD2	2.55	0.41
1:A:1017:SER:HA	1:A:1020:LEU:HG	2.03	0.41
1:A:1479:LYS:HB3	6:F:103:PRO:HB3	2.03	0.41
2:B:22:TRP:HD1	2:B:24:GLU:HB2	1.85	0.41
2:B:63:PRO:HB2	2:B:88:PHE:CD1	2.56	0.41
2:B:236:TRP:HB2	2:B:259:THR:HB	2.03	0.41
2:B:602:SER:OG	2:B:620:ARG:NH1	2.54	0.41
2:B:669:GLU:O	2:B:673:VAL:HG13	2.21	0.41
2:B:821:LYS:N	2:B:825:GLN:O	2.39	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1137:CYS:HB3	2:B:1142:ASN:CB	2.51	0.41
3:C:1:MET:SD	11:K:52:LYS:HE3	2.61	0.41
3:C:190:ASN:ND2	3:C:193:ARG:HA	2.36	0.41
8:H:64:LEU:O	8:H:83:SER:HB3	2.21	0.41
11:K:82:SER:HA	11:K:83:PRO:HD3	1.81	0.41
12:L:16:ILE:O	12:L:17:TYR:HD2	2.02	0.41
13:M:218:PHE:CD1	13:M:277:ILE:HG22	2.55	0.41
17:Q:170:LYS:HG3	17:Q:173:ALA:H	1.86	0.41
22:V:514:MET:HE2	22:V:664:SER:HB3	2.01	0.41
25:1:52:VAL:O	25:1:56:ARG:HG2	2.21	0.41
26:2:117:ASN:HB3	26:2:118:LEU:H	1.66	0.41
26:2:138:PRO:HD3	26:2:189:GLU:CD	2.40	0.41
26:2:171:VAL:CG1	26:2:216:MET:SD	3.06	0.41
26:2:188:THR:CG2	26:2:189:GLU:N	2.83	0.41
26:2:259:LEU:HD12	26:2:260:ASN:CA	2.50	0.41
27:3:14:VAL:HG22	27:3:162:LEU:O	2.21	0.41
27:3:42:MET:HE2	27:3:108:ASN:CG	2.41	0.41
1:A:16:ARG:N	2:B:1148:LEU:O	2.32	0.41
1:A:33:ARG:HB3	2:B:1139:GLY:HA2	2.02	0.41
1:A:204:HIS:O	1:A:206:ASN:N	2.43	0.41
1:A:549:THR:OG1	1:A:639:ILE:HG13	2.20	0.41
1:A:720:ALA:HB2	1:A:725:LEU:HD13	2.02	0.41
1:A:731:ASN:HD21	21:U:253:THR:HG22	1.78	0.41
1:A:1218:ARG:HA	1:A:1221:MET:HG2	2.03	0.41
2:B:68:GLN:OE1	2:B:135:GLU:HG3	2.21	0.41
2:B:194:LEU:HD13	2:B:467:SER:HB2	2.03	0.41
2:B:198:GLU:CD	2:B:524:LYS:HZ2	2.23	0.41
2:B:1123:GLY:HA3	2:B:1171:MET:H	1.85	0.41
4:D:64:THR:HG21	7:G:46:ILE:HG23	2.02	0.41
9:I:29:ASP:O	9:I:33:ARG:N	2.53	0.41
9:I:80:ARG:HE	9:I:115:THR:HG21	1.85	0.41
10:J:3:ILE:HD13	10:J:18:TRP:HB2	2.03	0.41
11:K:32:LEU:HD21	11:K:72:ILE:HB	2.02	0.41
11:K:35:ILE:N	11:K:35:ILE:HD12	2.36	0.41
12:L:17:TYR:O	12:L:45:TYR:CD2	2.74	0.41
13:M:128:ILE:HG13	13:M:130:LEU:HG	2.02	0.41
13:M:259:TYR:HD1	13:M:274:ILE:HD12	1.86	0.41
14:N:39:LEU:O	14:N:42:LEU:HB3	2.21	0.41
14:N:314:LEU:HD12	16:P:248:ALA:O	2.21	0.41
17:Q:37:LEU:HD13	17:Q:71:PHE:CE1	2.55	0.41
17:Q:106:LYS:NZ	18:R:219:LEU:CD1	2.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
17:Q:191:LEU:HD22	18:R:212:VAL:CB	2.50	0.41
20:T:143:GLN:HA	20:T:143:GLN:HE21	1.86	0.41
20:T:198:ASN:O	20:T:202:LEU:HG	2.21	0.41
20:T:227:GLY:C	28:X:30:DG:H5"	2.40	0.41
22:V:353:ALA:O	22:V:357:VAL:HG23	2.21	0.41
22:V:518:PHE:HB2	25:1:16:MET:SD	2.61	0.41
23:W:73:CYS:O	23:W:209:TYR:HE2	2.04	0.41
23:W:492:PRO:HG2	23:W:678:VAL:HG22	2.03	0.41
25:1:1:MET:N	26:2:418:PHE:CB	2.84	0.41
25:1:10:ILE:HG22	26:2:407:VAL:CG2	2.50	0.41
25:1:38:ILE:CB	25:1:44:PHE:CD1	3.04	0.41
26:2:93:LEU:CA	26:2:96:TRP:HD1	2.31	0.41
26:2:93:LEU:HD23	26:2:96:TRP:HE1	1.85	0.41
26:2:94:ARG:HD2	26:2:95:ILE:HD13	2.02	0.41
26:2:123:LEU:HD21	26:2:178:LEU:HD11	2.02	0.41
26:2:204:LEU:CD2	26:2:254:MET:HG3	2.50	0.41
27:3:8:LEU:CD2	27:3:54:SER:HB3	2.45	0.41
27:3:33:THR:HG22	27:3:36:LYS:CB	2.44	0.41
27:3:41:VAL:HG13	27:3:42:MET:N	2.35	0.41
27:3:100:LYS:HE2	27:3:100:LYS:HB2	1.89	0.41
27:3:222:SER:HB3	27:3:225:GLN:CG	2.51	0.41
28:X:57:DC:C2'	28:X:58:DT:H72	2.50	0.41
1:A:42:LYS:HD3	1:A:55:GLY:H	1.86	0.41
1:A:338:SER:O	1:A:342:ARG:HG3	2.21	0.41
1:A:470:MET:SD	1:A:521:VAL:HG23	2.61	0.41
1:A:702:ILE:O	1:A:706:ILE:HG12	2.21	0.41
1:A:1054:MET:O	1:A:1059:ARG:N	2.54	0.41
1:A:1165:THR:O	1:A:1169:VAL:HG23	2.21	0.41
1:A:1173:THR:HB	9:I:56:ASN:HB3	2.02	0.41
3:C:190:ASN:ND2	3:C:195:THR:O	2.51	0.41
5:E:142:HIS:HB3	5:E:145:VAL:HG23	2.02	0.41
6:F:44:ARG:H	6:F:45:PRO:CD	2.34	0.41
11:K:81:TYR:CE2	11:K:86:ALA:HB2	2.55	0.41
16:P:193:ASN:HA	16:P:194:PRO:HD2	1.92	0.41
17:Q:129:CYS:HB2	17:Q:154:CYS:HB2	2.02	0.41
22:V:297:PHE:CG	22:V:298:ARG:N	2.89	0.41
22:V:409:THR:H	22:V:418:LYS:HG3	1.86	0.41
25:1:10:ILE:O	25:1:10:ILE:HG23	2.21	0.41
27:3:60:ILE:CG2	27:3:61:ALA:N	2.83	0.41
27:3:174:TYR:CZ	27:3:178:MET:HG3	2.56	0.41
1:A:404:GLU:OE1	1:A:407:ARG:NH1	2.45	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:432:HIS:CG	1:A:433:PRO:HD2	2.56	0.40
1:A:864:LEU:HD22	1:A:1095:LEU:HD23	2.02	0.40
1:A:915:ALA:O	1:A:919:LYS:N	2.45	0.40
1:A:1053:ARG:NE	1:A:1057:GLU:OE1	2.53	0.40
2:B:474:THR:H	2:B:477:SER:HB2	1.85	0.40
2:B:761:THR:H	2:B:764:MET:CE	2.33	0.40
5:E:11:TRP:CZ2	5:E:15:LYS:HE3	2.56	0.40
5:E:17:ILE:O	5:E:20:LEU:HB3	2.21	0.40
8:H:97:TYR:CZ	8:H:115:TYR:HB3	2.56	0.40
9:I:24:LEU:HD11	9:I:44:TYR:HE2	1.86	0.40
12:L:34:ILE:HD12	12:L:42:ARG:HB3	2.03	0.40
13:M:178:LYS:C	20:T:154:LYS:CG	2.87	0.40
14:N:332:GLU:HA	15:O:92:LYS:O	2.21	0.40
15:O:70:ASN:HB3	15:O:99:ASP:HB3	2.02	0.40
16:P:200:VAL:HG12	16:P:213:ILE:HD13	2.02	0.40
18:R:195:PRO:HB2	18:R:199:LYS:CG	2.51	0.40
19:S:48:GLU:OE1	19:S:101:ARG:NH2	2.54	0.40
19:S:108:ARG:HA	19:S:108:ARG:HD3	1.97	0.40
22:V:413:LEU:H	22:V:417:THR:CG2	2.34	0.40
23:W:144:ALA:O	23:W:149:ASP:HB2	2.21	0.40
24:0:54:ARG:HA	27:3:209:ILE:HD13	1.06	0.40
26:2:236:PHE:HZ	26:2:258:LEU:CD1	2.34	0.40
27:3:217:VAL:HA	27:3:218:PRO:HD2	1.96	0.40
27:3:229:TRP:HD1	27:3:229:TRP:O	2.04	0.40
1:A:32:LYS:HG2	1:A:87:HIS:NE2	2.36	0.40
1:A:63:GLY:HA2	1:A:71:CYS:SG	2.62	0.40
1:A:240:PRO:HB3	1:A:244:ARG:HH11	1.87	0.40
1:A:337:LYS:O	1:A:341:GLN:HB3	2.21	0.40
1:A:416:ALA:HA	1:A:448:ARG:HA	2.03	0.40
1:A:587:THR:O	1:A:591:ILE:HG12	2.21	0.40
1:A:625:ASP:H	1:A:637:MET:CG	2.33	0.40
1:A:802:PHE:CZ	1:A:808:PRO:HB3	2.57	0.40
1:A:1161:LEU:HB3	1:A:1308:TYR:OH	2.21	0.40
2:B:607:ILE:HG21	9:I:72:VAL:N	2.36	0.40
2:B:1080:ARG:HG2	13:M:53:ARG:NH1	2.36	0.40
3:C:47:ILE:HG22	12:L:57:ALA:HB2	2.04	0.40
7:G:89:VAL:HA	7:G:99:THR:HA	2.03	0.40
7:G:163:LEU:HD23	7:G:163:LEU:O	2.21	0.40
9:I:27:LYS:HE3	9:I:38:ALA:HB2	2.03	0.40
16:P:203:ARG:HG3	16:P:203:ARG:HH21	1.87	0.40
18:R:195:PRO:HB2	18:R:199:LYS:HD2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
19:S:49:ARG:HD2	19:S:96:GLN:HB2	2.03	0.40
20:T:145:LEU:C	20:T:147:LYS:N	2.64	0.40
22:V:514:MET:SD	22:V:537:ASN:CG	2.99	0.40
23:W:428:ILE:HA	23:W:430:ASN:HD21	1.85	0.40
25:1:1:MET:CA	26:2:413:LEU:HA	2.48	0.40
26:2:34:LEU:CD2	26:2:34:LEU:N	2.84	0.40
26:2:159:VAL:HG11	26:2:161:HIS:CD2	2.49	0.40
26:2:219:TYR:CD1	26:2:219:TYR:C	2.95	0.40
26:2:221:GLN:O	26:2:268:PHE:CE1	2.74	0.40
26:2:236:PHE:CE1	26:2:258:LEU:HD12	2.57	0.40
27:3:17:ALA:CB	27:3:63:HIS:CD2	2.99	0.40
27:3:131:THR:CG2	27:3:133:LEU:CD1	2.95	0.40
27:3:144:ILE:HG23	27:3:145:HIS:N	2.36	0.40
1:A:309:LEU:HG	1:A:313:HIS:CD2	2.57	0.40
1:A:336:LEU:HG	1:A:338:SER:H	1.86	0.40
1:A:340:LYS:HG3	1:A:1436:VAL:HG21	2.03	0.40
1:A:452:ASP:OD1	1:A:476:ILE:HG12	2.21	0.40
1:A:550:LYS:HG2	1:A:552:ASP:H	1.86	0.40
1:A:790:GLN:OE1	1:A:822:PHE:HB2	2.22	0.40
1:A:962:ASP:OD2	1:A:1046:ARG:HD2	2.21	0.40
1:A:1173:THR:HA	1:A:1214:VAL:HA	2.03	0.40
2:B:481:HIS:HA	2:B:484:ARG:NH1	2.36	0.40
3:C:19:VAL:CG1	3:C:233:VAL:HB	2.51	0.40
5:E:120:ASP:O	5:E:122:ALA:N	2.54	0.40
6:F:99:ALA:HB1	6:F:101:LYS:HG3	2.01	0.40
13:M:179:GLU:HG2	20:T:154:LYS:CE	2.51	0.40
13:M:195:PHE:CZ	13:M:199:LEU:HD11	2.56	0.40
13:M:279:GLY:HA2	20:T:153:TYR:OH	2.21	0.40
13:M:289:TYR:HA	13:M:292:ILE:HG12	2.03	0.40
17:Q:104:LYS:HE3	18:R:238:LYS:NZ	2.36	0.40
18:R:225:VAL:HG13	18:R:226:ASP:CG	2.17	0.40
21:U:191:VAL:O	21:U:195:ILE:HG13	2.22	0.40
25:1:13:ASP:OD2	25:1:17:LYS:HB2	2.16	0.40
26:2:41:CYS:SG	26:2:42:LEU:N	2.95	0.40
26:2:61:PHE:HE1	26:2:99:GLN:NE2	2.19	0.40
26:2:223:ALA:C	26:2:225:SER:H	2.24	0.40
27:3:222:SER:O	27:3:226:TYR:CD2	2.75	0.40
1:A:15:LEU:HA	2:B:1148:LEU:HB3	2.02	0.40
1:A:312:PHE:CE2	1:A:326:PRO:HB2	2.55	0.40
2:B:225:LEU:O	2:B:230:ARG:HG2	2.20	0.40
2:B:249:LYS:C	2:B:251:ALA:N	2.75	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:834:ARG:HD2	2:B:840:MET:SD	2.61	0.40
3:C:54:ALA:O	3:C:160:ARG:N	2.36	0.40
5:E:82:VAL:HG21	5:E:106:VAL:HG22	2.03	0.40
5:E:172:ARG:NE	5:E:208:LEU:HD22	2.36	0.40
6:F:70:ALA:O	6:F:74:ALA:N	2.48	0.40
6:F:110:LEU:N	6:F:114:SER:O	2.55	0.40
9:I:27:LYS:O	9:I:35:LEU:HD12	2.22	0.40
17:Q:109:HIS:HB3	18:R:221:ARG:HB3	2.04	0.40
17:Q:124:ARG:HD3	17:Q:168:MET:SD	2.62	0.40
23:W:233:PHE:HB2	23:W:456:ILE:HG22	2.02	0.40
26:2:170:ALA:C	26:2:213:TRP:CZ3	2.94	0.40
26:2:195:CYS:SG	26:2:196:ILE:N	2.95	0.40
26:2:201:PHE:CZ	26:2:202:GLN:OE1	2.74	0.40
27:3:68:ARG:HG2	27:3:69:PHE:N	2.36	0.40
29:Y:89:DC:H2"	29:Y:90:DC:C5	2.57	0.40
1:A:364:ARG:HH12	1:A:461:GLN:HB3	1.86	0.40
1:A:420:ILE:HB	1:A:445:LYS:HB2	2.03	0.40
1:A:746:ASN:HA	1:A:749:ARG:HE	1.86	0.40
1:A:1323:THR:HG23	1:A:1325:ASP:N	2.31	0.40
2:B:88:PHE:CE2	2:B:128:ILE:HG12	2.56	0.40
2:B:990:SER:O	2:B:994:GLY:N	2.53	0.40
4:D:105:PRO:O	4:D:135:GLN:NE2	2.47	0.40
7:G:11:ILE:N	7:G:68:TYR:O	2.49	0.40
10:J:35:LEU:HB3	10:J:46:ARG:CZ	2.51	0.40
16:P:211:ALA:HA	16:P:220:VAL:O	2.21	0.40
16:P:237:TYR:O	16:P:240:VAL:HG23	2.22	0.40
16:P:295:MET:N	16:P:300:ILE:O	2.54	0.40
17:Q:104:LYS:NZ	18:R:238:LYS:CD	2.82	0.40
19:S:54:LYS:HE2	19:S:54:LYS:HB2	1.84	0.40
20:T:20:LEU:O	20:T:113:ARG:HA	2.21	0.40
20:T:154:LYS:HA	20:T:155:PRO:HD3	1.97	0.40
26:2:219:TYR:N	26:2:264:HIS:NE2	2.69	0.40
27:3:64:ILE:HD12	27:3:128:HIS:HB3	2.04	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	A	1450/1970 (74%)	1305 (90%)	97 (7%)	48 (3%)	4 26
2	B	1163/1174 (99%)	1049 (90%)	76 (6%)	38 (3%)	4 26
3	C	273/275 (99%)	241 (88%)	18 (7%)	14 (5%)	2 19
4	D	127/142 (89%)	118 (93%)	8 (6%)	1 (1%)	19 60
5	E	208/210 (99%)	195 (94%)	7 (3%)	6 (3%)	4 29
6	F	84/127 (66%)	78 (93%)	4 (5%)	2 (2%)	6 33
7	G	169/172 (98%)	158 (94%)	10 (6%)	1 (1%)	25 66
8	H	148/150 (99%)	123 (83%)	13 (9%)	12 (8%)	1 12
9	I	123/125 (98%)	100 (81%)	14 (11%)	9 (7%)	1 14
10	J	65/67 (97%)	53 (82%)	9 (14%)	3 (5%)	2 21
11	K	115/117 (98%)	112 (97%)	3 (3%)	0	100 100
12	L	44/58 (76%)	37 (84%)	3 (7%)	4 (9%)	1 11
13	M	256/316 (81%)	236 (92%)	12 (5%)	8 (3%)	4 27
14	N	109/376 (29%)	100 (92%)	5 (5%)	4 (4%)	3 24
15	O	97/109 (89%)	90 (93%)	7 (7%)	0	100 100
16	P	183/339 (54%)	170 (93%)	8 (4%)	5 (3%)	5 31
17	Q	176/439 (40%)	159 (90%)	11 (6%)	6 (3%)	3 26
18	R	163/291 (56%)	128 (78%)	22 (14%)	13 (8%)	1 12
19	S	134/517 (26%)	123 (92%)	7 (5%)	4 (3%)	4 28
20	T	218/249 (88%)	191 (88%)	17 (8%)	10 (5%)	2 21
21	U	168/301 (56%)	136 (81%)	21 (12%)	11 (6%)	1 16
22	V	473/782 (60%)	400 (85%)	46 (10%)	27 (6%)	1 18
23	W	661/760 (87%)	567 (86%)	69 (10%)	25 (4%)	3 24
24	0	186/395 (47%)	168 (90%)	13 (7%)	5 (3%)	5 31
25	1	60/71 (84%)	53 (88%)	5 (8%)	2 (3%)	4 26

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
26	2	264/462 (57%)	246 (93%)	14 (5%)	4 (2%)	10 46
27	3	187/308 (61%)	175 (94%)	9 (5%)	3 (2%)	9 44
All	All	7304/10302 (71%)	6511 (89%)	528 (7%)	265 (4%)	6 25

All (265) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	67	ARG
1	A	205	VAL
1	A	266	MET
1	A	267	GLN
1	A	531	ASN
1	A	605	THR
1	A	611	ASP
1	A	613	GLU
1	A	615	SER
1	A	623	PRO
1	A	911	PRO
1	A	929	ALA
1	A	932	ARG
1	A	1117	VAL
1	A	1275	VAL
1	A	1303	GLN
1	A	1306	LYS
2	B	61	ASP
2	B	79	GLU
2	B	232	THR
2	B	250	SER
2	B	491	ARG
2	B	498	PRO
2	B	500	GLN
2	B	549	SER
2	B	841	ARG
2	B	879	GLU
3	C	7	PRO
3	C	89	THR
3	C	126	ARG
3	C	147	ASP
3	C	213	GLU
3	C	218	ALA
5	E	52	ARG

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Mol	Chain	Res	Type
5	E	53	PRO
5	E	66	ASP
7	G	154	LYS
8	H	67	ASP
8	H	74	GLU
8	H	75	TYR
8	H	86	ASP
8	H	108	ALA
8	H	111	ARG
9	I	57	LYS
9	I	85	PRO
9	I	87	GLN
9	I	104	ALA
9	I	106	ASP
12	L	16	ILE
12	L	38	GLU
13	M	10	LEU
13	M	11	PRO
13	M	12	ARG
13	M	44	ARG
13	M	109	SER
16	P	160	GLY
16	P	161	ILE
16	P	206	GLU
18	R	134	ASP
18	R	163	LEU
18	R	195	PRO
18	R	206	LYS
20	T	139	VAL
20	T	147	LYS
20	T	156	VAL
21	U	251	ALA
21	U	257	GLN
22	V	385	ASP
22	V	427	MET
22	V	461	HIS
22	V	491	ALA
22	V	499	ASN
22	V	632	SER
22	V	648	LYS
22	V	649	GLY
23	W	67	VAL

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Mol	Chain	Res	Type
23	W	409	THR
23	W	411	ALA
23	W	419	GLU
23	W	420	PRO
23	W	421	PHE
23	W	424	ARG
23	W	430	ASN
23	W	504	ILE
23	W	573	ASP
23	W	595	ILE
23	W	630	SER
24	0	77	LYS
24	0	78	PRO
25	1	48	GLU
26	2	49	PRO
27	3	120	THR
27	3	209	ILE
1	A	44	PRO
1	A	273	GLN
1	A	338	SER
1	A	346	LYS
1	A	625	ASP
1	A	930	LEU
1	A	935	GLN
1	A	1101	GLN
1	A	1264	SER
1	A	1273	GLU
1	A	1282	ASP
1	A	1435	THR
2	B	76	GLY
2	B	243	GLY
2	B	428	ASP
2	B	460	HIS
2	B	649	ASN
2	B	791	GLU
2	B	875	GLU
2	B	881	GLU
2	B	882	SER
2	B	883	THR
2	B	889	LYS
3	C	91	GLU
3	C	143	VAL

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Mol	Chain	Res	Type
3	C	211	LEU
4	D	57	LEU
5	E	65	ASN
5	E	121	MET
8	H	3	GLY
8	H	21	LYS
8	H	107	GLU
10	J	14	VAL
12	L	17	TYR
12	L	18	ILE
17	Q	103	VAL
17	Q	169	PRO
18	R	157	GLN
18	R	164	GLY
18	R	212	VAL
20	T	146	ASP
20	T	181	GLN
21	U	227	GLU
21	U	233	LEU
21	U	267	LYS
22	V	254	GLN
22	V	404	SER
23	W	124	LEU
23	W	408	SER
23	W	646	ILE
26	2	223	ALA
26	2	231	VAL
1	A	156	GLY
1	A	1200	PRO
1	A	1305	SER
1	A	1417	HIS
2	B	73	HIS
2	B	75	SER
2	B	229	SER
2	B	456	GLN
2	B	497	LYS
2	B	651	TYR
2	B	863	ASP
2	B	898	THR
2	B	1129	ASN
2	B	1132	THR
3	C	144	GLU

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Mol	Chain	Res	Type
8	H	106	THR
9	I	92	LYS
9	I	119	CYS
13	M	106	THR
14	N	346	LYS
17	Q	163	GLU
18	R	196	ASP
19	S	170	VAL
20	T	124	TYR
21	U	222	ARG
21	U	226	GLU
21	U	256	THR
22	V	343	GLY
22	V	418	LYS
22	V	460	ALA
23	W	155	CYS
23	W	509	GLU
27	3	198	SER
1	A	72	GLN
1	A	184	CYS
1	A	461	GLN
1	A	479	TRP
1	A	981	CYS
2	B	257	VAL
2	B	495	LEU
2	B	873	LEU
2	B	1136	GLU
3	C	137	ASN
5	E	64	HIS
6	F	85	GLY
8	H	70	LEU
8	H	71	ASP
9	I	20	CYS
10	J	3	ILE
13	M	149	LYS
14	N	355	ASP
17	Q	124	ARG
17	Q	165	GLU
18	R	197	LYS
20	T	38	GLY
20	T	135	SER
20	T	140	ARG

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Mol	Chain	Res	Type
22	V	310	LEU
22	V	428	GLU
22	V	470	LEU
22	V	475	ASP
22	V	502	ILE
22	V	629	HIS
1	A	75	ALA
1	A	300	ALA
1	A	1106	THR
1	A	1265	ASP
1	A	1266	GLU
1	A	1342	SER
3	C	151	VAL
10	J	6	ARG
16	P	297	LYS
18	R	140	LYS
18	R	174	ALA
19	S	153	ARG
19	S	154	THR
19	S	160	ALA
21	U	229	ALA
21	U	266	CYS
21	U	295	GLY
22	V	650	MET
23	W	152	LEU
23	W	551	SER
24	0	79	ASN
26	2	430	VAL
1	A	1281	ASP
2	B	737	ILE
6	F	44	ARG
9	I	105	GLU
13	M	247	GLY
14	N	312	GLU
18	R	141	PRO
18	R	225	VAL
22	V	436	GLY
22	V	582	GLY
23	W	36	GLY
23	W	345	ARG
23	W	697	ILE
1	A	50	GLY

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Mol	Chain	Res	Type
2	B	493	GLY
22	V	311	LYS
22	V	651	VAL
1	A	51	ARG
1	A	498	GLY
22	V	426	VAL
22	V	457	ILE
23	W	495	ILE
24	0	216	GLY
3	C	6	GLN
3	C	78	ILE
17	Q	100	VAL
20	T	138	PRO
22	V	405	VAL
23	W	174	ILE
25	1	2	VAL
16	P	207	PRO
2	B	1008	VAL
14	N	313	PRO
23	W	45	GLY
24	0	56	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	A	1279/1748 (73%)	1247 (98%)	32 (2%)	47 68
2	B	1020/1028 (99%)	997 (98%)	23 (2%)	50 70
3	C	252/252 (100%)	246 (98%)	6 (2%)	49 69
4	D	119/126 (94%)	118 (99%)	1 (1%)	81 89
5	E	192/192 (100%)	186 (97%)	6 (3%)	40 62
6	F	74/111 (67%)	74 (100%)	0	100 100
7	G	152/153 (99%)	149 (98%)	3 (2%)	55 74
8	H	131/131 (100%)	127 (97%)	4 (3%)	40 62

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles
9	I	112/112 (100%)	106 (95%)	6 (5%)	22 47
10	J	56/56 (100%)	56 (100%)	0	100 100
11	K	106/106 (100%)	105 (99%)	1 (1%)	78 87
12	L	43/55 (78%)	43 (100%)	0	100 100
13	M	222/268 (83%)	212 (96%)	10 (4%)	27 52
14	N	105/324 (32%)	104 (99%)	1 (1%)	76 86
15	O	90/98 (92%)	89 (99%)	1 (1%)	73 84
16	P	159/293 (54%)	154 (97%)	5 (3%)	40 62
17	Q	164/373 (44%)	157 (96%)	7 (4%)	29 53
18	R	150/261 (58%)	138 (92%)	12 (8%)	12 35
19	S	121/448 (27%)	118 (98%)	3 (2%)	47 68
20	T	196/218 (90%)	187 (95%)	9 (5%)	27 52
21	U	148/266 (56%)	139 (94%)	9 (6%)	18 44
22	V	422/688 (61%)	403 (96%)	19 (4%)	27 52
23	W	577/664 (87%)	541 (94%)	36 (6%)	18 43
24	0	171/352 (49%)	163 (95%)	8 (5%)	26 51
25	1	56/64 (88%)	52 (93%)	4 (7%)	14 39
26	2	238/399 (60%)	229 (96%)	9 (4%)	33 57
27	3	171/272 (63%)	159 (93%)	12 (7%)	15 40
All	All	6526/9058 (72%)	6299 (96%)	227 (4%)	39 59

All (227) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	29	ASP
1	A	57	LEU
1	A	147	LEU
1	A	152	ASN
1	A	188	GLN
1	A	264	VAL
1	A	267	GLN
1	A	275	ASP
1	A	339	LEU
1	A	372	ASN
1	A	472	HIS

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Mol	Chain	Res	Type
1	A	484	LEU
1	A	611	ASP
1	A	613	GLU
1	A	614	ASP
1	A	615	SER
1	A	625	ASP
1	A	644	SER
1	A	647	THR
1	A	659	GLU
1	A	669	TYR
1	A	750	ASP
1	A	839	HIS
1	A	932	ARG
1	A	964	GLU
1	A	1152	GLU
1	A	1289	GLU
1	A	1306	LYS
1	A	1307	VAL
1	A	1311	LEU
1	A	1314	THR
1	A	1386	ILE
2	B	26	CYS
2	B	54	SER
2	B	79	GLU
2	B	97	THR
2	B	125	TYR
2	B	131	THR
2	B	169	ARG
2	B	249	LYS
2	B	250	SER
2	B	256	ILE
2	B	407	MET
2	B	442	ASP
2	B	446	TYR
2	B	499	ARG
2	B	546	GLU
2	B	588	ARG
2	B	604	ILE
2	B	664	TYR
2	B	666	ASP
2	B	814	TYR
2	B	880	LEU

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Mol	Chain	Res	Type
2	B	881	GLU
2	B	1080	ARG
3	C	35	ARG
3	C	61	ASP
3	C	113	ARG
3	C	212	ASP
3	C	215	GLU
3	C	217	GLN
4	D	43	HIS
5	E	23	ASP
5	E	50	GLU
5	E	62	VAL
5	E	64	HIS
5	E	129	GLN
5	E	172	ARG
7	G	63	ARG
7	G	144	ARG
7	G	163	LEU
8	H	55	LYS
8	H	65	TYR
8	H	84	ARG
8	H	107	GLU
9	I	27	LYS
9	I	58	ILE
9	I	71	ASP
9	I	72	VAL
9	I	84	HIS
9	I	103	ARG
11	K	8	GLU
13	M	7	LEU
13	M	10	LEU
13	M	31	ASP
13	M	39	LEU
13	M	53	ARG
13	M	107	MET
13	M	112	ARG
13	M	114	MET
13	M	120	GLU
13	M	126	ASP
14	N	319	ASP
15	O	10	THR
16	P	161	ILE

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Mol	Chain	Res	Type
16	P	206	GLU
16	P	271	GLU
16	P	297	LYS
16	P	299	ARG
17	Q	45	GLU
17	Q	101	ASN
17	Q	105	TYR
17	Q	123	ASN
17	Q	139	LEU
17	Q	142	ASN
17	Q	193	GLU
18	R	88	ARG
18	R	99	LEU
18	R	140	LYS
18	R	159	ASP
18	R	163	LEU
18	R	194	ARG
18	R	206	LYS
18	R	209	GLN
18	R	210	PHE
18	R	212	VAL
18	R	223	VAL
18	R	225	VAL
19	S	7	SER
19	S	163	GLU
19	S	166	ARG
20	T	143	GLN
20	T	145	LEU
20	T	149	VAL
20	T	154	LYS
20	T	160	GLN
20	T	161	TYR
20	T	162	ASN
20	T	177	ARG
20	T	180	LYS
21	U	179	GLU
21	U	187	TYR
21	U	194	ARG
21	U	218	ASP
21	U	222	ARG
21	U	223	MET
21	U	252	LYS

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Mol	Chain	Res	Type
21	U	253	THR
21	U	274	THR
22	V	246	MET
22	V	332	ARG
22	V	362	LEU
22	V	366	ASN
22	V	418	LYS
22	V	427	MET
22	V	429	TRP
22	V	458	VAL
22	V	471	VAL
22	V	479	ASP
22	V	482	PHE
22	V	492	ASN
22	V	517	GLU
22	V	530	ARG
22	V	566	PHE
22	V	568	LEU
22	V	581	TYR
22	V	590	MET
22	V	614	SER
23	W	37	HIS
23	W	64	PRO
23	W	95	GLU
23	W	101	LYS
23	W	112	ARG
23	W	122	THR
23	W	123	PRO
23	W	145	GLN
23	W	166	ARG
23	W	175	TYR
23	W	196	ARG
23	W	207	TYR
23	W	263	LEU
23	W	283	ASP
23	W	285	TYR
23	W	288	LEU
23	W	309	VAL
23	W	333	LEU
23	W	345	ARG
23	W	346	VAL
23	W	425	THR

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Mol	Chain	Res	Type
23	W	461	LEU
23	W	489	CYS
23	W	523	LEU
23	W	533	ASP
23	W	543	GLN
23	W	544	TYR
23	W	554	GLU
23	W	584	TYR
23	W	596	LEU
23	W	610	PHE
23	W	620	MET
23	W	647	ARG
23	W	654	PHE
23	W	669	ARG
23	W	676	LEU
24	0	77	LYS
24	0	103	GLN
24	0	125	ARG
24	0	137	MET
24	0	174	LEU
24	0	202	SER
24	0	218	THR
24	0	222	ILE
25	1	10	ILE
25	1	16	MET
25	1	18	GLN
25	1	38	ILE
26	2	61	PHE
26	2	77	LYS
26	2	181	GLN
26	2	202	GLN
26	2	402	ARG
26	2	407	VAL
26	2	426	ARG
26	2	430	VAL
26	2	452	LYS
27	3	56	LYS
27	3	66	GLU
27	3	109	GLU
27	3	121	LYS
27	3	124	ILE
27	3	133	LEU

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Mol	Chain	Res	Type
27	3	144	ILE
27	3	147	MET
27	3	157	MET
27	3	185	GLN
27	3	190	LEU
27	3	216	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (61) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	516	GLN
1	A	529	GLN
1	A	539	GLN
1	A	700	GLN
1	A	703	GLN
1	A	1310	HIS
1	A	1332	GLN
2	B	98	HIS
2	B	227	ASN
2	B	245	GLN
2	B	452	ASN
2	B	817	GLN
2	B	970	HIS
2	B	1040	GLN
2	B	1101	GLN
2	B	1117	HIS
2	B	1160	GLN
3	C	5	ASN
3	C	6	GLN
3	C	25	ASN
3	C	137	ASN
5	E	64	HIS
5	E	71	GLN
5	E	129	GLN
5	E	132	GLN
9	I	84	HIS
9	I	87	GLN
9	I	98	GLN
9	I	121	HIS
12	L	23	HIS
18	R	177	ASN
18	R	204	ASN

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Mol	Chain	Res	Type
18	R	209	GLN
22	V	281	GLN
22	V	286	HIS
22	V	366	ASN
22	V	415	HIS
22	V	539	ASN
22	V	677	GLN
23	W	187	GLN
23	W	430	ASN
23	W	434	HIS
23	W	590	ASN
24	0	60	HIS
24	0	103	GLN
25	1	51	ASN
26	2	117	ASN
26	2	161	HIS
26	2	181	GLN
26	2	202	GLN
26	2	221	GLN
26	2	239	GLN
26	2	263	GLN
26	2	273	GLN
27	3	52	ASN
27	3	63	HIS
27	3	148	ASN
27	3	155	GLN
27	3	185	GLN
27	3	187	GLN
27	3	225	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 13 ligands modelled in this entry, 13 are monoatomic - leaving 0 for Mogul analysis.

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

No monomer is involved in short contacts.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

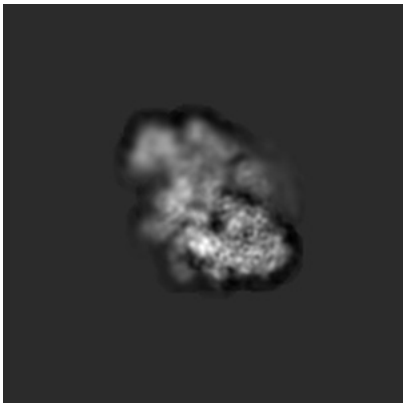
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-3307. These allow visual inspection of the internal detail of the map and identification of artifacts.

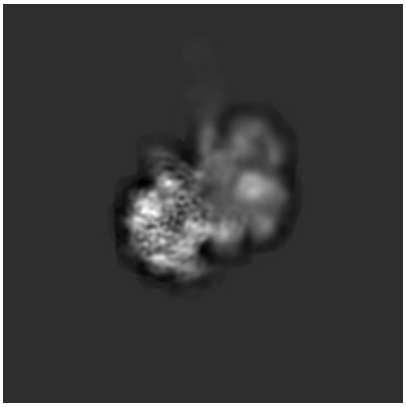
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

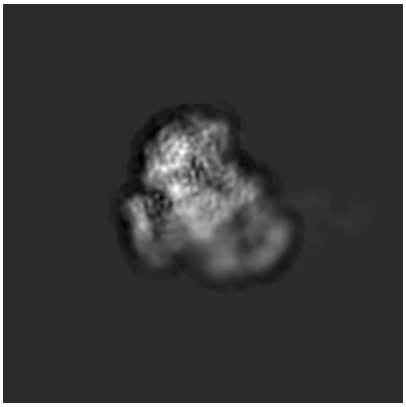
6.1.1 Primary map



X



Y

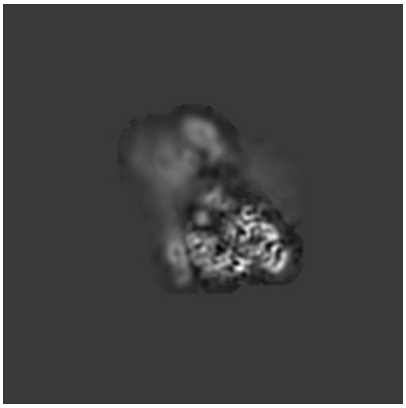


Z

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

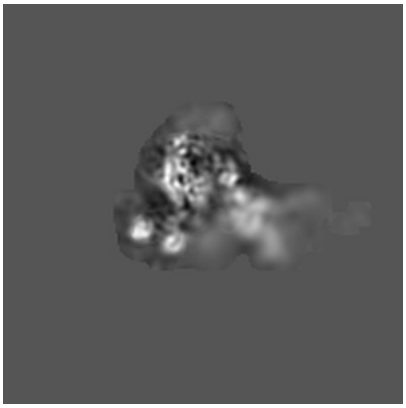
6.2 Central slices

6.2.1 Primary map



X Index: 96

Y Index: 96

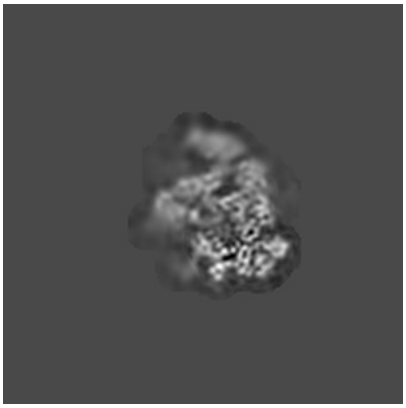


Z Index: 96

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

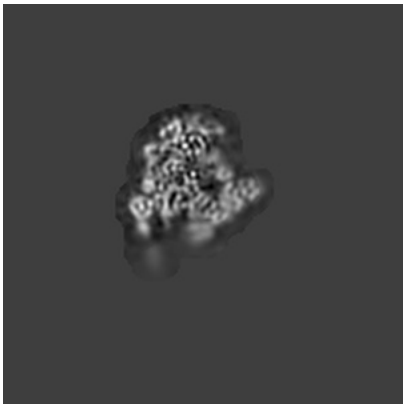
6.3 Largest variance slices (i)

6.3.1 Primary map



X Index: 83

Y Index: 96

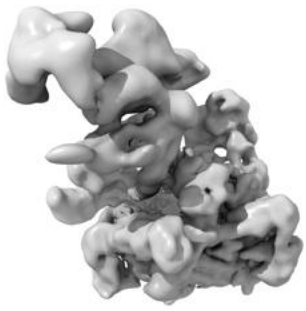


Z Index: 75

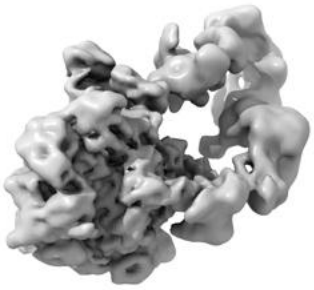
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

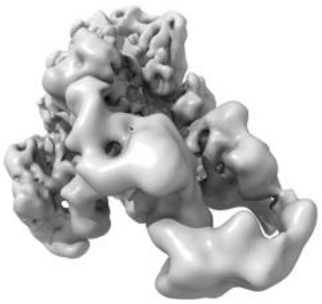
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.045. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

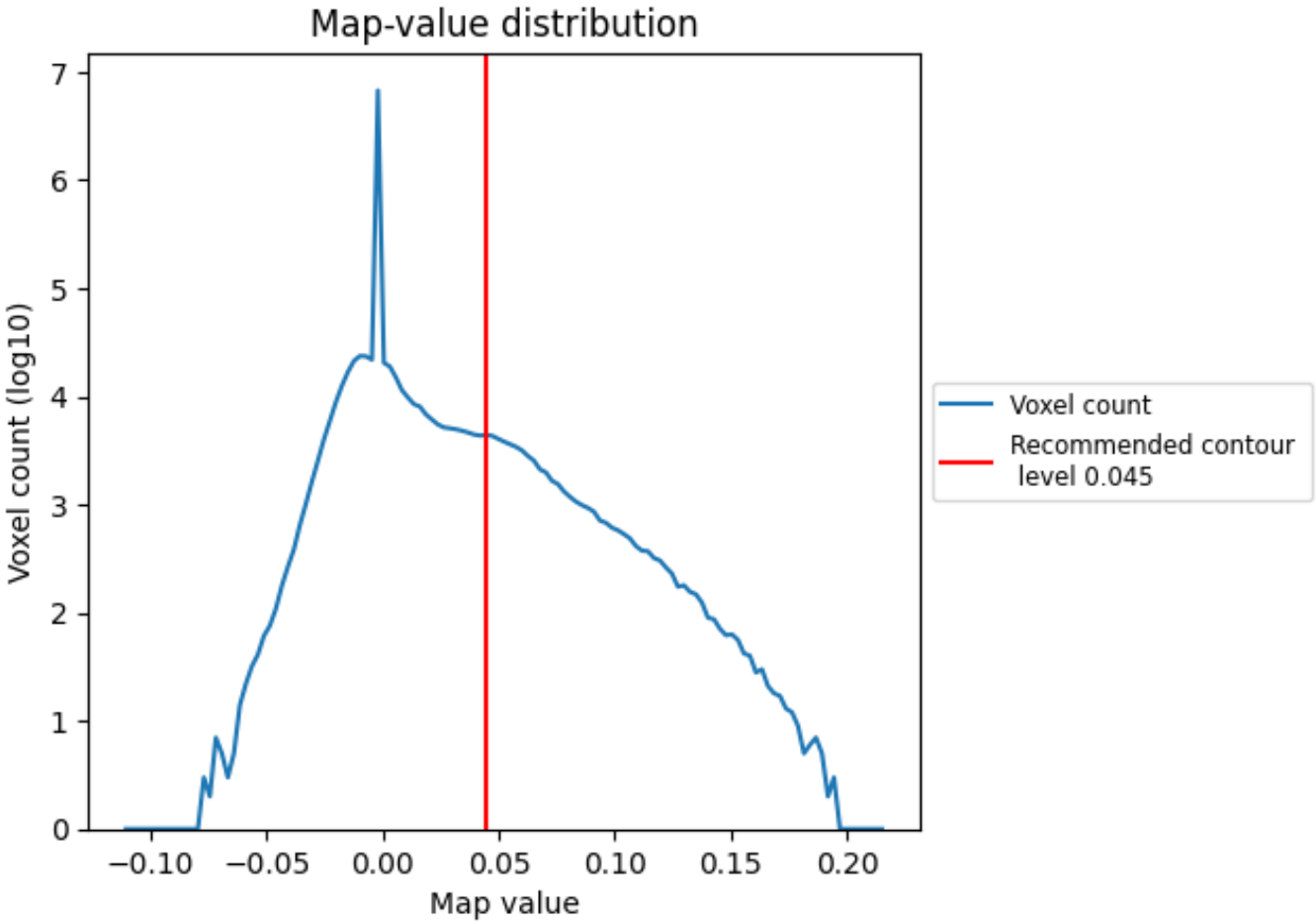
6.5 Mask visualisation (i)

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

7 Map analysis

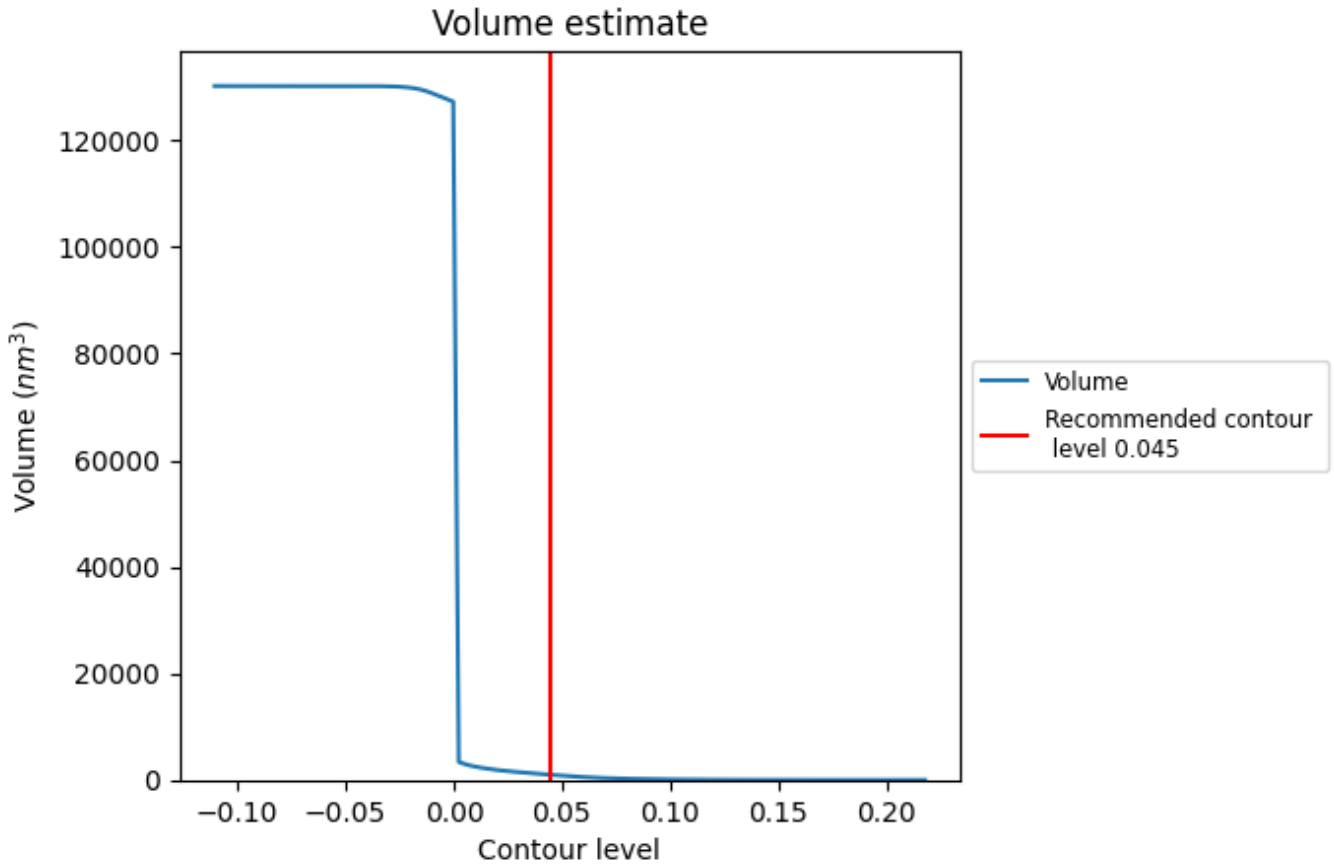
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

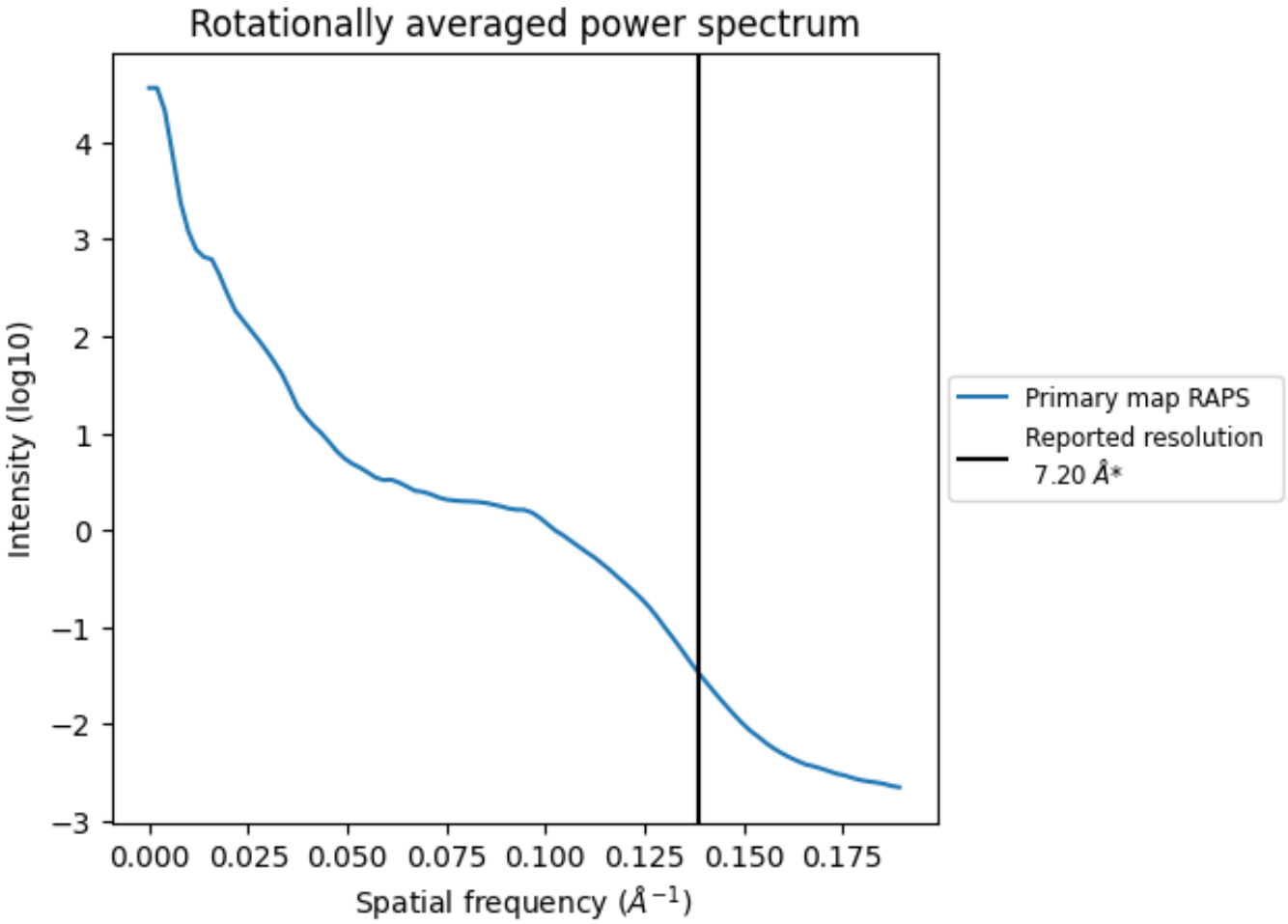
7.2 Volume estimate



The volume at the recommended contour level is 965 nm^3; this corresponds to an approximate mass of 872 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)

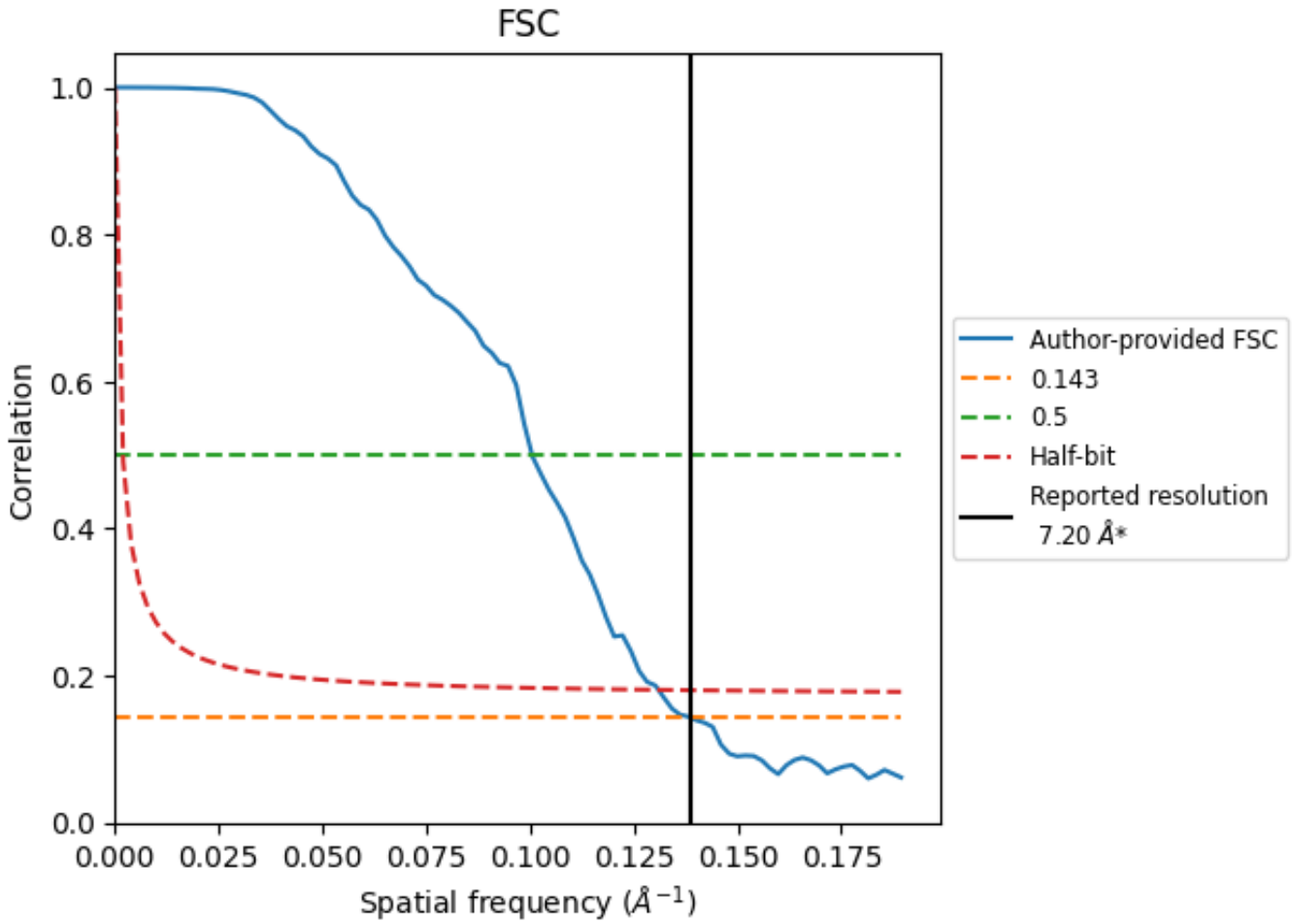


*Reported resolution corresponds to spatial frequency of 0.139 $Å^{-1}$

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 0.139 Å^{-1}

8.2 Resolution estimates (i)

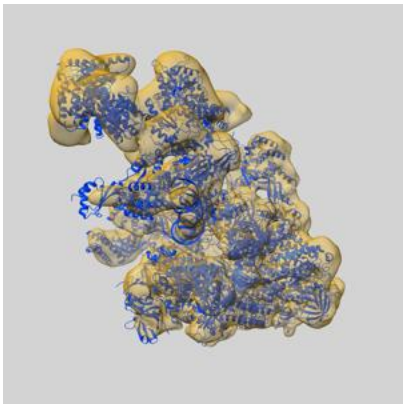
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	7.20	-	-
Author-provided FSC curve	7.23	9.95	7.64
Unmasked-calculated*	-	-	-

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

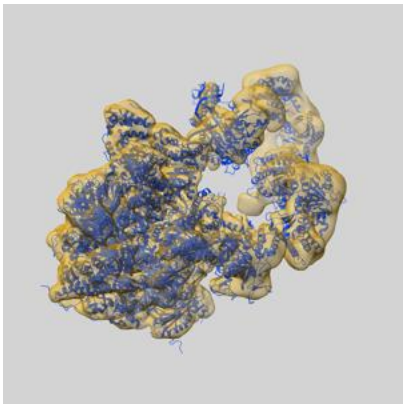
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-3307 and PDB model 5IY6. Per-residue inclusion information can be found in section 3 on page 9.

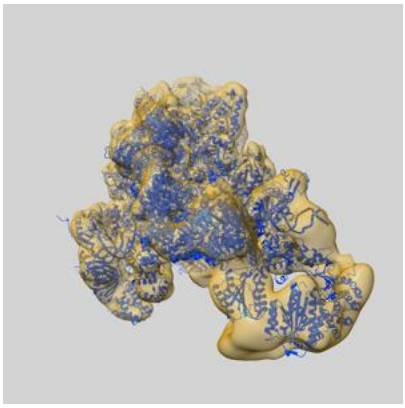
9.1 Map-model overlay



X



Y



Z

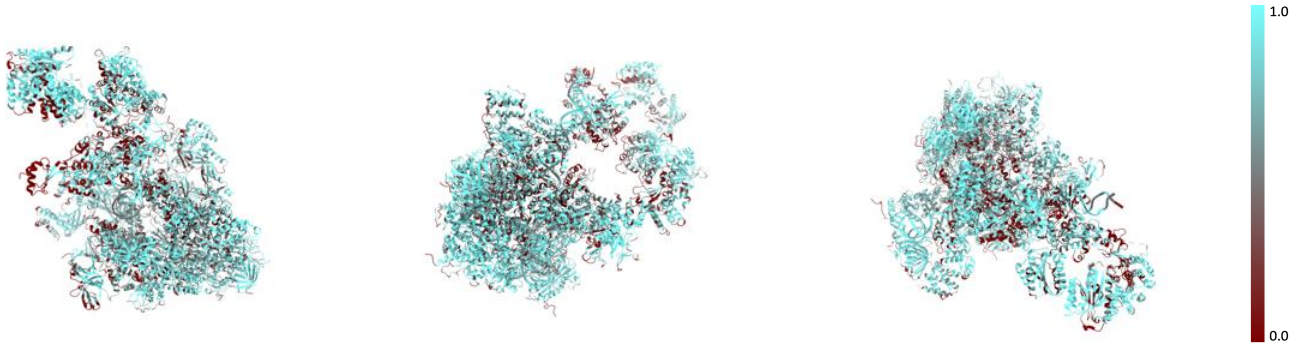
The images above show the 3D surface view of the map at the recommended contour level 0.045 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model

X Y Z

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

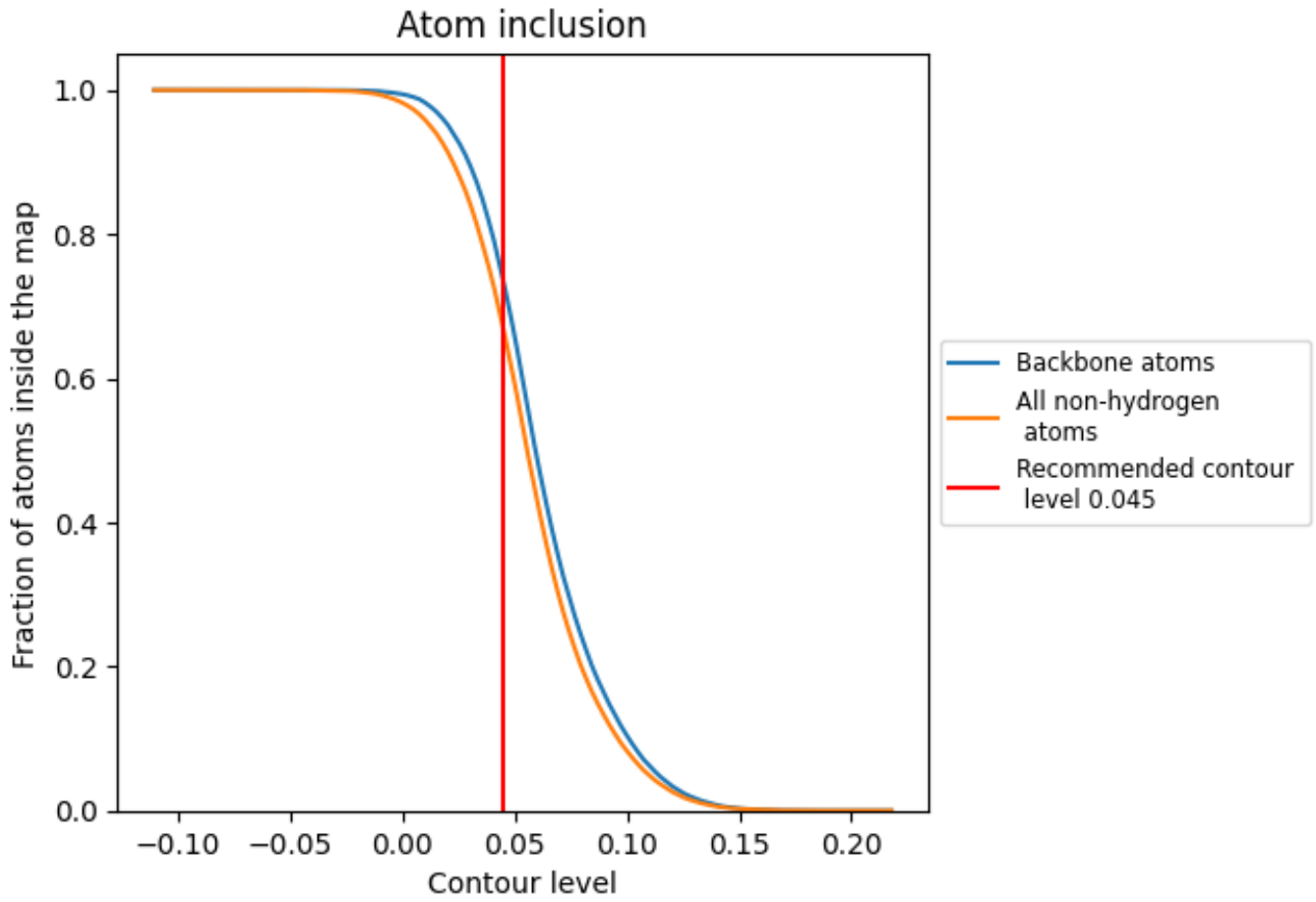
9.3 Atom inclusion mapped to coordinate model



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.045).

9.4 Atom inclusion (i)



At the recommended contour level, 73% of all backbone atoms, 67% 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 (0.045) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.6677	0.0820
0	0.7466	0.0510
1	0.3217	0.0670
2	0.5648	0.0700
3	0.6773	0.0530
A	0.6121	0.0730
B	0.6798	0.0860
C	0.8025	0.1000
D	0.7199	0.0820
E	0.6920	0.0870
F	0.6722	0.0400
G	0.7402	0.0860
H	0.7674	0.0850
I	0.7150	0.1000
J	0.7351	0.0790
K	0.7933	0.1260
L	0.8522	0.1250
M	0.7330	0.1110
N	0.7183	0.1030
O	0.8376	0.0950
P	0.8438	0.0960
Q	0.6607	0.0940
R	0.6831	0.0970
S	0.5537	0.0750
T	0.6241	0.0950
U	0.6095	0.0840
V	0.5560	0.0630
W	0.6283	0.0530
X	0.7803	0.1280
Y	0.7356	0.1290