Full wwPDB EM Validation Report ⓘ

Nov 29, 2022 – 03:11 AM JST

PDB ID	:	7VQ1
EMDB ID	:	EMD-32082
Title	:	Structure of Apo-hsTRPM2 channel
Authors	:	Yu, X.F.; Xie, Y.; Zhang, X.K.; Ma, C.; Guo, J.T.; Yang, F.; Yang, W.
Deposited on	:	2021-10-18
Resolution	:	3.76 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:

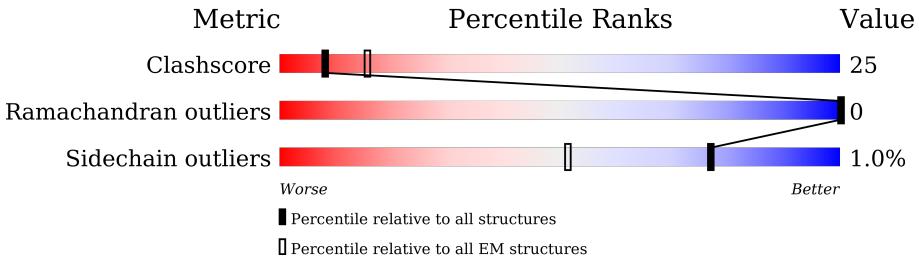
EMDB validation analysis	:	0.0.1.dev43
MolProbity	:	4.02b-467
Percentile statistics	:	20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ	:	1.9.9
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.31.3

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 3.76 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	1503	12% 53% 34% 13%
1	B	1503	12% 52% 34% 13%
1	C	1503	12% 52% 35% 13%
1	D	1503	13% 52% 34% 13%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 37804 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.

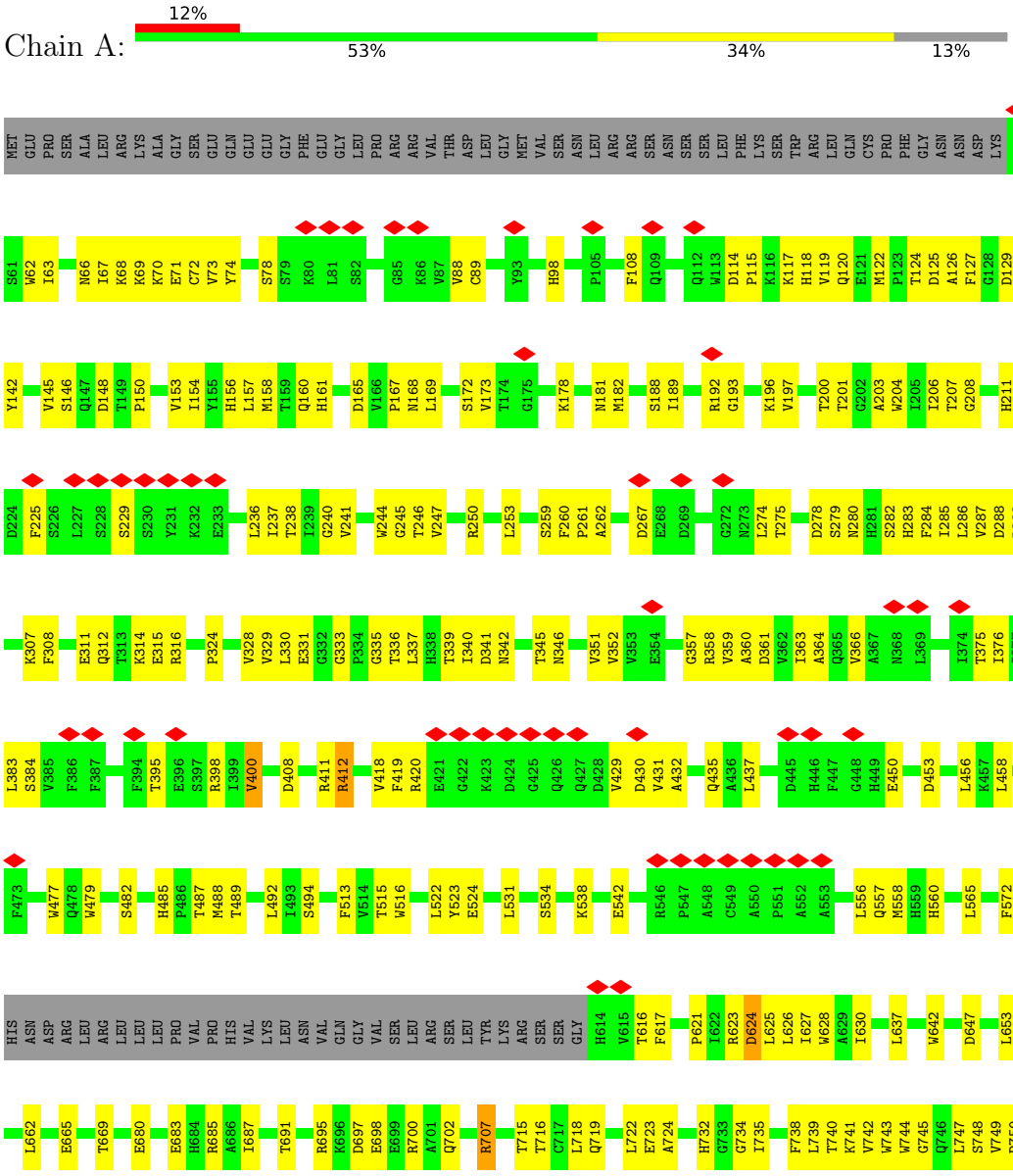
- Molecule 1 is a protein called Transient receptor potential cation channel subfamily M member 2.

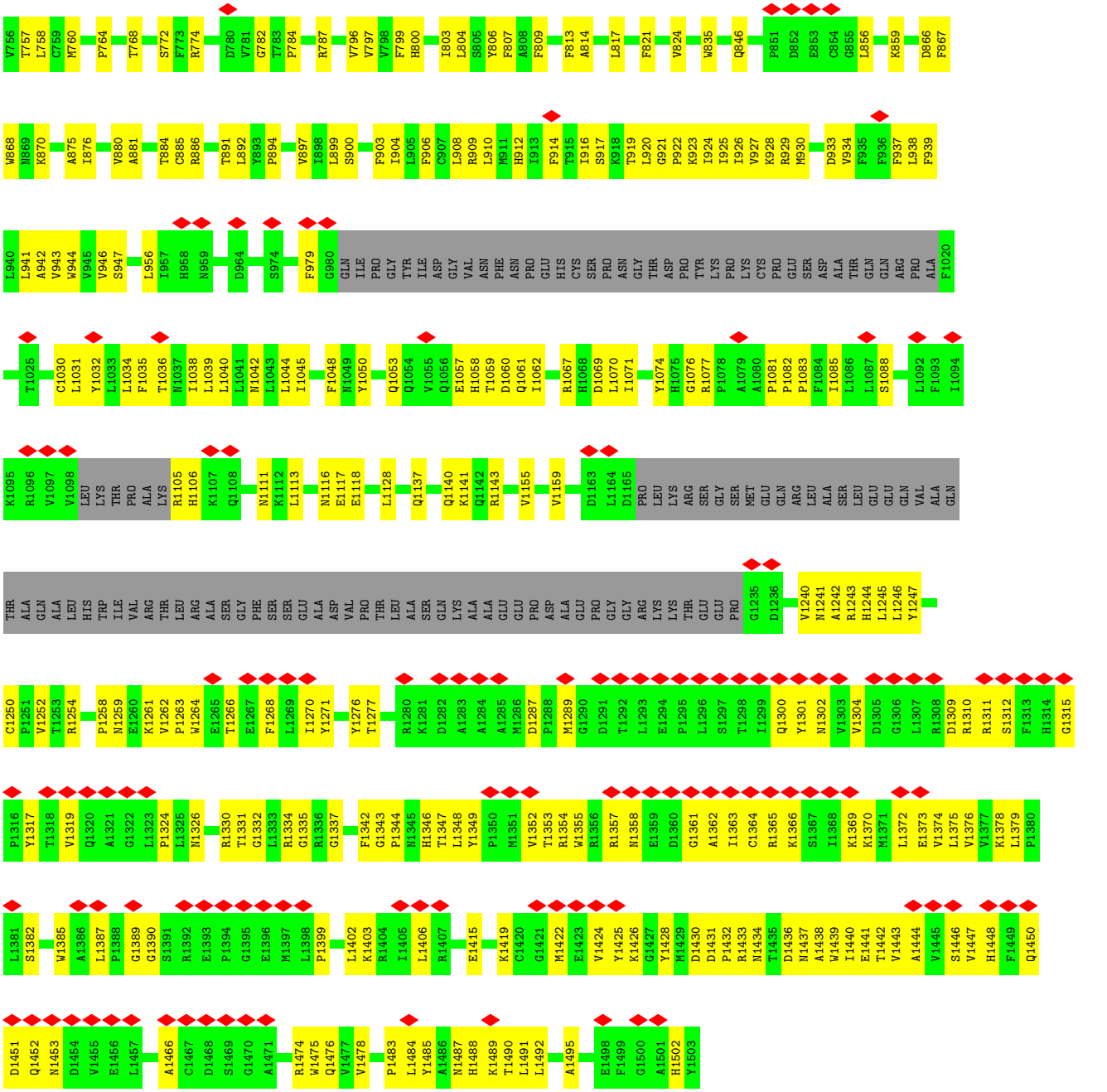
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1302	Total	C	N	O	S	0	0
			9451	6096	1670	1648	37		
1	B	1302	Total	C	N	O	S	0	0
			9451	6096	1670	1648	37		
1	C	1302	Total	C	N	O	S	0	0
			9451	6096	1670	1648	37		
1	D	1302	Total	C	N	O	S	0	0
			9451	6096	1670	1648	37		

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.

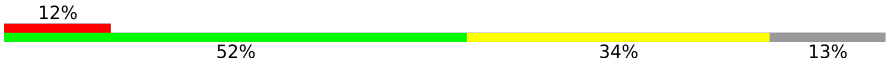
• Molecule 1: Transient receptor potential cation channel subfamily M member 2

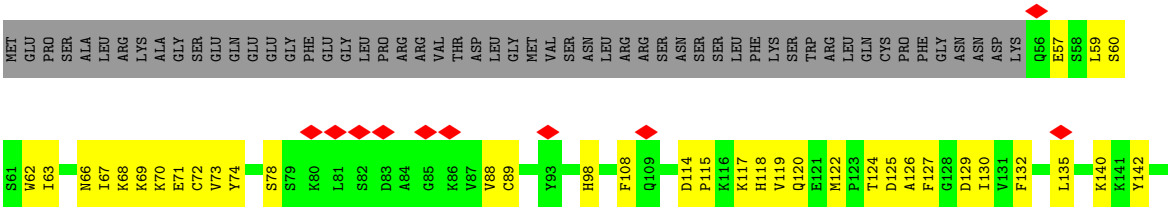


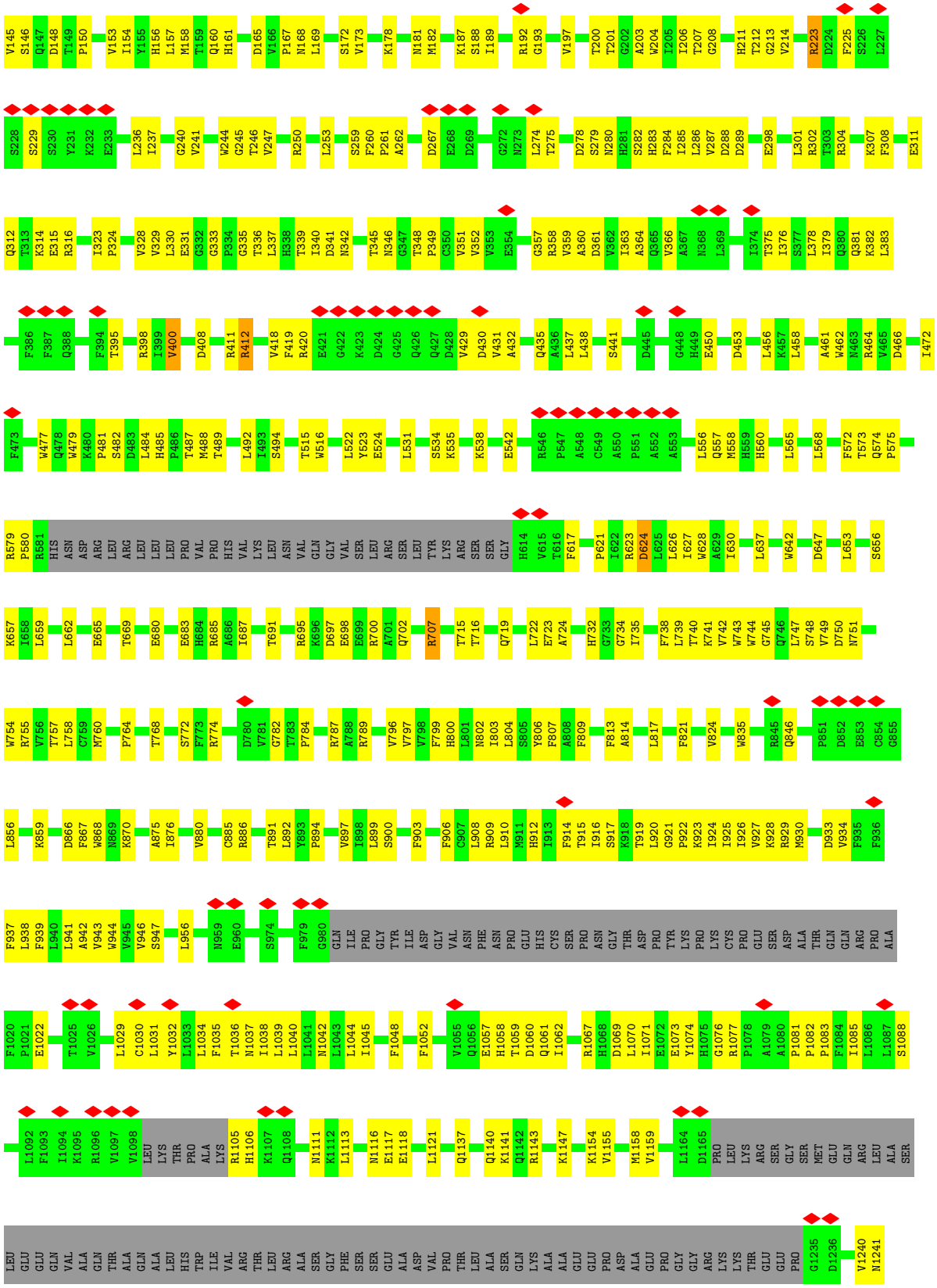


• Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain B:



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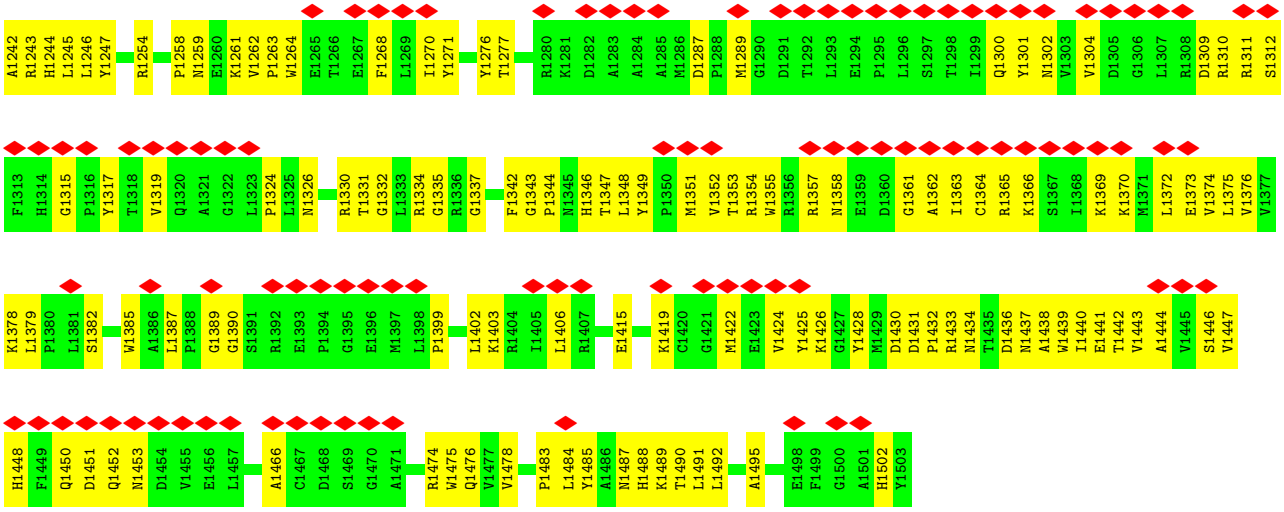
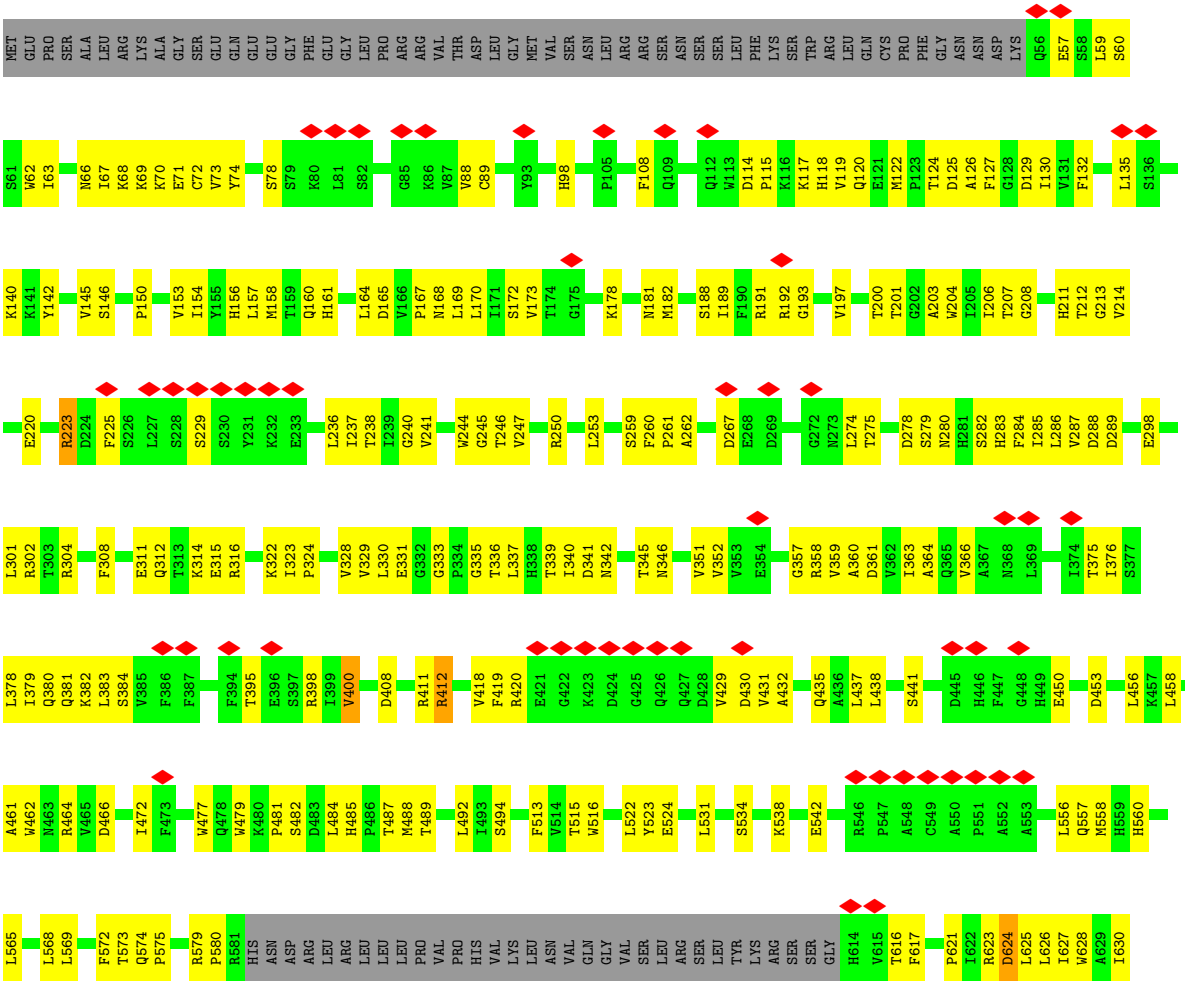
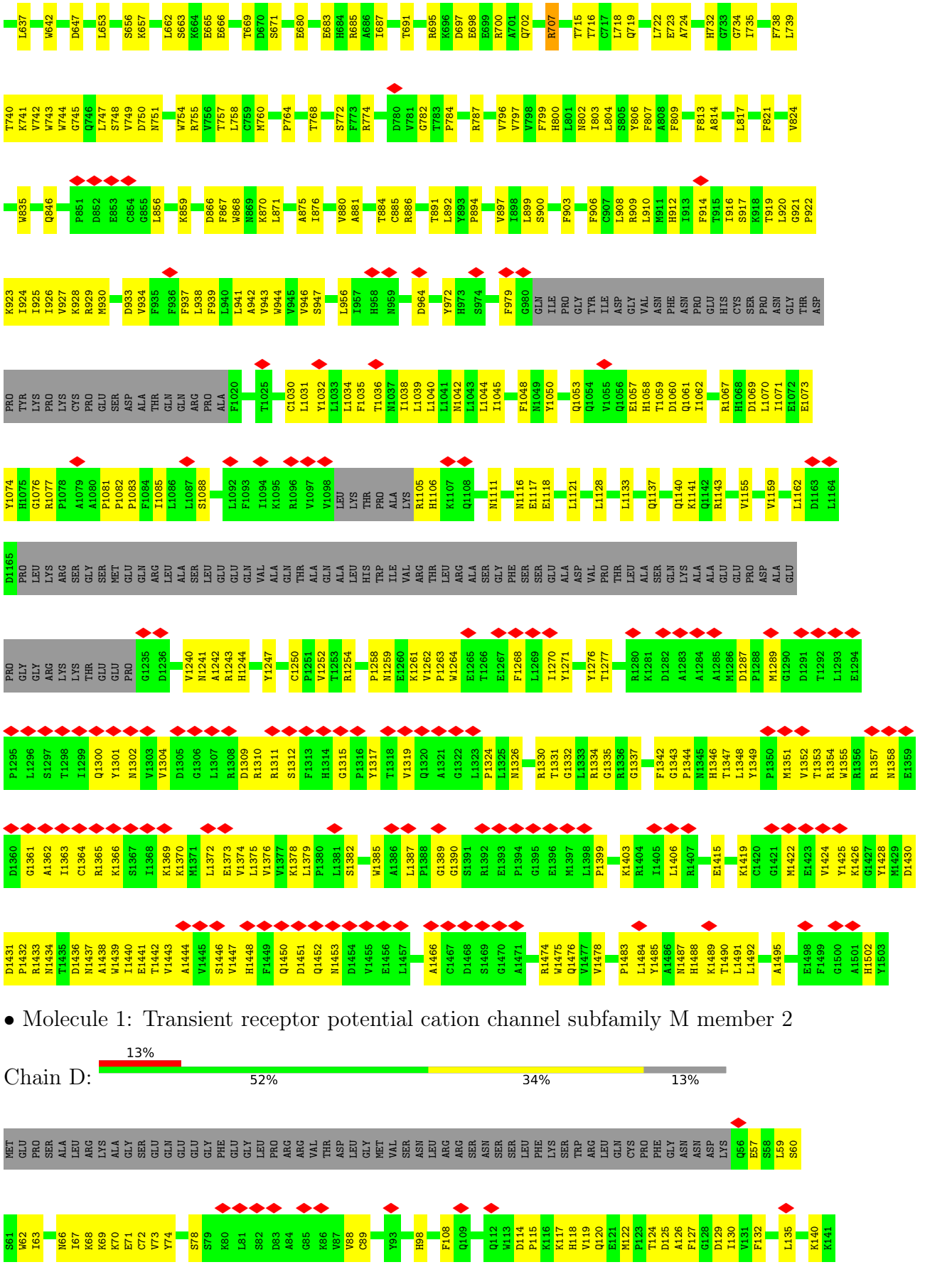
S228 S229 S230 Y231 K232 E233 L236 I237 G240 V241 W244 G245 T246 V247 R250 L253 S259 F260 P261 A262 D267 E268 D269 G272 N273 L274 T275 D278 S279 W280 H281 S282 H283 F284 I285 L286 V287 D288 D289 E298 L301 R302 T303 R304 K307 F308 E311
Q312 T313 K314 E315 R316 I323 P324 V328 V329 L330 E331 G332 G333 P334 G335 T336 L337 H338 T339 I340 D341 N342 T345 N346 G347 T348 P349 C350 V351 V352 V353 E354 G357 R358 V359 A360 D361 V362 I363 A364 Q365 V366 A367 N368 L369 I374 T375 I376 S377 L378 I379 Q380 Q381 K382 L383
F386 F387 Q388 F394 T395 R398 I399 V400 D408 R411 R412 V418 F419 R420 E421 G422 K423 D424 G425 Q426 Q427 D428 V429 D430 V431 A432 Q435 A436 L437 L438 S441 D445 G448 H449 E450 D453 L456 K457 L458 A461 W462 N463 R464 V465 D466 I472
F473 W477 Q478 W479 K480 P481 S482 D483 L484 H485 P486 T487 M488 T489 L492 I493 S494 T515 W516 L522 Y523 E524 L531 S534 K535 K538 E542 R546 P547 A548 C549 A550 P551 A552 A553 L556 Q557 M558 H559 H560 L565 L568 F572 T573 Q574 P575
R579 P580 R581 HIS ASN ASP ARG LEU ARG LEU LEU LEU PRO VAL PRO HIS VAL LYS LEU ASN VAL GLN GLY VAL SER LEU ARG SER LEU TYR LYS ARG SER SER GLY H614 V615 T616 F617 P621 I622 R623 D624 L625 L626 I627 W628 A629 I630 L637 W642 D647 L653 S656
K657 I658 L659 L662 E665 T669 E680 E683 H684 R685 A686 I687 T691 R695 K696 D697 E698 E699 R700 A701 Q702 R707 T715 T716 Q719 L722 E723 A724 H732 G733 G734 I735 F738 L739 T740 K741 V742 W743 W744 G745 Q746 L747 S748 V749 D750 N751
W754 R755 V756 T757 L758 C759 M760 P764 T768 S772 F773 R774 D780 V781 G782 T783 P784 R787 A788 R789 V796 V797 W798 F799 H800 L801 N802 I803 L804 S805 Y806 F807 A808 F809 F813 A814 L817 F821 V824 W835 R845 Q846 P851 D852 E853 C854 G855
L856 K859 D866 F867 W868 N869 K870 A875 I876 V880 C885 R886 T891 L892 Y893 P894 V897 I898 L899 S900 F903 F906 C907 L908 R909 L910 M911 H912 I913 F914 T915 I916 S917 K918 T919 L920 G921 P922 K923 I924 I925 I926 V927 K928 R929 M930 D933 V934 F935 F936
F937 L938 F939 L940 L941 A942 V943 W944 V945 V946 S947 L956 N959 E960 S974 F979 G980 GLN ILE PRO GLY TYR ILE ASP GLY VAL ASN PHE ASN PRO GLU HIS CYS SER PRO ASN GLY THR ASP PRO TYR LYS PRO LYS CYS PRO GLU SER ASP ALA THR GLN GLN ARG PRO ALA
F1020 P1021 E1022 T1025 V1026 L1029 C1030 L1031 Y1032 L1033 L1034 F1035 T1036 N1037 I1038 L1039 L1040 L1041 N1042 L1043 L1044 I1045 F1048 F1052 V1055 Q1056 E1057 H1058 T1059 D1060 Q1061 I1062 R1067 H1068 D1069 L1070 I1071 E1072 E1073 Y1074 H1075 G1076 R1077 P1078 A1079 A1080 P1081 P1082 P1083 F1084 I1085 L1086 L1087 S1088
L1092 F1093 I1094 K1095 R1096 V1097 V1098 LEU LYS THR PRO ALA LYS R1105 H1106 K1107 Q1108 N1111 K1112 L1113 N1116 E1117 E1118 L1121 Q1137 Q1140 K1141 Q1142 R1143 K1147 K1154 V1155 M1158 V1159 L1164 D1165 PRO LEU LYS ARG SER GLY SER MET GLU GLN GLN ARG LEU ALA SER
LEU GLU GLU GLN VAL ALA GLN THR ALA GLN ALA LEU HIS TRP ILE VAL ARG THR LEU ARG ALA SER GLY PHE SER SER GLU ALA ASP VAL PRO THR LEU ALA SER GLN LYS ALA ALA GLU GLU PRO ASP ALA GLU PRO GLY GLY ARG LYS LYS THR GLU GLU PRO G1235 D1236 V1240 N1241



• Molecule 1: Transient receptor potential cation channel subfamily M member 2

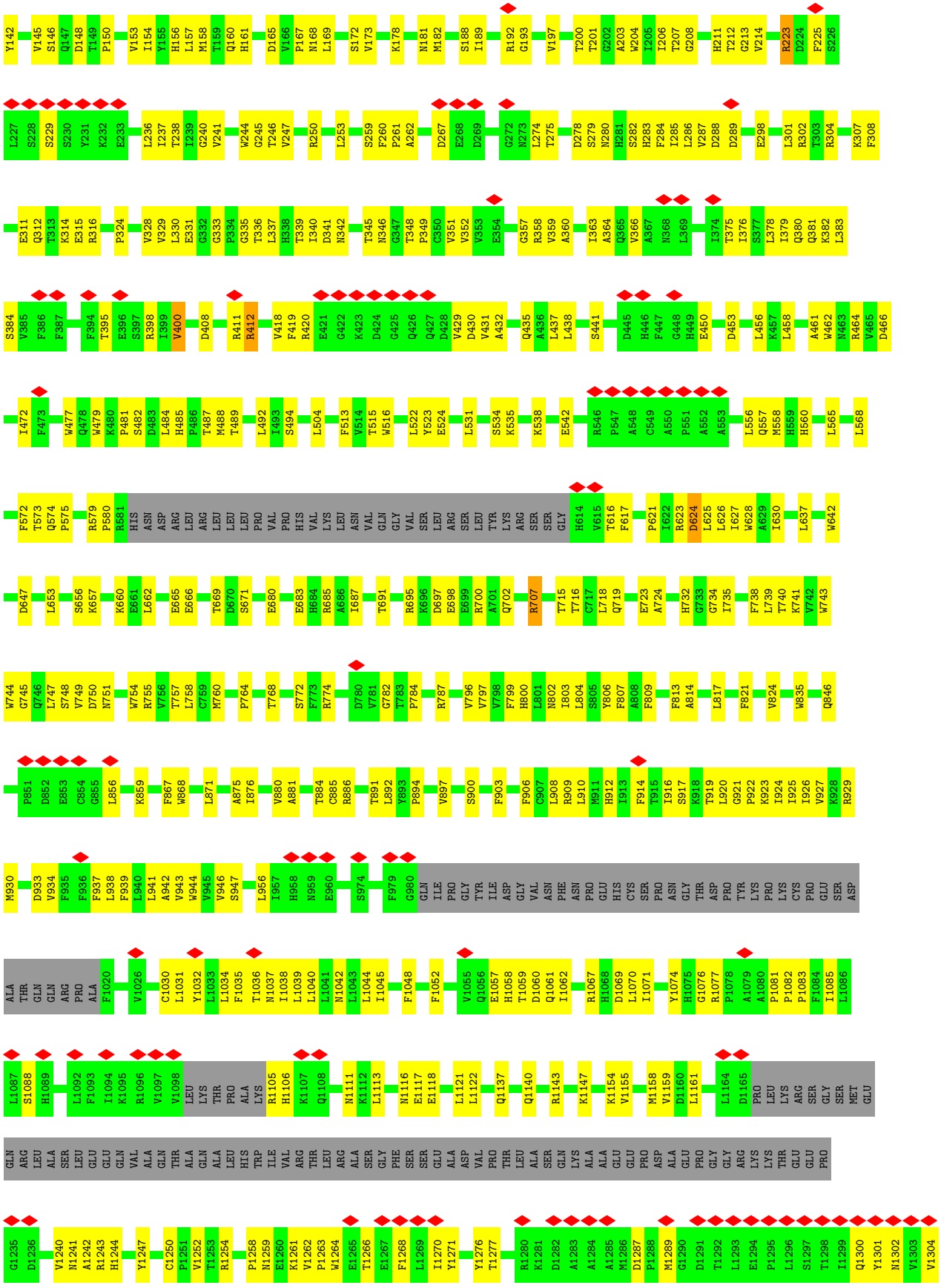
Chain C:

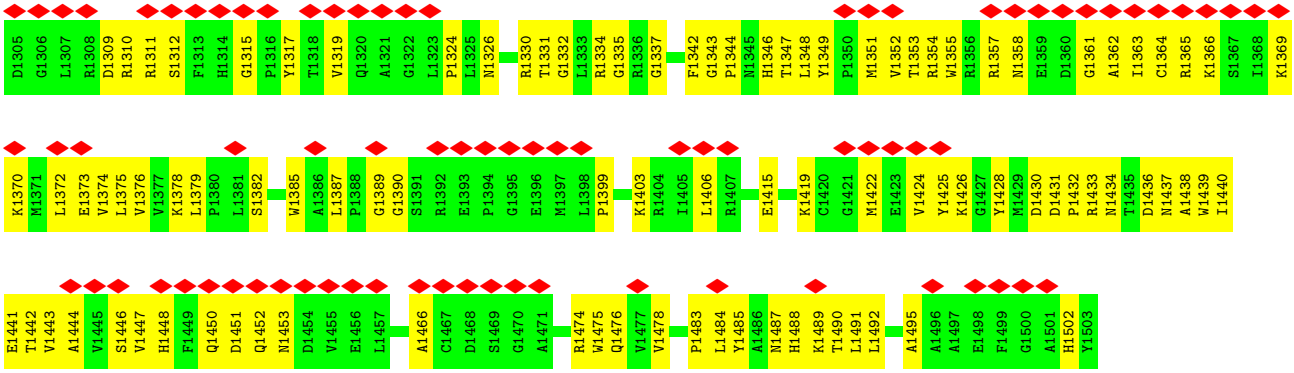




• Molecule 1: Transient receptor potential cation channel subfamily M member 2

Chain D:


Y142 V145 S146 Q147 D148 T149 P150 V153 I154 Y155 H156 L157 M158 T159 Q160 H161 D165 V166 P167 N168 L169 S172 V173 K178 N181 M182 S188 I189 R192 G193 V197 T200 T201 G202 A203 W204 I205 I206 T207 G208 H211 T212 G213 V214 R223 D224 F225 S226
L227 S228 S229 S230 Y231 K232 E233 L236 T237 T238 I239 G240 V241 W244 G245 T246 V247 R250 L253 S259 F260 P261 A262 D267 E268 D269 G272 N273 L274 T275 D278 S279 N280 H281 S282 H283 F284 I285 L286 V287 D288 D289 E298 L301 R302 T303 R304 K307 F308
E311 Q312 T313 K314 E315 R316 P324 V328 V329 L330 E331 G332 G333 P334 G335 T336 L337 H338 T339 I340 D341 N342 T345 N346 G347 T348 P349 C350 V351 V352 V353 E354 G357 R358 V359 A360 I363 A364 Q365 V366 A367 N368 L369 I374 T375 I376 S377 L378 I379 Q380 Q381 K382 L383
S384 V385 F386 F387 F394 T395 E396 S397 R398 I399 V400 D408 R411 R412 V418 F419 R420 E421 G422 K423 D424 G425 Q426 Q427 D428 V429 D430 V431 A432 Q435 A436 L437 L438 S441 D445 H446 F447 G448 H449 E450 D453 L456 K457 L458 A461 W462 N463 R464 V465 D466
I472 F473 W477 Q478 W479 K480 P481 S482 D483 L484 H485 P486 T487 M488 T489 L492 I493 S494 L504 F513 V514 T515 W516 L522 Y523 E524 L531 S534 K535 K538 E542 R546 P547 A548 C549 A550 P551 A552 A553 L556 Q557 M558 H559 H560 L565 L568
F572 T573 Q574 P575 R579 P580 R581 HIS ASN ASP ARG LEU ARG LEU LEU LEU PRO VAL PRO HIS VAL VAL LYS LEU ASN VAL GLN GLY VAL SER LEU ARG SER LEU TYR LYS ARG SER SER GLY H614 V615 T616 F617 P621 I622 R623 D624 L625 L626 I627 W628 A629 I630 L637 W642
D647 L653 S656 K657 K660 E661 L662 E665 E666 T669 D670 S671 E680 E683 H684 R685 A686 I687 T691 R695 K696 D697 E698 E699 R700 A701 Q702 R707 T715 T716 C717 L718 Q719 E723 A724 H732 G733 G734 I735 F738 L739 T740 K741 V742 W743
W744 G745 Q746 L747 S748 V749 D750 N751 W754 R755 V756 T757 L758 C759 M760 P764 T768 S772 F773 R774 D780 V781 G782 T783 P784 R787 V796 V797 V798 F799 H800 L801 N802 I803 L804 S805 Y806 F807 A808 F809 F813 A814 L817 F821 V824 W835 Q846
P851 D852 E853 C854 G855 L856 K859 F867 W868 L871 A875 I876 V880 A881 T884 C885 R886 T891 L892 Y893 P894 V897 S900 F903 F906 C907 L908 R909 L910 M911 H912 I913 F914 T915 I916 S917 K918 T919 L920 G921 P922 K923 I924 I925 I926 V927 K928 R929
M930 D933 V934 F935 F936 F937 L938 F939 L940 L941 A942 V943 W944 V945 V946 S947 L956 I957 H958 N959 E960 S974 F979 G980 GLN ILE PRO GLY TYR ILE ASP GLY VAL ASN PHE ASN PRO GLU HIS CYS SER PRO ASN GLY THR ASP PRO TYR LYS PRO LYS CYS PRO GLU SER ASP
ALA THR GLN GLN ARG PRO ALA F1020 V1026 C1030 L1031 Y1032 L1033 L1034 F1035 T1036 N1037 I1038 L1039 L1040 L1041 N1042 L1043 L1044 I1045 F1048 F1052 V1055 Q1056 E1057 H1058 T1059 D1060 Q1061 I1062 R1067 H1068 D1069 L1070 I1071 Y1074 H1075 G1076 R1077 P1078 A1079 A1080 P1081 P1082 P1083 F1084 I1085 L1086
L1087 S1088 H1089 L1092 F1093 I1094 K1095 R1096 V1097 V1098 LEU LYS THR PRO ALA LYS R1105 H1106 K1107 Q1108 N1111 K1112 L1113 N1116 E1117 E1118 L1121 L1122 Q1137 Q1140 R1143 K1147 K1154 V1155 M1158 V1159 D1160 L1161 L1164 D1165 PRO LEU LYS ARG SER GLY SER MET GLU
GLN ARG LEU ALA SER LEU GLU GLN VAL ALA GLN THR ALA GLN ALA LEU HIS TRP ILE VAL ARG THR LEU ARG ALA SER GLY PHE SER SER GLU ALA ASP VAL PRO THR LEU ALA SER GLN LYS ALA ALA ALA GLU GLU PRO ASP ALA GLU PRO LEU LYS THR GLU GLU PRO
G1235 D1236 V1240 N1241 A1242 R1243 H1244 Y1247 C1250 P1251 V1252 T1253 R1254 P1258 N1259 E1260 K1261 V1262 P1263 W1264 E1265 T1266 E1267 F1268 I1269 I1270 Y1271 Y1276 T1277 R1280 K1281 D1282 A1283 A1284 A1285 M1286 D1287 P1288 M1289 G1290 D1291 T1292 L1293 E1294 P1295 L1296 S1297 T1298 I1299 Q1300 Y1301 N1302 V1303 V1304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R1330 T1331 G1332 L1333 R1334 G1335 R1336 G1337
F1342 G1343 P1344 N1345 H1346 T1347 L1348 Y1349 P1350 M1351 V1352 T1353 R1354 W1355 R1356 R1357 M1358 E1359 D1360 G1361 A1362 I1363 C1364 R1365 K1366 S1367 I1368 K1369
K1370 M1371 L1372 E1373 V1374 L1375 V1376 V1377 K1378 L1379 P1380 L1381 S1382
W1385 A1386 L1387 P1388 G1389 G1390 S1391 R1392 E1393 P1394 G1395 E1396 M1397 L1398 P1399
K1403 R1404 T1405 L1406 R1407
E1415
K1419 C1420 G1421 M1422 E1423 V1424 Y1425 K1426 G1427 Y1428 M1429 D1430 D1431 P1432 R1433 N1434 T1435 D1436 N1437 A1438 W1439 I1440
E1441 T1442 V1443 A1444 V1445 S1446 V1447 H1448 F1449 Q1450 D1451 Q1452 N1453 D1454 V1455 E1456 L1457
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R1474 W1475 Q1476 V1477 V1478
P1483 L1484 Y1485 A1486 N1487 H1488 K1489 T1490 L1491 L1492
A1495 A1496 A1497 E1498 F1499 G1500 A1501 H1502 Y1503

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	68530	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 ($e^-/Å^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 (6k x 4k)	Depositor
Maximum map value	0.009	Depositor
Minimum map value	-0.004	Depositor
Average map value	-0.000	Depositor
Map value standard deviation	0.000	Depositor
Recommended contour level	0.0022	Depositor
Map size (Å)	342.0, 342.0, 342.0	wwPDB
Map dimensions	400, 400, 400	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.855, 0.855, 0.855	Depositor

5 Model quality

5.1 Standard geometry

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\#\|Z\| > 5$	RMSZ	$\#\|Z\| > 5$
1	A	0.50	0/9675	0.52	0/13228
1	B	0.50	0/9675	0.52	0/13228
1	C	0.50	0/9675	0.52	0/13228
1	D	0.50	0/9675	0.52	0/13228
All	All	0.50	0/38700	0.52	0/52912

There are no bond length outliers.

There are no bond angle outliers.

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts

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	9451	0	8720	455	0
1	B	9451	0	8720	449	0
1	C	9451	0	8720	461	0
1	D	9451	0	8720	459	0
All	All	37804	0	34880	1792	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 25.

All (1792) 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)
1:A:1038:ILE:HD13	1:B:938:LEU:HD11	1.56	0.88
1:B:1035:PHE:HA	1:B:1039:LEU:HD13	1.60	0.84
1:C:1035:PHE:HA	1:C:1039:LEU:HD13	1.60	0.83
1:A:846:GLN:HE22	1:A:1077:ARG:HH21	1.28	0.82
1:B:846:GLN:HE22	1:B:1077:ARG:HH21	1.28	0.82
1:D:1035:PHE:HA	1:D:1039:LEU:HD13	1.60	0.82
1:A:69:LYS:HE3	1:A:125:ASP:H	1.46	0.81
1:D:69:LYS:HE3	1:D:125:ASP:H	1.46	0.81
1:D:846:GLN:HE22	1:D:1077:ARG:HH21	1.28	0.81
1:C:846:GLN:HE22	1:C:1077:ARG:HH21	1.28	0.80
1:A:1035:PHE:HA	1:A:1039:LEU:HD13	1.60	0.80
1:B:69:LYS:HE3	1:B:125:ASP:H	1.46	0.79
1:C:69:LYS:HE3	1:C:125:ASP:H	1.46	0.78
1:C:707:ARG:NH2	1:C:1118:GLU:OE2	2.16	0.77
1:B:707:ARG:NH2	1:B:1118:GLU:OE2	2.16	0.77
1:C:72:CYS:HA	1:C:119:VAL:HA	1.66	0.77
1:C:745:GLY:O	1:C:774:ARG:NH1	2.18	0.77
1:B:72:CYS:HA	1:B:119:VAL:HA	1.66	0.77
1:A:707:ARG:NH2	1:A:1118:GLU:OE2	2.16	0.77
1:A:72:CYS:HA	1:A:119:VAL:HA	1.66	0.76
1:A:745:GLY:O	1:A:774:ARG:NH1	2.18	0.76
1:B:241:VAL:HG13	1:B:285:ILE:HD11	1.67	0.76
1:D:745:GLY:O	1:D:774:ARG:NH1	2.18	0.76
1:D:245:GLY:O	1:D:250:ARG:NH2	2.19	0.76
1:A:62:TRP:O	1:A:66:ASN:ND2	2.17	0.76
1:B:745:GLY:O	1:B:774:ARG:NH1	2.18	0.76
1:C:62:TRP:O	1:C:66:ASN:ND2	2.17	0.76
1:D:72:CYS:HA	1:D:119:VAL:HA	1.66	0.76
1:A:245:GLY:O	1:A:250:ARG:NH2	2.19	0.75
1:A:1399:PRO:O	1:A:1403:LYS:N	2.14	0.75
1:B:62:TRP:O	1:B:66:ASN:ND2	2.17	0.75
1:B:245:GLY:O	1:B:250:ARG:NH2	2.19	0.75
1:C:1399:PRO:O	1:C:1403:LYS:N	2.14	0.75
1:C:245:GLY:O	1:C:250:ARG:NH2	2.19	0.75
1:D:707:ARG:NH2	1:D:1118:GLU:OE2	2.16	0.75
1:C:241:VAL:HG13	1:C:285:ILE:HD11	1.67	0.75
1:D:241:VAL:HG13	1:D:285:ILE:HD11	1.67	0.74
1:A:740:THR:OG1	1:A:1067:ARG:NH2	2.21	0.74
1:C:740:THR:OG1	1:C:1067:ARG:NH2	2.21	0.74
1:A:241:VAL:HG13	1:A:285:ILE:HD11	1.67	0.74
1:C:78:SER:N	1:C:88:VAL:O	2.19	0.74
1:D:623:ARG:NH1	1:D:624:ASP:OD1	2.21	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:740:THR:OG1	1:D:1067:ARG:NH2	2.21	0.74
1:C:178:LYS:HE2	1:C:358:ARG:HD2	1.71	0.73
1:D:178:LYS:HE2	1:D:358:ARG:HD2	1.70	0.73
1:B:1399:PRO:O	1:B:1403:LYS:N	2.14	0.73
1:A:78:SER:N	1:A:88:VAL:O	2.19	0.73
1:C:623:ARG:NH1	1:C:624:ASP:OD1	2.21	0.73
1:B:740:THR:OG1	1:B:1067:ARG:NH2	2.21	0.73
1:C:919:THR:O	1:C:923:LYS:NZ	2.20	0.73
1:C:364:ALA:O	1:C:420:ARG:NH2	2.22	0.73
1:B:623:ARG:NH1	1:B:624:ASP:OD1	2.21	0.72
1:D:62:TRP:O	1:D:66:ASN:ND2	2.17	0.72
1:D:364:ALA:O	1:D:420:ARG:NH2	2.22	0.72
1:C:1038:ILE:HD13	1:D:938:LEU:HD11	1.71	0.72
1:A:623:ARG:NH1	1:A:624:ASP:OD1	2.21	0.72
1:D:78:SER:N	1:D:88:VAL:O	2.19	0.72
1:D:1399:PRO:O	1:D:1403:LYS:N	2.14	0.72
1:B:919:THR:O	1:B:923:LYS:NZ	2.20	0.72
1:B:364:ALA:O	1:B:420:ARG:NH2	2.22	0.72
1:B:178:LYS:HE2	1:B:358:ARG:HD2	1.70	0.71
1:B:357:GLY:HA3	1:B:360:ALA:HB3	1.72	0.71
1:A:178:LYS:HE2	1:A:358:ARG:HD2	1.71	0.71
1:C:357:GLY:HA3	1:C:360:ALA:HB3	1.72	0.71
1:B:1349:TYR:HD1	1:B:1389:GLY:HA3	1.55	0.71
1:C:1375:LEU:HA	1:C:1475:TRP:HA	1.72	0.71
1:D:1349:TYR:HD1	1:D:1389:GLY:HA3	1.55	0.71
1:B:63:ILE:HG23	1:B:67:ILE:HD12	1.73	0.71
1:D:653:LEU:O	1:D:656:SER:OG	2.09	0.71
1:A:364:ALA:O	1:A:420:ARG:NH2	2.22	0.71
1:B:363:ILE:HA	1:B:366:VAL:HG12	1.73	0.70
1:B:1375:LEU:HA	1:B:1475:TRP:HA	1.72	0.70
1:D:63:ILE:HG23	1:D:67:ILE:HD12	1.73	0.70
1:D:1375:LEU:HA	1:D:1475:TRP:HA	1.72	0.70
1:A:357:GLY:HA3	1:A:360:ALA:HB3	1.72	0.70
1:C:363:ILE:HA	1:C:366:VAL:HG12	1.73	0.70
1:D:260:PHE:HB2	1:D:261:PRO:HD3	1.74	0.70
1:A:916:ILE:HD13	1:A:1070:LEU:HD23	1.74	0.70
1:A:1349:TYR:HD1	1:A:1389:GLY:HA3	1.55	0.70
1:B:653:LEU:O	1:B:656:SER:OG	2.09	0.70
1:D:919:THR:O	1:D:923:LYS:NZ	2.20	0.70
1:A:260:PHE:HB2	1:A:261:PRO:HD3	1.74	0.70
1:C:1349:TYR:HD1	1:C:1389:GLY:HA3	1.55	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:933:ASP:OD1	1:D:934:VAL:N	2.25	0.70
1:D:1076:GLY:HA2	1:D:1106:HIS:HE1	1.57	0.70
1:C:260:PHE:HB2	1:C:261:PRO:HD3	1.74	0.70
1:B:916:ILE:HD13	1:B:1070:LEU:HD23	1.74	0.70
1:C:63:ILE:HG23	1:C:67:ILE:HD12	1.73	0.70
1:D:357:GLY:HA3	1:D:360:ALA:HB3	1.72	0.70
1:A:1375:LEU:HA	1:A:1475:TRP:HA	1.72	0.70
1:B:260:PHE:HB2	1:B:261:PRO:HD3	1.74	0.70
1:B:933:ASP:OD1	1:B:934:VAL:N	2.25	0.70
1:C:933:ASP:OD1	1:C:934:VAL:N	2.25	0.70
1:C:1038:ILE:O	1:C:1042:ASN:ND2	2.25	0.70
1:D:916:ILE:HD13	1:D:1070:LEU:HD23	1.74	0.70
1:A:1038:ILE:O	1:A:1042:ASN:ND2	2.25	0.69
1:A:1076:GLY:HA2	1:A:1106:HIS:HE1	1.57	0.69
1:C:916:ILE:HD13	1:C:1070:LEU:HD23	1.74	0.69
1:A:653:LEU:O	1:A:656:SER:OG	2.09	0.69
1:A:1347:THR:OG1	1:A:1390:GLY:O	2.10	0.69
1:C:73:VAL:N	1:C:118:HIS:O	2.23	0.69
1:C:1076:GLY:HA2	1:C:1106:HIS:HE1	1.57	0.69
1:C:1347:THR:OG1	1:C:1390:GLY:O	2.10	0.69
1:A:363:ILE:HA	1:A:366:VAL:HG12	1.73	0.69
1:C:1335:GLY:O	1:C:1437:ASN:ND2	2.26	0.69
1:D:363:ILE:HA	1:D:366:VAL:HG12	1.73	0.69
1:C:653:LEU:O	1:C:656:SER:OG	2.09	0.69
1:D:741:LYS:HG3	1:D:774:ARG:HH22	1.57	0.69
1:D:1335:GLY:O	1:D:1437:ASN:ND2	2.26	0.69
1:B:741:LYS:HG3	1:B:774:ARG:HH22	1.57	0.69
1:B:1038:ILE:O	1:B:1042:ASN:ND2	2.25	0.69
1:B:1347:THR:OG1	1:B:1390:GLY:O	2.11	0.69
1:C:522:LEU:O	1:C:628:TRP:NE1	2.26	0.69
1:A:63:ILE:HG23	1:A:67:ILE:HD12	1.73	0.69
1:A:200:THR:HG21	1:A:464:ARG:HH11	1.57	0.69
1:A:919:THR:O	1:A:923:LYS:NZ	2.20	0.69
1:B:1076:GLY:HA2	1:B:1106:HIS:HE1	1.57	0.69
1:D:522:LEU:O	1:D:628:TRP:NE1	2.26	0.69
1:D:1038:ILE:O	1:D:1042:ASN:ND2	2.25	0.69
1:A:933:ASP:OD1	1:A:934:VAL:N	2.25	0.69
1:B:522:LEU:O	1:B:628:TRP:NE1	2.26	0.69
1:D:73:VAL:N	1:D:118:HIS:O	2.22	0.69
1:C:741:LYS:HG3	1:C:774:ARG:HH22	1.57	0.69
1:D:1347:THR:OG1	1:D:1390:GLY:O	2.10	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:73:VAL:N	1:A:118:HIS:O	2.23	0.68
1:A:741:LYS:HG3	1:A:774:ARG:HH22	1.57	0.68
1:C:200:THR:HG21	1:C:464:ARG:HH11	1.57	0.68
1:D:1378:LYS:NZ	1:D:1382:SER:OG	2.26	0.68
1:D:1242:ALA:O	1:D:1254:ARG:NH1	2.27	0.68
1:B:923:LYS:HA	1:B:926:ILE:HD12	1.76	0.68
1:C:923:LYS:HA	1:C:926:ILE:HD12	1.76	0.68
1:C:168:ASN:OD1	1:C:314:LYS:NZ	2.26	0.68
1:D:168:ASN:OD1	1:D:314:LYS:NZ	2.26	0.68
1:A:1335:GLY:O	1:A:1437:ASN:ND2	2.26	0.68
1:C:1242:ALA:O	1:C:1254:ARG:NH1	2.27	0.68
1:A:168:ASN:OD1	1:A:314:LYS:NZ	2.26	0.67
1:A:522:LEU:O	1:A:628:TRP:NE1	2.26	0.67
1:C:157:LEU:HD12	1:C:161:HIS:HB2	1.77	0.67
1:B:1242:ALA:O	1:B:1254:ARG:NH1	2.27	0.67
1:C:1378:LYS:NZ	1:C:1382:SER:OG	2.26	0.67
1:D:200:THR:HG21	1:D:464:ARG:HH11	1.58	0.67
1:A:157:LEU:HD12	1:A:161:HIS:HB2	1.77	0.67
1:A:1242:ALA:O	1:A:1254:ARG:NH1	2.27	0.67
1:B:200:THR:HG21	1:B:464:ARG:HH11	1.57	0.67
1:A:1488:HIS:HA	1:A:1491:LEU:HD12	1.77	0.67
1:B:1335:GLY:O	1:B:1437:ASN:ND2	2.26	0.67
1:D:157:LEU:HD12	1:D:161:HIS:HB2	1.77	0.67
1:A:1366:LYS:N	1:A:1369:LYS:O	2.27	0.67
1:A:1378:LYS:NZ	1:A:1382:SER:OG	2.26	0.67
1:B:157:LEU:HD12	1:B:161:HIS:HB2	1.77	0.67
1:D:1488:HIS:HA	1:D:1491:LEU:HD12	1.77	0.67
1:C:1488:HIS:HA	1:C:1491:LEU:HD12	1.77	0.67
1:A:225:PHE:O	1:A:229:SER:N	2.28	0.66
1:D:923:LYS:HA	1:D:926:ILE:HD12	1.76	0.66
1:A:923:LYS:HA	1:A:926:ILE:HD12	1.76	0.66
1:B:168:ASN:OD1	1:B:314:LYS:NZ	2.26	0.66
1:B:73:VAL:N	1:B:118:HIS:O	2.23	0.66
1:B:1301:TYR:HD2	1:B:1319:VAL:HG22	1.61	0.66
1:A:938:LEU:HD11	1:D:1038:ILE:HD13	1.76	0.66
1:B:642:TRP:CZ3	1:B:685:ARG:HD3	2.31	0.66
1:C:1366:LYS:N	1:C:1369:LYS:O	2.27	0.66
1:A:1301:TYR:HD2	1:A:1319:VAL:HG22	1.61	0.66
1:D:642:TRP:CZ3	1:D:685:ARG:HD3	2.31	0.66
1:B:1488:HIS:HA	1:B:1491:LEU:HD12	1.77	0.66
1:A:642:TRP:CZ3	1:A:685:ARG:HD3	2.31	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1261:LYS:O	1:A:1330:ARG:NH1	2.30	0.65
1:B:1366:LYS:N	1:B:1369:LYS:O	2.27	0.65
1:C:642:TRP:CZ3	1:C:685:ARG:HD3	2.31	0.65
1:B:1354:ARG:NE	1:B:1373:GLU:OE1	2.30	0.65
1:B:78:SER:N	1:B:88:VAL:O	2.19	0.65
1:B:1261:LYS:O	1:B:1330:ARG:NH1	2.30	0.65
1:D:1301:TYR:HD2	1:D:1319:VAL:HG22	1.61	0.65
1:D:1366:LYS:N	1:D:1369:LYS:O	2.27	0.65
1:B:1378:LYS:NZ	1:B:1382:SER:OG	2.26	0.65
1:A:130:ILE:HA	1:A:262:ALA:HB3	1.79	0.65
1:C:1301:TYR:HD2	1:C:1319:VAL:HG22	1.61	0.65
1:C:1261:LYS:O	1:C:1330:ARG:NH1	2.30	0.65
1:A:1354:ARG:NE	1:A:1373:GLU:OE1	2.30	0.65
1:C:225:PHE:O	1:C:229:SER:N	2.28	0.65
1:C:1241:ASN:N	1:C:1430:ASP:OD2	2.24	0.64
1:C:408:ASP:HB3	1:C:412:ARG:HH22	1.62	0.64
1:A:408:ASP:HB3	1:A:412:ARG:HH22	1.62	0.64
1:A:797:VAL:O	1:A:800:HIS:N	2.30	0.64
1:D:408:ASP:HB3	1:D:412:ARG:HH22	1.62	0.64
1:D:797:VAL:O	1:D:800:HIS:N	2.30	0.64
1:B:1331:THR:N	1:B:1436:ASP:OD1	2.28	0.64
1:C:797:VAL:O	1:C:800:HIS:N	2.30	0.64
1:C:1354:ARG:NE	1:C:1373:GLU:OE1	2.30	0.64
1:B:408:ASP:HB3	1:B:412:ARG:HH22	1.62	0.64
1:D:1261:LYS:O	1:D:1330:ARG:NH1	2.29	0.64
1:B:130:ILE:HA	1:B:262:ALA:HB3	1.79	0.64
1:D:1354:ARG:NE	1:D:1373:GLU:OE1	2.30	0.64
1:B:797:VAL:O	1:B:800:HIS:N	2.30	0.64
1:C:897:VAL:O	1:C:900:SER:OG	2.15	0.64
1:D:130:ILE:HA	1:D:262:ALA:HB3	1.79	0.64
1:A:856:LEU:HA	1:A:859:LYS:HE3	1.81	0.63
1:B:856:LEU:HA	1:B:859:LYS:HE3	1.80	0.63
1:B:1241:ASN:N	1:B:1430:ASP:OD2	2.24	0.63
1:B:301:LEU:HD12	1:B:304:ARG:HH12	1.63	0.63
1:D:856:LEU:HA	1:D:859:LYS:HE3	1.80	0.63
1:A:301:LEU:HD12	1:A:304:ARG:HH12	1.63	0.63
1:B:897:VAL:O	1:B:900:SER:OG	2.15	0.63
1:B:938:LEU:HD13	1:B:941:LEU:HD21	1.81	0.63
1:D:246:THR:HG22	1:D:275:THR:HG22	1.81	0.63
1:A:1038:ILE:HG21	1:B:938:LEU:HD21	1.80	0.63
1:B:1354:ARG:HB2	1:B:1452:GLN:HE22	1.64	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1354:ARG:HB2	1:D:1452:GLN:HE22	1.64	0.63
1:A:1354:ARG:HB2	1:A:1452:GLN:HE22	1.64	0.63
1:C:246:THR:HG22	1:C:275:THR:HG22	1.81	0.63
1:C:856:LEU:HA	1:C:859:LYS:HE3	1.81	0.63
1:C:130:ILE:HA	1:C:262:ALA:HB3	1.79	0.63
1:C:1354:ARG:HB2	1:C:1452:GLN:HE22	1.64	0.63
1:D:225:PHE:O	1:D:229:SER:N	2.28	0.63
1:B:246:THR:HG22	1:B:275:THR:HG22	1.81	0.62
1:B:800:HIS:O	1:B:803:ILE:HG22	1.99	0.62
1:D:301:LEU:HD12	1:D:304:ARG:HH12	1.63	0.62
1:D:1379:LEU:HB2	1:D:1382:SER:HB3	1.81	0.62
1:A:375:THR:HG23	1:A:378:LEU:H	1.64	0.62
1:B:1037:ASN:ND2	1:C:979:PHE:O	2.32	0.62
1:D:375:THR:HG23	1:D:378:LEU:H	1.64	0.62
1:A:897:VAL:O	1:A:900:SER:OG	2.15	0.62
1:A:1379:LEU:HB2	1:A:1382:SER:HB3	1.81	0.62
1:B:375:THR:HG23	1:B:378:LEU:H	1.64	0.62
1:C:301:LEU:HD12	1:C:304:ARG:HH12	1.63	0.62
1:A:1140:GLN:HA	1:A:1143:ARG:HH22	1.65	0.62
1:A:1365:ARG:HA	1:A:1370:LYS:HA	1.82	0.62
1:C:938:LEU:HD13	1:C:941:LEU:HD21	1.81	0.62
1:C:1140:GLN:HA	1:C:1143:ARG:HH22	1.65	0.62
1:D:1353:THR:OG1	1:D:1448:HIS:ND1	2.32	0.62
1:A:1353:THR:OG1	1:A:1448:HIS:ND1	2.32	0.62
1:B:430:ASP:OD1	1:B:430:ASP:N	2.32	0.62
1:C:800:HIS:O	1:C:803:ILE:HG22	1.99	0.62
1:D:324:PRO:HB2	1:D:437:LEU:HD21	1.82	0.62
1:D:1365:ARG:HA	1:D:1370:LYS:HA	1.82	0.62
1:B:573:THR:OG1	1:B:574:GLN:N	2.33	0.62
1:C:324:PRO:HB2	1:C:437:LEU:HD21	1.82	0.62
1:C:1105:ARG:CZ	1:C:1106:HIS:H	2.13	0.62
1:D:813:PHE:HE2	1:D:903:PHE:HD2	1.47	0.62
1:A:315:GLU:O	1:A:316:ARG:NE	2.31	0.62
1:B:324:PRO:HB2	1:B:437:LEU:HD21	1.82	0.62
1:B:1140:GLN:HA	1:B:1143:ARG:HH22	1.65	0.62
1:C:885:CYS:O	1:C:891:THR:OG1	2.13	0.62
1:A:924:ILE:H	1:A:924:ILE:HD12	1.64	0.62
1:B:1379:LEU:HB2	1:B:1382:SER:HB3	1.81	0.62
1:C:375:THR:HG23	1:C:378:LEU:H	1.64	0.62
1:D:938:LEU:HD13	1:D:941:LEU:HD21	1.81	0.62
1:D:1241:ASN:N	1:D:1430:ASP:OD2	2.24	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:246:THR:HG22	1:A:275:THR:HG22	1.81	0.62
1:B:1365:ARG:HA	1:B:1370:LYS:HA	1.82	0.62
1:A:324:PRO:HB2	1:A:437:LEU:HD21	1.82	0.61
1:B:813:PHE:HE2	1:B:903:PHE:HD2	1.47	0.61
1:D:917:SER:OG	1:D:921:GLY:N	2.33	0.61
1:D:924:ILE:H	1:D:924:ILE:HD12	1.65	0.61
1:D:1270:ILE:H	1:D:1270:ILE:HD12	1.65	0.61
1:A:430:ASP:N	1:A:430:ASP:OD1	2.32	0.61
1:A:938:LEU:HD13	1:A:941:LEU:HD21	1.81	0.61
1:B:1270:ILE:H	1:B:1270:ILE:HD12	1.65	0.61
1:B:1105:ARG:CZ	1:B:1106:HIS:H	2.13	0.61
1:C:813:PHE:HE2	1:C:903:PHE:HD2	1.47	0.61
1:A:813:PHE:HE2	1:A:903:PHE:HD2	1.47	0.61
1:B:813:PHE:CE2	1:B:903:PHE:HB2	2.35	0.61
1:C:1270:ILE:H	1:C:1270:ILE:HD12	1.65	0.61
1:D:813:PHE:CE2	1:D:903:PHE:HB2	2.35	0.61
1:A:800:HIS:O	1:A:803:ILE:HG22	1.99	0.61
1:B:885:CYS:O	1:B:891:THR:OG1	2.13	0.61
1:C:914:PHE:HA	1:C:917:SER:HB3	1.83	0.61
1:C:1379:LEU:HB2	1:C:1382:SER:HB3	1.81	0.61
1:D:800:HIS:O	1:D:803:ILE:HG22	1.99	0.61
1:B:917:SER:OG	1:B:921:GLY:N	2.33	0.61
1:D:1105:ARG:CZ	1:D:1106:HIS:H	2.13	0.61
1:A:813:PHE:CE2	1:A:903:PHE:HB2	2.35	0.61
1:A:917:SER:OG	1:A:921:GLY:N	2.33	0.61
1:A:1105:ARG:CZ	1:A:1106:HIS:H	2.13	0.61
1:C:1353:THR:OG1	1:C:1448:HIS:ND1	2.32	0.61
1:C:1365:ARG:HA	1:C:1370:LYS:HA	1.82	0.61
1:D:914:PHE:HA	1:D:917:SER:HB3	1.83	0.61
1:A:1270:ILE:H	1:A:1270:ILE:HD12	1.65	0.61
1:C:430:ASP:N	1:C:430:ASP:OD1	2.32	0.61
1:A:885:CYS:O	1:A:891:THR:OG1	2.13	0.61
1:A:914:PHE:HA	1:A:917:SER:HB3	1.83	0.61
1:C:813:PHE:CE2	1:C:903:PHE:HB2	2.35	0.61
1:D:430:ASP:N	1:D:430:ASP:OD1	2.32	0.61
1:B:225:PHE:O	1:B:229:SER:N	2.28	0.61
1:B:914:PHE:HA	1:B:917:SER:HB3	1.83	0.61
1:A:376:ILE:HD13	1:A:400:VAL:HG23	1.83	0.60
1:A:1353:THR:HG1	1:A:1448:HIS:HD1	1.47	0.60
1:C:1140:GLN:HA	1:C:1143:ARG:NH2	2.16	0.60
1:C:868:TRP:CZ3	1:C:912:HIS:HB2	2.37	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:924:ILE:H	1:C:924:ILE:HD12	1.64	0.60
1:A:381:GLN:HE22	1:A:382:LYS:HE3	1.67	0.60
1:B:868:TRP:CZ3	1:B:912:HIS:HB2	2.36	0.60
1:B:924:ILE:H	1:B:924:ILE:HD12	1.64	0.60
1:B:1353:THR:HG1	1:B:1448:HIS:HD1	1.47	0.60
1:B:1353:THR:OG1	1:B:1448:HIS:ND1	2.32	0.60
1:D:573:THR:OG1	1:D:574:GLN:N	2.33	0.60
1:A:695:ARG:HD2	1:D:669:THR:HG21	1.84	0.60
1:B:376:ILE:HD13	1:B:400:VAL:HG23	1.84	0.60
1:B:381:GLN:HE22	1:B:382:LYS:HE3	1.67	0.60
1:A:1243:ARG:NH2	1:A:1259:ASN:OD1	2.34	0.60
1:C:917:SER:OG	1:C:921:GLY:N	2.33	0.60
1:D:376:ILE:HD13	1:D:400:VAL:HG23	1.83	0.60
1:A:1241:ASN:N	1:A:1430:ASP:OD2	2.24	0.60
1:A:1331:THR:N	1:A:1436:ASP:OD1	2.28	0.60
1:C:376:ILE:HD13	1:C:400:VAL:HG23	1.83	0.60
1:C:573:THR:OG1	1:C:574:GLN:N	2.33	0.60
1:C:1276:TYR:N	1:C:1334:ARG:O	2.32	0.60
1:C:1353:THR:HG1	1:C:1448:HIS:HD1	1.47	0.60
1:D:1140:GLN:HA	1:D:1143:ARG:HH22	1.65	0.60
1:D:1276:TYR:N	1:D:1334:ARG:O	2.32	0.60
1:A:1422:MET:O	1:A:1446:SER:N	2.35	0.60
1:C:381:GLN:HE22	1:C:382:LYS:HE3	1.67	0.60
1:D:868:TRP:CZ3	1:D:912:HIS:HB2	2.36	0.60
1:A:1276:TYR:N	1:A:1334:ARG:O	2.32	0.60
1:B:197:VAL:HB	1:B:430:ASP:HB3	1.83	0.60
1:D:381:GLN:HE22	1:D:382:LYS:HE3	1.67	0.60
1:A:944:TRP:O	1:A:947:SER:OG	2.20	0.60
1:C:181:ASN:OD1	1:C:182:MET:N	2.29	0.60
1:A:129:ASP:OD1	1:A:130:ILE:N	2.35	0.59
1:B:1422:MET:O	1:B:1446:SER:N	2.35	0.59
1:C:835:TRP:CZ2	1:C:1082:PRO:HB2	2.37	0.59
1:A:197:VAL:HB	1:A:430:ASP:HB3	1.83	0.59
1:A:1140:GLN:HA	1:A:1143:ARG:NH2	2.16	0.59
1:B:211:HIS:O	1:B:211:HIS:ND1	2.36	0.59
1:B:1276:TYR:H	1:B:1335:GLY:HA3	1.67	0.59
1:B:1448:HIS:O	1:B:1450:GLN:NE2	2.35	0.59
1:D:315:GLU:O	1:D:316:ARG:NE	2.31	0.59
1:D:1331:THR:N	1:D:1436:ASP:OD1	2.28	0.59
1:D:1448:HIS:O	1:D:1450:GLN:NE2	2.35	0.59
1:A:835:TRP:CZ2	1:A:1082:PRO:HB2	2.37	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1331:THR:N	1:C:1436:ASP:OD1	2.28	0.59
1:D:1243:ARG:NH2	1:D:1259:ASN:OD1	2.34	0.59
1:D:1422:MET:O	1:D:1446:SER:N	2.35	0.59
1:A:1448:HIS:O	1:A:1450:GLN:NE2	2.35	0.59
1:B:1140:GLN:HA	1:B:1143:ARG:NH2	2.16	0.59
1:C:197:VAL:HB	1:C:430:ASP:HB3	1.83	0.59
1:A:181:ASN:OD1	1:A:182:MET:N	2.29	0.59
1:B:799:PHE:HD1	1:B:1074:TYR:CE2	2.21	0.59
1:C:1422:MET:O	1:C:1446:SER:N	2.35	0.59
1:A:211:HIS:ND1	1:A:211:HIS:O	2.36	0.59
1:A:868:TRP:CZ3	1:A:912:HIS:HB2	2.37	0.59
1:A:1276:TYR:H	1:A:1335:GLY:HA3	1.67	0.59
1:D:835:TRP:CZ2	1:D:1082:PRO:HB2	2.37	0.59
1:D:1140:GLN:HA	1:D:1143:ARG:NH2	2.17	0.59
1:C:173:VAL:HG23	1:C:328:VAL:HG13	1.85	0.59
1:C:799:PHE:HD1	1:C:1074:TYR:CE2	2.21	0.59
1:C:1276:TYR:H	1:C:1335:GLY:HA3	1.67	0.59
1:D:71:GLU:O	1:D:120:GLN:N	2.35	0.59
1:D:197:VAL:HB	1:D:430:ASP:HB3	1.83	0.59
1:D:181:ASN:OD1	1:D:182:MET:N	2.29	0.59
1:D:799:PHE:HD1	1:D:1074:TYR:CE2	2.21	0.59
1:A:573:THR:OG1	1:A:574:GLN:N	2.33	0.59
1:B:835:TRP:CZ2	1:B:1082:PRO:HB2	2.37	0.59
1:C:1448:HIS:O	1:C:1450:GLN:NE2	2.35	0.59
1:B:1276:TYR:N	1:B:1334:ARG:O	2.32	0.59
1:C:1487:ASN:O	1:C:1490:THR:OG1	2.20	0.59
1:D:308:PHE:O	1:D:312:GLN:NE2	2.30	0.59
1:D:329:VAL:HG11	1:D:340:ILE:HD11	1.85	0.58
1:B:129:ASP:OD1	1:B:130:ILE:N	2.35	0.58
1:C:211:HIS:ND1	1:C:211:HIS:O	2.36	0.58
1:C:329:VAL:HG11	1:C:340:ILE:HD11	1.85	0.58
1:D:211:HIS:ND1	1:D:211:HIS:O	2.36	0.58
1:D:813:PHE:HE2	1:D:903:PHE:CD2	2.22	0.58
1:D:897:VAL:O	1:D:900:SER:OG	2.15	0.58
1:B:244:TRP:O	1:B:250:ARG:NH1	2.36	0.58
1:B:757:THR:HA	1:B:760:MET:HE2	1.86	0.58
1:D:1348:LEU:HD23	1:D:1399:PRO:HD3	1.85	0.58
1:A:244:TRP:O	1:A:250:ARG:NH1	2.36	0.58
1:A:813:PHE:HE2	1:A:903:PHE:CD2	2.22	0.58
1:A:1358:ASN:OD1	1:A:1362:ALA:N	2.37	0.58
1:C:71:GLU:O	1:C:120:GLN:N	2.35	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:885:CYS:O	1:D:891:THR:OG1	2.13	0.58
1:D:1353:THR:HG1	1:D:1448:HIS:HD1	1.46	0.58
1:A:329:VAL:HG11	1:A:340:ILE:HD11	1.85	0.58
1:A:524:GLU:HG2	1:A:556:LEU:HD23	1.86	0.58
1:B:173:VAL:HG23	1:B:328:VAL:HG13	1.85	0.58
1:B:329:VAL:HG11	1:B:340:ILE:HD11	1.85	0.58
1:D:244:TRP:O	1:D:250:ARG:NH1	2.36	0.58
1:A:623:ARG:HG3	1:A:624:ASP:N	2.19	0.58
1:C:1243:ARG:NH2	1:C:1259:ASN:OD1	2.34	0.58
1:C:1355:TRP:HA	1:C:1372:LEU:HD13	1.86	0.58
1:A:400:VAL:HG22	1:A:1258:PRO:HG2	1.86	0.58
1:B:1348:LEU:HD23	1:B:1399:PRO:HD3	1.85	0.58
1:B:1355:TRP:HA	1:B:1372:LEU:HD13	1.86	0.58
1:D:129:ASP:OD1	1:D:130:ILE:N	2.35	0.58
1:D:400:VAL:HG22	1:D:1258:PRO:HG2	1.85	0.58
1:D:524:GLU:HG2	1:D:556:LEU:HD23	1.86	0.58
1:D:1276:TYR:H	1:D:1335:GLY:HA3	1.67	0.58
1:A:71:GLU:O	1:A:120:GLN:N	2.35	0.58
1:A:751:ASN:HB3	1:A:772:SER:OG	2.04	0.58
1:A:799:PHE:HD1	1:A:1074:TYR:CE2	2.21	0.58
1:A:1348:LEU:HD23	1:A:1399:PRO:HD3	1.85	0.58
1:A:1487:ASN:O	1:A:1490:THR:OG1	2.20	0.58
1:C:1348:LEU:HD23	1:C:1399:PRO:HD3	1.85	0.58
1:D:751:ASN:HB3	1:D:772:SER:OG	2.04	0.58
1:A:173:VAL:HG23	1:A:328:VAL:HG13	1.85	0.57
1:C:813:PHE:HE2	1:C:903:PHE:CD2	2.22	0.57
1:C:1358:ASN:OD1	1:C:1362:ALA:N	2.37	0.57
1:B:89:CYS:CB	1:B:98:HIS:H	2.17	0.57
1:B:400:VAL:HG22	1:B:1258:PRO:HG2	1.85	0.57
1:B:1349:TYR:CD1	1:B:1389:GLY:HA3	2.39	0.57
1:B:1358:ASN:OD1	1:B:1362:ALA:N	2.37	0.57
1:C:337:LEU:HB2	1:C:359:VAL:HG21	1.86	0.57
1:D:173:VAL:HG23	1:D:328:VAL:HG13	1.85	0.57
1:C:244:TRP:O	1:C:250:ARG:NH1	2.36	0.57
1:C:524:GLU:HG2	1:C:556:LEU:HD23	1.86	0.57
1:A:337:LEU:HB2	1:A:359:VAL:HG21	1.86	0.57
1:B:337:LEU:HB2	1:B:359:VAL:HG21	1.86	0.57
1:B:626:LEU:O	1:B:630:ILE:HG12	2.04	0.57
1:B:813:PHE:CE2	1:B:903:PHE:HD2	2.23	0.57
1:C:315:GLU:O	1:C:316:ARG:NE	2.31	0.57
1:A:1355:TRP:HA	1:A:1372:LEU:HD13	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:PHE:HE2	1:B:903:PHE:CD2	2.21	0.57
1:C:814:ALA:O	1:C:817:LEU:HG	2.05	0.57
1:C:944:TRP:O	1:C:947:SER:OG	2.20	0.57
1:D:89:CYS:CB	1:D:98:HIS:H	2.17	0.57
1:D:1324:PRO:HG2	1:D:1342:PHE:HB3	1.87	0.57
1:D:1358:ASN:OD1	1:D:1362:ALA:N	2.37	0.57
1:A:626:LEU:O	1:A:630:ILE:HG12	2.05	0.57
1:A:813:PHE:CE2	1:A:903:PHE:HD2	2.23	0.57
1:C:129:ASP:OD1	1:C:130:ILE:N	2.35	0.57
1:D:1076:GLY:HA2	1:D:1106:HIS:CE1	2.39	0.57
1:B:315:GLU:O	1:B:316:ARG:NE	2.31	0.57
1:C:531:LEU:O	1:C:534:SER:OG	2.23	0.57
1:D:337:LEU:HB2	1:D:359:VAL:HG21	1.86	0.57
1:D:757:THR:HA	1:D:760:MET:HE2	1.86	0.57
1:D:814:ALA:O	1:D:817:LEU:HG	2.05	0.57
1:D:1355:TRP:HA	1:D:1372:LEU:HD13	1.86	0.57
1:A:1042:ASN:HA	1:A:1045:ILE:HD12	1.87	0.57
1:C:89:CYS:CB	1:C:98:HIS:H	2.17	0.57
1:C:400:VAL:HG22	1:C:1258:PRO:HG2	1.86	0.57
1:D:623:ARG:HG3	1:D:624:ASP:N	2.19	0.57
1:A:244:TRP:HB3	1:A:288:ASP:HB2	1.87	0.57
1:A:757:THR:HA	1:A:760:MET:HE2	1.87	0.57
1:B:244:TRP:HB3	1:B:288:ASP:HB2	1.87	0.57
1:B:1311:ARG:HA	1:B:1317:TYR:HE1	1.70	0.57
1:C:813:PHE:CE2	1:C:903:PHE:HD2	2.23	0.57
1:A:466:ASP:N	1:A:466:ASP:OD1	2.38	0.57
1:A:814:ALA:O	1:A:817:LEU:HG	2.05	0.57
1:A:1059:THR:O	1:A:1062:ILE:N	2.38	0.57
1:B:814:ALA:O	1:B:817:LEU:HG	2.05	0.57
1:B:920:LEU:HA	1:B:923:LYS:HD3	1.87	0.57
1:D:523:TYR:CZ	1:D:628:TRP:HB2	2.40	0.57
1:D:920:LEU:HA	1:D:923:LYS:HD3	1.87	0.57
1:A:579:ARG:HD3	1:A:580:PRO:HD2	1.87	0.56
1:B:524:GLU:HG2	1:B:556:LEU:HD23	1.86	0.56
1:B:1042:ASN:HA	1:B:1045:ILE:HD12	1.87	0.56
1:C:626:LEU:O	1:C:630:ILE:HG12	2.05	0.56
1:B:1324:PRO:HG2	1:B:1342:PHE:HB3	1.87	0.56
1:C:172:SER:HB2	1:C:302:ARG:HH21	1.71	0.56
1:D:165:ASP:N	1:D:165:ASP:OD1	2.38	0.56
1:D:626:LEU:O	1:D:630:ILE:HG12	2.04	0.56
1:D:813:PHE:CE2	1:D:903:PHE:HD2	2.23	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1374:VAL:O	1:D:1476:GLN:N	2.38	0.56
1:A:920:LEU:HA	1:A:923:LYS:HD3	1.87	0.56
1:B:466:ASP:OD1	1:B:466:ASP:N	2.38	0.56
1:B:523:TYR:CZ	1:B:628:TRP:HB2	2.40	0.56
1:C:244:TRP:HB3	1:C:288:ASP:HB2	1.87	0.56
1:C:751:ASN:HB3	1:C:772:SER:OG	2.04	0.56
1:C:920:LEU:HA	1:C:923:LYS:HD3	1.87	0.56
1:C:1059:THR:O	1:C:1062:ILE:N	2.38	0.56
1:C:1324:PRO:HG2	1:C:1342:PHE:HB3	1.87	0.56
1:D:244:TRP:HB3	1:D:288:ASP:HB2	1.87	0.56
1:D:944:TRP:O	1:D:947:SER:OG	2.20	0.56
1:D:1431:ASP:OD1	1:D:1433:ARG:NH2	2.39	0.56
1:A:89:CYS:CB	1:A:98:HIS:H	2.17	0.56
1:A:1374:VAL:O	1:A:1476:GLN:N	2.39	0.56
1:B:751:ASN:HB3	1:B:772:SER:OG	2.04	0.56
1:C:1311:ARG:HA	1:C:1317:TYR:HE1	1.70	0.56
1:A:172:SER:HB2	1:A:302:ARG:HH21	1.71	0.56
1:B:172:SER:HB2	1:B:302:ARG:HH21	1.71	0.56
1:B:623:ARG:HG3	1:B:624:ASP:N	2.19	0.56
1:B:867:PHE:HD2	1:B:868:TRP:CD1	2.24	0.56
1:B:1243:ARG:NH2	1:B:1259:ASN:OD1	2.34	0.56
1:C:1431:ASP:OD1	1:C:1433:ARG:NH2	2.39	0.56
1:A:1311:ARG:HA	1:A:1317:TYR:HE1	1.70	0.56
1:B:181:ASN:OD1	1:B:182:MET:N	2.29	0.56
1:B:214:VAL:HB	1:B:330:LEU:HD12	1.88	0.56
1:B:531:LEU:O	1:B:534:SER:OG	2.23	0.56
1:D:115:PRO:HA	1:D:119:VAL:HG23	1.87	0.56
1:A:379:ILE:HG22	1:A:383:LEU:HD23	1.88	0.56
1:A:523:TYR:CZ	1:A:628:TRP:HB2	2.40	0.56
1:D:531:LEU:O	1:D:534:SER:OG	2.23	0.56
1:D:867:PHE:HD2	1:D:868:TRP:CD1	2.24	0.56
1:C:1030:CYS:SG	1:C:1031:LEU:N	2.79	0.56
1:D:172:SER:HB2	1:D:302:ARG:HH21	1.71	0.56
1:D:379:ILE:HG22	1:D:383:LEU:HD23	1.88	0.56
1:D:1042:ASN:HA	1:D:1045:ILE:HD12	1.87	0.56
1:D:1342:PHE:HA	1:D:1438:ALA:HB2	1.88	0.56
1:A:214:VAL:HB	1:A:330:LEU:HD12	1.88	0.56
1:B:124:THR:HG22	1:B:126:ALA:H	1.70	0.56
1:C:1349:TYR:CD1	1:C:1389:GLY:HA3	2.39	0.56
1:D:89:CYS:H	1:D:98:HIS:N	2.04	0.56
1:D:1059:THR:O	1:D:1062:ILE:N	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1050:TYR:HA	1:B:1052:PHE:HZ	1.71	0.56
1:A:1276:TYR:O	1:A:1337:GLY:N	2.39	0.56
1:B:1030:CYS:SG	1:B:1031:LEU:N	2.79	0.56
1:C:523:TYR:CZ	1:C:628:TRP:HB2	2.40	0.56
1:D:579:ARG:HD3	1:D:580:PRO:HD2	1.87	0.56
1:B:115:PRO:HA	1:B:119:VAL:HG23	1.88	0.55
1:B:579:ARG:HD3	1:B:580:PRO:HD2	1.87	0.55
1:B:1059:THR:O	1:B:1062:ILE:N	2.38	0.55
1:B:1348:LEU:HD13	1:B:1443:VAL:HB	1.88	0.55
1:C:623:ARG:HG3	1:C:624:ASP:N	2.19	0.55
1:C:867:PHE:HD2	1:C:868:TRP:CD1	2.24	0.55
1:D:214:VAL:HB	1:D:330:LEU:HD12	1.88	0.55
1:A:1324:PRO:HG2	1:A:1342:PHE:HB3	1.87	0.55
1:C:89:CYS:H	1:C:98:HIS:N	2.04	0.55
1:C:124:THR:HG22	1:C:126:ALA:H	1.70	0.55
1:C:466:ASP:OD1	1:C:466:ASP:N	2.38	0.55
1:C:1268:PHE:CD2	1:C:1271:TYR:HB2	2.41	0.55
1:C:1276:TYR:O	1:C:1337:GLY:N	2.39	0.55
1:D:124:THR:HG22	1:D:126:ALA:H	1.70	0.55
1:A:867:PHE:HD2	1:A:868:TRP:CD1	2.24	0.55
1:A:1030:CYS:SG	1:A:1031:LEU:N	2.79	0.55
1:A:1431:ASP:OD1	1:A:1433:ARG:NH2	2.39	0.55
1:B:1276:TYR:O	1:B:1337:GLY:N	2.39	0.55
1:A:89:CYS:H	1:A:98:HIS:N	2.04	0.55
1:A:167:PRO:HG3	1:A:204:TRP:CD2	2.41	0.55
1:B:167:PRO:HG3	1:B:204:TRP:CD2	2.42	0.55
1:B:381:GLN:NE2	1:B:382:LYS:HG2	2.22	0.55
1:B:1076:GLY:HA2	1:B:1106:HIS:CE1	2.39	0.55
1:C:1042:ASN:HA	1:C:1045:ILE:HD12	1.87	0.55
1:C:1348:LEU:HD13	1:C:1443:VAL:HB	1.88	0.55
1:D:167:PRO:HG3	1:D:204:TRP:CD2	2.42	0.55
1:A:59:LEU:HD13	1:A:161:HIS:HB3	1.89	0.55
1:A:124:THR:HG22	1:A:126:ALA:H	1.70	0.55
1:A:204:TRP:CD1	1:A:237:ILE:HD11	2.42	0.55
1:A:432:ALA:HA	1:A:435:GLN:OE1	2.07	0.55
1:B:1268:PHE:CD2	1:B:1271:TYR:HB2	2.41	0.55
1:B:1374:VAL:O	1:B:1476:GLN:N	2.39	0.55
1:C:1076:GLY:HA2	1:C:1106:HIS:CE1	2.39	0.55
1:D:381:GLN:NE2	1:D:382:LYS:HG2	2.22	0.55
1:B:809:PHE:CD1	1:B:835:TRP:CD1	2.95	0.55
1:C:1374:VAL:O	1:C:1476:GLN:N	2.39	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1311:ARG:HA	1:D:1317:TYR:HE1	1.70	0.55
1:B:71:GLU:O	1:B:120:GLN:N	2.35	0.55
1:B:89:CYS:H	1:B:98:HIS:N	2.04	0.55
1:B:204:TRP:CD1	1:B:237:ILE:HD11	2.42	0.55
1:B:944:TRP:O	1:B:947:SER:OG	2.20	0.55
1:C:809:PHE:CD1	1:C:835:TRP:CD1	2.95	0.55
1:D:432:ALA:HA	1:D:435:GLN:OE1	2.07	0.55
1:D:1030:CYS:SG	1:D:1031:LEU:N	2.79	0.55
1:D:1263:PRO:O	1:D:1330:ARG:NH1	2.40	0.55
1:A:115:PRO:HA	1:A:119:VAL:HG23	1.87	0.55
1:A:1263:PRO:O	1:A:1330:ARG:NH1	2.40	0.55
1:A:1268:PHE:CD2	1:A:1271:TYR:HB2	2.41	0.55
1:A:1342:PHE:HA	1:A:1438:ALA:HB2	1.88	0.55
1:B:1263:PRO:O	1:B:1330:ARG:NH1	2.40	0.55
1:C:214:VAL:HB	1:C:330:LEU:HD12	1.88	0.55
1:C:381:GLN:NE2	1:C:382:LYS:HG2	2.22	0.55
1:C:943:VAL:HA	1:C:946:VAL:HG22	1.89	0.55
1:A:381:GLN:NE2	1:A:382:LYS:HG2	2.22	0.55
1:A:868:TRP:HZ3	1:A:912:HIS:HB2	1.72	0.55
1:B:1038:ILE:HD13	1:C:938:LEU:HD11	1.89	0.55
1:C:1343:GLY:O	1:C:1439:TRP:N	2.27	0.55
1:D:466:ASP:N	1:D:466:ASP:OD1	2.38	0.55
1:A:341:ASP:O	1:A:345:THR:HG23	2.08	0.55
1:A:1357:ARG:NH2	1:A:1450:GLN:O	2.40	0.55
1:C:1342:PHE:HA	1:C:1438:ALA:HB2	1.88	0.55
1:D:204:TRP:CD1	1:D:237:ILE:HD11	2.42	0.55
1:D:868:TRP:HZ3	1:D:912:HIS:HB2	1.72	0.55
1:B:868:TRP:HZ3	1:B:912:HIS:HB2	1.72	0.54
1:C:115:PRO:HA	1:C:119:VAL:HG23	1.87	0.54
1:C:167:PRO:HG3	1:C:204:TRP:CD2	2.41	0.54
1:C:379:ILE:HG22	1:C:383:LEU:HD23	1.88	0.54
1:D:1268:PHE:CD2	1:D:1271:TYR:HB2	2.41	0.54
1:B:379:ILE:HG22	1:B:383:LEU:HD23	1.88	0.54
1:B:1431:ASP:OD1	1:B:1433:ARG:NH2	2.39	0.54
1:C:204:TRP:CD1	1:C:237:ILE:HD11	2.42	0.54
1:C:669:THR:HG21	1:D:695:ARG:HD2	1.89	0.54
1:D:1348:LEU:HD13	1:D:1443:VAL:HB	1.88	0.54
1:A:806:TYR:OH	1:A:909:ARG:NH1	2.41	0.54
1:A:1076:GLY:HA2	1:A:1106:HIS:CE1	2.39	0.54
1:B:165:ASP:OD1	1:B:165:ASP:N	2.38	0.54
1:B:813:PHE:HE2	1:B:903:PHE:HB2	1.72	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1271:TYR:OH	1:B:1436:ASP:OD2	2.26	0.54
1:C:579:ARG:HD3	1:C:580:PRO:HD2	1.87	0.54
1:C:1357:ARG:NH2	1:C:1450:GLN:O	2.40	0.54
1:D:1140:GLN:HB3	1:D:1143:ARG:HH12	1.72	0.54
1:D:1276:TYR:O	1:D:1337:GLY:N	2.39	0.54
1:A:809:PHE:CD1	1:A:835:TRP:CD1	2.95	0.54
1:B:1140:GLN:HB3	1:B:1143:ARG:HH12	1.72	0.54
1:B:1357:ARG:NH2	1:B:1450:GLN:O	2.40	0.54
1:A:937:PHE:CE2	1:A:1044:LEU:HD11	2.42	0.54
1:B:59:LEU:HD13	1:B:161:HIS:HB3	1.89	0.54
1:B:784:PRO:HA	1:B:787:ARG:HB2	1.90	0.54
1:B:943:VAL:HA	1:B:946:VAL:HG22	1.89	0.54
1:B:1342:PHE:HA	1:B:1438:ALA:HB2	1.88	0.54
1:C:806:TYR:OH	1:C:909:ARG:NH1	2.41	0.54
1:A:1348:LEU:HD13	1:A:1443:VAL:HB	1.88	0.54
1:B:341:ASP:O	1:B:345:THR:HG23	2.08	0.54
1:B:937:PHE:CE2	1:B:1044:LEU:HD11	2.42	0.54
1:C:341:ASP:O	1:C:345:THR:HG23	2.08	0.54
1:D:937:PHE:CE2	1:D:1044:LEU:HD11	2.42	0.54
1:D:943:VAL:HA	1:D:946:VAL:HG22	1.89	0.54
1:D:1243:ARG:HH12	1:D:1259:ASN:HA	1.73	0.54
1:D:1357:ARG:NH2	1:D:1450:GLN:O	2.40	0.54
1:A:1140:GLN:HB3	1:A:1143:ARG:HH12	1.72	0.54
1:C:813:PHE:HE2	1:C:903:PHE:HB2	1.73	0.54
1:D:380:GLN:O	1:D:384:SER:OG	2.17	0.54
1:D:809:PHE:CD1	1:D:835:TRP:CD1	2.95	0.54
1:A:1038:ILE:CD1	1:B:938:LEU:HD11	2.32	0.54
1:B:432:ALA:HA	1:B:435:GLN:OE1	2.07	0.54
1:B:938:LEU:O	1:B:941:LEU:HG	2.08	0.54
1:C:784:PRO:HA	1:C:787:ARG:HB2	1.90	0.54
1:C:1243:ARG:HH12	1:C:1259:ASN:HA	1.73	0.54
1:D:59:LEU:HD13	1:D:161:HIS:HB3	1.89	0.54
1:A:1243:ARG:HH12	1:A:1259:ASN:HA	1.73	0.54
1:C:1140:GLN:HB3	1:C:1143:ARG:HH12	1.72	0.54
1:C:1271:TYR:OH	1:C:1436:ASP:OD2	2.26	0.54
1:A:165:ASP:OD1	1:A:165:ASP:N	2.38	0.54
1:A:784:PRO:HA	1:A:787:ARG:HB2	1.90	0.54
1:A:943:VAL:HA	1:A:946:VAL:HG22	1.89	0.54
1:C:937:PHE:CE2	1:C:1044:LEU:HD11	2.42	0.54
1:D:938:LEU:O	1:D:941:LEU:HG	2.08	0.54
1:D:784:PRO:HA	1:D:787:ARG:HB2	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1349:TYR:CD1	1:D:1389:GLY:HA3	2.39	0.53
1:B:1415:GLU:O	1:B:1419:LYS:N	2.41	0.53
1:C:59:LEU:HD13	1:C:161:HIS:HB3	1.89	0.53
1:C:1415:GLU:O	1:C:1419:LYS:N	2.42	0.53
1:D:341:ASP:O	1:D:345:THR:HG23	2.07	0.53
1:A:531:LEU:O	1:A:534:SER:OG	2.23	0.53
1:A:1415:GLU:O	1:A:1419:LYS:N	2.42	0.53
1:C:868:TRP:HZ3	1:C:912:HIS:HB2	1.72	0.53
1:C:1263:PRO:O	1:C:1330:ARG:NH1	2.40	0.53
1:D:806:TYR:OH	1:D:909:ARG:NH1	2.41	0.53
1:A:1244:HIS:O	1:A:1254:ARG:NE	2.42	0.53
1:C:621:PRO:HA	1:C:624:ASP:OD2	2.08	0.53
1:C:938:LEU:O	1:C:941:LEU:HG	2.08	0.53
1:D:1415:GLU:O	1:D:1419:LYS:N	2.42	0.53
1:A:813:PHE:HE2	1:A:903:PHE:HB2	1.73	0.53
1:B:1243:ARG:HH12	1:B:1259:ASN:HA	1.73	0.53
1:C:432:ALA:HA	1:C:435:GLN:OE1	2.07	0.53
1:C:1244:HIS:O	1:C:1254:ARG:NE	2.42	0.53
1:D:193:GLY:HA3	1:D:429:VAL:HB	1.91	0.53
1:A:621:PRO:HA	1:A:624:ASP:OD2	2.08	0.53
1:A:1271:TYR:OH	1:A:1436:ASP:OD2	2.26	0.53
1:B:1304:VAL:HA	1:B:1309:ASP:HA	1.91	0.53
1:D:621:PRO:HA	1:D:624:ASP:OD2	2.08	0.53
1:B:747:LEU:HD12	1:B:748:SER:O	2.09	0.53
1:B:806:TYR:OH	1:B:909:ARG:NH1	2.41	0.53
1:B:1244:HIS:O	1:B:1254:ARG:NE	2.42	0.53
1:A:287:VAL:HG21	1:A:298:GLU:HA	1.91	0.53
1:A:1354:ARG:HG2	1:A:1373:GLU:HB2	1.91	0.53
1:C:287:VAL:HG21	1:C:298:GLU:HA	1.91	0.53
1:C:331:GLU:HA	1:C:357:GLY:HA2	1.91	0.53
1:C:757:THR:HA	1:C:760:MET:HE2	1.90	0.53
1:A:1304:VAL:HA	1:A:1309:ASP:HA	1.91	0.53
1:B:621:PRO:HA	1:B:624:ASP:OD2	2.08	0.53
1:B:669:THR:HG21	1:C:695:ARG:HD2	1.89	0.53
1:B:1287:ASP:C	1:B:1289:MET:H	2.12	0.53
1:B:1487:ASN:O	1:B:1490:THR:OG1	2.20	0.53
1:C:193:GLY:HA3	1:C:429:VAL:HB	1.91	0.53
1:C:1354:ARG:HG2	1:C:1373:GLU:HB2	1.91	0.53
1:D:1287:ASP:C	1:D:1289:MET:H	2.12	0.53
1:D:1312:SER:OG	1:D:1315:GLY:O	2.27	0.53
1:A:308:PHE:O	1:A:312:GLN:NE2	2.30	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:331:GLU:HA	1:D:357:GLY:HA2	1.91	0.53
1:D:747:LEU:HD12	1:D:748:SER:O	2.09	0.53
1:D:1271:TYR:OH	1:D:1436:ASP:OD2	2.26	0.53
1:B:287:VAL:HG21	1:B:298:GLU:HA	1.91	0.52
1:D:1244:HIS:O	1:D:1254:ARG:NE	2.42	0.52
1:D:1487:ASN:O	1:D:1490:THR:OG1	2.20	0.52
1:A:747:LEU:HD12	1:A:748:SER:O	2.09	0.52
1:A:938:LEU:O	1:A:941:LEU:HG	2.08	0.52
1:B:1040:LEU:HD12	1:B:1040:LEU:H	1.75	0.52
1:C:1040:LEU:H	1:C:1040:LEU:HD12	1.74	0.52
1:D:813:PHE:HE2	1:D:903:PHE:HB2	1.72	0.52
1:A:331:GLU:HA	1:A:357:GLY:HA2	1.91	0.52
1:B:456:LEU:HD13	1:B:472:ILE:HG21	1.92	0.52
1:C:747:LEU:HD12	1:C:748:SER:O	2.09	0.52
1:C:1304:VAL:HA	1:C:1309:ASP:HA	1.91	0.52
1:D:1304:VAL:HA	1:D:1309:ASP:HA	1.91	0.52
1:A:193:GLY:HA3	1:A:429:VAL:HB	1.91	0.52
1:A:914:PHE:HD2	1:A:920:LEU:HD13	1.75	0.52
1:B:1312:SER:OG	1:B:1315:GLY:O	2.27	0.52
1:C:914:PHE:HD2	1:C:920:LEU:HD13	1.75	0.52
1:D:697:ASP:OD1	1:D:700:ARG:N	2.39	0.52
1:D:1474:ARG:NE	1:D:1476:GLN:OE1	2.43	0.52
1:A:750:ASP:OD1	1:A:750:ASP:N	2.42	0.52
1:C:1111:ASN:N	1:C:1111:ASN:OD1	2.41	0.52
1:A:1349:TYR:CD1	1:A:1389:GLY:HA3	2.39	0.52
1:B:657:LYS:HD3	1:B:724:ALA:HB2	1.91	0.52
1:C:1287:ASP:C	1:C:1289:MET:H	2.12	0.52
1:D:657:LYS:HD3	1:D:724:ALA:HB2	1.91	0.52
1:A:1040:LEU:H	1:A:1040:LEU:HD12	1.74	0.52
1:B:331:GLU:HA	1:B:357:GLY:HA2	1.91	0.52
1:D:1040:LEU:H	1:D:1040:LEU:HD12	1.74	0.52
1:D:1085:ILE:O	1:D:1088:SER:OG	2.24	0.52
1:D:1354:ARG:HG2	1:D:1373:GLU:HB2	1.91	0.52
1:A:456:LEU:HD13	1:A:472:ILE:HG21	1.92	0.52
1:A:1312:SER:OG	1:A:1315:GLY:O	2.27	0.52
1:A:1474:ARG:NE	1:A:1476:GLN:OE1	2.43	0.52
1:B:308:PHE:O	1:B:312:GLN:NE2	2.30	0.52
1:B:1474:ARG:NE	1:B:1476:GLN:OE1	2.43	0.52
1:B:1484:LEU:HD23	1:B:1489:LYS:HG2	1.92	0.52
1:C:1484:LEU:HD23	1:C:1489:LYS:HG2	1.92	0.52
1:B:193:GLY:HA3	1:B:429:VAL:HB	1.91	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1277:THR:HA	1:C:1337:GLY:H	1.75	0.51
1:C:1312:SER:OG	1:C:1315:GLY:O	2.27	0.51
1:D:287:VAL:HG21	1:D:298:GLU:HA	1.91	0.51
1:D:1111:ASN:OD1	1:D:1111:ASN:N	2.41	0.51
1:A:1057:GLU:OE1	1:A:1057:GLU:N	2.43	0.51
1:A:1484:LEU:HD23	1:A:1489:LYS:HG2	1.92	0.51
1:C:1240:VAL:N	1:C:1430:ASP:OD2	2.44	0.51
1:A:697:ASP:OD1	1:A:700:ARG:N	2.39	0.51
1:D:914:PHE:HD2	1:D:920:LEU:HD13	1.75	0.51
1:A:647:ASP:OD1	1:A:647:ASP:N	2.43	0.51
1:B:1240:VAL:N	1:B:1430:ASP:OD2	2.44	0.51
1:D:456:LEU:HD13	1:D:472:ILE:HG21	1.92	0.51
1:A:1240:VAL:N	1:A:1430:ASP:OD2	2.44	0.51
1:D:1057:GLU:OE1	1:D:1057:GLU:N	2.43	0.51
1:A:169:LEU:HB3	1:A:203:ALA:HB2	1.92	0.51
1:A:657:LYS:HD3	1:A:724:ALA:HB2	1.91	0.51
1:A:917:SER:HG	1:A:921:GLY:N	2.09	0.51
1:A:1085:ILE:O	1:A:1088:SER:OG	2.24	0.51
1:A:1111:ASN:OD1	1:A:1111:ASN:N	2.41	0.51
1:B:378:LEU:HD12	1:B:381:GLN:NE2	2.26	0.51
1:B:647:ASP:OD1	1:B:647:ASP:N	2.43	0.51
1:B:1082:PRO:HA	1:B:1085:ILE:HB	1.92	0.51
1:B:1140:GLN:HG2	1:B:1143:ARG:HH22	1.76	0.51
1:C:657:LYS:HD3	1:C:724:ALA:HB2	1.91	0.51
1:C:1376:VAL:HG21	1:C:1385:TRP:HB3	1.93	0.51
1:C:1474:ARG:NE	1:C:1476:GLN:OE1	2.43	0.51
1:D:378:LEU:HD12	1:D:381:GLN:NE2	2.26	0.51
1:A:1287:ASP:C	1:A:1289:MET:H	2.12	0.51
1:B:914:PHE:HD2	1:B:920:LEU:HD13	1.75	0.51
1:B:1057:GLU:OE1	1:B:1057:GLU:N	2.44	0.51
1:B:1343:GLY:O	1:B:1439:TRP:N	2.27	0.51
1:C:456:LEU:HD13	1:C:472:ILE:HG21	1.92	0.51
1:A:938:LEU:HD21	1:D:1038:ILE:HG21	1.93	0.51
1:A:1140:GLN:HG2	1:A:1143:ARG:HH22	1.76	0.51
1:D:482:SER:O	1:D:482:SER:OG	2.28	0.51
1:D:1277:THR:HA	1:D:1337:GLY:H	1.75	0.51
1:A:1060:ASP:OD1	1:A:1061:GLN:N	2.44	0.51
1:B:169:LEU:HB3	1:B:203:ALA:HB2	1.92	0.51
1:B:697:ASP:OD1	1:B:700:ARG:N	2.39	0.51
1:B:1354:ARG:HG2	1:B:1373:GLU:HB2	1.91	0.51
1:B:1376:VAL:HG21	1:B:1385:TRP:HB3	1.93	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1057:GLU:OE1	1:C:1057:GLU:N	2.43	0.51
1:A:1045:ILE:HD13	1:B:1048:PHE:CD2	2.46	0.51
1:B:1346:HIS:ND1	1:B:1441:GLU:HB2	2.26	0.51
1:C:308:PHE:O	1:C:312:GLN:NE2	2.30	0.51
1:C:378:LEU:HD12	1:C:381:GLN:NE2	2.26	0.51
1:C:1060:ASP:OD1	1:C:1061:GLN:N	2.44	0.51
1:A:378:LEU:HD12	1:A:381:GLN:NE2	2.26	0.50
1:A:1346:HIS:ND1	1:A:1441:GLU:HB2	2.26	0.50
1:C:70:LYS:HD2	1:C:289:ASP:HA	1.94	0.50
1:C:1082:PRO:HA	1:C:1085:ILE:HB	1.92	0.50
1:B:922:PRO:O	1:B:925:ILE:HB	2.11	0.50
1:D:1082:PRO:HA	1:D:1085:ILE:HB	1.92	0.50
1:D:1484:LEU:HD23	1:D:1489:LYS:HG2	1.92	0.50
1:A:557:GLN:HB3	1:A:560:HIS:CE1	2.46	0.50
1:C:697:ASP:OD1	1:C:700:ARG:N	2.39	0.50
1:C:1346:HIS:ND1	1:C:1441:GLU:HB2	2.26	0.50
1:D:1346:HIS:ND1	1:D:1441:GLU:HB2	2.26	0.50
1:D:1376:VAL:HG21	1:D:1385:TRP:HB3	1.93	0.50
1:A:70:LYS:HD2	1:A:289:ASP:HA	1.94	0.50
1:A:1082:PRO:HA	1:A:1085:ILE:HB	1.92	0.50
1:B:167:PRO:HG3	1:B:204:TRP:CG	2.47	0.50
1:C:169:LEU:HB3	1:C:203:ALA:HB2	1.92	0.50
1:C:647:ASP:OD1	1:C:647:ASP:N	2.43	0.50
1:C:922:PRO:O	1:C:925:ILE:HB	2.11	0.50
1:D:169:LEU:HB3	1:D:203:ALA:HB2	1.92	0.50
1:D:1240:VAL:N	1:D:1430:ASP:OD2	2.44	0.50
1:A:167:PRO:HG3	1:A:204:TRP:CG	2.47	0.50
1:A:188:SER:HB2	1:A:192:ARG:HH22	1.77	0.50
1:B:557:GLN:HB3	1:B:560:HIS:CE1	2.46	0.50
1:B:1277:THR:HA	1:B:1337:GLY:H	1.75	0.50
1:C:917:SER:OG	1:C:917:SER:O	2.29	0.50
1:D:647:ASP:OD1	1:D:647:ASP:N	2.42	0.50
1:D:750:ASP:OD1	1:D:750:ASP:N	2.42	0.50
1:A:1376:VAL:HG21	1:A:1385:TRP:HB3	1.93	0.50
1:B:245:GLY:HA2	1:B:250:ARG:HH12	1.77	0.50
1:B:1111:ASN:OD1	1:B:1111:ASN:N	2.41	0.50
1:C:167:PRO:HG3	1:C:204:TRP:CG	2.47	0.50
1:C:207:THR:OG1	1:C:208:GLY:N	2.45	0.50
1:C:245:GLY:HA2	1:C:250:ARG:HH12	1.77	0.50
1:C:482:SER:O	1:C:482:SER:OG	2.28	0.50
1:C:1140:GLN:HG2	1:C:1143:ARG:HH22	1.76	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:167:PRO:HG3	1:D:204:TRP:CG	2.47	0.50
1:D:188:SER:HB2	1:D:192:ARG:HH22	1.77	0.50
1:A:669:THR:HG21	1:B:695:ARG:HD2	1.93	0.50
1:A:922:PRO:O	1:A:925:ILE:HB	2.11	0.50
1:B:329:VAL:HG12	1:B:352:VAL:HG12	1.94	0.50
1:B:917:SER:OG	1:B:917:SER:O	2.29	0.50
1:D:329:VAL:HG12	1:D:352:VAL:HG12	1.94	0.50
1:A:207:THR:OG1	1:A:208:GLY:N	2.45	0.50
1:B:750:ASP:OD1	1:B:750:ASP:N	2.42	0.50
1:C:557:GLN:HB3	1:C:560:HIS:CE1	2.46	0.50
1:D:207:THR:OG1	1:D:208:GLY:N	2.45	0.50
1:D:741:LYS:HG3	1:D:774:ARG:NH2	2.27	0.50
1:A:245:GLY:HA2	1:A:250:ARG:HH12	1.77	0.49
1:A:1277:THR:HA	1:A:1337:GLY:H	1.75	0.49
1:B:378:LEU:HD12	1:B:381:GLN:HE21	1.77	0.49
1:C:329:VAL:HG12	1:C:352:VAL:HG12	1.94	0.49
1:D:378:LEU:HD12	1:D:381:GLN:HE21	1.77	0.49
1:A:378:LEU:HD12	1:A:381:GLN:HE21	1.77	0.49
1:C:208:GLY:HA2	1:C:241:VAL:O	2.13	0.49
1:D:148:ASP:OD1	1:D:148:ASP:N	2.44	0.49
1:D:557:GLN:H	1:D:560:HIS:CD2	2.30	0.49
1:D:557:GLN:HB3	1:D:560:HIS:CE1	2.46	0.49
1:A:1354:ARG:HB2	1:A:1452:GLN:NE2	2.27	0.49
1:B:1485:TYR:O	1:B:1489:LYS:NZ	2.43	0.49
1:C:917:SER:HG	1:C:921:GLY:N	2.10	0.49
1:D:245:GLY:HA2	1:D:250:ARG:HH12	1.77	0.49
1:A:557:GLN:H	1:A:560:HIS:CD2	2.30	0.49
1:A:1137:GLN:O	1:A:1140:GLN:HB2	2.13	0.49
1:B:1029:LEU:HD11	1:C:972:TYR:HA	1.94	0.49
1:D:208:GLY:HA2	1:D:241:VAL:O	2.12	0.49
1:D:922:PRO:O	1:D:925:ILE:HB	2.11	0.49
1:B:188:SER:HB2	1:B:192:ARG:HH22	1.77	0.49
1:B:894:PRO:HA	1:B:897:VAL:HG22	1.94	0.49
1:B:1069:ASP:OD1	1:B:1070:LEU:N	2.46	0.49
1:C:1137:GLN:O	1:C:1140:GLN:HB2	2.13	0.49
1:D:70:LYS:HD2	1:D:289:ASP:HA	1.94	0.49
1:D:130:ILE:HB	1:D:142:TYR:CD1	2.48	0.49
1:D:1140:GLN:HG2	1:D:1143:ARG:HH22	1.76	0.49
1:C:130:ILE:HB	1:C:142:TYR:CD1	2.48	0.49
1:C:278:ASP:OD1	1:C:280:ASN:N	2.46	0.49
1:C:1069:ASP:OD1	1:C:1070:LEU:N	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:894:PRO:HA	1:D:897:VAL:HG22	1.94	0.49
1:D:1137:GLN:O	1:D:1140:GLN:HB2	2.13	0.49
1:A:246:THR:HG23	1:A:274:LEU:HA	1.95	0.49
1:B:130:ILE:HB	1:B:142:TYR:CD1	2.48	0.49
1:B:482:SER:O	1:B:482:SER:OG	2.28	0.49
1:C:188:SER:HB2	1:C:192:ARG:HH22	1.77	0.49
1:C:894:PRO:HA	1:C:897:VAL:HG22	1.94	0.49
1:D:917:SER:HG	1:D:921:GLY:N	2.09	0.49
1:A:130:ILE:HB	1:A:142:TYR:CD1	2.48	0.49
1:B:74:TYR:HE1	1:B:108:PHE:O	1.96	0.49
1:B:132:PHE:CZ	1:B:279:SER:HA	2.48	0.49
1:A:208:GLY:HA2	1:A:241:VAL:O	2.13	0.49
1:A:329:VAL:HG12	1:A:352:VAL:HG12	1.94	0.49
1:A:1425:TYR:H	1:A:1444:ALA:HB3	1.78	0.49
1:B:207:THR:OG1	1:B:208:GLY:N	2.45	0.49
1:B:557:GLN:H	1:B:560:HIS:CD2	2.30	0.49
1:B:1137:GLN:O	1:B:1140:GLN:HB2	2.13	0.49
1:D:1424:VAL:N	1:D:1444:ALA:O	2.46	0.49
1:A:57:GLU:HA	1:A:60:SER:HB2	1.95	0.49
1:A:894:PRO:HA	1:A:897:VAL:HG22	1.94	0.49
1:C:246:THR:HG23	1:C:274:LEU:HA	1.95	0.49
1:C:1346:HIS:HA	1:C:1441:GLU:O	2.13	0.49
1:D:114:ASP:O	1:D:117:LYS:N	2.46	0.49
1:D:246:THR:HG23	1:D:274:LEU:HA	1.95	0.49
1:D:1355:TRP:HB2	1:D:1357:ARG:HE	1.78	0.49
1:A:132:PHE:CZ	1:A:279:SER:HA	2.48	0.48
1:A:1355:TRP:HB2	1:A:1357:ARG:HE	1.78	0.48
1:A:1426:LYS:HG3	1:A:1442:THR:O	2.13	0.48
1:B:70:LYS:HD2	1:B:289:ASP:HA	1.93	0.48
1:B:278:ASP:OD1	1:B:280:ASN:N	2.46	0.48
1:B:282:SER:HG	1:B:283:HIS:CD2	2.31	0.48
1:B:378:LEU:O	1:B:381:GLN:NE2	2.46	0.48
1:B:1060:ASP:OD1	1:B:1061:GLN:N	2.44	0.48
1:B:1352:VAL:HA	1:B:1447:VAL:O	2.13	0.48
1:C:557:GLN:H	1:C:560:HIS:CD2	2.30	0.48
1:C:1085:ILE:O	1:C:1088:SER:OG	2.24	0.48
1:D:1346:HIS:HA	1:D:1441:GLU:O	2.13	0.48
1:A:74:TYR:HE1	1:A:108:PHE:O	1.96	0.48
1:A:282:SER:HG	1:A:283:HIS:CD2	2.31	0.48
1:A:342:ASN:O	1:A:346:ASN:ND2	2.46	0.48
1:A:378:LEU:O	1:A:381:GLN:NE2	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1426:LYS:HG3	1:B:1442:THR:O	2.13	0.48
1:C:132:PHE:CZ	1:C:279:SER:HA	2.48	0.48
1:C:342:ASN:O	1:C:346:ASN:ND2	2.46	0.48
1:D:311:GLU:HB2	1:D:312:GLN:NE2	2.29	0.48
1:D:1276:TYR:N	1:D:1335:GLY:HA3	2.28	0.48
1:A:278:ASP:OD1	1:A:280:ASN:N	2.46	0.48
1:B:917:SER:HG	1:B:921:GLY:N	2.10	0.48
1:B:1346:HIS:HA	1:B:1441:GLU:O	2.13	0.48
1:C:1354:ARG:HB2	1:C:1452:GLN:NE2	2.27	0.48
1:C:1424:VAL:N	1:C:1444:ALA:O	2.46	0.48
1:D:57:GLU:HA	1:D:60:SER:HB2	1.95	0.48
1:A:743:TRP:CE2	1:A:796:VAL:HG22	2.49	0.48
1:A:1364:CYS:SG	1:A:1365:ARG:N	2.87	0.48
1:B:208:GLY:HA2	1:B:241:VAL:O	2.12	0.48
1:B:1425:TYR:H	1:B:1444:ALA:HB3	1.78	0.48
1:C:69:LYS:HD3	1:C:124:THR:HG23	1.95	0.48
1:C:378:LEU:HD12	1:C:381:GLN:HE21	1.77	0.48
1:A:311:GLU:HB2	1:A:312:GLN:NE2	2.29	0.48
1:A:1276:TYR:N	1:A:1335:GLY:HA3	2.28	0.48
1:A:1347:THR:OG1	1:A:1348:LEU:N	2.46	0.48
1:B:246:THR:HG23	1:B:274:LEU:HA	1.95	0.48
1:B:1276:TYR:N	1:B:1335:GLY:HA3	2.28	0.48
1:C:282:SER:HG	1:C:283:HIS:CD2	2.31	0.48
1:C:485:HIS:O	1:C:489:THR:OG1	2.31	0.48
1:C:1355:TRP:HB2	1:C:1357:ARG:HE	1.78	0.48
1:C:1364:CYS:SG	1:C:1365:ARG:N	2.87	0.48
1:D:172:SER:HA	1:D:206:ILE:HG23	1.95	0.48
1:D:1039:LEU:HA	1:D:1042:ASN:HD21	1.79	0.48
1:A:132:PHE:CE2	1:A:279:SER:HA	2.49	0.48
1:A:1352:VAL:HA	1:A:1447:VAL:O	2.14	0.48
1:B:538:LYS:O	1:B:542:GLU:HG2	2.14	0.48
1:C:74:TYR:HE1	1:C:108:PHE:O	1.96	0.48
1:D:132:PHE:CZ	1:D:279:SER:HA	2.48	0.48
1:D:1364:CYS:SG	1:D:1365:ARG:N	2.87	0.48
1:A:1039:LEU:HA	1:A:1042:ASN:HD21	1.79	0.48
1:B:311:GLU:HB2	1:B:312:GLN:NE2	2.29	0.48
1:B:1364:CYS:SG	1:B:1365:ARG:N	2.87	0.48
1:C:172:SER:HA	1:C:206:ILE:HG23	1.95	0.48
1:C:1039:LEU:HA	1:C:1042:ASN:HD21	1.79	0.48
1:D:342:ASN:O	1:D:346:ASN:ND2	2.46	0.48
1:A:1069:ASP:OD1	1:A:1070:LEU:N	2.46	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:342:ASN:O	1:B:346:ASN:ND2	2.46	0.48
1:B:937:PHE:CE2	1:B:941:LEU:HD23	2.49	0.48
1:C:132:PHE:CE2	1:C:279:SER:HA	2.49	0.48
1:C:169:LEU:HD12	1:C:169:LEU:HA	1.64	0.48
1:A:1346:HIS:HA	1:A:1441:GLU:O	2.13	0.48
1:B:743:TRP:CE2	1:B:796:VAL:HG22	2.49	0.48
1:D:282:SER:HG	1:D:283:HIS:CD2	2.31	0.48
1:D:557:GLN:OE1	1:D:558:MET:N	2.43	0.48
1:D:743:TRP:CE2	1:D:796:VAL:HG22	2.49	0.48
1:D:1262:VAL:HG13	1:D:1263:PRO:HD3	1.96	0.48
1:D:1352:VAL:HA	1:D:1447:VAL:O	2.14	0.48
1:D:1425:TYR:H	1:D:1444:ALA:HB3	1.78	0.48
1:A:538:LYS:O	1:A:542:GLU:HG2	2.14	0.48
1:B:1347:THR:OG1	1:B:1348:LEU:N	2.46	0.48
1:B:1355:TRP:HB2	1:B:1357:ARG:HE	1.78	0.48
1:C:1347:THR:OG1	1:C:1348:LEU:N	2.46	0.48
1:C:1426:LYS:HG3	1:C:1442:THR:O	2.13	0.48
1:D:1354:ARG:HB2	1:D:1452:GLN:NE2	2.27	0.48
1:A:1262:VAL:HG13	1:A:1263:PRO:HD3	1.96	0.47
1:B:57:GLU:HA	1:B:60:SER:HB2	1.95	0.47
1:B:132:PHE:CE2	1:B:279:SER:HA	2.49	0.47
1:B:148:ASP:N	1:B:148:ASP:OD1	2.44	0.47
1:B:1354:ARG:HB2	1:B:1452:GLN:NE2	2.27	0.47
1:C:1425:TYR:H	1:C:1444:ALA:HB3	1.78	0.47
1:D:485:HIS:O	1:D:489:THR:OG1	2.31	0.47
1:D:1069:ASP:OD1	1:D:1070:LEU:N	2.46	0.47
1:A:937:PHE:CE2	1:A:941:LEU:HD23	2.49	0.47
1:C:311:GLU:HB2	1:C:312:GLN:NE2	2.29	0.47
1:C:743:TRP:CE2	1:C:796:VAL:HG22	2.49	0.47
1:D:69:LYS:HD3	1:D:124:THR:HG23	1.95	0.47
1:D:132:PHE:CE2	1:D:279:SER:HA	2.49	0.47
1:C:132:PHE:HB3	1:C:135:LEU:HD12	1.96	0.47
1:C:732:HIS:CD2	1:C:734:GLY:H	2.32	0.47
1:C:741:LYS:HG3	1:C:774:ARG:NH2	2.27	0.47
1:C:1352:VAL:HA	1:C:1447:VAL:O	2.14	0.47
1:D:378:LEU:O	1:D:381:GLN:NE2	2.46	0.47
1:D:1426:LYS:HG3	1:D:1442:THR:O	2.13	0.47
1:A:132:PHE:HB3	1:A:135:LEU:HD12	1.96	0.47
1:B:732:HIS:CD2	1:B:734:GLY:H	2.33	0.47
1:B:764:PRO:O	1:B:768:THR:N	2.48	0.47
1:D:917:SER:OG	1:D:917:SER:O	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:69:LYS:HD3	1:A:124:THR:HG23	1.95	0.47
1:A:73:VAL:HG12	1:A:118:HIS:O	2.15	0.47
1:A:732:HIS:CD2	1:A:734:GLY:H	2.32	0.47
1:A:917:SER:OG	1:A:917:SER:O	2.29	0.47
1:B:73:VAL:HG12	1:B:118:HIS:O	2.15	0.47
1:B:132:PHE:HB3	1:B:135:LEU:HD12	1.96	0.47
1:C:142:TYR:CE2	1:C:253:LEU:HD13	2.50	0.47
1:C:538:LYS:O	1:C:542:GLU:HG2	2.14	0.47
1:D:142:TYR:CE2	1:D:253:LEU:HD13	2.50	0.47
1:D:732:HIS:CD2	1:D:734:GLY:H	2.32	0.47
1:D:1347:THR:OG1	1:D:1348:LEU:N	2.46	0.47
1:A:698:GLU:O	1:A:702:GLN:HG2	2.15	0.47
1:A:1081:PRO:HB2	1:A:1083:PRO:HD2	1.96	0.47
1:B:1085:ILE:O	1:B:1088:SER:OG	2.24	0.47
1:C:1262:VAL:HG13	1:C:1263:PRO:HD3	1.96	0.47
1:C:1484:LEU:O	1:C:1489:LYS:NZ	2.39	0.47
1:D:333:GLY:O	1:D:336:THR:OG1	2.31	0.47
1:D:1060:ASP:OD1	1:D:1061:GLN:N	2.44	0.47
1:A:172:SER:HA	1:A:206:ILE:HG23	1.95	0.47
1:A:246:THR:HG22	1:A:275:THR:H	1.80	0.47
1:A:565:LEU:HD11	1:A:627:ILE:HG21	1.97	0.47
1:A:1446:SER:O	1:A:1446:SER:OG	2.33	0.47
1:B:172:SER:HA	1:B:206:ILE:HG23	1.95	0.47
1:B:579:ARG:HG3	1:B:580:PRO:O	2.15	0.47
1:B:1032:TYR:O	1:B:1036:THR:HG23	2.15	0.47
1:B:1081:PRO:HB2	1:B:1083:PRO:HD2	1.96	0.47
1:B:1424:VAL:N	1:B:1444:ALA:O	2.46	0.47
1:C:57:GLU:HA	1:C:60:SER:HB2	1.95	0.47
1:C:378:LEU:O	1:C:381:GLN:NE2	2.46	0.47
1:C:579:ARG:HG3	1:C:580:PRO:O	2.15	0.47
1:C:1276:TYR:N	1:C:1335:GLY:HA3	2.28	0.47
1:B:1022:GLU:CB	1:C:964:ASP:HA	2.45	0.47
1:B:1121:LEU:HD12	1:B:1121:LEU:HA	1.69	0.47
1:D:74:TYR:HE1	1:D:108:PHE:O	1.96	0.47
1:D:132:PHE:HB3	1:D:135:LEU:HD12	1.96	0.47
1:D:538:LYS:O	1:D:542:GLU:HG2	2.14	0.47
1:D:579:ARG:HG3	1:D:580:PRO:O	2.15	0.47
1:D:937:PHE:CE2	1:D:941:LEU:HD23	2.49	0.47
1:D:1326:ASN:HA	1:D:1439:TRP:CE3	2.50	0.47
1:A:1424:VAL:N	1:A:1444:ALA:O	2.46	0.47
1:B:69:LYS:HD3	1:B:124:THR:HG23	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:THR:HG22	1:B:275:THR:H	1.80	0.47
1:B:565:LEU:HD11	1:B:627:ILE:HG21	1.97	0.47
1:D:1378:LYS:HB2	1:D:1385:TRP:CH2	2.50	0.47
1:A:979:PHE:O	1:D:1037:ASN:ND2	2.48	0.47
1:B:169:LEU:HA	1:B:169:LEU:HD12	1.64	0.47
1:B:1039:LEU:HA	1:B:1042:ASN:HD21	1.79	0.47
1:B:1326:ASN:HA	1:B:1439:TRP:CE3	2.50	0.47
1:D:246:THR:HG22	1:D:275:THR:H	1.80	0.47
1:D:278:ASP:OD1	1:D:280:ASN:N	2.46	0.47
1:D:698:GLU:O	1:D:702:GLN:HG2	2.15	0.47
1:D:732:HIS:HB3	1:D:735:ILE:HG12	1.97	0.47
1:D:1081:PRO:HB2	1:D:1083:PRO:HD2	1.96	0.47
1:A:142:TYR:CE2	1:A:253:LEU:HD13	2.50	0.46
1:A:240:GLY:N	1:A:283:HIS:O	2.44	0.46
1:A:732:HIS:HB3	1:A:735:ILE:HG12	1.97	0.46
1:A:744:TRP:CZ3	1:A:796:VAL:HG11	2.50	0.46
1:A:1264:TRP:HH2	1:A:1436:ASP:HB3	1.80	0.46
1:A:1378:LYS:HB2	1:A:1385:TRP:CH2	2.50	0.46
1:B:142:TYR:CE2	1:B:253:LEU:HD13	2.50	0.46
1:C:744:TRP:CZ3	1:C:796:VAL:HG11	2.50	0.46
1:C:924:ILE:HA	1:C:927:VAL:HG22	1.96	0.46
1:C:937:PHE:CE2	1:C:941:LEU:HD23	2.49	0.46
1:C:1378:LYS:HB2	1:C:1385:TRP:CH2	2.50	0.46
1:D:764:PRO:O	1:D:768:THR:N	2.48	0.46
1:A:579:ARG:HG3	1:A:580:PRO:O	2.15	0.46
1:A:1032:TYR:O	1:A:1036:THR:HG23	2.15	0.46
1:A:1326:ASN:HA	1:A:1439:TRP:CE3	2.50	0.46
1:B:568:LEU:HD23	1:B:568:LEU:HA	1.63	0.46
1:B:938:LEU:HA	1:B:941:LEU:HD21	1.97	0.46
1:C:285:ILE:O	1:C:285:ILE:HG13	2.15	0.46
1:C:687:ILE:O	1:C:691:THR:HG22	2.16	0.46
1:C:764:PRO:O	1:C:768:THR:N	2.48	0.46
1:C:1081:PRO:HB2	1:C:1083:PRO:HD2	1.96	0.46
1:D:687:ILE:O	1:D:691:THR:HG22	2.16	0.46
1:A:285:ILE:O	1:A:285:ILE:HG13	2.15	0.46
1:A:924:ILE:HA	1:A:927:VAL:HG22	1.96	0.46
1:B:114:ASP:O	1:B:118:HIS:N	2.48	0.46
1:B:154:ILE:O	1:B:158:MET:HG3	2.16	0.46
1:B:653:LEU:HD23	1:B:653:LEU:HA	1.51	0.46
1:B:782:GLY:O	1:B:784:PRO:HD3	2.15	0.46
1:C:246:THR:HG22	1:C:275:THR:H	1.80	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1032:TYR:O	1:C:1036:THR:HG23	2.15	0.46
1:D:114:ASP:O	1:D:118:HIS:N	2.48	0.46
1:A:114:ASP:O	1:A:117:LYS:N	2.46	0.46
1:B:741:LYS:HG3	1:B:774:ARG:NH2	2.27	0.46
1:B:1262:VAL:HG13	1:B:1263:PRO:HD3	1.96	0.46
1:B:1378:LYS:HB2	1:B:1385:TRP:CH2	2.50	0.46
1:C:114:ASP:O	1:C:118:HIS:N	2.49	0.46
1:C:1038:ILE:HG21	1:D:938:LEU:HD21	1.97	0.46
1:A:523:TYR:CD1	1:A:628:TRP:HD1	2.33	0.46
1:A:764:PRO:O	1:A:768:THR:N	2.48	0.46
1:A:938:LEU:HA	1:A:941:LEU:HD21	1.97	0.46
1:A:1116:ASN:OD1	1:A:1117:GLU:N	2.49	0.46
1:A:1343:GLY:O	1:A:1439:TRP:N	2.27	0.46
1:B:1031:LEU:O	1:B:1034:LEU:HB3	2.16	0.46
1:B:1431:ASP:OD2	1:B:1433:ARG:N	2.34	0.46
1:C:223:ARG:HB2	1:C:280:ASN:CG	2.36	0.46
1:C:568:LEU:HD23	1:C:568:LEU:HA	1.63	0.46
1:C:1155:VAL:HG13	1:D:1154:LYS:HD2	1.97	0.46
1:A:68:LYS:O	1:A:146:SER:HB3	2.15	0.46
1:A:565:LEU:HA	1:A:565:LEU:HD23	1.62	0.46
1:A:875:ALA:HB1	1:A:906:PHE:CE1	2.51	0.46
1:C:165:ASP:OD1	1:C:165:ASP:N	2.38	0.46
1:C:1247:TYR:HA	1:C:1254:ARG:HH21	1.81	0.46
1:A:557:GLN:OE1	1:A:558:MET:N	2.43	0.46
1:A:659:LEU:HA	1:A:659:LEU:HD23	1.69	0.46
1:B:744:TRP:CZ3	1:B:796:VAL:HG11	2.50	0.46
1:C:328:VAL:HG23	1:C:351:VAL:HG13	1.98	0.46
1:C:565:LEU:HD11	1:C:627:ILE:HG21	1.97	0.46
1:C:1116:ASN:OD1	1:C:1117:GLU:N	2.49	0.46
1:C:1326:ASN:HA	1:C:1439:TRP:CE3	2.50	0.46
1:D:565:LEU:HA	1:D:565:LEU:HD23	1.61	0.46
1:D:1116:ASN:OD1	1:D:1117:GLU:N	2.49	0.46
1:A:1448:HIS:CD2	1:A:1450:GLN:HG3	2.51	0.46
1:B:68:LYS:O	1:B:146:SER:HB3	2.16	0.46
1:B:285:ILE:HG13	1:B:285:ILE:O	2.15	0.46
1:B:687:ILE:O	1:B:691:THR:HG22	2.16	0.46
1:B:698:GLU:O	1:B:702:GLN:HG2	2.15	0.46
1:B:782:GLY:HA2	1:B:787:ARG:HD2	1.98	0.46
1:B:1448:HIS:CD2	1:B:1450:GLN:HG3	2.51	0.46
1:C:73:VAL:HG12	1:C:118:HIS:O	2.15	0.46
1:C:875:ALA:HB1	1:C:906:PHE:CE1	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1264:TRP:HH2	1:C:1436:ASP:HB3	1.80	0.46
1:D:223:ARG:HB2	1:D:280:ASN:CG	2.36	0.46
1:D:926:ILE:O	1:D:930:MET:HG2	2.16	0.46
1:A:223:ARG:HB2	1:A:280:ASN:CG	2.36	0.46
1:B:328:VAL:HG23	1:B:351:VAL:HG13	1.98	0.46
1:B:924:ILE:HA	1:B:927:VAL:HG22	1.96	0.46
1:D:73:VAL:HG12	1:D:118:HIS:O	2.15	0.46
1:D:523:TYR:CD1	1:D:628:TRP:HD1	2.33	0.46
1:D:924:ILE:HA	1:D:927:VAL:HG22	1.96	0.46
1:D:1343:GLY:O	1:D:1439:TRP:N	2.27	0.46
1:D:1448:HIS:CD2	1:D:1450:GLN:HG3	2.51	0.46
1:A:531:LEU:HD21	1:A:665:GLU:HG3	1.98	0.46
1:A:687:ILE:O	1:A:691:THR:HG22	2.16	0.46
1:A:866:ASP:O	1:A:870:LYS:N	2.46	0.46
1:A:908:LEU:O	1:A:910:LEU:N	2.49	0.46
1:B:114:ASP:O	1:B:117:LYS:N	2.46	0.46
1:B:127:PHE:O	1:B:142:TYR:OH	2.34	0.46
1:B:523:TYR:CD1	1:B:628:TRP:HD1	2.33	0.46
1:B:732:HIS:HB3	1:B:735:ILE:HG12	1.97	0.46
1:B:926:ILE:O	1:B:930:MET:HG2	2.16	0.46
1:C:698:GLU:O	1:C:702:GLN:HG2	2.15	0.46
1:C:732:HIS:HB3	1:C:735:ILE:HG12	1.97	0.46
1:C:1264:TRP:NE1	1:C:1326:ASN:O	2.44	0.46
1:C:1448:HIS:CD2	1:C:1450:GLN:HG3	2.51	0.46
1:D:285:ILE:O	1:D:285:ILE:HG13	2.15	0.46
1:D:531:LEU:HD21	1:D:665:GLU:HG3	1.98	0.46
1:D:565:LEU:HD11	1:D:627:ILE:HG21	1.97	0.46
1:D:875:ALA:HB1	1:D:906:PHE:CE1	2.51	0.46
1:D:1264:TRP:HH2	1:D:1436:ASP:HB3	1.81	0.46
1:A:114:ASP:O	1:A:118:HIS:N	2.49	0.45
1:B:142:TYR:OH	1:B:259:SER:OG	2.34	0.45
1:C:154:ILE:O	1:C:158:MET:HG3	2.16	0.45
1:C:487:THR:OG1	1:C:488:MET:N	2.49	0.45
1:C:739:LEU:HA	1:C:739:LEU:HD23	1.74	0.45
1:C:938:LEU:HA	1:C:941:LEU:HD21	1.97	0.45
1:D:68:LYS:O	1:D:146:SER:HB3	2.15	0.45
1:D:142:TYR:OH	1:D:259:SER:OG	2.35	0.45
1:D:240:GLY:N	1:D:283:HIS:O	2.44	0.45
1:D:782:GLY:O	1:D:784:PRO:HD3	2.16	0.45
1:D:1031:LEU:O	1:D:1034:LEU:HB3	2.16	0.45
1:D:1406:LEU:O	1:D:1466:ALA:HA	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:142:TYR:OH	1:A:259:SER:OG	2.35	0.45
1:B:535:LYS:HE3	1:B:535:LYS:HB3	1.83	0.45
1:B:1247:TYR:HA	1:B:1254:ARG:HH21	1.81	0.45
1:B:1406:LEU:O	1:B:1466:ALA:HA	2.16	0.45
1:B:1450:GLN:H	1:B:1450:GLN:CD	2.20	0.45
1:C:68:LYS:O	1:C:146:SER:HB3	2.15	0.45
1:C:782:GLY:HA2	1:C:787:ARG:HD2	1.98	0.45
1:C:1031:LEU:O	1:C:1034:LEU:HB3	2.16	0.45
1:C:1057:GLU:HG2	1:C:1058:HIS:N	2.32	0.45
1:D:487:THR:OG1	1:D:488:MET:N	2.49	0.45
1:D:782:GLY:HA2	1:D:787:ARG:HD2	1.98	0.45
1:D:1032:TYR:O	1:D:1036:THR:HG23	2.15	0.45
1:A:154:ILE:O	1:A:158:MET:HG3	2.16	0.45
1:A:204:TRP:HD1	1:A:237:ILE:HD11	1.81	0.45
1:B:487:THR:OG1	1:B:488:MET:N	2.49	0.45
1:B:908:LEU:C	1:B:910:LEU:H	2.20	0.45
1:C:523:TYR:CD1	1:C:628:TRP:HD1	2.33	0.45
1:C:565:LEU:HD23	1:C:565:LEU:HA	1.62	0.45
1:C:876:ILE:O	1:C:880:VAL:HG12	2.16	0.45
1:C:1343:GLY:HA2	1:C:1439:TRP:CH2	2.51	0.45
1:C:1406:LEU:O	1:C:1466:ALA:HA	2.16	0.45
1:D:59:LEU:HD22	1:D:161:HIS:HB3	1.98	0.45
1:D:744:TRP:CZ3	1:D:796:VAL:HG11	2.50	0.45
1:D:908:LEU:O	1:D:910:LEU:N	2.49	0.45
1:D:1450:GLN:H	1:D:1450:GLN:CD	2.20	0.45
1:A:804:LEU:O	1:A:807:PHE:N	2.50	0.45
1:A:1247:TYR:HA	1:A:1254:ARG:HH21	1.81	0.45
1:B:531:LEU:HD21	1:B:665:GLU:HG3	1.98	0.45
1:C:59:LEU:HD22	1:C:161:HIS:HB3	1.98	0.45
1:C:357:GLY:N	1:C:361:ASP:OD2	2.40	0.45
1:C:531:LEU:HD21	1:C:665:GLU:HG3	1.98	0.45
1:C:867:PHE:CD2	1:C:868:TRP:CD1	3.04	0.45
1:C:926:ILE:O	1:C:930:MET:HG2	2.16	0.45
1:C:1241:ASN:ND2	1:C:1432:PRO:HD3	2.32	0.45
1:C:1450:GLN:CD	1:C:1450:GLN:H	2.20	0.45
1:D:154:ILE:O	1:D:158:MET:HG3	2.16	0.45
1:A:782:GLY:HA2	1:A:787:ARG:HD2	1.98	0.45
1:A:1406:LEU:O	1:A:1466:ALA:HA	2.16	0.45
1:A:1431:ASP:HB3	1:A:1434:ASN:OD1	2.17	0.45
1:B:450:GLU:O	1:B:453:ASP:HB2	2.16	0.45
1:B:920:LEU:O	1:B:923:LYS:N	2.50	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:557:GLN:OE1	1:C:558:MET:N	2.43	0.45
1:C:637:LEU:HD23	1:C:637:LEU:HA	1.67	0.45
1:C:782:GLY:O	1:C:784:PRO:HD3	2.15	0.45
1:C:866:ASP:O	1:C:870:LYS:N	2.46	0.45
1:D:450:GLU:O	1:D:453:ASP:HB2	2.17	0.45
1:D:938:LEU:HA	1:D:941:LEU:HD21	1.97	0.45
1:A:59:LEU:HD22	1:A:161:HIS:HB3	1.98	0.45
1:A:169:LEU:HA	1:A:169:LEU:HD12	1.64	0.45
1:A:782:GLY:O	1:A:784:PRO:HD3	2.15	0.45
1:A:1053:GLN:CD	1:B:1052:PHE:HE2	2.19	0.45
1:B:223:ARG:HB2	1:B:280:ASN:CG	2.36	0.45
1:B:1140:GLN:CB	1:B:1143:ARG:HH12	2.30	0.45
1:C:920:LEU:O	1:C:923:LYS:N	2.50	0.45
1:C:1140:GLN:CB	1:C:1143:ARG:HH12	2.30	0.45
1:C:1162:LEU:HG	1:D:1161:LEU:HD22	1.97	0.45
1:D:285:ILE:O	1:D:286:LEU:HD23	2.17	0.45
1:D:335:GLY:O	1:D:339:THR:HG23	2.17	0.45
1:D:1247:TYR:HA	1:D:1254:ARG:HH21	1.81	0.45
1:D:1343:GLY:HA2	1:D:1439:TRP:CH2	2.51	0.45
1:A:335:GLY:O	1:A:339:THR:HG23	2.17	0.45
1:A:739:LEU:HD23	1:A:739:LEU:HA	1.74	0.45
1:A:741:LYS:HG3	1:A:774:ARG:NH2	2.27	0.45
1:A:754:TRP:O	1:A:758:LEU:HG	2.17	0.45
1:A:1375:LEU:HG	1:A:1474:ARG:C	2.37	0.45
1:A:1428:TYR:CD1	1:A:1439:TRP:HB2	2.52	0.45
1:B:1343:GLY:HA2	1:B:1439:TRP:CH2	2.51	0.45
1:B:1428:TYR:CD1	1:B:1439:TRP:HB2	2.52	0.45
1:C:130:ILE:HG13	1:C:262:ALA:HB3	1.99	0.45
1:C:142:TYR:OH	1:C:259:SER:OG	2.35	0.45
1:C:1375:LEU:HG	1:C:1474:ARG:C	2.37	0.45
1:C:1431:ASP:HB3	1:C:1434:ASN:OD1	2.17	0.45
1:D:130:ILE:HG13	1:D:262:ALA:HB3	1.99	0.45
1:D:1140:GLN:CB	1:D:1143:ARG:HH12	2.30	0.45
1:D:1241:ASN:ND2	1:D:1432:PRO:HD3	2.32	0.45
1:A:328:VAL:HG23	1:A:351:VAL:HG13	1.98	0.45
1:A:926:ILE:O	1:A:930:MET:HG2	2.16	0.45
1:B:875:ALA:HB1	1:B:906:PHE:CE1	2.51	0.45
1:C:333:GLY:O	1:C:336:THR:OG1	2.31	0.45
1:D:1375:LEU:HG	1:D:1474:ARG:C	2.37	0.45
1:D:1378:LYS:HB2	1:D:1385:TRP:CZ3	2.52	0.45
1:A:908:LEU:C	1:A:910:LEU:H	2.20	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:307:LYS:HE2	1:B:307:LYS:HB3	1.76	0.45
1:B:739:LEU:HD23	1:B:739:LEU:HA	1.74	0.45
1:B:867:PHE:CD2	1:B:868:TRP:CD1	3.04	0.45
1:B:1264:TRP:NE1	1:B:1326:ASN:O	2.43	0.45
1:C:718:LEU:HD12	1:C:718:LEU:HA	1.70	0.45
1:C:1378:LYS:HB2	1:C:1385:TRP:CZ3	2.52	0.45
1:D:328:VAL:HG23	1:D:351:VAL:HG13	1.98	0.45
1:D:876:ILE:O	1:D:880:VAL:HG12	2.16	0.45
1:A:487:THR:OG1	1:A:488:MET:N	2.49	0.45
1:A:1057:GLU:HG2	1:A:1058:HIS:N	2.32	0.45
1:A:1264:TRP:NE1	1:A:1326:ASN:O	2.44	0.45
1:B:1264:TRP:HH2	1:B:1436:ASP:HB3	1.80	0.45
1:B:1433:ARG:NH1	1:B:1433:ARG:HB2	2.32	0.45
1:B:1492:LEU:HD12	1:B:1495:ALA:HB3	1.99	0.45
1:C:1433:ARG:NH1	1:C:1433:ARG:HB2	2.32	0.45
1:D:1354:ARG:CG	1:D:1373:GLU:HB2	2.47	0.45
1:A:485:HIS:O	1:A:489:THR:OG1	2.31	0.44
1:A:867:PHE:CD2	1:A:868:TRP:CD1	3.04	0.44
1:A:916:ILE:HD12	1:A:916:ILE:HA	1.80	0.44
1:A:1241:ASN:ND2	1:A:1432:PRO:HD3	2.32	0.44
1:B:458:LEU:HD22	1:B:462:TRP:CZ2	2.53	0.44
1:B:804:LEU:O	1:B:807:PHE:N	2.50	0.44
1:B:876:ILE:O	1:B:880:VAL:HG12	2.16	0.44
1:B:908:LEU:O	1:B:910:LEU:N	2.49	0.44
1:B:1057:GLU:HG2	1:B:1058:HIS:N	2.32	0.44
1:B:1241:ASN:ND2	1:B:1432:PRO:HD3	2.32	0.44
1:B:1364:CYS:O	1:B:1370:LYS:NZ	2.42	0.44
1:C:335:GLY:O	1:C:339:THR:HG23	2.17	0.44
1:C:477:TRP:CD2	1:C:479:TRP:HB3	2.53	0.44
1:C:1492:LEU:HD12	1:C:1495:ALA:HB3	1.99	0.44
1:D:1057:GLU:HG2	1:D:1058:HIS:N	2.32	0.44
1:A:285:ILE:O	1:A:286:LEU:HD23	2.16	0.44
1:A:1031:LEU:O	1:A:1034:LEU:HB3	2.16	0.44
1:A:1044:LEU:HB3	1:A:1048:PHE:CE2	2.53	0.44
1:A:1343:GLY:HA2	1:A:1439:TRP:CH2	2.51	0.44
1:A:1378:LYS:HB2	1:A:1385:TRP:CZ3	2.52	0.44
1:C:285:ILE:O	1:C:286:LEU:HD23	2.16	0.44
1:C:1044:LEU:HB3	1:C:1048:PHE:CE2	2.53	0.44
1:C:1428:TYR:CD1	1:C:1439:TRP:HB2	2.52	0.44
1:D:236:LEU:HA	1:D:236:LEU:HD23	1.73	0.44
1:D:477:TRP:CD2	1:D:479:TRP:HB3	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:804:LEU:O	1:D:807:PHE:N	2.50	0.44
1:D:1344:PRO:HB2	1:D:1346:HIS:CE1	2.53	0.44
1:A:718:LEU:HD12	1:A:718:LEU:HA	1.70	0.44
1:A:876:ILE:O	1:A:880:VAL:HG12	2.16	0.44
1:A:942:ALA:O	1:A:946:VAL:HG13	2.17	0.44
1:A:1354:ARG:CG	1:A:1373:GLU:HB2	2.47	0.44
1:B:1044:LEU:HB3	1:B:1048:PHE:CE2	2.53	0.44
1:B:1116:ASN:OD1	1:B:1117:GLU:N	2.49	0.44
1:C:204:TRP:HD1	1:C:237:ILE:HD11	1.81	0.44
1:D:535:LYS:HE3	1:D:535:LYS:HB3	1.83	0.44
1:D:754:TRP:O	1:D:758:LEU:HG	2.17	0.44
1:D:1385:TRP:O	1:D:1484:LEU:HA	2.17	0.44
1:D:1428:TYR:CD1	1:D:1439:TRP:HB2	2.52	0.44
1:D:1431:ASP:OD2	1:D:1433:ARG:N	2.34	0.44
1:A:127:PHE:O	1:A:142:TYR:OH	2.34	0.44
1:A:450:GLU:O	1:A:453:ASP:HB2	2.17	0.44
1:A:1428:TYR:HA	1:A:1440:ILE:O	2.17	0.44
1:A:1450:GLN:CD	1:A:1450:GLN:H	2.20	0.44
1:A:1485:TYR:O	1:A:1489:LYS:HG3	2.17	0.44
1:B:59:LEU:HD22	1:B:161:HIS:HB3	1.98	0.44
1:B:477:TRP:CD2	1:B:479:TRP:HB3	2.53	0.44
1:B:925:ILE:HD13	1:B:925:ILE:HA	1.83	0.44
1:C:804:LEU:O	1:C:807:PHE:N	2.50	0.44
1:C:908:LEU:O	1:C:910:LEU:N	2.49	0.44
1:D:150:PRO:O	1:D:153:VAL:HG12	2.18	0.44
1:D:942:ALA:O	1:D:946:VAL:HG13	2.17	0.44
1:D:1044:LEU:HB3	1:D:1048:PHE:CE2	2.53	0.44
1:D:1428:TYR:HA	1:D:1440:ILE:O	2.17	0.44
1:A:821:PHE:HE2	1:A:892:LEU:HD21	1.83	0.44
1:A:920:LEU:O	1:A:923:LYS:N	2.50	0.44
1:A:1247:TYR:CE2	1:A:1433:ARG:HA	2.53	0.44
1:A:1492:LEU:HD12	1:A:1495:ALA:HB3	1.99	0.44
1:B:285:ILE:O	1:B:286:LEU:HD23	2.17	0.44
1:B:492:LEU:O	1:B:494:SER:N	2.51	0.44
1:B:754:TRP:O	1:B:758:LEU:HG	2.17	0.44
1:B:1300:GLN:O	1:B:1310:ARG:HD3	2.18	0.44
1:B:1431:ASP:HB3	1:B:1434:ASN:OD1	2.17	0.44
1:C:450:GLU:O	1:C:453:ASP:HB2	2.17	0.44
1:D:168:ASN:ND2	1:D:201:THR:O	2.51	0.44
1:D:169:LEU:HD12	1:D:169:LEU:HA	1.64	0.44
1:D:1431:ASP:HB3	1:D:1434:ASN:OD1	2.17	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1492:LEU:HD12	1:D:1495:ALA:HB3	1.99	0.44
1:A:796:VAL:O	1:A:799:PHE:HB3	2.18	0.44
1:B:130:ILE:HG13	1:B:262:ALA:HB3	1.99	0.44
1:C:754:TRP:O	1:C:758:LEU:HG	2.17	0.44
1:C:1247:TYR:CE2	1:C:1433:ARG:HA	2.53	0.44
1:C:1344:PRO:HB2	1:C:1346:HIS:CE1	2.53	0.44
1:C:1428:TYR:HA	1:C:1440:ILE:O	2.17	0.44
1:A:357:GLY:N	1:A:361:ASP:OD2	2.40	0.44
1:A:1140:GLN:CB	1:A:1143:ARG:HH12	2.30	0.44
1:A:1344:PRO:HB2	1:A:1346:HIS:CE1	2.53	0.44
1:B:335:GLY:O	1:B:339:THR:HG23	2.17	0.44
1:B:910:LEU:HD12	1:B:910:LEU:HA	1.78	0.44
1:B:922:PRO:O	1:B:926:ILE:HG13	2.18	0.44
1:B:942:ALA:O	1:B:946:VAL:HG13	2.17	0.44
1:B:1378:LYS:HB2	1:B:1385:TRP:CZ3	2.52	0.44
1:C:824:VAL:C	1:C:886:ARG:HH22	2.21	0.44
1:C:922:PRO:O	1:C:926:ILE:HG13	2.18	0.44
1:D:382:LYS:HD3	1:D:382:LYS:HA	1.76	0.44
1:D:458:LEU:O	1:D:461:ALA:N	2.51	0.44
1:D:1433:ARG:NH1	1:D:1433:ARG:HB2	2.32	0.44
1:A:130:ILE:HG13	1:A:262:ALA:HB3	1.99	0.44
1:A:168:ASN:ND2	1:A:201:THR:O	2.51	0.44
1:A:307:LYS:HE2	1:A:307:LYS:HB3	1.76	0.44
1:A:333:GLY:O	1:A:336:THR:OG1	2.31	0.44
1:A:395:THR:HG22	1:A:398:ARG:HD2	2.00	0.44
1:B:197:VAL:HA	1:B:200:THR:HG22	2.00	0.44
1:B:1378:LYS:HD3	1:B:1385:TRP:CE2	2.53	0.44
1:B:1385:TRP:HB2	1:B:1483:PRO:O	2.18	0.44
1:C:150:PRO:O	1:C:153:VAL:HG12	2.18	0.44
1:C:750:ASP:OD1	1:C:750:ASP:N	2.42	0.44
1:C:925:ILE:HD13	1:C:925:ILE:HA	1.83	0.44
1:D:492:LEU:O	1:D:494:SER:N	2.51	0.44
1:D:821:PHE:HE2	1:D:892:LEU:HD21	1.83	0.44
1:D:824:VAL:C	1:D:886:ARG:HH22	2.21	0.44
1:D:908:LEU:C	1:D:910:LEU:H	2.20	0.44
1:D:956:LEU:HD23	1:D:956:LEU:HA	1.80	0.44
1:D:1121:LEU:HD12	1:D:1121:LEU:HA	1.69	0.44
1:A:236:LEU:HA	1:A:236:LEU:HD23	1.73	0.44
1:A:301:LEU:HD12	1:A:304:ARG:NH1	2.31	0.44
1:A:1385:TRP:HB2	1:A:1483:PRO:O	2.18	0.44
1:B:168:ASN:ND2	1:B:201:THR:O	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:PHE:CZ	1:B:903:PHE:HB2	2.53	0.44
1:B:1354:ARG:CG	1:B:1373:GLU:HB2	2.47	0.44
1:B:1478:VAL:HG13	1:B:1502:HIS:NE2	2.33	0.44
1:B:1485:TYR:O	1:B:1489:LYS:HG3	2.17	0.44
1:C:458:LEU:HD22	1:C:462:TRP:CZ2	2.53	0.44
1:C:821:PHE:HE2	1:C:892:LEU:HD21	1.83	0.44
1:C:942:ALA:O	1:C:946:VAL:HG13	2.17	0.44
1:C:1271:TYR:HE1	1:C:1332:GLY:HA2	1.83	0.44
1:D:142:TYR:HA	1:D:284:PHE:O	2.18	0.44
1:D:922:PRO:O	1:D:926:ILE:HG13	2.18	0.44
1:D:1264:TRP:CE3	1:D:1330:ARG:HG2	2.53	0.44
1:A:477:TRP:CD2	1:A:479:TRP:HB3	2.53	0.43
1:A:1385:TRP:O	1:A:1484:LEU:HA	2.17	0.43
1:B:142:TYR:HA	1:B:284:PHE:O	2.18	0.43
1:B:716:THR:HG23	1:B:719:GLN:H	1.83	0.43
1:B:796:VAL:O	1:B:799:PHE:HB3	2.18	0.43
1:B:824:VAL:C	1:B:886:ARG:HH22	2.21	0.43
1:B:1428:TYR:HA	1:B:1440:ILE:O	2.17	0.43
1:C:492:LEU:O	1:C:494:SER:N	2.51	0.43
1:C:716:THR:HG23	1:C:719:GLN:H	1.83	0.43
1:C:1385:TRP:O	1:C:1484:LEU:HA	2.17	0.43
1:C:1434:ASN:HD22	1:C:1439:TRP:HA	1.83	0.43
1:A:492:LEU:O	1:A:494:SER:N	2.51	0.43
1:A:716:THR:HG23	1:A:719:GLN:H	1.83	0.43
1:A:1271:TYR:HE1	1:A:1332:GLY:HA2	1.83	0.43
1:A:1378:LYS:HD3	1:A:1385:TRP:CE2	2.53	0.43
1:A:1433:ARG:NH1	1:A:1433:ARG:HB2	2.32	0.43
1:B:1344:PRO:HB2	1:B:1346:HIS:CE1	2.53	0.43
1:C:1264:TRP:CE3	1:C:1330:ARG:HG2	2.53	0.43
1:D:189:ILE:HG12	1:D:192:ARG:NH1	2.34	0.43
1:D:867:PHE:CD2	1:D:868:TRP:CD1	3.04	0.43
1:D:1271:TYR:HE1	1:D:1332:GLY:HA2	1.83	0.43
1:D:1300:GLN:O	1:D:1310:ARG:HD3	2.18	0.43
1:A:225:PHE:CD2	1:A:236:LEU:HD12	2.54	0.43
1:A:458:LEU:O	1:A:461:ALA:N	2.51	0.43
1:A:458:LEU:HD22	1:A:462:TRP:CZ2	2.53	0.43
1:A:1264:TRP:CE3	1:A:1330:ARG:HG2	2.53	0.43
1:B:150:PRO:O	1:B:153:VAL:HG12	2.18	0.43
1:B:189:ILE:HG12	1:B:192:ARG:NH1	2.34	0.43
1:B:240:GLY:N	1:B:283:HIS:O	2.44	0.43
1:B:395:THR:HG22	1:B:398:ARG:HD2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:866:ASP:O	1:B:870:LYS:N	2.46	0.43
1:B:1343:GLY:HA2	1:B:1439:TRP:CZ3	2.53	0.43
1:B:1385:TRP:O	1:B:1484:LEU:HA	2.17	0.43
1:C:168:ASN:ND2	1:C:201:THR:O	2.51	0.43
1:D:438:LEU:O	1:D:441:SER:OG	2.27	0.43
1:D:716:THR:HG23	1:D:719:GLN:H	1.84	0.43
1:D:813:PHE:CZ	1:D:903:PHE:HB2	2.53	0.43
1:D:1485:TYR:O	1:D:1489:LYS:HG3	2.17	0.43
1:A:515:THR:OG1	1:A:516:TRP:N	2.52	0.43
1:A:662:LEU:HA	1:A:662:LEU:HD12	1.80	0.43
1:A:1113:LEU:HD23	1:A:1113:LEU:HA	1.81	0.43
1:A:1343:GLY:HA2	1:A:1439:TRP:CZ3	2.53	0.43
1:B:333:GLY:O	1:B:336:THR:OG1	2.30	0.43
1:B:637:LEU:HD23	1:B:637:LEU:HA	1.67	0.43
1:C:114:ASP:O	1:C:117:LYS:N	2.46	0.43
1:C:225:PHE:CD2	1:C:236:LEU:HD12	2.54	0.43
1:C:735:ILE:O	1:C:738:PHE:N	2.52	0.43
1:C:1478:VAL:HG13	1:C:1502:HIS:NE2	2.33	0.43
1:D:124:THR:HG22	1:D:126:ALA:N	2.34	0.43
1:D:307:LYS:HE2	1:D:307:LYS:HB3	1.76	0.43
1:A:482:SER:O	1:A:482:SER:OG	2.28	0.43
1:B:357:GLY:N	1:B:361:ASP:OD2	2.40	0.43
1:C:189:ILE:HG12	1:C:192:ARG:NH1	2.34	0.43
1:C:323:ILE:H	1:C:323:ILE:HG13	1.70	0.43
1:C:625:LEU:HD12	1:C:625:LEU:HA	1.63	0.43
1:C:813:PHE:CZ	1:C:903:PHE:HB2	2.53	0.43
1:C:908:LEU:C	1:C:910:LEU:H	2.20	0.43
1:C:1300:GLN:O	1:C:1310:ARG:HD3	2.18	0.43
1:D:395:THR:HG22	1:D:398:ARG:HD2	2.00	0.43
1:D:637:LEU:HD23	1:D:637:LEU:HA	1.67	0.43
1:D:1378:LYS:HD3	1:D:1385:TRP:CE2	2.53	0.43
1:A:124:THR:HG22	1:A:126:ALA:N	2.34	0.43
1:A:899:LEU:HA	1:A:899:LEU:HD13	1.75	0.43
1:A:1300:GLN:O	1:A:1310:ARG:HD3	2.18	0.43
1:B:1247:TYR:CE2	1:B:1433:ARG:HA	2.53	0.43
1:B:1375:LEU:HG	1:B:1474:ARG:C	2.38	0.43
1:B:1446:SER:O	1:B:1446:SER:OG	2.33	0.43
1:C:458:LEU:O	1:C:461:ALA:N	2.51	0.43
1:D:458:LEU:HD22	1:D:462:TRP:CZ2	2.53	0.43
1:D:1434:ASN:HD22	1:D:1439:TRP:HA	1.83	0.43
1:A:148:ASP:N	1:A:148:ASP:OD1	2.44	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:189:ILE:HG12	1:A:192:ARG:NH1	2.34	0.43
1:A:1155:VAL:HG13	1:B:1154:LYS:HD2	2.01	0.43
1:B:225:PHE:CD2	1:B:236:LEU:HD12	2.54	0.43
1:B:1434:ASN:HD22	1:B:1439:TRP:HA	1.83	0.43
1:C:1378:LYS:HD3	1:C:1385:TRP:CE2	2.53	0.43
1:D:572:PHE:CZ	1:D:723:GLU:HG3	2.54	0.43
1:D:1060:ASP:OD1	1:D:1060:ASP:N	2.51	0.43
1:D:1247:TYR:CE2	1:D:1433:ARG:HA	2.53	0.43
1:D:1343:GLY:HA2	1:D:1439:TRP:CZ3	2.53	0.43
1:A:922:PRO:O	1:A:926:ILE:HG13	2.18	0.43
1:B:458:LEU:O	1:B:461:ALA:N	2.51	0.43
1:C:142:TYR:HA	1:C:284:PHE:O	2.18	0.43
1:C:170:LEU:HD12	1:C:170:LEU:HA	1.78	0.43
1:C:197:VAL:HA	1:C:200:THR:HG22	2.00	0.43
1:C:662:LEU:HA	1:C:662:LEU:HD12	1.80	0.43
1:C:666:GLU:OE1	1:C:671:SER:OG	2.37	0.43
1:C:796:VAL:O	1:C:799:PHE:HB3	2.18	0.43
1:C:802:ASN:ND2	1:C:1074:TYR:OH	2.51	0.43
1:C:1343:GLY:HA2	1:C:1439:TRP:CZ3	2.53	0.43
1:C:1354:ARG:CG	1:C:1373:GLU:HB2	2.47	0.43
1:D:225:PHE:CD2	1:D:236:LEU:HD12	2.54	0.43
1:D:515:THR:HA	1:D:617:PHE:CD1	2.54	0.43
1:D:799:PHE:CD1	1:D:1074:TYR:CE2	3.05	0.43
1:D:1385:TRP:HB2	1:D:1483:PRO:O	2.18	0.43
1:A:515:THR:HA	1:A:617:PHE:CD1	2.54	0.43
1:A:680:GLU:O	1:A:683:GLU:HG2	2.19	0.43
1:A:1128:LEU:HD23	1:A:1128:LEU:HA	1.74	0.43
1:A:1355:TRP:HB3	1:A:1363:ILE:HG23	2.01	0.43
1:B:348:THR:HA	1:B:349:PRO:HD3	1.87	0.43
1:B:735:ILE:O	1:B:738:PHE:N	2.52	0.43
1:B:1155:VAL:O	1:B:1159:VAL:HG23	2.19	0.43
1:B:1264:TRP:CE3	1:B:1330:ARG:HG2	2.53	0.43
1:C:395:THR:HG22	1:C:398:ARG:HD2	2.00	0.43
1:C:1060:ASP:OD1	1:C:1060:ASP:N	2.51	0.43
1:C:1155:VAL:O	1:C:1159:VAL:HG23	2.19	0.43
1:C:1485:TYR:O	1:C:1489:LYS:HG3	2.17	0.43
1:D:680:GLU:O	1:D:683:GLU:HG2	2.19	0.43
1:D:1250:CYS:O	1:D:1252:VAL:N	2.46	0.43
1:D:1266:THR:O	1:D:1330:ARG:NH2	2.51	0.43
1:A:813:PHE:CZ	1:A:903:PHE:HB2	2.53	0.43
1:A:824:VAL:C	1:A:886:ARG:HH22	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1478:VAL:HG13	1:A:1502:HIS:NE2	2.33	0.43
1:B:515:THR:HA	1:B:617:PHE:CD1	2.54	0.43
1:B:662:LEU:HD12	1:B:662:LEU:HA	1.80	0.43
1:B:1484:LEU:HB3	1:B:1489:LYS:HE3	2.01	0.43
1:C:515:THR:OG1	1:C:516:TRP:N	2.52	0.43
1:C:715:THR:OG1	1:C:716:THR:N	2.52	0.43
1:C:799:PHE:CD1	1:C:1074:TYR:CE2	3.05	0.43
1:C:1038:ILE:CD1	1:D:938:LEU:HD11	2.45	0.43
1:D:796:VAL:O	1:D:799:PHE:HB3	2.18	0.43
1:A:150:PRO:O	1:A:153:VAL:HG12	2.18	0.42
1:A:572:PHE:CZ	1:A:723:GLU:HG3	2.54	0.42
1:A:1155:VAL:O	1:A:1159:VAL:HG23	2.19	0.42
1:B:515:THR:OG1	1:B:516:TRP:N	2.52	0.42
1:B:1355:TRP:HB3	1:B:1363:ILE:HG23	2.01	0.42
1:C:680:GLU:O	1:C:683:GLU:HG2	2.19	0.42
1:C:804:LEU:HA	1:C:804:LEU:HD13	1.86	0.42
1:D:1478:VAL:HG13	1:D:1502:HIS:NE2	2.33	0.42
1:A:382:LYS:HA	1:A:382:LYS:HD3	1.76	0.42
1:A:637:LEU:HD23	1:A:637:LEU:HA	1.67	0.42
1:B:789:ARG:HE	1:B:789:ARG:HB2	1.68	0.42
1:B:821:PHE:HE2	1:B:892:LEU:HD21	1.83	0.42
1:B:1060:ASP:OD1	1:B:1060:ASP:N	2.51	0.42
1:C:211:HIS:CD2	1:C:278:ASP:HA	2.54	0.42
1:D:735:ILE:O	1:D:738:PHE:N	2.52	0.42
1:D:1147:LYS:HE2	1:D:1147:LYS:HB2	1.84	0.42
1:D:1155:VAL:O	1:D:1159:VAL:HG23	2.19	0.42
1:A:456:LEU:HD12	1:A:456:LEU:HA	1.81	0.42
1:A:1141:LYS:HE2	1:A:1141:LYS:HB2	1.82	0.42
1:B:1426:LYS:HG3	1:B:1443:VAL:HA	2.02	0.42
1:C:477:TRP:HB3	1:C:479:TRP:HE3	1.84	0.42
1:C:515:THR:HA	1:C:617:PHE:CD1	2.54	0.42
1:C:719:GLN:O	1:C:723:GLU:HG2	2.20	0.42
1:C:1484:LEU:HB3	1:C:1489:LYS:HE3	2.01	0.42
1:D:211:HIS:CD2	1:D:278:ASP:HA	2.54	0.42
1:D:715:THR:OG1	1:D:716:THR:N	2.52	0.42
1:B:572:PHE:CZ	1:B:723:GLU:HG3	2.54	0.42
1:C:1053:GLN:NE2	1:D:1052:PHE:HE2	2.16	0.42
1:D:169:LEU:HB3	1:D:203:ALA:CB	2.50	0.42
1:D:197:VAL:HA	1:D:200:THR:HG22	2.00	0.42
1:D:376:ILE:H	1:D:376:ILE:HG13	1.59	0.42
1:D:718:LEU:HA	1:D:718:LEU:HD12	1.70	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:719:GLN:O	1:D:723:GLU:HG2	2.20	0.42
1:A:142:TYR:HA	1:A:284:PHE:O	2.18	0.42
1:A:244:TRP:CD1	1:A:288:ASP:HB2	2.55	0.42
1:A:380:GLN:O	1:A:384:SER:OG	2.17	0.42
1:A:1250:CYS:O	1:A:1252:VAL:N	2.46	0.42
1:A:1301:TYR:O	1:A:1302:ASN:ND2	2.52	0.42
1:A:1484:LEU:HB3	1:A:1489:LYS:HE3	2.01	0.42
1:B:211:HIS:CD2	1:B:278:ASP:HA	2.54	0.42
1:B:244:TRP:CD1	1:B:288:ASP:HB2	2.55	0.42
1:B:680:GLU:O	1:B:683:GLU:HG2	2.19	0.42
1:B:875:ALA:HB1	1:B:906:PHE:HE1	1.85	0.42
1:C:145:VAL:HG12	1:C:286:LEU:O	2.20	0.42
1:C:572:PHE:CZ	1:C:723:GLU:HG3	2.54	0.42
1:C:653:LEU:HA	1:C:653:LEU:HD23	1.51	0.42
1:C:1159:VAL:HG22	1:D:1158:MET:HE3	2.01	0.42
1:D:477:TRP:HB3	1:D:479:TRP:HE3	1.84	0.42
1:D:754:TRP:CD1	1:D:755:ARG:N	2.88	0.42
1:A:69:LYS:HE3	1:A:124:THR:HA	2.01	0.42
1:A:341:ASP:OD1	1:A:412:ARG:NH1	2.53	0.42
1:A:1434:ASN:HD22	1:A:1439:TRP:HA	1.83	0.42
1:A:1478:VAL:O	1:A:1502:HIS:NE2	2.52	0.42
1:B:477:TRP:HB3	1:B:479:TRP:HE3	1.84	0.42
1:B:1113:LEU:HD23	1:B:1113:LEU:HA	1.81	0.42
1:C:301:LEU:HD12	1:C:304:ARG:NH1	2.31	0.42
1:C:341:ASP:OD1	1:C:412:ARG:NH1	2.53	0.42
1:C:1478:VAL:O	1:C:1502:HIS:NE2	2.52	0.42
1:D:69:LYS:HE3	1:D:124:THR:HA	2.01	0.42
1:D:204:TRP:HD1	1:D:237:ILE:HD11	1.81	0.42
1:D:244:TRP:CD1	1:D:288:ASP:HB2	2.55	0.42
1:D:1301:TYR:O	1:D:1302:ASN:ND2	2.52	0.42
1:D:1484:LEU:HB3	1:D:1489:LYS:HE3	2.01	0.42
1:A:212:THR:OG1	1:A:213:GLY:N	2.53	0.42
1:A:492:LEU:HA	1:A:492:LEU:HD23	1.78	0.42
1:A:910:LEU:HA	1:A:910:LEU:HD12	1.78	0.42
1:B:557:GLN:OE1	1:B:558:MET:N	2.43	0.42
1:B:956:LEU:HA	1:B:956:LEU:HD23	1.80	0.42
1:B:1038:ILE:HG21	1:C:938:LEU:HD21	2.01	0.42
1:B:1271:TYR:HE1	1:B:1332:GLY:HA2	1.83	0.42
1:C:438:LEU:O	1:C:441:SER:OG	2.27	0.42
1:C:740:THR:O	1:C:743:TRP:N	2.53	0.42
1:C:1128:LEU:HD23	1:C:1128:LEU:HA	1.74	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:666:GLU:OE1	1:D:671:SER:OG	2.37	0.42
1:D:871:LEU:HD13	1:D:871:LEU:HA	1.88	0.42
1:A:477:TRP:HB3	1:A:479:TRP:HE3	1.84	0.42
1:A:735:ILE:O	1:A:738:PHE:N	2.52	0.42
1:B:145:VAL:HG12	1:B:286:LEU:O	2.20	0.42
1:B:212:THR:OG1	1:B:213:GLY:N	2.53	0.42
1:B:301:LEU:HD12	1:B:304:ARG:NH1	2.31	0.42
1:B:744:TRP:HB2	1:B:749:VAL:HG12	2.02	0.42
1:B:1067:ARG:O	1:B:1071:ILE:HG12	2.20	0.42
1:B:1301:TYR:O	1:B:1302:ASN:ND2	2.53	0.42
1:B:1358:ASN:OD1	1:B:1361:GLY:N	2.53	0.42
1:C:408:ASP:O	1:C:411:ARG:HB3	2.20	0.42
1:C:754:TRP:CD1	1:C:755:ARG:N	2.88	0.42
1:C:871:LEU:HD13	1:C:871:LEU:HA	1.88	0.42
1:C:1053:GLN:CD	1:D:1052:PHE:HE2	2.23	0.42
1:D:739:LEU:HD23	1:D:739:LEU:HA	1.74	0.42
1:D:740:THR:O	1:D:743:TRP:N	2.53	0.42
1:A:719:GLN:O	1:A:723:GLU:HG2	2.20	0.42
1:A:741:LYS:HE3	1:A:741:LYS:HB2	1.70	0.42
1:B:204:TRP:HD1	1:B:237:ILE:HD11	1.81	0.42
1:B:341:ASP:OD1	1:B:412:ARG:NH1	2.53	0.42
1:B:929:ARG:HB2	1:B:929:ARG:CZ	2.50	0.42
1:B:1073:GLU:O	1:B:1076:GLY:N	2.51	0.42
1:C:124:THR:HG22	1:C:126:ALA:N	2.34	0.42
1:C:574:GLN:HB3	1:C:575:PRO:HD2	2.02	0.42
1:C:875:ALA:HB1	1:C:906:PHE:HE1	1.85	0.42
1:C:1050:TYR:HA	1:D:1052:PHE:HZ	1.84	0.42
1:C:1358:ASN:OD1	1:C:1361:GLY:N	2.53	0.42
1:D:331:GLU:O	1:D:359:VAL:HG12	2.20	0.42
1:D:662:LEU:HA	1:D:662:LEU:HD12	1.80	0.42
1:D:1259:ASN:O	1:D:1262:VAL:HG12	2.20	0.42
1:D:1355:TRP:HB3	1:D:1363:ILE:HG23	2.01	0.42
1:A:408:ASP:O	1:A:411:ARG:HB3	2.20	0.42
1:B:69:LYS:HG2	1:B:124:THR:HA	2.02	0.42
1:B:659:LEU:HA	1:B:659:LEU:HD23	1.69	0.42
1:C:244:TRP:CD1	1:C:288:ASP:HB2	2.55	0.42
1:C:336:THR:OG1	1:C:359:VAL:HG11	2.20	0.42
1:C:937:PHE:CD2	1:C:1044:LEU:HD21	2.55	0.42
1:C:1385:TRP:HB2	1:C:1483:PRO:O	2.18	0.42
1:C:1426:LYS:HG3	1:C:1443:VAL:HA	2.01	0.42
1:C:1485:TYR:O	1:C:1489:LYS:NZ	2.43	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:69:LYS:HG2	1:D:124:THR:HA	2.02	0.42
1:D:336:THR:OG1	1:D:359:VAL:HG11	2.20	0.42
1:D:938:LEU:HA	1:D:941:LEU:CD2	2.50	0.42
1:D:1484:LEU:O	1:D:1489:LYS:NZ	2.39	0.42
1:A:211:HIS:CD2	1:A:278:ASP:HA	2.54	0.41
1:A:754:TRP:CD1	1:A:755:ARG:N	2.88	0.41
1:A:1067:ARG:O	1:A:1071:ILE:HG12	2.20	0.41
1:C:68:LYS:HB3	1:C:122:MET:N	2.35	0.41
1:C:1355:TRP:HB3	1:C:1363:ILE:HG23	2.01	0.41
1:D:660:LYS:HE3	1:D:660:LYS:HB2	1.95	0.41
1:D:929:ARG:CZ	1:D:929:ARG:HB2	2.50	0.41
1:A:69:LYS:HG2	1:A:124:THR:HA	2.02	0.41
1:A:420:ARG:HA	1:A:420:ARG:HD3	1.78	0.41
1:A:799:PHE:CD1	1:A:1074:TYR:CE2	3.05	0.41
1:A:956:LEU:HD23	1:A:956:LEU:HA	1.80	0.41
1:B:938:LEU:HA	1:B:941:LEU:CD2	2.50	0.41
1:C:127:PHE:O	1:C:142:TYR:OH	2.34	0.41
1:C:920:LEU:O	1:C:924:ILE:HD12	2.21	0.41
1:D:127:PHE:O	1:D:142:TYR:OH	2.34	0.41
1:D:341:ASP:OD1	1:D:412:ARG:NH1	2.53	0.41
1:D:741:LYS:HB2	1:D:741:LYS:HE3	1.71	0.41
1:A:929:ARG:CZ	1:A:929:ARG:HB2	2.50	0.41
1:A:1159:VAL:HG13	1:B:1158:MET:HE1	2.02	0.41
1:B:68:LYS:HB3	1:B:122:MET:N	2.35	0.41
1:B:485:HIS:O	1:B:489:THR:OG1	2.31	0.41
1:B:719:GLN:O	1:B:723:GLU:HG2	2.20	0.41
1:B:802:ASN:ND2	1:B:1074:TYR:OH	2.51	0.41
1:B:937:PHE:CD2	1:B:1044:LEU:HD21	2.55	0.41
1:C:331:GLU:O	1:C:359:VAL:HG12	2.20	0.41
1:C:956:LEU:HD23	1:C:956:LEU:HA	1.80	0.41
1:C:1250:CYS:O	1:C:1252:VAL:N	2.46	0.41
1:D:515:THR:OG1	1:D:516:TRP:N	2.52	0.41
1:A:197:VAL:HA	1:A:200:THR:HG22	2.00	0.41
1:A:331:GLU:O	1:A:359:VAL:HG12	2.20	0.41
1:A:715:THR:OG1	1:A:716:THR:N	2.52	0.41
1:A:904:ILE:HD13	1:A:904:ILE:HA	1.85	0.41
1:A:925:ILE:HD13	1:A:925:ILE:HA	1.83	0.41
1:A:1426:LYS:HG3	1:A:1443:VAL:HA	2.01	0.41
1:B:69:LYS:HE3	1:B:124:THR:HA	2.01	0.41
1:B:408:ASP:O	1:B:411:ARG:HB3	2.20	0.41
1:B:740:THR:O	1:B:743:TRP:N	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1141:LYS:HE2	1:B:1141:LYS:HB2	1.82	0.41
1:C:169:LEU:HB3	1:C:203:ALA:CB	2.50	0.41
1:C:212:THR:OG1	1:C:213:GLY:N	2.53	0.41
1:C:1067:ARG:O	1:C:1071:ILE:HG12	2.20	0.41
1:C:1301:TYR:O	1:C:1302:ASN:ND2	2.52	0.41
1:D:574:GLN:HB3	1:D:575:PRO:HD2	2.02	0.41
1:D:625:LEU:HD12	1:D:625:LEU:HA	1.62	0.41
1:D:1301:TYR:CD2	1:D:1319:VAL:HG22	2.49	0.41
1:D:1387:LEU:HG	1:D:1488:HIS:HB3	2.02	0.41
1:D:1446:SER:O	1:D:1446:SER:OG	2.33	0.41
1:A:267:ASP:OD1	1:A:267:ASP:N	2.53	0.41
1:A:515:THR:HA	1:A:617:PHE:HD1	1.85	0.41
1:A:653:LEU:HD23	1:A:653:LEU:HA	1.51	0.41
1:A:740:THR:O	1:A:743:TRP:N	2.53	0.41
1:A:920:LEU:O	1:A:924:ILE:HD12	2.21	0.41
1:B:574:GLN:HB3	1:B:575:PRO:HD2	2.02	0.41
1:B:719:GLN:O	1:B:722:LEU:N	2.54	0.41
1:B:739:LEU:O	1:B:742:VAL:N	2.51	0.41
1:C:69:LYS:HG2	1:C:124:THR:HA	2.02	0.41
1:C:513:PHE:O	1:C:515:THR:N	2.54	0.41
1:C:929:ARG:HB2	1:C:929:ARG:CZ	2.50	0.41
1:C:1387:LEU:HG	1:C:1488:HIS:HB3	2.02	0.41
1:D:881:ALA:O	1:D:884:THR:HG22	2.21	0.41
1:D:1067:ARG:O	1:D:1071:ILE:HG12	2.20	0.41
1:D:1358:ASN:OD1	1:D:1361:GLY:N	2.53	0.41
1:D:1426:LYS:HG3	1:D:1443:VAL:HA	2.01	0.41
1:A:169:LEU:HB3	1:A:203:ALA:CB	2.50	0.41
1:A:247:VAL:O	1:A:274:LEU:HD12	2.21	0.41
1:A:937:PHE:CD2	1:A:1044:LEU:HD21	2.55	0.41
1:A:1259:ASN:O	1:A:1262:VAL:HG12	2.20	0.41
1:B:336:THR:OG1	1:B:359:VAL:HG11	2.20	0.41
1:B:754:TRP:CD1	1:B:755:ARG:N	2.88	0.41
1:C:69:LYS:HE3	1:C:124:THR:HA	2.01	0.41
1:C:420:ARG:HD3	1:C:420:ARG:HA	1.78	0.41
1:C:899:LEU:HA	1:C:899:LEU:HD13	1.75	0.41
1:C:1073:GLU:O	1:C:1076:GLY:N	2.51	0.41
1:C:1453:ASN:OD1	1:C:1453:ASN:N	2.53	0.41
1:D:568:LEU:HD23	1:D:568:LEU:HA	1.63	0.41
1:D:744:TRP:HB2	1:D:749:VAL:HG12	2.02	0.41
1:D:937:PHE:CD2	1:D:1044:LEU:HD21	2.55	0.41
1:D:1378:LYS:HA	1:D:1378:LYS:HD2	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:1426:LYS:HB2	1:D:1426:LYS:HE2	1.80	0.41
1:A:574:GLN:HB3	1:A:575:PRO:HD2	2.02	0.41
1:B:741:LYS:HB2	1:B:741:LYS:HE3	1.71	0.41
1:B:899:LEU:HD13	1:B:899:LEU:HA	1.75	0.41
1:C:938:LEU:HA	1:C:941:LEU:CD2	2.50	0.41
1:C:1034:LEU:O	1:C:1038:ILE:HB	2.21	0.41
1:D:68:LYS:HB3	1:D:122:MET:N	2.35	0.41
1:D:212:THR:OG1	1:D:213:GLY:N	2.53	0.41
1:D:348:THR:HA	1:D:349:PRO:HD3	1.87	0.41
1:D:920:LEU:O	1:D:923:LYS:N	2.50	0.41
1:A:1442:THR:OG1	1:A:1443:VAL:N	2.54	0.41
1:B:1478:VAL:O	1:B:1502:HIS:NE2	2.52	0.41
1:C:130:ILE:HG22	1:C:140:LYS:O	2.21	0.41
1:C:739:LEU:O	1:C:742:VAL:N	2.51	0.41
1:C:1162:LEU:CG	1:D:1161:LEU:HD22	2.50	0.41
1:C:1259:ASN:O	1:C:1262:VAL:HG12	2.20	0.41
1:C:1262:VAL:CG1	1:C:1263:PRO:HD3	2.51	0.41
1:D:135:LEU:HD23	1:D:135:LEU:HA	1.89	0.41
1:D:145:VAL:HG12	1:D:286:LEU:O	2.20	0.41
1:D:1122:LEU:HD23	1:D:1122:LEU:HA	1.86	0.41
1:A:68:LYS:HB3	1:A:122:MET:N	2.35	0.41
1:A:196:LYS:HE2	1:A:196:LYS:HB3	1.85	0.41
1:A:881:ALA:O	1:A:884:THR:HG22	2.21	0.41
1:A:938:LEU:HA	1:A:941:LEU:CD2	2.50	0.41
1:A:1034:LEU:O	1:A:1038:ILE:HB	2.21	0.41
1:A:1358:ASN:OD1	1:A:1361:GLY:N	2.53	0.41
1:A:1387:LEU:HG	1:A:1488:HIS:HB3	2.02	0.41
1:A:1425:TYR:O	1:A:1426:LYS:HD3	2.21	0.41
1:A:1453:ASN:OD1	1:A:1453:ASN:N	2.53	0.41
1:B:267:ASP:N	1:B:267:ASP:OD1	2.53	0.41
1:B:323:ILE:H	1:B:323:ILE:HG13	1.70	0.41
1:B:438:LEU:O	1:B:441:SER:OG	2.27	0.41
1:B:1147:LYS:HE2	1:B:1147:LYS:HB2	1.84	0.41
1:B:1375:LEU:HD23	1:B:1376:VAL:N	2.36	0.41
1:C:240:GLY:N	1:C:283:HIS:O	2.44	0.41
1:C:267:ASP:N	1:C:267:ASP:OD1	2.53	0.41
1:C:803:ILE:HA	1:C:803:ILE:HD12	1.84	0.41
1:C:867:PHE:CG	1:C:928:LYS:HE3	2.56	0.41
1:C:881:ALA:O	1:C:884:THR:HG22	2.21	0.41
1:C:910:LEU:HD12	1:C:910:LEU:HA	1.78	0.41
1:C:1426:LYS:HE2	1:C:1426:LYS:HB2	1.80	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:D:130:ILE:HG22	1:D:140:LYS:O	2.21	0.41
1:D:408:ASP:O	1:D:411:ARG:HB3	2.20	0.41
1:D:504:LEU:HD23	1:D:504:LEU:HA	1.86	0.41
1:D:630:ILE:HD13	1:D:630:ILE:HA	1.87	0.41
1:D:802:ASN:ND2	1:D:1074:TYR:OH	2.51	0.41
1:D:910:LEU:HA	1:D:910:LEU:HD12	1.78	0.41
1:D:1262:VAL:CG1	1:D:1263:PRO:HD3	2.51	0.41
1:A:625:LEU:HD12	1:A:625:LEU:HA	1.63	0.41
1:A:744:TRP:HB2	1:A:749:VAL:HG12	2.02	0.41
1:A:1262:VAL:CG1	1:A:1263:PRO:HD3	2.51	0.41
1:B:481:PRO:HA	1:B:484:LEU:HD13	2.03	0.41
1:B:1442:THR:OG1	1:B:1443:VAL:N	2.54	0.41
1:C:247:VAL:O	1:C:274:LEU:HD12	2.21	0.41
1:C:380:GLN:O	1:C:384:SER:OG	2.17	0.41
1:C:741:LYS:HB2	1:C:741:LYS:HE3	1.70	0.41
1:C:1045:ILE:HD13	1:D:1048:PHE:CD2	2.55	0.41
1:D:301:LEU:HD12	1:D:304:ARG:NH1	2.31	0.41
1:D:1034:LEU:O	1:D:1038:ILE:HB	2.21	0.41
1:D:1264:TRP:NE1	1:D:1326:ASN:O	2.43	0.41
1:A:145:VAL:HG12	1:A:286:LEU:O	2.20	0.40
1:A:238:THR:H	1:A:282:SER:HB3	1.86	0.40
1:A:719:GLN:O	1:A:722:LEU:N	2.54	0.40
1:A:867:PHE:CG	1:A:928:LYS:HE3	2.56	0.40
1:A:1060:ASP:OD1	1:A:1060:ASP:N	2.51	0.40
1:B:130:ILE:HG22	1:B:140:LYS:O	2.21	0.40
1:B:331:GLU:O	1:B:359:VAL:HG12	2.20	0.40
1:B:1425:TYR:O	1:B:1426:LYS:HD3	2.21	0.40
1:C:481:PRO:HA	1:C:484:LEU:HD13	2.03	0.40
1:C:569:LEU:HD12	1:C:569:LEU:HA	1.92	0.40
1:C:1121:LEU:HD12	1:C:1121:LEU:HA	1.69	0.40
1:D:267:ASP:N	1:D:267:ASP:OD1	2.53	0.40
1:D:515:THR:HA	1:D:617:PHE:HD1	1.85	0.40
1:D:702:GLN:OE1	1:D:738:PHE:HB2	2.21	0.40
1:D:1431:ASP:OD1	1:D:1432:PRO:HD2	2.21	0.40
1:D:1453:ASN:OD1	1:D:1453:ASN:N	2.53	0.40
1:A:336:THR:OG1	1:A:359:VAL:HG11	2.20	0.40
1:A:418:VAL:HG22	1:A:419:PHE:N	2.36	0.40
1:A:450:GLU:HA	1:A:453:ASP:OD2	2.22	0.40
1:A:1266:THR:O	1:A:1330:ARG:NH2	2.51	0.40
1:A:1348:LEU:HD12	1:A:1349:TYR:N	2.37	0.40
1:A:1390:GLY:HA3	1:A:1402:LEU:N	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:124:THR:HG22	1:B:126:ALA:N	2.34	0.40
1:B:132:PHE:HB3	1:B:135:LEU:HB2	2.03	0.40
1:B:169:LEU:HB3	1:B:203:ALA:CB	2.50	0.40
1:B:247:VAL:O	1:B:274:LEU:HD12	2.21	0.40
1:B:515:THR:HA	1:B:617:PHE:HD1	1.85	0.40
1:B:912:HIS:O	1:B:915:THR:OG1	2.33	0.40
1:B:920:LEU:O	1:B:924:ILE:HD12	2.21	0.40
1:B:1259:ASN:O	1:B:1262:VAL:HG12	2.20	0.40
1:B:1351:MET:SD	1:B:1495:ALA:HB2	2.62	0.40
1:B:1390:GLY:HA3	1:B:1402:LEU:N	2.36	0.40
1:C:62:TRP:CZ3	1:C:157:LEU:HB2	2.56	0.40
1:C:238:THR:H	1:C:282:SER:HB3	1.86	0.40
1:C:322:LYS:HB3	1:C:322:LYS:HE3	1.86	0.40
1:C:663:SER:O	1:C:663:SER:OG	2.36	0.40
1:C:702:GLN:OE1	1:C:738:PHE:HB2	2.21	0.40
1:C:744:TRP:HB2	1:C:749:VAL:HG12	2.02	0.40
1:C:754:TRP:O	1:C:757:THR:OG1	2.31	0.40
1:C:1133:LEU:HD23	1:C:1133:LEU:HA	1.93	0.40
1:C:1351:MET:SD	1:C:1495:ALA:HB2	2.62	0.40
1:C:1431:ASP:OD1	1:C:1432:PRO:HD2	2.21	0.40
1:D:450:GLU:HA	1:D:453:ASP:OD2	2.21	0.40
1:D:513:PHE:O	1:D:515:THR:N	2.54	0.40
1:D:747:LEU:H	1:D:747:LEU:HG	1.73	0.40
1:D:1113:LEU:HD23	1:D:1113:LEU:HA	1.81	0.40
1:D:1351:MET:SD	1:D:1495:ALA:HB2	2.62	0.40
1:D:1425:TYR:O	1:D:1426:LYS:HD3	2.21	0.40
1:A:62:TRP:CZ3	1:A:157:LEU:HB2	2.56	0.40
1:A:513:PHE:O	1:A:515:THR:N	2.54	0.40
1:A:630:ILE:HD13	1:A:630:ILE:HA	1.87	0.40
1:A:742:VAL:O	1:A:745:GLY:N	2.41	0.40
1:A:804:LEU:HA	1:A:804:LEU:HD13	1.86	0.40
1:B:715:THR:OG1	1:B:716:THR:N	2.52	0.40
1:B:1245:LEU:HD23	1:B:1246:LEU:HB2	2.03	0.40
1:C:382:LYS:HA	1:C:382:LYS:HD3	1.76	0.40
1:C:719:GLN:O	1:C:722:LEU:N	2.54	0.40
1:C:1141:LYS:HE2	1:C:1141:LYS:HB2	1.82	0.40
1:D:418:VAL:HG22	1:D:419:PHE:N	2.36	0.40
1:D:420:ARG:HA	1:D:420:ARG:HD3	1.78	0.40
1:D:481:PRO:HA	1:D:484:LEU:HD13	2.03	0.40
1:D:1478:VAL:O	1:D:1502:HIS:NE2	2.52	0.40
1:A:156:HIS:CD2	1:A:160:GLN:HG3	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:875:ALA:HB1	1:A:906:PHE:HE1	1.85	0.40
1:A:1053:GLN:NE2	1:B:1052:PHE:HE2	2.20	0.40
1:A:1354:ARG:HD3	1:A:1475:TRP:CZ2	2.57	0.40
1:B:156:HIS:CD2	1:B:160:GLN:HG3	2.56	0.40
1:B:418:VAL:HG22	1:B:419:PHE:N	2.36	0.40
1:B:867:PHE:CG	1:B:928:LYS:HE3	2.56	0.40
1:B:1034:LEU:O	1:B:1038:ILE:HB	2.21	0.40
1:B:1301:TYR:CD2	1:B:1319:VAL:HG22	2.49	0.40
1:C:164:LEU:HD23	1:C:164:LEU:HA	1.80	0.40
1:D:156:HIS:CD2	1:D:160:GLN:HG3	2.56	0.40
1:D:238:THR:H	1:D:282:SER:HB3	1.86	0.40
1:D:247:VAL:O	1:D:274:LEU:HD12	2.21	0.40
1:D:735:ILE:HG12	1:D:735:ILE:H	1.63	0.40
1:D:920:LEU:O	1:D:924:ILE:HD12	2.21	0.40
1:D:1348:LEU:HD12	1:D:1349:TYR:N	2.36	0.40
1:A:735:ILE:HG12	1:A:735:ILE:H	1.63	0.40
1:A:813:PHE:CE2	1:A:903:PHE:CD2	3.05	0.40
1:A:1245:LEU:HD23	1:A:1246:LEU:HB2	2.03	0.40
1:A:1431:ASP:OD2	1:A:1433:ARG:N	2.34	0.40
1:B:187:LYS:HE3	1:B:187:LYS:HB2	1.88	0.40
1:B:1387:LEU:HG	1:B:1488:HIS:HB3	2.02	0.40
1:B:1453:ASN:OD1	1:B:1453:ASN:N	2.53	0.40
1:C:132:PHE:HB3	1:C:135:LEU:HB2	2.03	0.40
1:C:156:HIS:CD2	1:C:160:GLN:HG3	2.56	0.40
1:C:191:ARG:NH2	1:C:220:GLU:HB3	2.37	0.40
1:C:418:VAL:HG22	1:C:419:PHE:N	2.36	0.40
1:D:62:TRP:CZ3	1:D:157:LEU:HB2	2.56	0.40
1:D:1442:THR:OG1	1:D:1443:VAL:N	2.54	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	1292/1503 (86%)	1107 (86%)	185 (14%)	0	100	100
1	B	1292/1503 (86%)	1106 (86%)	186 (14%)	0	100	100
1	C	1292/1503 (86%)	1107 (86%)	185 (14%)	0	100	100
1	D	1292/1503 (86%)	1106 (86%)	186 (14%)	0	100	100
All	All	5168/6012 (86%)	4426 (86%)	742 (14%)	0	100	100

There are no Ramachandran outliers to report.

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	855/1318 (65%)	846 (99%)	9 (1%)	73	85
1	B	855/1318 (65%)	847 (99%)	8 (1%)	78	88
1	C	855/1318 (65%)	846 (99%)	9 (1%)	73	85
1	D	855/1318 (65%)	846 (99%)	9 (1%)	73	85
All	All	3420/5272 (65%)	3385 (99%)	35 (1%)	77	86

All (35) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	223	ARG
1	A	400	VAL
1	A	412	ARG
1	A	431	VAL
1	A	616	THR
1	A	624	ASP
1	A	707	ARG
1	A	939	PHE
1	A	1451	ASP
1	B	223	ARG
1	B	400	VAL
1	B	412	ARG
1	B	431	VAL

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Mol	Chain	Res	Type
1	B	624	ASP
1	B	707	ARG
1	B	939	PHE
1	B	1451	ASP
1	C	223	ARG
1	C	400	VAL
1	C	412	ARG
1	C	431	VAL
1	C	616	THR
1	C	624	ASP
1	C	707	ARG
1	C	939	PHE
1	C	1451	ASP
1	D	223	ARG
1	D	400	VAL
1	D	412	ARG
1	D	431	VAL
1	D	616	THR
1	D	624	ASP
1	D	707	ARG
1	D	939	PHE
1	D	1451	ASP

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (54) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	156	HIS
1	A	381	GLN
1	A	463	ASN
1	A	537	GLN
1	A	574	GLN
1	A	732	HIS
1	A	846	GLN
1	A	1042	ASN
1	A	1068	HIS
1	A	1089	HIS
1	A	1139	GLN
1	A	1302	ASN
1	A	1452	GLN
1	B	156	HIS
1	B	381	GLN
1	B	463	ASN

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Mol	Chain	Res	Type
1	B	537	GLN
1	B	574	GLN
1	B	732	HIS
1	B	846	GLN
1	B	1042	ASN
1	B	1068	HIS
1	B	1089	HIS
1	B	1139	GLN
1	B	1302	ASN
1	B	1452	GLN
1	C	156	HIS
1	C	381	GLN
1	C	463	ASN
1	C	537	GLN
1	C	574	GLN
1	C	732	HIS
1	C	846	GLN
1	C	1042	ASN
1	C	1068	HIS
1	C	1089	HIS
1	C	1139	GLN
1	C	1302	ASN
1	C	1450	GLN
1	C	1452	GLN
1	D	156	HIS
1	D	381	GLN
1	D	463	ASN
1	D	537	GLN
1	D	574	GLN
1	D	732	HIS
1	D	846	GLN
1	D	1042	ASN
1	D	1068	HIS
1	D	1089	HIS
1	D	1139	GLN
1	D	1302	ASN
1	D	1450	GLN
1	D	1452	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

5.4 Non-standard residues in protein, DNA, RNA chains (i)

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

5.5 Carbohydrates (i)

There are no monosaccharides in this entry.

5.6 Ligand geometry (i)

There are no ligands in this entry.

5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

There are no chain breaks in this entry.

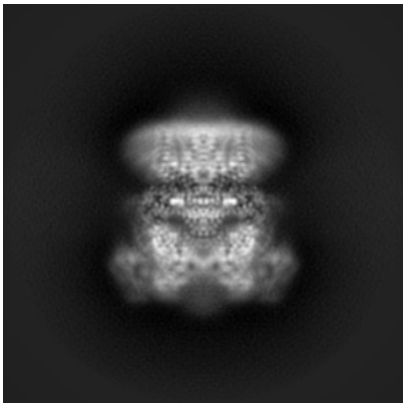
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-32082. These allow visual inspection of the internal detail of the map and identification of artifacts.

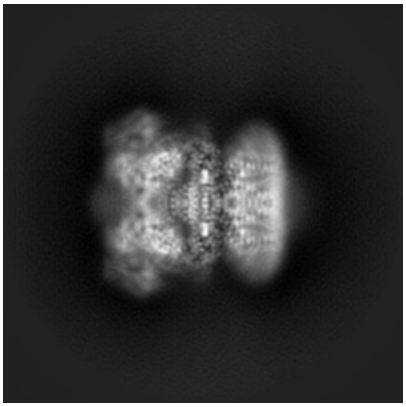
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

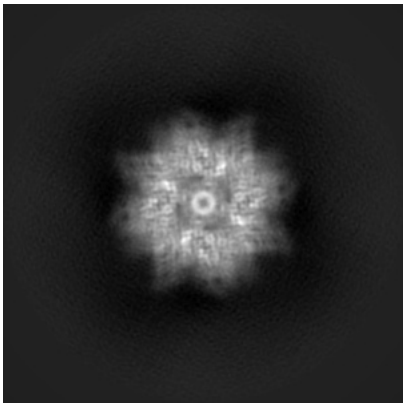
6.1.1 Primary map



X



Y

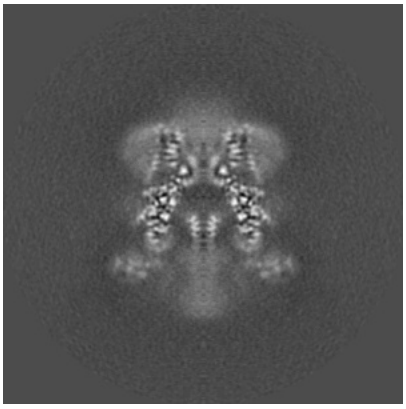


Z

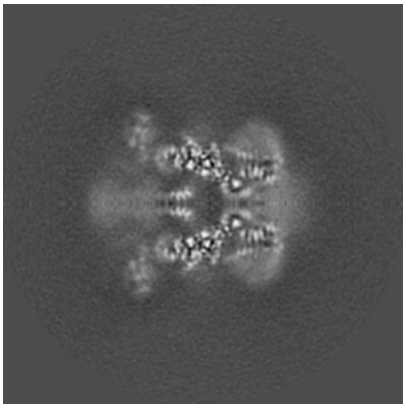
The images above show the map projected in three orthogonal directions.

6.2 Central slices

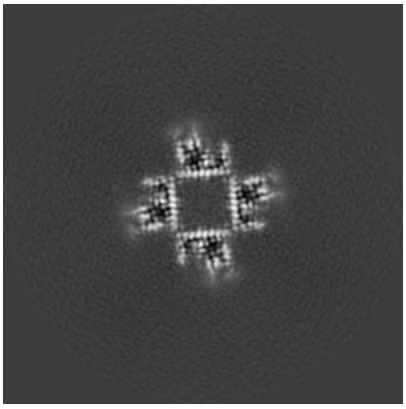
6.2.1 Primary map



X Index: 200



Y Index: 200

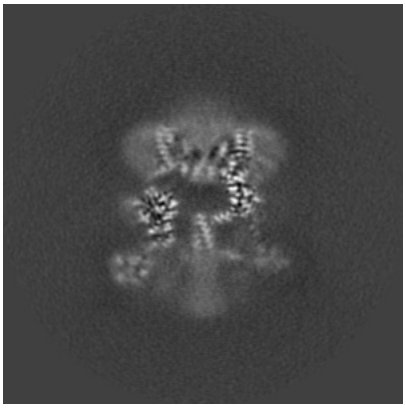


Z Index: 200

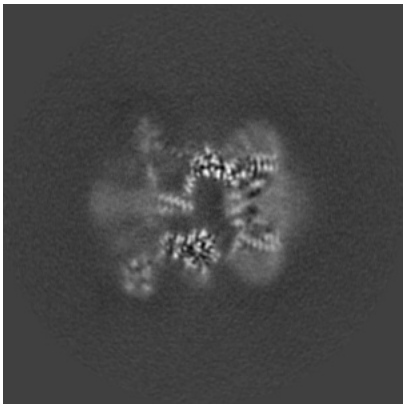
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

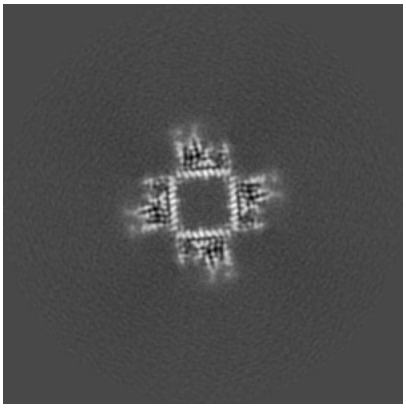
6.3.1 Primary map



X Index: 208



Y Index: 192

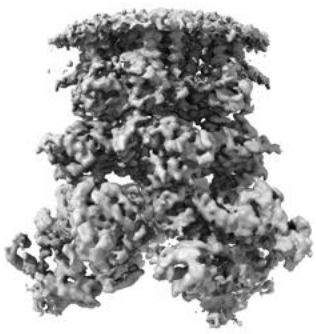


Z Index: 202

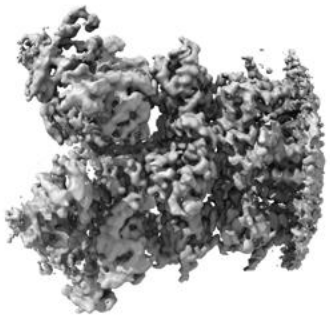
The images above show the largest variance slices of the map in three orthogonal directions.

6.4 Orthogonal surface views (i)

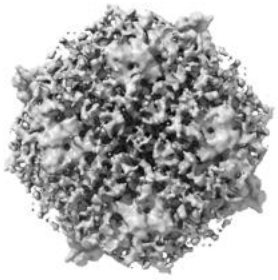
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0022. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

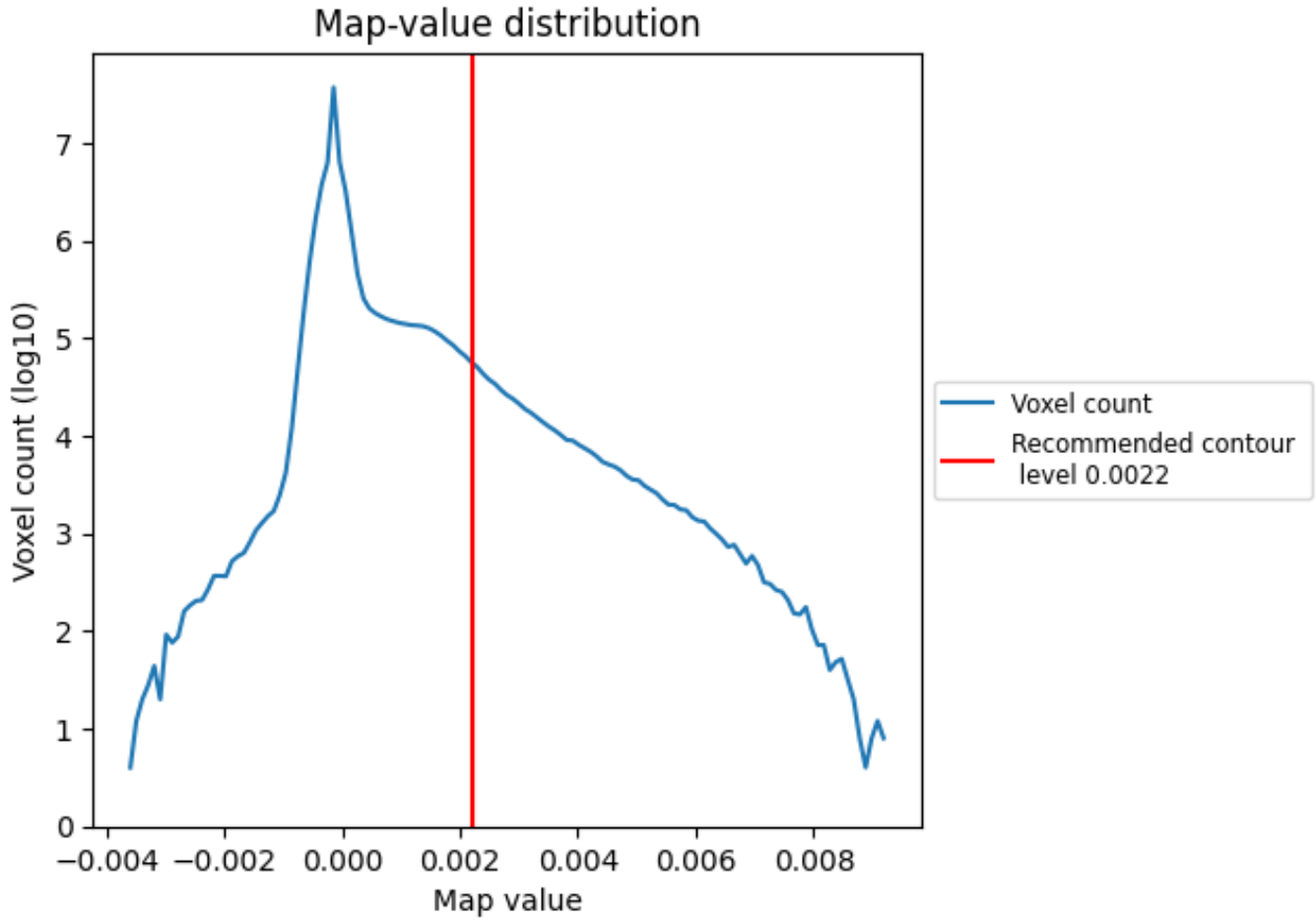
6.5 Mask visualisation (i)

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

7 Map analysis

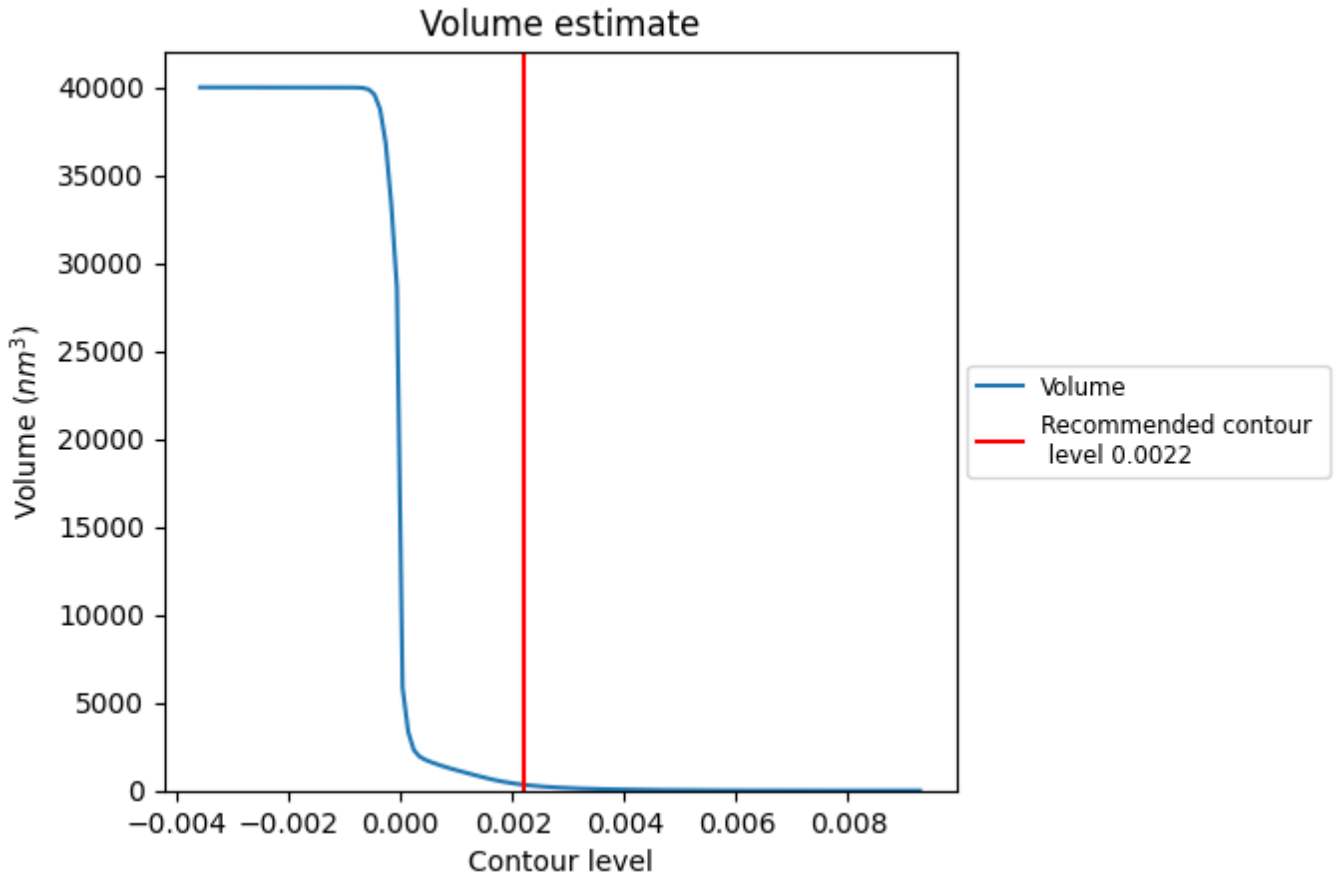
This section contains the results of statistical analysis of the map.

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.

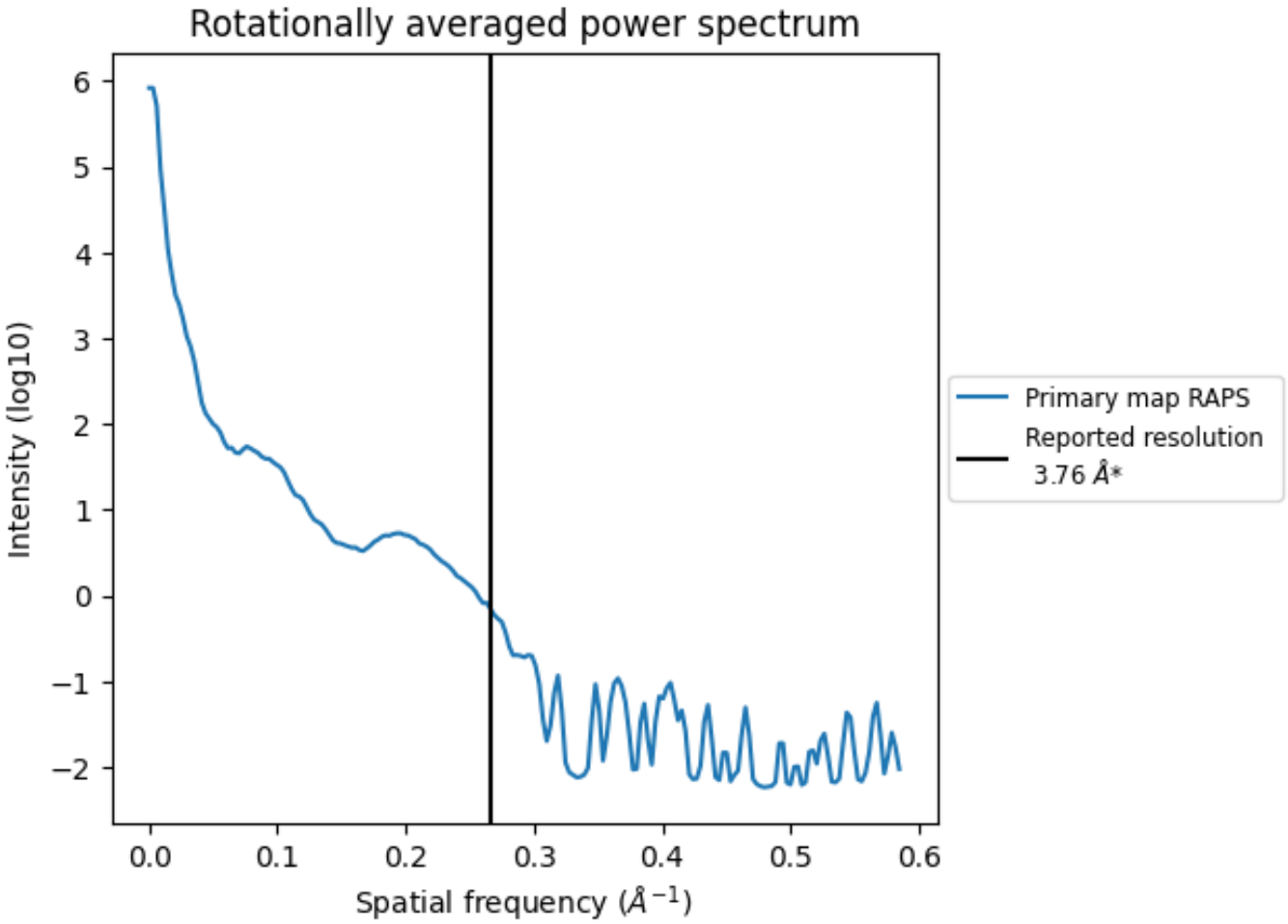
7.2 Volume estimate



The volume at the recommended contour level is 330 nm^3; this corresponds to an approximate mass of 298 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 0.266 Å^{-1}

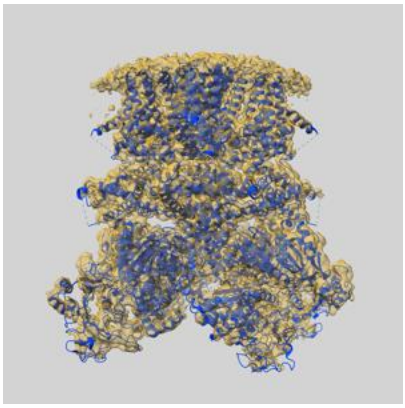
8 Fourier-Shell correlation (i)

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

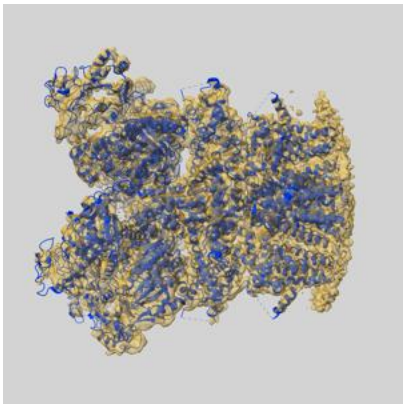
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-32082 and PDB model 7VQ1. Per-residue inclusion information can be found in section 3 on page 4.

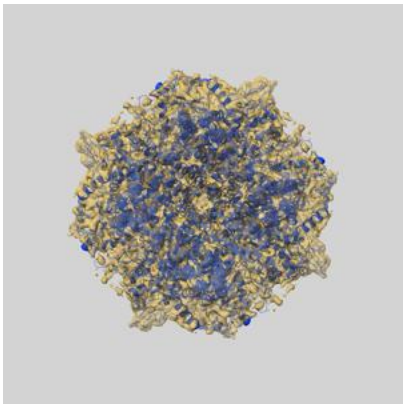
9.1 Map-model overlay



X



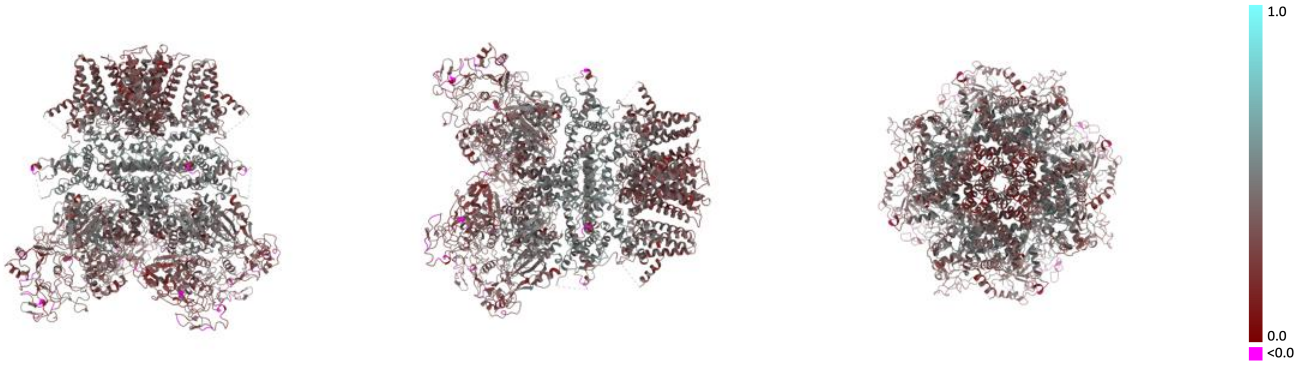
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0022 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

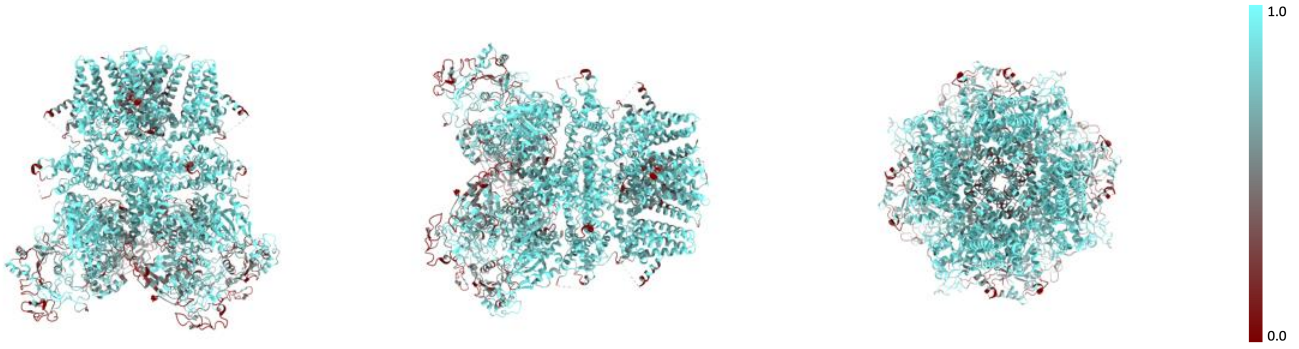
9.2 Q-score mapped to coordinate model (i)



X Y Z

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

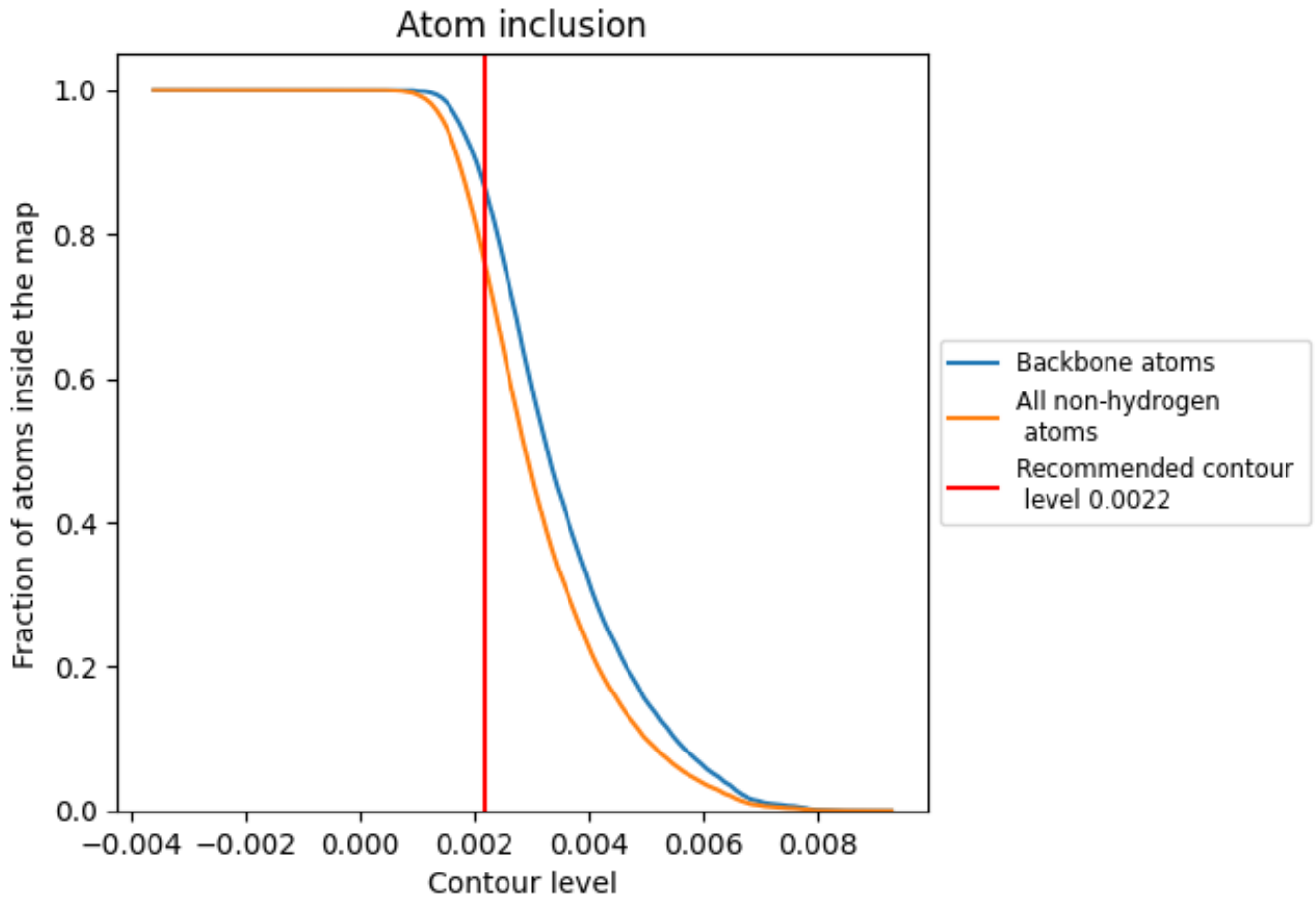
9.3 Atom inclusion mapped to coordinate model (i)



X Y Z

The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.0022).

9.4 Atom inclusion (i)



At the recommended contour level, 86% of all backbone atoms, 75% 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 (0.0022) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.7537	0.3830
A	0.7536	0.3830
B	0.7531	0.3820
C	0.7536	0.3830
D	0.7547	0.3830