Full wwPDB EM Validation Report ⓘ

Mar 24, 2026 – 11:38 PM UTC

PDB ID	:	9J9F / pdb_00009j9f
EMDB ID	:	EMD-61270
Title	:	Bovine ABCC1 conformation 1
Authors	:	Zhong, C.; Wang, F.; Liu, Z.; Yu, G.
Deposited on	:	2024-08-22
Resolution	:	3.13 Å(reported)

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

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

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

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

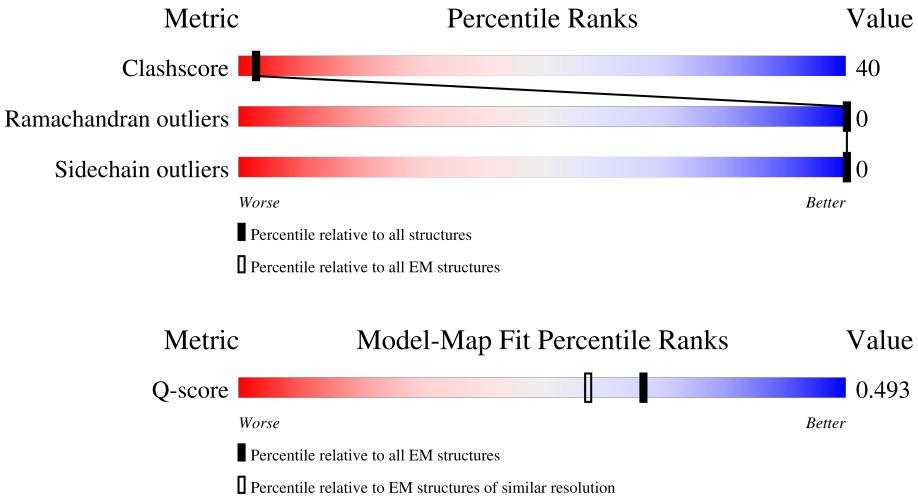
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data in the EMDB archive up until May 2025)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.13 Å.

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



Metric	Whole archive (#Entries)	EM structures (#Entries)	Similar EM resolution (#Entries, resolution range(Å))
Clashscore	229148	23984	-
Ramachandran outliers	224038	23583	-
Sidechain outliers	223484	23102	-
Q-score	-	25397	14478 (2.63 - 3.63)

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	1530	20% 46% 45% 8%

2 Entry composition

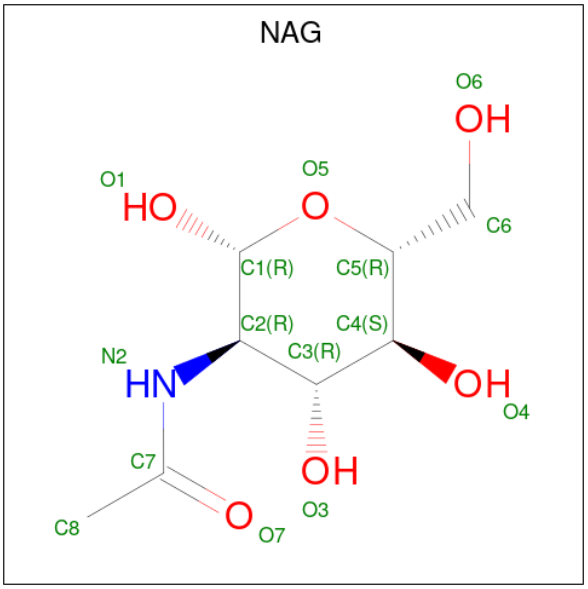
There are 2 unique types of molecules in this entry. The entry contains 10487 atoms, of which 0 are hydrogens and 0 are deuteriums.

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 Multidrug resistance-associated protein 1.

Mol	Chain	Residues	Atoms					AltConf	Trace
			Total	C	N	O	S		
1	A	1400	10473	6779	1759	1883	52	0	0

- Molecule 2 is 2-acetamido-2-deoxy-beta-D-glucopyranose (CCD ID: NAG) (formula: $C_8H_{15}NO_6$).



Mol	Chain	Residues	Atoms				AltConf
			Total	C	N	O	
2	A	1	14	8	1	5	0

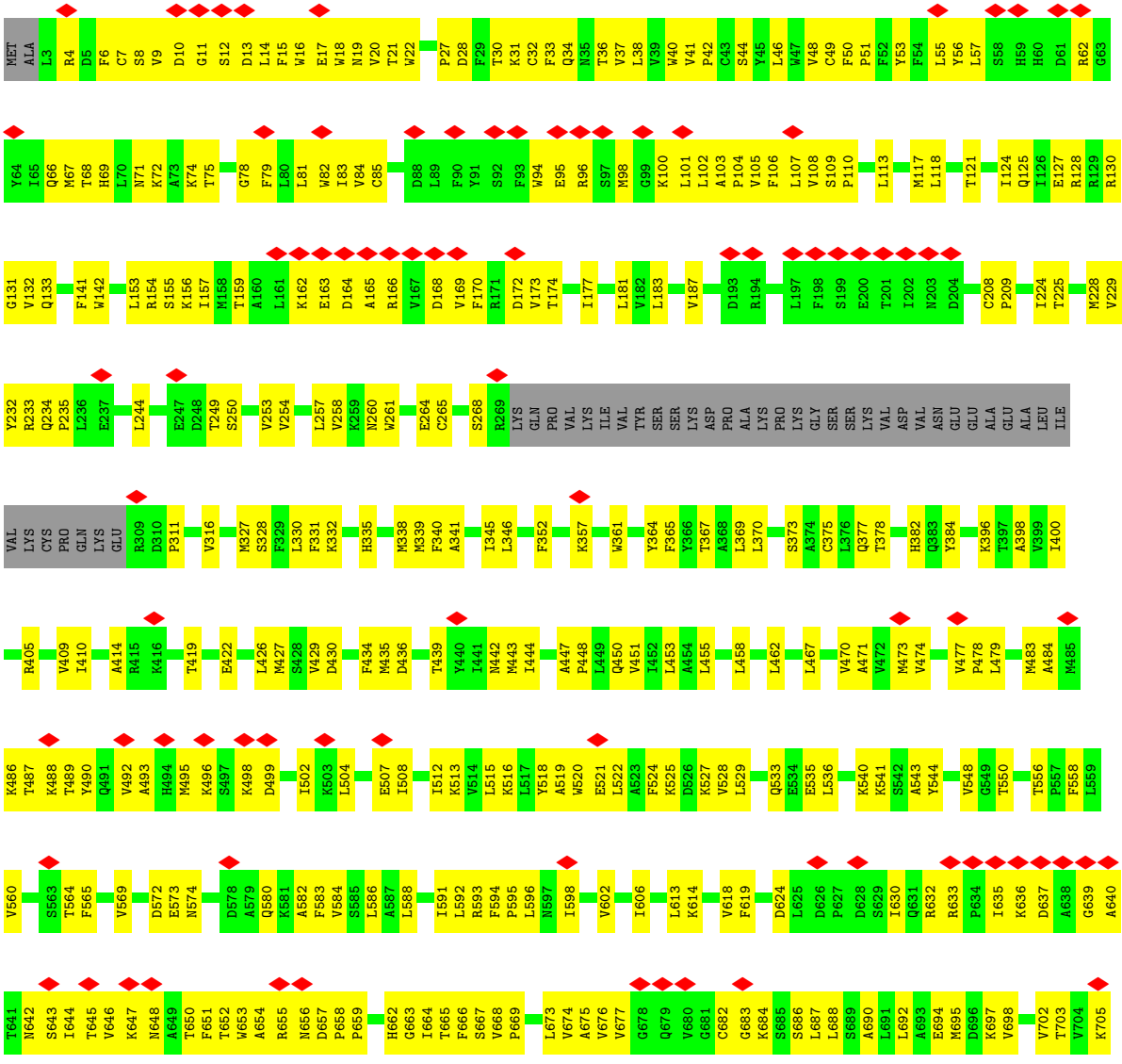
3 Residue-property plots (i)

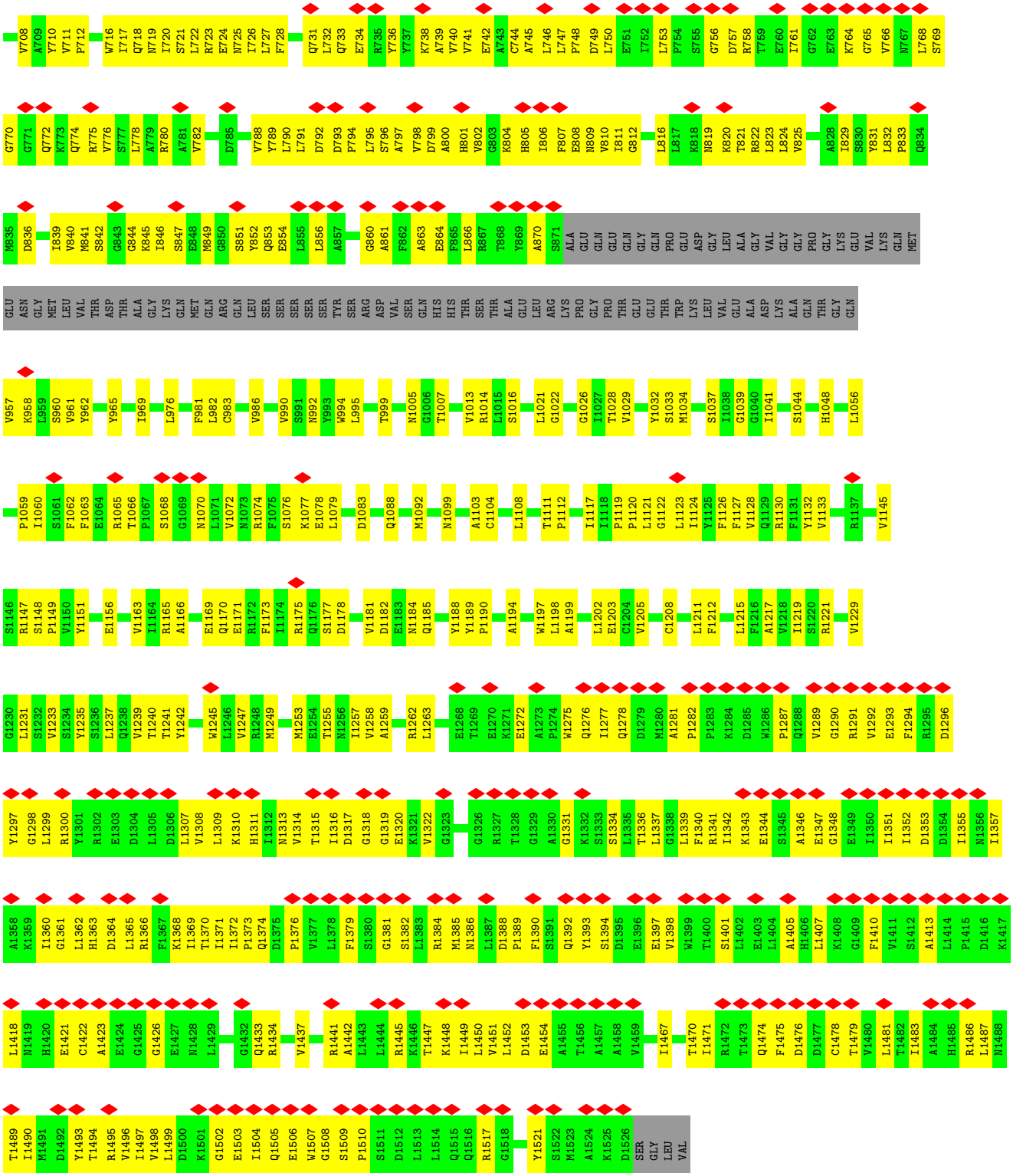
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion in map density. Residues are color-coded according to the number of geometric quality criteria for which they contain at least one outlier: green = 0, yellow = 1, orange = 2 and red = 3 or more. A red diamond above a residue indicates a poor fit to the EM map for this residue (all-atom inclusion < 40%). Stretches of 2 or more consecutive residues without any outlier are shown as a green connector. Residues present in the sample, but not in the model, are shown in grey.

• Molecule 1: Multidrug resistance-associated protein 1

Chain A:






V708 A709 Y710 V711 P712 W716 I717 Q718 N719 I720 S721 L722 R723 E724 N725 I726 L727 F728 Q731 L732 Q733 E734 R735 Y736 Y737 K738 A739 V740 V741 E742 A743 C744 A745 L746 L747 P748 D749 L750 E751 I752 L753 P754 S755 G756 D757 R758 T759 E760 I761 G762 E763 K764 G765 V766 N767 L768 S769
G770 G771 Q772 K773 Q774 R775 V776 S777 L778 A779 R780 A781 V782 D785 V788 Y789 L790 L791 D792 D793 P794 L795 S796 A797 V798 D799 A800 H801 V802 Q803 K804 H805 I806 F807 E808 N809 V810 I811 G812 L816 L817 K818 N819 K820 T821 R822 L823 L824 V825 A828 I829 S830 Y831 L832 P833 Q834
M835 D836 I839 V840 M841 S842 G843 G844 K845 I846 S847 E848 M849 G850 S851 Y852 Q853 E854 L855 L856 A857 G860 A861 F862 A863 E864 F865 L866 R867 T868 Y869 A870 S871 ALA GLU GLN GLU GLN GLY GLN PRO GLU ASP GLY LEU ALA GLY VAL GLY GLY PRO GLY LYS GLU VAL LYS GLN MET
GLU ASN GLY MET LEU VAL THR ASP THR ALA GLY LYS GLN MET GLN ARG GLN LEU SER SER SER SER SER TYR SER ARG ASP VAL SER GLN HIS HIS THR SER THR ALA GLU LEU ARG LYS PRO GLY PRO THR GLU GLU THR TRP LYS LEU VAL GLU ALA ASP LYS ALA GLN THR GLY GLN
V957 K958 L959 S960 V961 Y962 Y965 I969 L976 F981 L982 C983 V986 V990 S991 N992 Y993 W994 L995 T999 N1005 G1006 T1007 V1013 R1014 L1015 S1016 L1021 G1022 G1026 I1027 T1028 V1029 Y1032 S1033 M1034 S1037 I1038 G1039 G1040 I1041 S1044 H1048 L1056
P1059 I1060 S1061 F1062 F1063 E1064 R1065 T1066 P1067 S1068 G1069 N1070 L1071 V1072 N1073 R1074 F1075 S1076 K1077 E1078 L1079 D1083 Q1088 M1092 N1099 A1103 C1104 L1108 T1111 P1112 I1117 I1118 P1119 P1120 L1121 G1122 L1123 I1124 Y1125 F1126 F1127 V1128 Q1129 R1130 F1131 Y1132 V1133 R1137 V1145
S1146 R1147 S1148 P1149 V1150 Y1151 E1156 V1163 I1164 R1165 A1166 E1169 Q1170 E1171 R1172 F1173 I1174 R1175 Q1176 S1177 D1178 V1181 D1182 E1183 N1184 Q1185 Y1188 Y1189 P1190 A1194 W1197 L1198 A1199 L1202 E1203 C1204 V1205 C1208 L1211 F1212 L1215 F1216 A1217 V1218 I1219 S1220 R1221 V1229
G1230 L1231 S1232 V1233 S1234 Y1235 S1236 L1237 Q1238 V1239 T1240 T1241 Y1242 W1245 L1246 V1247 R1248 M1249 M1253 E1254 T1255 N1256 I1257 V1258 A1259 R1262 L1263 E1268 T1269 E1270 K1271 E1272 A1273 P1274 W1275 Q1276 I1277 Q1278 D1279 M1280 A1281 P1282 P1283 K1284 D1285 W1286 P1287 Q1288 V1289 G1290 R1291 V1292 E1293 F1294 R1295 D1296
Y1297 G1298 L1299 R1300 Y1301 R1302 E1303 D1304 L1305 D1306 L1307 V1308 L1309 K1310 H1311 I1312 N1313 V1314 T1315 I1316 D1317 G1318 G1319 E1320 K1321 V1322 G1323 G1326 R1327 T1328 G1329 A1330 G1331 K1332 S1333 S1334 L1335 T1336 L1337 G1338 L1339 F1340 R1341 I1342 K1343 E1344 S1345 A1346 E1347 G1348 E1349 I1350 T1351 I1352 D1353 D1354 I1355 N1356 I1357
A1358 K1359 I1360 G1361 L1362 H1363 D1364 L1365 R1366 F1367 K1368 I1369 T1370 I1371 I1372 P1373 Q1374 D1375 P1376 V1377 L1378 F1379 S1380 G1381 S1382 L1383 R1384 M1385 N1386 L1387 D1388 P1389 F1390 S1391 Q1392 Y1393 S1394 D1395 E1396 E1397 V1398 W1399 T1400 S1401 L1402 E1403 L1404 A1405 H1406 L1407 K1408 G1409 F1410 V1411 S1412 A1413 L1414 P1415 D1416 K1417
L1418 N1419 H1420 E1421 C1422 A1423 E1424 G1425 G1426 E1427 N1428 L1429 G1432 Q1433 R1434 V1437 R1441 A1442 L1443 L1444 R1445 K1446 T1447 K1448 I1449 L1450 V1451 L1452 D1453 E1454 A1455 T1456 A1457 A1458 V1459 I1467 T1470 I1471 R1472 T1473 Q1474 F1475 D1476 D1477 C1478 T1479 V1480 L1481 T1482 I1483 A1484 H1485 R1486 L1487 N1488
T1489 I1490 M1491 D1492 Y1493 T1494 R1495 V1496 I1497 V1498 L1499 D1500 K1501 G1502 E1503 I1504 Q1505 E1506 W1507 G1508 S1509 P1510 S1511 D1512 L1513 L1514 Q1515 Q1516 R1517 G1518 Y1521 S1522 M1523 A1524 K1525 D1526 SER GLY LEU VAL

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	149514	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 ($e^-/Å^2$)	80	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	1800	Depositor
Magnification	105000	Depositor
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	1.773	Depositor
Minimum map value	-0.024	Depositor
Average map value	0.001	Depositor
Map value standard deviation	0.024	Depositor
Recommended contour level	0.25	Depositor
Map size (Å)	265.6, 265.6, 265.6	wwPDB
Map dimensions	320, 320, 320	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.83000004, 0.83000004, 0.83000004	Depositor

5 Model quality

5.1 Standard geometry

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

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	0.32	0/10705	0.39	0/14593

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	10473	0	10103	817	0
2	A	14	0	13	2	0
All	All	10487	0	10116	817	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 40.

All (817) 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:328:SER:O	1:A:384:TYR:CE1	1.91	1.24
1:A:1297:TYR:HA	1:A:1348:GLY:HA3	1.19	1.18

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1292:VAL:HB	1:A:1316:ILE:HB	1.24	1.17
1:A:742:GLU:HA	1:A:747:LEU:HD11	1.32	1.09
1:A:328:SER:C	1:A:384:TYR:HE1	1.62	1.07
1:A:1298:GLY:HA2	1:A:1309:LEU:HB2	1.31	1.06
1:A:410:ILE:HG23	1:A:414:ALA:HB3	1.36	1.05
1:A:384:TYR:OH	1:A:442:ASN:ND2	1.91	1.03
1:A:1449:ILE:HG22	1:A:1479:THR:HB	1.41	1.01
1:A:668:VAL:HG12	1:A:674:VAL:HG21	1.42	0.99
1:A:328:SER:C	1:A:384:TYR:CE1	2.37	0.98
1:A:328:SER:O	1:A:384:TYR:CD1	2.16	0.98
1:A:558:PHE:CZ	1:A:1022:GLY:HA3	1.99	0.98
1:A:636:LYS:HE3	1:A:636:LYS:HA	1.47	0.97
1:A:384:TYR:OH	1:A:442:ASN:CG	2.07	0.97
1:A:965:TYR:CE2	1:A:969:ILE:HD11	2.00	0.97
1:A:778:LEU:O	1:A:782:VAL:HG23	1.65	0.96
1:A:1276:GLN:HE22	1:A:1363:HIS:HB2	1.28	0.96
1:A:1282:PRO:HG3	1:A:1364:ASP:HB3	1.46	0.96
1:A:646:VAL:HG12	1:A:702:VAL:HG23	1.45	0.96
1:A:352:PHE:CE2	1:A:1221:ARG:HD3	2.02	0.94
1:A:507:GLU:OE2	1:A:1379:PHE:HA	1.67	0.94
1:A:162:LYS:HE3	1:A:162:LYS:HA	1.50	0.93
1:A:744:CYS:SG	1:A:746:LEU:HG	2.09	0.92
1:A:1433:GLN:O	1:A:1437:VAL:HG23	1.69	0.92
1:A:719:ASN:HD21	1:A:764:LYS:HA	1.36	0.91
1:A:1382:SER:HA	1:A:1421:GLU:HA	1.51	0.90
1:A:409:VAL:HG12	1:A:624:ASP:HB3	1.52	0.89
1:A:841:MET:HA	1:A:847:SER:H	1.37	0.89
1:A:1401:SER:O	1:A:1405:ALA:N	2.06	0.89
1:A:630:ILE:HG23	1:A:702:VAL:HG13	1.55	0.88
1:A:804:LYS:O	1:A:808:GLU:HG2	1.74	0.88
1:A:467:LEU:HA	1:A:470:VAL:HG12	1.58	0.86
1:A:1390:PHE:HB3	1:A:1392:GLN:HG2	1.55	0.85
1:A:1471:ILE:O	1:A:1476:ASP:N	2.10	0.85
1:A:462:LEU:HD21	1:A:564:THR:HG22	1.56	0.85
1:A:1470:THR:O	1:A:1475:PHE:N	2.10	0.85
1:A:444:ILE:HD11	1:A:606:ILE:CD1	2.07	0.84
1:A:499:ASP:O	1:A:502:ILE:HG22	1.76	0.84
1:A:651:PHE:HE1	1:A:697:LYS:HG3	1.42	0.84
1:A:1454:GLU:N	1:A:1483:ILE:O	2.09	0.84
1:A:328:SER:HB2	1:A:384:TYR:CE1	2.13	0.83
1:A:742:GLU:HA	1:A:747:LEU:CD1	2.08	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:264:GLU:HG3	1:A:316:VAL:HG22	1.59	0.83
1:A:520:TRP:CE2	1:A:1389:PRO:HG3	2.13	0.83
1:A:676:VAL:HG13	1:A:825:VAL:HG23	1.60	0.83
1:A:722:LEU:HD11	1:A:776:VAL:HG21	1.59	0.83
1:A:34:GLN:OE1	1:A:155:SER:OG	1.97	0.83
1:A:68:THR:O	1:A:72:LYS:HE2	1.78	0.82
1:A:410:ILE:CG2	1:A:414:ALA:HB3	2.09	0.82
1:A:565:PHE:O	1:A:569:VAL:HG22	1.80	0.81
1:A:646:VAL:HG23	1:A:665:THR:HA	1.61	0.81
1:A:1297:TYR:HA	1:A:1348:GLY:CA	2.07	0.81
1:A:1298:GLY:N	1:A:1347:GLU:O	2.13	0.81
1:A:27:PRO:O	1:A:154:ARG:NH2	2.13	0.81
1:A:1092:MET:HE2	1:A:1249:MET:HE3	1.60	0.81
1:A:810:VAL:HG23	1:A:811:ILE:HG13	1.60	0.81
1:A:1068:SER:O	1:A:1072:VAL:HG23	1.81	0.81
1:A:382:HIS:NE2	1:A:1199:ALA:HB1	1.96	0.80
1:A:1299:LEU:HA	1:A:1346:ALA:HB3	1.60	0.80
1:A:995:LEU:O	1:A:999:THR:HG23	1.80	0.80
1:A:1297:TYR:CA	1:A:1348:GLY:HA3	2.07	0.80
1:A:686:SER:HB3	1:A:695:MET:HE1	1.64	0.80
1:A:688:LEU:HD12	1:A:792:ASP:HB2	1.64	0.80
1:A:1070:ASN:O	1:A:1074:ARG:CD	2.31	0.79
1:A:1343:LYS:HD3	1:A:1344:GLU:N	1.96	0.79
1:A:992:ASN:ND2	1:A:1235:TYR:OH	2.15	0.79
1:A:1471:ILE:HA	1:A:1475:PHE:CB	2.12	0.79
1:A:992:ASN:HB3	1:A:1231:LEU:HD11	1.65	0.79
1:A:1495:ARG:HH21	1:A:1507:TRP:HB2	1.46	0.78
1:A:462:LEU:HD21	1:A:564:THR:CG2	2.14	0.78
1:A:1217:ALA:HB1	1:A:1229:VAL:HG22	1.66	0.78
1:A:657:ASP:HB3	1:A:658:PRO:HD2	1.65	0.77
1:A:722:LEU:HD11	1:A:776:VAL:CG2	2.14	0.77
1:A:651:PHE:CE1	1:A:697:LYS:HG3	2.20	0.77
1:A:682:CYS:O	1:A:844:GLY:N	2.17	0.76
1:A:444:ILE:HD11	1:A:606:ILE:HD11	1.64	0.76
1:A:1059:PRO:HA	1:A:1272:GLU:OE2	1.85	0.76
1:A:37:VAL:O	1:A:41:VAL:HG23	1.85	0.76
1:A:750:LEU:HA	1:A:753:LEU:HG	1.67	0.76
1:A:723:ARG:O	1:A:727:LEU:HG	1.86	0.76
1:A:1060:ILE:HG13	1:A:1342:ILE:HG23	1.67	0.76
1:A:556:THR:O	1:A:560:VAL:HG23	1.87	0.75
1:A:384:TYR:OH	1:A:442:ASN:CB	2.35	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:841:MET:HG2	1:A:846:ILE:HA	1.69	0.75
1:A:400:ILE:HG23	1:A:427:MET:HE2	1.69	0.75
1:A:633:ARG:HH22	1:A:639:GLY:HA3	1.51	0.74
1:A:1029:VAL:HA	1:A:1032:TYR:CE1	2.22	0.74
1:A:1294:PHE:N	1:A:1314:VAL:O	2.19	0.74
1:A:1298:GLY:O	1:A:1347:GLU:N	2.21	0.74
1:A:14:LEU:HD13	1:A:17:GLU:OE1	1.88	0.74
1:A:8:SER:HB2	1:A:13:ASP:OD1	1.87	0.74
1:A:68:THR:HG22	1:A:71:ASN:ND2	2.03	0.74
1:A:498:LYS:HB3	1:A:535:GLU:OE2	1.87	0.73
1:A:643:SER:OG	1:A:821:THR:HG21	1.88	0.73
1:A:1316:ILE:HG23	1:A:1320:GLU:OE1	1.89	0.73
1:A:686:SER:CB	1:A:695:MET:HE1	2.19	0.73
1:A:1029:VAL:HA	1:A:1032:TYR:CD1	2.24	0.73
1:A:265:CYS:O	1:A:268:SER:OG	2.06	0.73
1:A:1357:ILE:O	1:A:1360:ILE:HG22	1.89	0.73
1:A:802:VAL:O	1:A:806:ILE:HG12	1.88	0.72
1:A:1070:ASN:O	1:A:1074:ARG:HD2	1.89	0.72
1:A:846:ILE:HD11	1:A:849:MET:SD	2.29	0.72
1:A:444:ILE:HD11	1:A:602:VAL:HG12	1.70	0.72
1:A:794:PRO:HG2	1:A:795:LEU:HD12	1.72	0.72
1:A:427:MET:HB3	1:A:1151:TYR:HE1	1.55	0.72
1:A:708:VAL:HG12	1:A:788:VAL:CG1	2.20	0.72
1:A:711:VAL:HG23	1:A:711:VAL:O	1.88	0.72
1:A:504:LEU:O	1:A:508:ILE:HG13	1.90	0.71
1:A:95:GLU:OE2	1:A:100:LYS:HG3	1.90	0.71
1:A:522:LEU:HD21	1:A:1275:TRP:HZ3	1.53	0.71
1:A:1394:SER:HB3	1:A:1397:GLU:OE2	1.90	0.71
1:A:1499:LEU:CB	1:A:1504:ILE:HA	2.19	0.71
1:A:846:ILE:HD11	1:A:849:MET:CG	2.20	0.71
1:A:328:SER:HA	1:A:384:TYR:CD1	2.25	0.71
1:A:522:LEU:HD21	1:A:1275:TRP:CZ3	2.25	0.71
1:A:104:PRO:O	1:A:108:VAL:HG23	1.91	0.71
1:A:328:SER:CA	1:A:384:TYR:CE1	2.73	0.71
1:A:470:VAL:HA	1:A:473:MET:CE	2.19	0.71
1:A:1296:ASP:HA	1:A:1311:HIS:C	2.14	0.71
1:A:810:VAL:HG23	1:A:811:ILE:CG1	2.20	0.71
1:A:230:GLN:OE1	1:A:233:ARG:NH2	2.23	0.70
1:A:1294:PHE:HB2	1:A:1314:VAL:H	1.54	0.70
1:A:328:SER:CB	1:A:384:TYR:CE1	2.75	0.70
1:A:819:ASN:O	1:A:820:LYS:HD3	1.91	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:TYR:HA	1:A:367:THR:HG22	1.72	0.70
1:A:792:ASP:HA	1:A:825:VAL:HG12	1.73	0.70
1:A:75:THR:HG22	1:A:79:PHE:CE2	2.26	0.70
1:A:1070:ASN:O	1:A:1074:ARG:HD3	1.91	0.70
1:A:738:LYS:O	1:A:742:GLU:HG3	1.92	0.70
1:A:636:LYS:HA	1:A:636:LYS:CE	2.17	0.69
1:A:1119:PRO:HB2	1:A:1120:PRO:HD3	1.74	0.69
1:A:1294:PHE:O	1:A:1313:ASN:HA	1.92	0.69
1:A:69:HIS:HA	1:A:72:LYS:HE2	1.74	0.69
1:A:170:PHE:O	1:A:174:THR:HG23	1.93	0.69
1:A:682:CYS:SG	1:A:684:LYS:HG3	2.32	0.69
1:A:829:ILE:HA	1:A:832:LEU:CD1	2.22	0.69
1:A:1029:VAL:HG23	1:A:1032:TYR:CE1	2.28	0.69
1:A:1123:LEU:C	1:A:1124:ILE:HD13	2.18	0.69
1:A:1308:VAL:O	1:A:1309:LEU:HD23	1.91	0.69
1:A:384:TYR:HH	1:A:442:ASN:CG	1.99	0.68
1:A:645:THR:HG22	1:A:703:THR:CG2	2.23	0.68
1:A:515:LEU:HD23	1:A:520:TRP:HB2	1.74	0.68
1:A:81:LEU:HB3	1:A:117:MET:HG3	1.74	0.68
1:A:328:SER:CA	1:A:384:TYR:CD1	2.77	0.68
1:A:1026:GLY:O	1:A:1029:VAL:HG12	1.94	0.68
1:A:1282:PRO:HG3	1:A:1360:ILE:HD11	1.74	0.68
1:A:162:LYS:HE3	1:A:162:LYS:CA	2.18	0.68
1:A:444:ILE:CD1	1:A:606:ILE:CD1	2.72	0.68
1:A:806:ILE:O	1:A:810:VAL:HG22	1.93	0.68
1:A:653:TRP:CZ2	1:A:695:MET:HE2	2.29	0.68
1:A:761:ILE:CG2	1:A:765:GLY:HA2	2.24	0.68
1:A:640:ALA:O	1:A:705:LYS:NZ	2.16	0.68
1:A:742:GLU:CA	1:A:747:LEU:HD11	2.18	0.68
1:A:1300:ARG:CB	1:A:1307:LEU:HA	2.24	0.68
1:A:444:ILE:CD1	1:A:606:ILE:HD11	2.23	0.67
1:A:10:ASP:OD1	1:A:12:SER:HB3	1.93	0.67
1:A:493:ALA:HA	1:A:496:LYS:HG2	1.75	0.67
1:A:644:ILE:HB	1:A:668:VAL:HG22	1.75	0.67
1:A:761:ILE:O	1:A:766:VAL:N	2.18	0.67
1:A:228:MET:HE1	1:A:1194:ALA:HB1	1.77	0.67
1:A:732:LEU:HD23	1:A:733:GLN:N	2.10	0.67
1:A:694:GLU:OE1	1:A:1165:ARG:NH1	2.28	0.67
1:A:746:LEU:HA	1:A:749:ASP:OD2	1.94	0.67
1:A:1390:PHE:CB	1:A:1392:GLN:HG2	2.25	0.67
1:A:1357:ILE:HA	1:A:1360:ILE:HG22	1.75	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1434:ARG:HA	1:A:1437:VAL:CG2	2.24	0.67
1:A:516:LYS:HE3	1:A:1272:GLU:OE2	1.95	0.66
1:A:642:ASN:ND2	1:A:667:SER:OG	2.27	0.66
1:A:853:GLN:O	1:A:856:LEU:HG	1.95	0.66
1:A:462:LEU:CD2	1:A:564:THR:CG2	2.74	0.66
1:A:801:HIS:O	1:A:804:LYS:HG3	1.95	0.66
1:A:1498:VAL:O	1:A:1505:GLN:N	2.23	0.66
1:A:327:MET:HE1	1:A:330:LEU:HD13	1.75	0.66
1:A:1495:ARG:NH2	1:A:1507:TRP:HB2	2.08	0.66
1:A:839:ILE:HG22	1:A:849:MET:CG	2.26	0.66
1:A:717:ILE:HD12	1:A:761:ILE:HG21	1.77	0.66
1:A:642:ASN:OD1	1:A:669:PRO:HA	1.96	0.66
1:A:1117:ILE:HG21	1:A:1212:PHE:CD2	2.31	0.66
1:A:635:ILE:HG23	1:A:636:LYS:HD2	1.79	0.65
1:A:405:ARG:HG3	1:A:405:ARG:HH11	1.60	0.65
1:A:793:ASP:OD1	1:A:796:SER:HB2	1.96	0.65
1:A:57:LEU:O	1:A:130:ARG:HD2	1.97	0.65
1:A:719:ASN:ND2	1:A:764:LYS:HA	2.10	0.65
1:A:444:ILE:HD11	1:A:606:ILE:HD12	1.77	0.65
1:A:455:LEU:HD21	1:A:473:MET:HE1	1.79	0.65
1:A:1282:PRO:CG	1:A:1360:ILE:HD11	2.26	0.65
1:A:69:HIS:HA	1:A:72:LYS:CE	2.27	0.65
1:A:470:VAL:HA	1:A:473:MET:HE3	1.79	0.65
1:A:473:MET:HG2	1:A:596:LEU:CD1	2.27	0.65
1:A:1310:LYS:N	1:A:1502:GLY:O	2.29	0.65
1:A:15:PHE:O	1:A:30:THR:HG21	1.97	0.64
1:A:825:VAL:HG13	1:A:825:VAL:O	1.97	0.64
1:A:1496:VAL:C	1:A:1497:ILE:HD12	2.22	0.64
1:A:515:LEU:HD21	1:A:524:PHE:CE2	2.33	0.64
1:A:1199:ALA:O	1:A:1203:GLU:HG2	1.97	0.64
1:A:490:TYR:CE2	1:A:541:LYS:HB3	2.32	0.64
1:A:261:TRP:HE3	1:A:316:VAL:HG21	1.63	0.64
1:A:1044:SER:HB2	1:A:1083:ASP:OD2	1.98	0.64
1:A:357:LYS:HE3	1:A:357:LYS:HA	1.79	0.64
1:A:1340:PHE:CZ	1:A:1371:ILE:HB	2.33	0.64
1:A:1437:VAL:O	1:A:1441:ARG:HG3	1.98	0.64
1:A:839:ILE:HG22	1:A:849:MET:HG2	1.79	0.63
1:A:840:VAL:HG23	1:A:847:SER:HB3	1.78	0.63
1:A:1451:VAL:HG13	1:A:1481:LEU:O	1.98	0.63
1:A:1117:ILE:HD12	1:A:1212:PHE:CE2	2.33	0.63
1:A:462:LEU:CD2	1:A:564:THR:HG21	2.29	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:747:LEU:HB2	1:A:748:PRO:HD3	1.81	0.63
1:A:676:VAL:CG1	1:A:825:VAL:HG23	2.27	0.63
1:A:104:PRO:O	1:A:107:LEU:HG	1.99	0.63
1:A:67:MET:SD	1:A:128:ARG:NH1	2.71	0.63
1:A:162:LYS:HA	1:A:162:LYS:CE	2.20	0.63
1:A:409:VAL:CG1	1:A:624:ASP:HB3	2.28	0.63
1:A:232:TYR:OH	1:A:1130:ARG:NH2	2.32	0.63
1:A:467:LEU:HA	1:A:470:VAL:CG1	2.27	0.63
1:A:1148:SER:OG	1:A:1149:PRO:HD3	1.98	0.63
1:A:1308:VAL:O	1:A:1308:VAL:HG12	1.98	0.63
1:A:1397:GLU:OE1	1:A:1397:GLU:N	2.17	0.63
1:A:1517:ARG:HA	1:A:1521:TYR:CB	2.29	0.63
1:A:427:MET:HB3	1:A:1151:TYR:CE1	2.32	0.62
1:A:653:TRP:CE2	1:A:695:MET:HE2	2.33	0.62
1:A:1382:SER:O	1:A:1385:MET:HG3	1.98	0.62
1:A:1299:LEU:HA	1:A:1346:ALA:CB	2.30	0.62
1:A:1029:VAL:HG23	1:A:1032:TYR:HE1	1.63	0.62
1:A:677:VAL:O	1:A:840:VAL:HA	1.99	0.62
1:A:860:GLY:O	1:A:863:ALA:HB3	1.98	0.62
1:A:1388:ASP:OD2	1:A:1393:TYR:N	2.28	0.62
1:A:6:PHE:CE1	1:A:104:PRO:HB2	2.35	0.62
1:A:30:THR:O	1:A:34:GLN:HG3	1.98	0.62
1:A:1099:ASN:HB3	1:A:1242:TYR:CD2	2.35	0.62
1:A:1497:ILE:HA	1:A:1506:GLU:O	2.00	0.62
1:A:673:LEU:HB2	1:A:822:ARG:NH2	2.15	0.61
1:A:493:ALA:HA	1:A:496:LYS:HZ2	1.65	0.61
1:A:6:PHE:O	1:A:104:PRO:HD2	2.00	0.61
1:A:261:TRP:CH2	1:A:311:PRO:HB2	2.35	0.61
1:A:1322:VAL:HG13	1:A:1495:ARG:C	2.25	0.61
1:A:127:GLU:O	1:A:132:VAL:HG12	1.99	0.61
1:A:708:VAL:HG12	1:A:788:VAL:HG11	1.83	0.61
1:A:507:GLU:CD	1:A:1379:PHE:HD1	2.08	0.61
1:A:328:SER:HA	1:A:384:TYR:HD1	1.63	0.61
1:A:338:MET:HE1	1:A:373:SER:HA	1.82	0.61
1:A:852:TYR:CD1	1:A:856:LEU:HD23	2.36	0.61
1:A:261:TRP:CE3	1:A:316:VAL:HG21	2.36	0.61
1:A:264:GLU:HG3	1:A:316:VAL:CG2	2.31	0.61
1:A:467:LEU:CA	1:A:470:VAL:HG12	2.30	0.61
1:A:164:ASP:O	1:A:166:ARG:NH1	2.34	0.60
1:A:66:GLN:HG2	1:A:67:MET:N	2.16	0.60
1:A:1486:ARG:O	1:A:1489:THR:N	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:103:ALA:HB1	1:A:104:PRO:CD	2.32	0.60
1:A:1099:ASN:HB3	1:A:1242:TYR:CE2	2.37	0.60
1:A:1407:LEU:HG	1:A:1407:LEU:O	2.00	0.60
1:A:74:LYS:HB3	1:A:124:ILE:HD13	1.84	0.60
1:A:447:ALA:HB3	1:A:448:PRO:HD3	1.84	0.60
1:A:473:MET:HG2	1:A:596:LEU:HD11	1.84	0.59
1:A:1495:ARG:HA	1:A:1509:SER:HA	1.84	0.59
1:A:444:ILE:CG1	1:A:606:ILE:HD11	2.32	0.59
1:A:1198:LEU:HD11	1:A:1247:VAL:HG11	1.82	0.59
1:A:1282:PRO:CG	1:A:1364:ASP:HB3	2.25	0.59
1:A:1352:ILE:HG22	1:A:1353:ASP:OD2	2.02	0.59
1:A:790:LEU:CD2	1:A:823:LEU:HD12	2.32	0.59
1:A:156:LYS:HD3	1:A:172:ASP:OD2	2.02	0.59
1:A:467:LEU:HD23	1:A:470:VAL:HG11	1.84	0.59
1:A:688:LEU:HD12	1:A:792:ASP:CB	2.32	0.59
1:A:1255:THR:O	1:A:1258:VAL:HG22	2.02	0.59
1:A:1289:VAL:O	1:A:1318:GLY:HA3	2.02	0.59
1:A:1294:PHE:HB2	1:A:1314:VAL:N	2.18	0.59
1:A:1177:SER:O	1:A:1181:VAL:HG23	2.02	0.59
1:A:1278:GLN:HA	1:A:1281:ALA:HB2	1.84	0.59
1:A:832:LEU:H	1:A:832:LEU:HD12	1.67	0.59
1:A:1060:ILE:HG13	1:A:1342:ILE:CG2	2.31	0.59
1:A:499:ASP:C	1:A:502:ILE:HG22	2.27	0.59
1:A:632:ARG:O	1:A:633:ARG:HG3	2.03	0.59
1:A:807:PHE:O	1:A:812:GLY:N	2.32	0.59
1:A:841:MET:HA	1:A:847:SER:N	2.13	0.59
1:A:483:MET:HE3	1:A:548:VAL:HG11	1.84	0.59
1:A:1365:LEU:HD21	1:A:1369:ILE:HD12	1.85	0.59
1:A:614:LYS:O	1:A:618:VAL:HG23	2.03	0.58
1:A:435:MET:HE2	1:A:1188:TYR:CZ	2.38	0.58
1:A:654:ALA:HB3	1:A:657:ASP:OD1	2.02	0.58
1:A:367:THR:OG1	1:A:1211:LEU:HD12	2.02	0.58
1:A:800:ALA:O	1:A:804:LYS:HG2	2.03	0.58
1:A:708:VAL:HG23	1:A:1166:ALA:O	2.02	0.58
1:A:810:VAL:CG2	1:A:811:ILE:HG13	2.30	0.58
1:A:593:ARG:HG3	1:A:594:PHE:N	2.17	0.58
1:A:630:ILE:HD11	1:A:690:ALA:O	2.04	0.58
1:A:162:LYS:HB3	1:A:164:ASP:OD2	2.04	0.58
1:A:866:LEU:HD12	1:A:870:ALA:CB	2.33	0.58
1:A:75:THR:HG22	1:A:79:PHE:HE2	1.69	0.58
1:A:364:TYR:OH	1:A:1219:ILE:HD13	2.03	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:982:LEU:O	1:A:986:VAL:HG23	2.04	0.57
1:A:744:CYS:O	1:A:775:ARG:HD2	2.04	0.57
1:A:722:LEU:HD13	1:A:768:LEU:HD11	1.86	0.57
1:A:78:GLY:HA3	1:A:121:THR:HG22	1.86	0.57
1:A:761:ILE:HG23	1:A:765:GLY:HA2	1.87	0.57
1:A:7:CYS:HA	1:A:105:VAL:HG11	1.85	0.57
1:A:750:LEU:HA	1:A:753:LEU:CG	2.34	0.57
1:A:1185:GLN:OE1	1:A:1185:GLN:HA	2.05	0.57
1:A:1449:ILE:HG22	1:A:1479:THR:CB	2.24	0.57
1:A:169:VAL:O	1:A:173:VAL:HG23	2.05	0.57
1:A:410:ILE:HD11	1:A:619:PHE:CZ	2.40	0.57
1:A:809:ASN:O	1:A:816:LEU:N	2.35	0.57
1:A:1331:GLY:O	1:A:1334:SER:N	2.37	0.57
1:A:717:ILE:HG13	1:A:717:ILE:O	2.02	0.57
1:A:375:CYS:HA	1:A:378:THR:HG22	1.87	0.57
1:A:718:GLN:HG2	1:A:1156:GLU:OE2	2.04	0.57
1:A:1360:ILE:HG13	1:A:1361:GLY:N	2.19	0.57
1:A:105:VAL:HG13	1:A:106:PHE:CD1	2.39	0.57
1:A:499:ASP:HA	1:A:502:ILE:HG22	1.87	0.57
1:A:516:LYS:HG3	1:A:1060:ILE:HD11	1.87	0.57
1:A:30:THR:HG23	1:A:33:PHE:H	1.69	0.57
1:A:647:LYS:NZ	1:A:648:ASN:HB2	2.20	0.57
1:A:676:VAL:HG23	1:A:839:ILE:HG13	1.87	0.57
1:A:1291:ARG:O	1:A:1352:ILE:HG23	2.05	0.57
1:A:1371:ILE:CD1	1:A:1451:VAL:HB	2.34	0.57
1:A:1371:ILE:HD12	1:A:1451:VAL:HB	1.85	0.57
1:A:753:LEU:HD12	1:A:756:GLY:H	1.70	0.56
1:A:375:CYS:O	1:A:378:THR:HG22	2.05	0.56
1:A:633:ARG:NH2	1:A:639:GLY:HA3	2.20	0.56
1:A:168:ASP:OD1	1:A:170:PHE:N	2.37	0.56
1:A:493:ALA:CA	1:A:496:LYS:HZ2	2.18	0.56
1:A:769:SER:O	1:A:772:GLN:N	2.39	0.56
1:A:866:LEU:HD12	1:A:870:ALA:HB3	1.87	0.56
1:A:572:ASP:OD1	1:A:574:ASN:N	2.39	0.56
1:A:1121:LEU:HD21	1:A:1205:VAL:HG13	1.87	0.56
1:A:156:LYS:HA	1:A:159:THR:HG22	1.88	0.56
1:A:747:LEU:HD12	1:A:747:LEU:H	1.70	0.56
1:A:819:ASN:C	1:A:820:LYS:HD3	2.31	0.56
1:A:1343:LYS:HD3	1:A:1343:LYS:C	2.30	0.56
1:A:435:MET:HE2	1:A:1188:TYR:CE2	2.40	0.56
1:A:594:PHE:HB3	1:A:595:PRO:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:ARG:HH22	1:A:708:VAL:CG1	2.19	0.56
1:A:1119:PRO:CB	1:A:1120:PRO:HD3	2.36	0.56
1:A:1299:LEU:H	1:A:1309:LEU:HG	1.71	0.56
1:A:711:VAL:HG22	1:A:791:LEU:HA	1.86	0.56
1:A:861:ALA:O	1:A:864:GLU:N	2.39	0.56
1:A:471:ALA:O	1:A:474:VAL:HG12	2.05	0.56
1:A:668:VAL:CG1	1:A:674:VAL:HG21	2.29	0.56
1:A:62:ARG:NH2	1:A:133:GLN:HG3	2.20	0.55
1:A:1448:LYS:O	1:A:1478:CYS:HA	2.06	0.55
1:A:81:LEU:HD21	1:A:181:LEU:HB3	1.87	0.55
1:A:789:TYR:HB3	1:A:791:LEU:CD1	2.36	0.55
1:A:1308:VAL:C	1:A:1309:LEU:HD23	2.32	0.55
1:A:1362:LEU:HD22	1:A:1366:ARG:HH21	1.71	0.55
1:A:19:ASN:HB3	2:A:1601:NAG:N2	2.21	0.55
1:A:636:LYS:HE3	1:A:636:LYS:CA	2.22	0.55
1:A:655:ARG:HG3	1:A:656:ASN:ND2	2.21	0.55
1:A:778:LEU:HD21	1:A:810:VAL:HG21	1.89	0.55
1:A:840:VAL:O	1:A:847:SER:N	2.38	0.55
1:A:1351:ILE:HA	1:A:1355:ILE:O	2.05	0.55
1:A:1398:VAL:O	1:A:1401:SER:OG	2.25	0.55
1:A:16:TRP:CE2	1:A:21:THR:HG21	2.42	0.55
1:A:726:ILE:HD11	1:A:746:LEU:HD11	1.89	0.55
1:A:958:LYS:O	1:A:960:SER:N	2.40	0.55
1:A:1198:LEU:CD1	1:A:1247:VAL:HG11	2.35	0.55
1:A:1362:LEU:O	1:A:1366:ARG:HG3	2.07	0.55
1:A:1233:VAL:O	1:A:1237:LEU:HD13	2.05	0.55
1:A:1287:PRO:HG3	1:A:1368:LYS:CB	2.37	0.55
1:A:462:LEU:HD23	1:A:564:THR:HG21	1.89	0.55
1:A:1292:VAL:O	1:A:1316:ILE:N	2.35	0.55
1:A:1422:CYS:SG	1:A:1423:ALA:N	2.80	0.55
1:A:78:GLY:HA3	1:A:121:THR:CG2	2.37	0.55
1:A:646:VAL:HG12	1:A:702:VAL:CG2	2.30	0.55
1:A:1060:ILE:CG1	1:A:1342:ILE:HG23	2.37	0.55
1:A:573:GLU:CD	1:A:573:GLU:H	2.15	0.55
1:A:851:SER:HB3	1:A:854:GLU:OE1	2.06	0.55
1:A:4:ARG:O	1:A:11:GLY:HA2	2.07	0.55
1:A:6:PHE:HA	1:A:104:PRO:HD2	1.88	0.55
1:A:107:LEU:C	1:A:107:LEU:HD12	2.32	0.55
1:A:467:LEU:O	1:A:470:VAL:HG12	2.08	0.54
1:A:515:LEU:HD11	1:A:524:PHE:CE2	2.42	0.54
1:A:1382:SER:O	1:A:1385:MET:N	2.38	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD21	1:A:181:LEU:CB	2.37	0.54
1:A:62:ARG:HH22	1:A:133:GLN:HG3	1.72	0.54
1:A:228:MET:CE	1:A:1194:ALA:HB1	2.36	0.54
1:A:666:PHE:HA	1:A:849:MET:HE1	1.90	0.54
1:A:1202:LEU:HD11	1:A:1247:VAL:HG21	1.89	0.54
1:A:520:TRP:CD2	1:A:1389:PRO:HG3	2.42	0.54
1:A:1361:GLY:O	1:A:1364:ASP:N	2.39	0.54
1:A:109:SER:HB3	1:A:110:PRO:HD3	1.88	0.54
1:A:153:LEU:HD11	1:A:157:ILE:HD11	1.90	0.54
1:A:647:LYS:HZ2	1:A:648:ASN:HB2	1.73	0.54
1:A:652:THR:HB	1:A:659:PRO:HA	1.88	0.54
1:A:462:LEU:HG	1:A:462:LEU:O	2.07	0.54
1:A:774:GLN:HG3	1:A:797:ALA:HB3	1.89	0.54
1:A:795:LEU:HD12	1:A:795:LEU:H	1.73	0.54
1:A:1394:SER:HB3	1:A:1397:GLU:CD	2.33	0.54
1:A:405:ARG:HG3	1:A:405:ARG:NH1	2.24	0.53
1:A:721:SER:O	1:A:724:GLU:N	2.41	0.53
1:A:961:VAL:HG12	1:A:1257:ILE:HG13	1.90	0.53
1:A:345:ILE:HB	1:A:370:LEU:HD13	1.90	0.53
1:A:163:GLU:C	1:A:166:ARG:HH22	2.16	0.53
1:A:410:ILE:HG23	1:A:414:ALA:CB	2.25	0.53
1:A:630:ILE:HG23	1:A:702:VAL:CG1	2.34	0.53
1:A:983:CYS:HB3	1:A:1028:THR:HG21	1.90	0.53
1:A:1382:SER:HA	1:A:1421:GLU:CA	2.31	0.53
1:A:361:TRP:HA	1:A:364:TYR:HD2	1.74	0.53
1:A:382:HIS:CE1	1:A:1199:ALA:HB1	2.44	0.53
1:A:520:TRP:HH2	1:A:1441:ARG:HH11	1.55	0.53
1:A:664:ILE:HG21	1:A:666:PHE:HE1	1.74	0.53
1:A:234:GLN:HB2	1:A:235:PRO:HD2	1.91	0.53
1:A:1123:LEU:O	1:A:1124:ILE:HD13	2.09	0.53
1:A:41:VAL:HB	1:A:42:PRO:HD3	1.90	0.53
1:A:94:TRP:O	1:A:98:MET:HB2	2.08	0.53
1:A:673:LEU:O	1:A:836:ASP:HB3	2.08	0.53
1:A:829:ILE:HA	1:A:832:LEU:HD13	1.90	0.53
1:A:692:LEU:HD11	1:A:710:TYR:CG	2.44	0.53
1:A:327:MET:HE3	1:A:327:MET:HA	1.91	0.52
1:A:338:MET:CE	1:A:373:SER:HA	2.38	0.52
1:A:444:ILE:CD1	1:A:602:VAL:HG12	2.38	0.52
1:A:582:ALA:O	1:A:583:PHE:HB2	2.09	0.52
1:A:1384:ARG:HB2	1:A:1418:LEU:O	2.09	0.52
1:A:477:VAL:CG2	1:A:478:PRO:HD3	2.39	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1293:GLU:HA	1:A:1315:THR:HA	1.90	0.52
1:A:543:ALA:HB1	1:A:1037:SER:HB3	1.91	0.52
1:A:1117:ILE:C	1:A:1120:PRO:HD2	2.33	0.52
1:A:521:GLU:OE2	1:A:1363:HIS:HE1	1.92	0.52
1:A:1117:ILE:HD12	1:A:1212:PHE:CZ	2.45	0.52
1:A:676:VAL:HA	1:A:839:ILE:O	2.10	0.52
1:A:716:TRP:CZ3	1:A:1163:VAL:HB	2.44	0.52
1:A:327:MET:O	1:A:331:PHE:HD2	1.93	0.52
1:A:1361:GLY:HA3	1:A:1364:ASP:OD2	2.10	0.52
1:A:507:GLU:OE2	1:A:1379:PHE:HD1	1.92	0.52
1:A:1322:VAL:O	1:A:1481:LEU:HA	2.10	0.52
1:A:683:GLY:C	1:A:841:MET:HE1	2.35	0.52
1:A:85:CYS:SG	1:A:113:LEU:HD23	2.50	0.52
1:A:357:LYS:HE3	1:A:357:LYS:CA	2.40	0.51
1:A:738:LYS:O	1:A:741:VAL:HG12	2.10	0.51
1:A:957:VAL:HG23	1:A:957:VAL:O	2.10	0.51
1:A:183:LEU:O	1:A:187:VAL:HG23	2.10	0.51
1:A:484:ALA:O	1:A:487:THR:HG22	2.11	0.51
1:A:504:LEU:CD2	1:A:527:LYS:HG2	2.40	0.51
1:A:508:ILE:HG23	1:A:515:LEU:HD13	1.91	0.51
1:A:346:LEU:HD13	1:A:1233:VAL:HG11	1.93	0.51
1:A:467:LEU:CD2	1:A:470:VAL:HG11	2.40	0.51
1:A:470:VAL:HA	1:A:473:MET:HE2	1.90	0.51
1:A:474:VAL:O	1:A:477:VAL:HG22	2.10	0.51
1:A:516:LYS:HG3	1:A:1060:ILE:CD1	2.39	0.51
1:A:650:THR:HG22	1:A:662:HIS:HA	1.92	0.51
1:A:666:PHE:CB	1:A:849:MET:HE1	2.39	0.51
1:A:958:LYS:C	1:A:960:SER:H	2.19	0.51
1:A:1369:ILE:HG12	1:A:1449:ILE:HD11	1.92	0.51
1:A:332:LYS:HB2	1:A:384:TYR:CZ	2.46	0.51
1:A:741:VAL:HG23	1:A:746:LEU:HD12	1.93	0.51
1:A:1434:ARG:HA	1:A:1437:VAL:HG23	1.91	0.51
1:A:14:LEU:HD12	1:A:14:LEU:H	1.75	0.51
1:A:384:TYR:HH	1:A:442:ASN:CB	2.23	0.51
1:A:518:TYR:O	1:A:519:ALA:HB3	2.10	0.51
1:A:163:GLU:N	1:A:163:GLU:OE1	2.43	0.51
1:A:1171:GLU:OE2	1:A:1171:GLU:HA	2.10	0.51
1:A:56:TYR:HD1	1:A:57:LEU:HD12	1.75	0.51
1:A:364:TYR:HA	1:A:367:THR:CG2	2.39	0.51
1:A:477:VAL:HG23	1:A:478:PRO:HD3	1.92	0.51
1:A:676:VAL:HA	1:A:839:ILE:HG13	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:515:LEU:HD23	1:A:520:TRP:CB	2.40	0.51
1:A:1189:TYR:HB3	1:A:1190:PRO:HD3	1.92	0.51
1:A:586:LEU:HD11	1:A:995:LEU:HD23	1.93	0.50
1:A:769:SER:H	1:A:772:GLN:HG3	1.75	0.50
1:A:544:TYR:HD1	1:A:1034:MET:SD	2.34	0.50
1:A:647:LYS:HZ2	1:A:648:ASN:CB	2.24	0.50
1:A:1175:ARG:HB3	1:A:1175:ARG:NH1	2.26	0.50
1:A:757:ASP:OD1	1:A:758:ARG:N	2.45	0.50
1:A:805:HIS:O	1:A:808:GLU:HG3	2.11	0.50
1:A:1181:VAL:O	1:A:1185:GLN:HG2	2.12	0.50
1:A:82:TRP:CD1	1:A:118:LEU:HG	2.47	0.50
1:A:666:PHE:HB3	1:A:849:MET:HE1	1.92	0.50
1:A:1362:LEU:HD22	1:A:1366:ARG:HE	1.76	0.50
1:A:20:VAL:HG12	1:A:28:ASP:O	2.11	0.49
1:A:1215:LEU:O	1:A:1219:ILE:HG12	2.12	0.49
1:A:173:VAL:O	1:A:177:ILE:HG12	2.12	0.49
1:A:645:THR:HG22	1:A:703:THR:HG22	1.91	0.49
1:A:811:ILE:O	1:A:822:ARG:NH1	2.45	0.49
1:A:443:MET:HE2	1:A:594:PHE:HE2	1.78	0.49
1:A:664:ILE:HG22	1:A:666:PHE:CD1	2.47	0.49
1:A:745:ALA:O	1:A:749:ASP:OD2	2.30	0.49
1:A:1215:LEU:O	1:A:1215:LEU:HD23	2.12	0.49
1:A:477:VAL:N	1:A:478:PRO:HD2	2.28	0.49
1:A:648:ASN:OD1	1:A:663:GLY:HA2	2.13	0.49
1:A:839:ILE:CG2	1:A:849:MET:SD	3.00	0.49
1:A:1245:TRP:HA	1:A:1245:TRP:CE3	2.48	0.49
1:A:1275:TRP:HB3	1:A:1363:HIS:HD2	1.77	0.49
1:A:1470:THR:O	1:A:1474:GLN:N	2.45	0.49
1:A:961:VAL:CG1	1:A:1257:ILE:HG13	2.43	0.49
1:A:1317:ASP:O	1:A:1320:GLU:HG3	2.12	0.49
1:A:55:LEU:C	1:A:55:LEU:HD23	2.38	0.49
1:A:95:GLU:HG3	1:A:100:LYS:HB2	1.95	0.49
1:A:253:VAL:HG12	1:A:398:ALA:HB2	1.95	0.49
1:A:396:LYS:HD2	1:A:435:MET:SD	2.52	0.49
1:A:790:LEU:HD22	1:A:823:LEU:HD12	1.94	0.49
1:A:1005:ASN:O	1:A:1007:THR:HG22	2.11	0.49
1:A:1351:ILE:C	1:A:1352:ILE:HD12	2.38	0.49
1:A:1370:THR:HG23	1:A:1447:THR:CB	2.42	0.49
1:A:1374:GLN:N	1:A:1453:ASP:OD2	2.45	0.49
1:A:328:SER:C	1:A:384:TYR:CD1	2.77	0.49
1:A:340:PHE:CE1	1:A:591:ILE:HD11	2.47	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:444:ILE:HG13	1:A:606:ILE:HD11	1.93	0.49
1:A:493:ALA:HB1	1:A:496:LYS:NZ	2.27	0.49
1:A:525:LYS:O	1:A:528:VAL:HG12	2.12	0.49
1:A:667:SER:O	1:A:669:PRO:HD3	2.12	0.49
1:A:722:LEU:CD1	1:A:761:ILE:HD11	2.42	0.49
1:A:846:ILE:HD11	1:A:849:MET:HG2	1.94	0.49
1:A:1175:ARG:HB3	1:A:1175:ARG:CZ	2.42	0.49
1:A:489:THR:O	1:A:492:VAL:HG12	2.13	0.49
1:A:791:LEU:HD22	1:A:811:ILE:HD13	1.94	0.49
1:A:507:GLU:OE2	1:A:1379:PHE:CD1	2.66	0.48
1:A:675:ALA:HA	1:A:824:LEU:O	2.13	0.48
1:A:1467:ILE:HA	1:A:1470:THR:OG1	2.12	0.48
1:A:633:ARG:NH2	1:A:637:ASP:OD2	2.46	0.48
1:A:1299:LEU:CA	1:A:1346:ALA:HB3	2.37	0.48
1:A:66:GLN:HG2	1:A:67:MET:H	1.77	0.48
1:A:692:LEU:HD11	1:A:710:TYR:CD1	2.48	0.48
1:A:1497:ILE:HG13	1:A:1507:TRP:HA	1.94	0.48
1:A:493:ALA:HA	1:A:496:LYS:NZ	2.27	0.48
1:A:1065:ARG:NH1	1:A:1065:ARG:HB2	2.28	0.48
1:A:1495:ARG:HH21	1:A:1508:GLY:H	1.61	0.48
1:A:1503:GLU:O	1:A:1503:GLU:HG2	2.13	0.48
1:A:257:LEU:HD12	1:A:257:LEU:O	2.14	0.48
1:A:593:ARG:CG	1:A:594:PHE:N	2.77	0.48
1:A:666:PHE:HB3	1:A:849:MET:CE	2.44	0.48
1:A:839:ILE:HG22	1:A:849:MET:SD	2.53	0.48
1:A:1385:MET:SD	1:A:1386:ASN:N	2.86	0.48
1:A:673:LEU:HD12	1:A:822:ARG:O	2.13	0.48
1:A:365:PHE:O	1:A:369:LEU:HD13	2.13	0.48
1:A:508:ILE:HD13	1:A:524:PHE:HB3	1.95	0.48
1:A:515:LEU:HD11	1:A:524:PHE:CD2	2.49	0.48
1:A:852:TYR:CE1	1:A:856:LEU:HD23	2.49	0.48
1:A:684:LYS:HB3	1:A:825:VAL:CG2	2.44	0.48
1:A:736:TYR:O	1:A:740:VAL:HG12	2.14	0.48
1:A:15:PHE:O	1:A:30:THR:CG2	2.62	0.47
1:A:702:VAL:HG22	1:A:703:THR:N	2.29	0.47
1:A:1076:SER:OG	1:A:1077:LYS:N	2.46	0.47
1:A:9:VAL:HG13	1:A:10:ASP:N	2.29	0.47
1:A:254:VAL:O	1:A:258:VAL:HG23	2.14	0.47
1:A:644:ILE:HB	1:A:668:VAL:CG2	2.44	0.47
1:A:1240:THR:HG23	1:A:1241:THR:HG23	1.96	0.47
1:A:1451:VAL:HG12	1:A:1452:LEU:N	2.29	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:81:LEU:HD23	1:A:181:LEU:HD23	1.97	0.47
1:A:495:MET:HA	1:A:498:LYS:HG2	1.95	0.47
1:A:648:ASN:N	1:A:664:ILE:O	2.44	0.47
1:A:831:TYR:C	1:A:833:PRO:HD2	2.39	0.47
1:A:16:TRP:CZ2	1:A:21:THR:HG21	2.50	0.47
1:A:1127:PHE:CD2	1:A:1130:ARG:HD2	2.49	0.47
1:A:1308:VAL:O	1:A:1308:VAL:CG1	2.62	0.47
1:A:504:LEU:HD21	1:A:527:LYS:HG2	1.95	0.47
1:A:795:LEU:HD23	1:A:806:ILE:HB	1.96	0.47
1:A:1119:PRO:HB2	1:A:1120:PRO:CD	2.43	0.47
1:A:62:ARG:HB2	1:A:131:GLY:O	2.15	0.47
1:A:829:ILE:HA	1:A:832:LEU:HD11	1.95	0.47
1:A:1062:PHE:CE1	1:A:1066:THR:HG21	2.50	0.47
1:A:1340:PHE:HZ	1:A:1371:ILE:HB	1.79	0.47
1:A:1372:ILE:HD11	1:A:1442:ALA:CB	2.45	0.47
1:A:18:TRP:HE3	1:A:22:TRP:HB3	1.78	0.47
1:A:44:SER:O	1:A:48:VAL:HG12	2.15	0.47
1:A:164:ASP:OD2	1:A:164:ASP:N	2.45	0.47
1:A:716:TRP:HE3	1:A:1163:VAL:HG21	1.79	0.47
1:A:728:PHE:CD1	1:A:780:ARG:HD2	2.49	0.47
1:A:1292:VAL:O	1:A:1315:THR:HA	2.14	0.47
1:A:1357:ILE:CA	1:A:1360:ILE:HG22	2.41	0.47
1:A:84:VAL:HG22	1:A:84:VAL:O	2.15	0.47
1:A:419:THR:OG1	1:A:422:GLU:HG3	2.14	0.47
1:A:665:THR:O	1:A:849:MET:HE1	2.15	0.47
1:A:1357:ILE:HA	1:A:1360:ILE:CG2	2.42	0.47
1:A:429:VAL:HG23	1:A:430:ASP:N	2.29	0.47
1:A:664:ILE:HG22	1:A:666:PHE:HD1	1.80	0.47
1:A:434:PHE:CZ	1:A:613:LEU:HB2	2.50	0.47
1:A:451:VAL:HA	1:A:592:LEU:HD11	1.97	0.47
1:A:794:PRO:HG2	1:A:795:LEU:CD1	2.44	0.47
1:A:801:HIS:NE2	1:A:805:HIS:NE2	2.63	0.47
1:A:1441:ARG:O	1:A:1445:ARG:HG2	2.15	0.47
1:A:31:LYS:HE3	1:A:34:GLN:NE2	2.30	0.46
1:A:68:THR:HG22	1:A:71:ASN:HD21	1.77	0.46
1:A:375:CYS:O	1:A:378:THR:CG2	2.63	0.46
1:A:499:ASP:O	1:A:502:ILE:CG2	2.56	0.46
1:A:665:THR:O	1:A:849:MET:CE	2.62	0.46
1:A:666:PHE:CA	1:A:849:MET:HE1	2.45	0.46
1:A:846:ILE:HG23	1:A:846:ILE:O	2.15	0.46
1:A:493:ALA:CB	1:A:496:LYS:NZ	2.77	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:651:PHE:HB3	1:A:695:MET:SD	2.55	0.46
1:A:594:PHE:CZ	1:A:598:ILE:HG13	2.50	0.46
1:A:1371:ILE:HG13	1:A:1373:PRO:HD3	1.97	0.46
1:A:6:PHE:O	1:A:105:VAL:HG12	2.15	0.46
1:A:458:LEU:O	1:A:462:LEU:HB3	2.15	0.46
1:A:1316:ILE:HG23	1:A:1320:GLU:CD	2.40	0.46
1:A:486:LYS:HA	1:A:489:THR:HB	1.97	0.46
1:A:515:LEU:HD21	1:A:524:PHE:CZ	2.51	0.46
1:A:969:ILE:HG23	1:A:1039:GLY:HA3	1.97	0.46
1:A:434:PHE:HZ	1:A:613:LEU:HB2	1.80	0.46
1:A:513:LYS:HE2	1:A:513:LYS:HB3	1.71	0.46
1:A:1044:SER:HB2	1:A:1083:ASP:CG	2.41	0.46
1:A:1048:HIS:HB2	1:A:1079:LEU:HD21	1.96	0.46
1:A:82:TRP:CE3	1:A:83:ILE:HG13	2.51	0.46
1:A:487:THR:HG23	1:A:488:LYS:N	2.30	0.46
1:A:841:MET:HB2	1:A:841:MET:HE3	1.85	0.46
1:A:1357:ILE:C	1:A:1360:ILE:HG22	2.41	0.46
1:A:332:LYS:HB2	1:A:384:TYR:CE1	2.51	0.46
1:A:352:PHE:CZ	1:A:1221:ARG:HD3	2.46	0.46
1:A:1203:GLU:OE1	1:A:1240:THR:OG1	2.34	0.46
1:A:36:THR:HB	1:A:40:TRP:CZ3	2.50	0.46
1:A:550:THR:HG21	1:A:1033:SER:OG	2.14	0.46
1:A:694:GLU:OE1	1:A:694:GLU:HA	2.16	0.46
1:A:1336:THR:OG1	1:A:1337:LEU:N	2.49	0.46
1:A:1362:LEU:HD22	1:A:1366:ARG:NH2	2.29	0.46
1:A:1434:ARG:HA	1:A:1437:VAL:HG21	1.97	0.46
1:A:594:PHE:CE1	1:A:598:ILE:HG13	2.51	0.46
1:A:630:ILE:HG12	1:A:702:VAL:HG11	1.97	0.46
1:A:732:LEU:HD23	1:A:732:LEU:C	2.40	0.46
1:A:105:VAL:HG13	1:A:106:PHE:N	2.31	0.45
1:A:249:THR:O	1:A:253:VAL:HG23	2.15	0.45
1:A:741:VAL:HG23	1:A:746:LEU:CB	2.45	0.45
1:A:825:VAL:O	1:A:825:VAL:CG1	2.63	0.45
1:A:529:LEU:O	1:A:533:GLN:HG2	2.16	0.45
1:A:9:VAL:HG13	1:A:10:ASP:H	1.82	0.45
1:A:664:ILE:HG21	1:A:666:PHE:CE1	2.50	0.45
1:A:753:LEU:HD12	1:A:753:LEU:O	2.16	0.45
1:A:1276:GLN:NE2	1:A:1363:HIS:HB2	2.12	0.45
1:A:7:CYS:HA	1:A:105:VAL:CG1	2.45	0.45
1:A:1132:TYR:O	1:A:1133:VAL:C	2.58	0.45
1:A:1292:VAL:N	1:A:1316:ILE:O	2.35	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1322:VAL:HG22	1:A:1494:THR:HG1	1.82	0.45
1:A:260:ASN:HB3	1:A:316:VAL:HG13	1.98	0.45
1:A:633:ARG:NE	1:A:637:ASP:OD1	2.47	0.45
1:A:1336:THR:O	1:A:1339:LEU:N	2.49	0.45
1:A:1372:ILE:HD11	1:A:1442:ALA:HB2	1.99	0.45
1:A:335:HIS:HE1	1:A:377:GLN:HE21	1.63	0.45
1:A:558:PHE:CE1	1:A:1022:GLY:HA3	2.50	0.45
1:A:473:MET:SD	1:A:596:LEU:HD11	2.57	0.45
1:A:976:LEU:HD12	1:A:976:LEU:HA	1.81	0.45
1:A:1077:LYS:N	1:A:1077:LYS:HD3	2.32	0.45
1:A:1103:ALA:CB	1:A:1239:VAL:HG22	2.47	0.45
1:A:225:THR:O	1:A:229:VAL:HG23	2.17	0.45
1:A:364:TYR:CA	1:A:367:THR:HG22	2.45	0.45
1:A:710:TYR:CD2	1:A:712:PRO:HD3	2.52	0.45
1:A:335:HIS:ND1	1:A:377:GLN:HG3	2.31	0.45
1:A:630:ILE:HG12	1:A:702:VAL:CG1	2.47	0.45
1:A:646:VAL:CG1	1:A:702:VAL:HG23	2.31	0.45
1:A:684:LYS:HB3	1:A:825:VAL:HG21	1.99	0.45
1:A:1370:THR:OG1	1:A:1450:LEU:HA	2.17	0.45
1:A:467:LEU:C	1:A:470:VAL:HG12	2.41	0.44
1:A:1104:CYS:O	1:A:1108:LEU:HD13	2.17	0.44
1:A:109:SER:CB	1:A:110:PRO:HD3	2.47	0.44
1:A:795:LEU:CD2	1:A:806:ILE:HB	2.47	0.44
1:A:477:VAL:CG2	1:A:478:PRO:CD	2.95	0.44
1:A:842:SER:N	1:A:845:LYS:O	2.48	0.44
1:A:499:ASP:CA	1:A:502:ILE:HG22	2.46	0.44
1:A:533:GLN:OE1	1:A:533:GLN:HA	2.17	0.44
1:A:808:GLU:HG3	1:A:809:ASN:OD1	2.18	0.44
1:A:990:VAL:CG1	1:A:1021:LEU:HD22	2.47	0.44
1:A:1495:ARG:NE	1:A:1508:GLY:HA2	2.32	0.44
1:A:643:SER:HG	1:A:821:THR:HG21	1.80	0.44
1:A:1361:GLY:O	1:A:1364:ASP:HB2	2.17	0.44
1:A:1422:CYS:SG	1:A:1426:GLY:HA2	2.57	0.44
1:A:46:LEU:HD22	1:A:141:PHE:CE2	2.52	0.44
1:A:75:THR:OG1	1:A:125:GLN:NE2	2.50	0.44
1:A:443:MET:HE2	1:A:594:PHE:CE2	2.52	0.44
1:A:451:VAL:HA	1:A:592:LEU:CD1	2.48	0.44
1:A:405:ARG:HH22	1:A:1178:ASP:CG	2.24	0.44
1:A:720:ILE:HG13	1:A:725:ASN:OD1	2.17	0.44
1:A:1259:ALA:O	1:A:1263:LEU:HG	2.17	0.44
1:A:68:THR:OG1	1:A:69:HIS:N	2.51	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1078:GLU:HG3	1:A:1262:ARG:HD2	2.00	0.44
1:A:1319:GLY:N	1:A:1479:THR:OG1	2.51	0.44
1:A:1121:LEU:HD11	1:A:1208:CYS:HB2	2.00	0.43
1:A:1145:VAL:HG12	1:A:1145:VAL:O	2.18	0.43
1:A:341:ALA:O	1:A:345:ILE:HG13	2.17	0.43
1:A:741:VAL:HG23	1:A:746:LEU:CD1	2.47	0.43
1:A:836:ASP:OD2	1:A:836:ASP:C	2.61	0.43
1:A:840:VAL:O	1:A:847:SER:HB3	2.17	0.43
1:A:981:PHE:CZ	1:A:1032:TYR:CE2	3.07	0.43
1:A:1467:ILE:O	1:A:1470:THR:OG1	2.30	0.43
1:A:761:ILE:CG2	1:A:761:ILE:O	2.67	0.43
1:A:6:PHE:CE2	1:A:105:VAL:HB	2.53	0.43
1:A:499:ASP:HA	1:A:502:ILE:CG2	2.48	0.43
1:A:508:ILE:CD1	1:A:524:PHE:HB3	2.48	0.43
1:A:1299:LEU:H	1:A:1309:LEU:CG	2.31	0.43
1:A:1381:GLY:HA3	1:A:1385:MET:HG2	2.00	0.43
1:A:15:PHE:HD1	1:A:32:CYS:SG	2.42	0.43
1:A:676:VAL:CB	1:A:839:ILE:HG13	2.48	0.43
1:A:741:VAL:CG2	1:A:746:LEU:HB2	2.48	0.43
1:A:1056:LEU:HD13	1:A:1056:LEU:HA	1.86	0.43
1:A:665:THR:O	1:A:665:THR:HG23	2.18	0.43
1:A:750:LEU:HA	1:A:753:LEU:CD2	2.49	0.43
1:A:774:GLN:CD	1:A:794:PRO:O	2.62	0.43
1:A:791:LEU:CD2	1:A:811:ILE:HD13	2.49	0.43
1:A:1410:PHE:O	1:A:1413:ALA:HB3	2.17	0.43
1:A:794:PRO:HD2	1:A:824:LEU:HD11	2.00	0.43
1:A:1122:GLY:O	1:A:1126:PHE:HB3	2.18	0.43
1:A:1486:ARG:O	1:A:1487:LEU:C	2.61	0.43
1:A:1496:VAL:O	1:A:1497:ILE:HG13	2.18	0.43
1:A:632:ARG:HH22	1:A:708:VAL:HG11	1.83	0.43
1:A:658:PRO:HA	1:A:659:PRO:HD2	1.91	0.43
1:A:687:LEU:HD12	1:A:687:LEU:HA	1.82	0.43
1:A:1336:THR:O	1:A:1337:LEU:C	2.62	0.43
1:A:56:TYR:CD1	1:A:57:LEU:HD12	2.54	0.42
1:A:580:GLN:O	1:A:584:VAL:HB	2.19	0.42
1:A:582:ALA:C	1:A:584:VAL:H	2.26	0.42
1:A:1203:GLU:OE2	1:A:1240:THR:O	2.37	0.42
1:A:1240:THR:HG23	1:A:1241:THR:N	2.34	0.42
1:A:1362:LEU:HD22	1:A:1366:ARG:NE	2.34	0.42
1:A:1376:PRO:HB2	1:A:1434:ARG:CB	2.49	0.42
1:A:244:LEU:HD11	1:A:1185:GLN:HB2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:GLU:O	1:A:426:LEU:HD13	2.19	0.42
1:A:436:ASP:O	1:A:439:THR:HG22	2.19	0.42
1:A:515:LEU:HD21	1:A:524:PHE:CD2	2.54	0.42
1:A:536:LEU:HD23	1:A:536:LEU:HA	1.79	0.42
1:A:1372:ILE:O	1:A:1372:ILE:HG22	2.19	0.42
1:A:67:MET:HE2	1:A:67:MET:HB2	1.91	0.42
1:A:684:LYS:C	1:A:686:SER:H	2.28	0.42
1:A:846:ILE:CD1	1:A:849:MET:SD	3.06	0.42
1:A:965:TYR:CZ	1:A:969:ILE:HD11	2.52	0.42
1:A:1275:TRP:CG	1:A:1363:HIS:CD2	3.08	0.42
1:A:339:MET:HE1	1:A:450:GLN:OE1	2.20	0.42
1:A:753:LEU:HD11	1:A:756:GLY:CA	2.49	0.42
1:A:789:TYR:HB3	1:A:791:LEU:HD11	2.01	0.42
1:A:479:LEU:O	1:A:483:MET:HG2	2.20	0.42
1:A:558:PHE:CE2	1:A:1022:GLY:HA3	2.51	0.42
1:A:657:ASP:HB3	1:A:658:PRO:CD	2.42	0.42
1:A:1079:LEU:HD12	1:A:1079:LEU:HA	1.84	0.42
1:A:1499:LEU:HA	1:A:1505:GLN:CB	2.48	0.42
1:A:81:LEU:HA	1:A:84:VAL:HG12	2.02	0.42
1:A:710:TYR:CE2	1:A:712:PRO:HB3	2.55	0.42
1:A:798:VAL:HG11	1:A:802:VAL:HG12	2.02	0.42
1:A:1088:GLN:N	1:A:1088:GLN:OE1	2.53	0.42
1:A:1108:LEU:O	1:A:1112:PRO:HA	2.19	0.42
1:A:162:LYS:HE3	1:A:163:GLU:OE1	2.20	0.42
1:A:654:ALA:CB	1:A:657:ASP:OD1	2.68	0.42
1:A:664:ILE:CG2	1:A:666:PHE:CE1	3.03	0.42
1:A:49:CYS:O	1:A:53:TYR:HB2	2.20	0.42
1:A:493:ALA:HB1	1:A:496:LYS:HZ1	1.84	0.42
1:A:19:ASN:CB	2:A:1601:NAG:N2	2.83	0.42
1:A:13:ASP:OD1	1:A:13:ASP:O	2.38	0.41
1:A:364:TYR:O	1:A:367:THR:HG22	2.20	0.41
1:A:434:PHE:HZ	1:A:613:LEU:CB	2.33	0.41
1:A:644:ILE:HD12	1:A:668:VAL:HG21	2.02	0.41
1:A:731:GLN:O	1:A:731:GLN:OE1	2.38	0.41
1:A:994:TRP:CZ2	1:A:1014:ARG:HD3	2.54	0.41
1:A:1322:VAL:CA	1:A:1493:TYR:HD2	2.33	0.41
1:A:1495:ARG:HA	1:A:1510:PRO:HD3	2.02	0.41
1:A:118:LEU:HD23	1:A:118:LEU:HA	1.84	0.41
1:A:165:ALA:O	1:A:166:ARG:NH2	2.52	0.41
1:A:250:SER:OG	1:A:1182:ASP:OD1	2.21	0.41
1:A:327:MET:HA	1:A:327:MET:CE	2.50	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:652:THR:HG22	1:A:698:VAL:HG23	2.02	0.41
1:A:722:LEU:HD11	1:A:776:VAL:HG22	2.00	0.41
1:A:733:GLN:O	1:A:734:GLU:C	2.63	0.41
1:A:832:LEU:N	1:A:833:PRO:CD	2.83	0.41
1:A:995:LEU:O	1:A:995:LEU:HD12	2.20	0.41
1:A:1296:ASP:HA	1:A:1311:HIS:O	2.19	0.41
1:A:1497:ILE:HD12	1:A:1497:ILE:N	2.35	0.41
1:A:6:PHE:O	1:A:103:ALA:HB1	2.20	0.41
1:A:81:LEU:HD23	1:A:181:LEU:CD2	2.50	0.41
1:A:127:GLU:CB	1:A:132:VAL:CG1	2.98	0.41
1:A:224:ILE:HG12	1:A:224:ILE:O	2.20	0.41
1:A:722:LEU:HD13	1:A:761:ILE:HD11	2.02	0.41
1:A:746:LEU:HD23	1:A:749:ASP:OD2	2.20	0.41
1:A:958:LYS:C	1:A:960:SER:N	2.79	0.41
1:A:962:TYR:HE1	1:A:1253:MET:HE3	1.84	0.41
1:A:1165:ARG:HG3	1:A:1170:GLN:NE2	2.34	0.41
1:A:1341:ARG:NH1	1:A:1357:ILE:O	2.53	0.41
1:A:1360:ILE:CG1	1:A:1361:GLY:N	2.83	0.41
1:A:1490:ILE:O	1:A:1493:TYR:HB2	2.20	0.41
1:A:330:LEU:C	1:A:330:LEU:HD23	2.45	0.41
1:A:761:ILE:HG22	1:A:765:GLY:H	1.83	0.41
1:A:1111:THR:O	1:A:1111:THR:OG1	2.35	0.41
1:A:1494:THR:OG1	1:A:1495:ARG:N	2.52	0.41
1:A:473:MET:CG	1:A:596:LEU:HD11	2.50	0.41
1:A:832:LEU:HD12	1:A:832:LEU:N	2.34	0.41
1:A:1013:VAL:O	1:A:1016:SER:OG	2.33	0.41
1:A:1433:GLN:C	1:A:1437:VAL:HG23	2.42	0.41
1:A:346:LEU:HD13	1:A:1233:VAL:CG1	2.50	0.41
1:A:444:ILE:CD1	1:A:606:ILE:HD12	2.45	0.41
1:A:524:PHE:N	1:A:524:PHE:CD1	2.88	0.41
1:A:583:PHE:HE1	1:A:1231:LEU:HD12	1.86	0.41
1:A:738:LYS:C	1:A:741:VAL:HG12	2.46	0.41
1:A:1277:ILE:O	1:A:1281:ALA:HA	2.19	0.41
1:A:1347:GLU:OE1	1:A:1347:GLU:HA	2.21	0.41
1:A:96:ARG:HH11	1:A:96:ARG:HG2	1.86	0.41
1:A:142:TRP:CE3	1:A:142:TRP:HA	2.56	0.41
1:A:734:GLU:OE1	1:A:734:GLU:N	2.51	0.41
1:A:38:LEU:HD23	1:A:38:LEU:HA	1.85	0.41
1:A:613:LEU:C	1:A:613:LEU:HD23	2.45	0.41
1:A:753:LEU:HD11	1:A:756:GLY:HA2	2.03	0.41
1:A:1117:ILE:CG2	1:A:1212:PHE:CD2	3.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1128:VAL:CG2	1:A:1197:TRP:CZ3	3.03	0.41
1:A:71:ASN:OD1	1:A:72:LYS:N	2.54	0.41
1:A:101:LEU:C	1:A:102:LEU:HD12	2.45	0.41
1:A:544:TYR:CD1	1:A:1034:MET:SD	3.14	0.41
1:A:799:ASP:OD1	1:A:799:ASP:C	2.63	0.41
1:A:866:LEU:HD12	1:A:870:ALA:HB2	2.02	0.41
1:A:1147:ARG:HG3	1:A:1184:ASN:HD21	1.86	0.41
1:A:1352:ILE:O	1:A:1355:ILE:HG13	2.21	0.41
1:A:1475:PHE:O	1:A:1478:CYS:N	2.42	0.41
1:A:40:TRP:O	1:A:44:SER:HB3	2.21	0.41
1:A:409:VAL:HG12	1:A:409:VAL:O	2.21	0.41
1:A:722:LEU:HD12	1:A:761:ILE:HD11	2.02	0.41
1:A:493:ALA:HA	1:A:496:LYS:CE	2.51	0.40
1:A:540:LYS:HA	1:A:1041:ILE:HD11	2.03	0.40
1:A:6:PHE:CD2	1:A:105:VAL:HB	2.57	0.40
1:A:208:CYS:HA	1:A:209:PRO:HD3	1.90	0.40
1:A:726:ILE:HD11	1:A:746:LEU:CD1	2.50	0.40
1:A:769:SER:O	1:A:770:GLY:C	2.64	0.40
1:A:810:VAL:HG23	1:A:811:ILE:HG12	2.02	0.40
1:A:832:LEU:CD1	1:A:832:LEU:H	2.32	0.40
1:A:453:LEU:HD23	1:A:453:LEU:HA	1.86	0.40
1:A:664:ILE:CG2	1:A:666:PHE:CD1	3.04	0.40
1:A:673:LEU:HB2	1:A:822:ARG:CZ	2.51	0.40
1:A:739:ALA:HA	1:A:742:GLU:HG3	2.04	0.40
1:A:1148:SER:OG	1:A:1149:PRO:CD	2.67	0.40
1:A:1169:GLU:O	1:A:1173:PHE:HD1	2.03	0.40
1:A:1290:GLY:O	1:A:1318:GLY:HA2	2.21	0.40
1:A:1499:LEU:HA	1:A:1505:GLN:N	2.36	0.40
1:A:50:PHE:HB3	1:A:51:PRO:HD3	2.02	0.40
1:A:125:GLN:OE1	1:A:125:GLN:HA	2.21	0.40
1:A:512:ILE:HG12	1:A:1063:PHE:CD2	2.56	0.40
1:A:588:LEU:O	1:A:592:LEU:HB2	2.22	0.40
1:A:646:VAL:O	1:A:665:THR:HA	2.22	0.40
1:A:668:VAL:O	1:A:668:VAL:HG23	2.20	0.40
1:A:1322:VAL:HG22	1:A:1494:THR:OG1	2.21	0.40
1:A:1372:ILE:O	1:A:1373:PRO:C	2.64	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	1394/1530 (91%)	1280 (92%)	114 (8%)	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	1053/1336 (79%)	1053 (100%)	0	100 100

There are no protein residues with a non-rotameric sidechain to report.

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (18) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	133	GLN
1	A	377	GLN
1	A	412	ASN
1	A	442	ASN
1	A	491	GLN
1	A	590	ASN
1	A	631	GLN
1	A	656	ASN
1	A	719	ASN
1	A	992	ASN
1	A	1053	HIS

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Mol	Chain	Res	Type
1	A	1170	GLN
1	A	1184	ASN
1	A	1238	GLN
1	A	1244	ASN
1	A	1276	GLN
1	A	1363	HIS
1	A	1420	HIS

5.3.3 RNA (i)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

1 ligand is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	1601	1	14,14,15	2.24	5 (35%)	17,19,21	1.44	3 (17%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	1601	1	-	0/6/23/26	0/1/1/1

All (5) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	A	1601	NAG	O5-C1	5.40	1.52	1.43
2	A	1601	NAG	C7-N2	4.17	1.47	1.34
2	A	1601	NAG	C2-N2	3.02	1.51	1.46
2	A	1601	NAG	O7-C7	-2.17	1.18	1.23
2	A	1601	NAG	O5-C5	2.06	1.47	1.43

All (3) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	1601	NAG	C1-O5-C5	3.97	117.51	112.19
2	A	1601	NAG	C8-C7-N2	2.31	119.96	116.12
2	A	1601	NAG	C2-N2-C7	-2.25	119.88	122.90

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	1601	NAG	2	0

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-61270. These allow visual inspection of the internal detail of the map and identification of artifacts.

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

6.1 Orthogonal projections

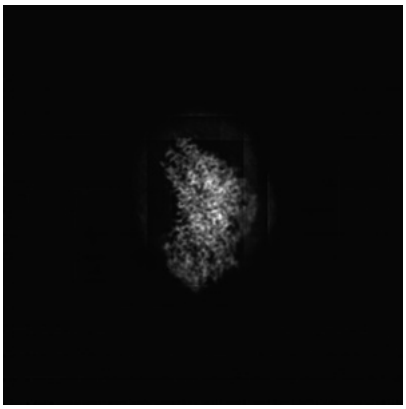
6.1.1 Primary map



X

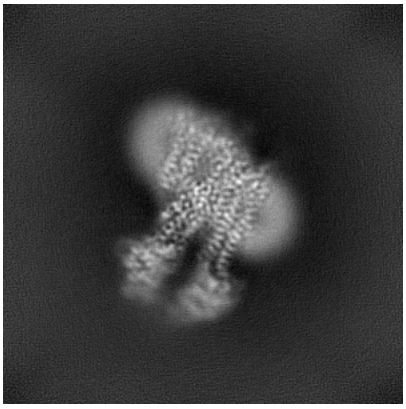


Y

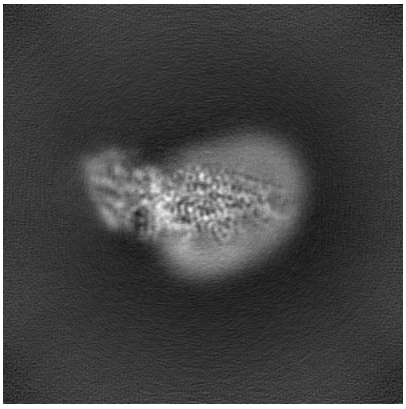


Z

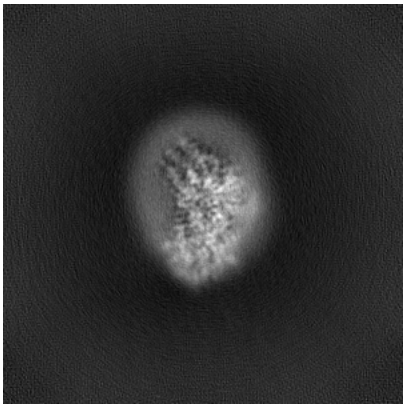
6.1.2 Raw map



X



Y



Z

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

6.2 Central slices (i)

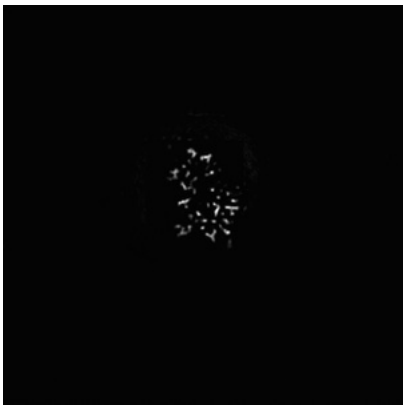
6.2.1 Primary map



X Index: 160

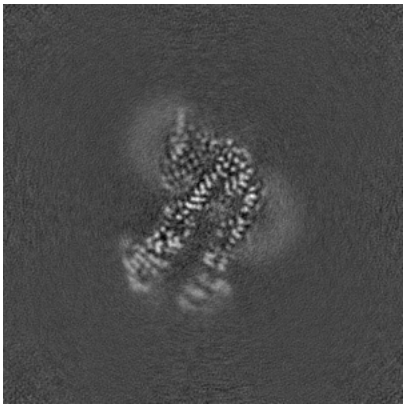


Y Index: 160

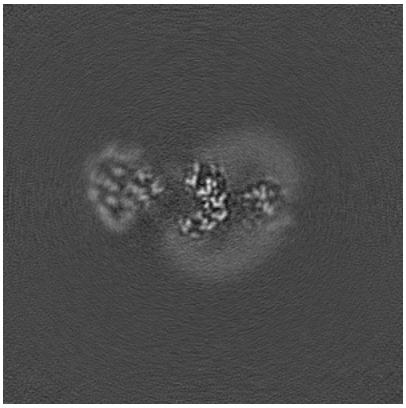


Z Index: 160

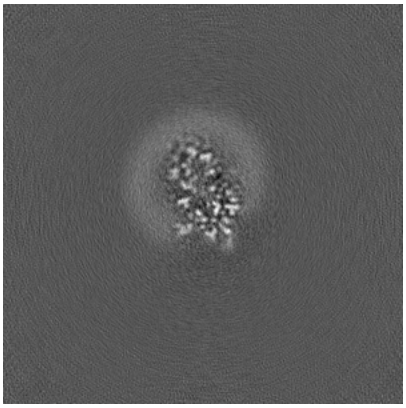
6.2.2 Raw map



X Index: 160



Y Index: 160



Z Index: 160

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: 169

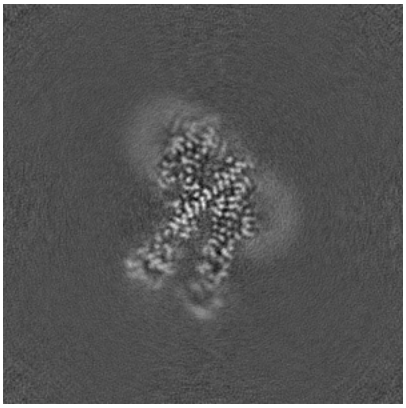


Y Index: 178

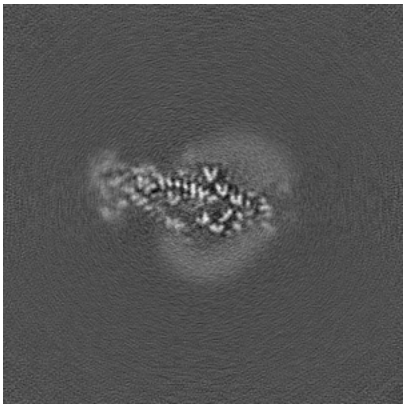


Z Index: 164

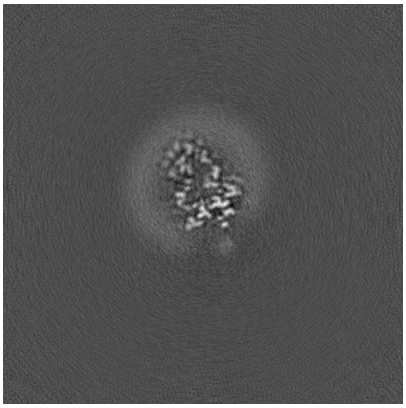
6.3.2 Raw map



X Index: 169



Y Index: 173

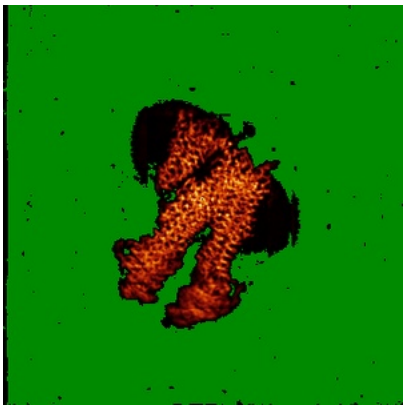


Z Index: 164

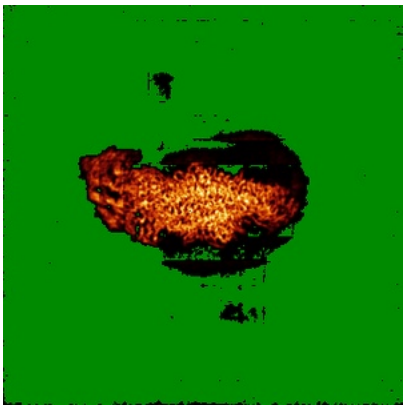
The images above show the largest variance slices of the map in three orthogonal directions.

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

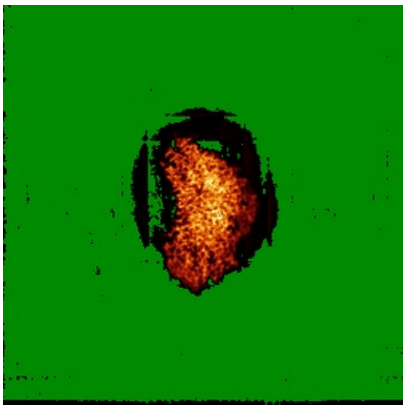
6.4.1 Primary map



X

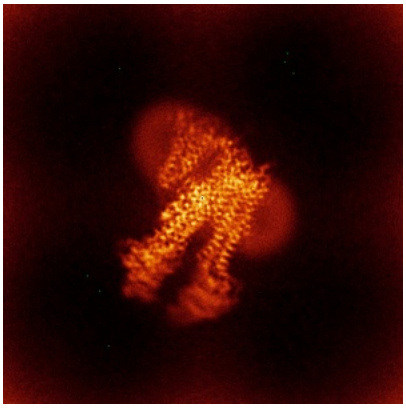


Y

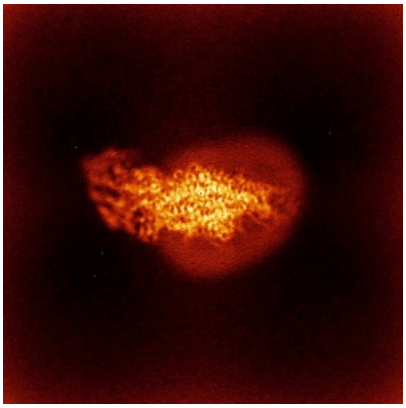


Z

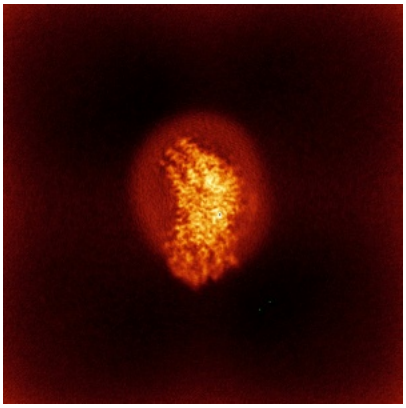
6.4.2 Raw map



X



Y



Z

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

6.5 Orthogonal surface views (i)

6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.25. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

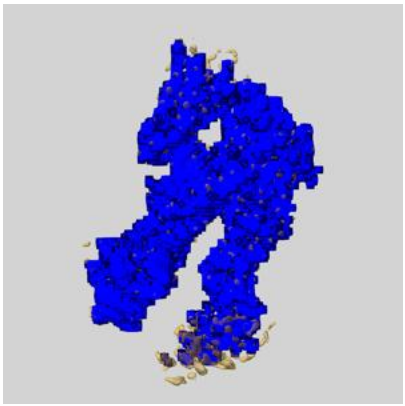
6.6 Mask visualisation (i)

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

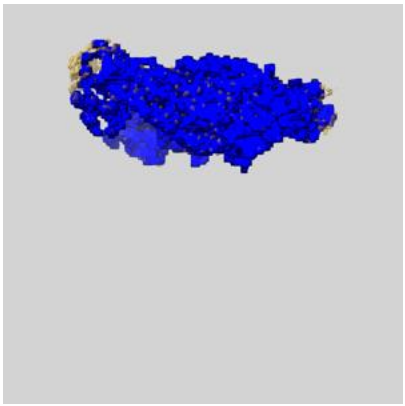
A mask typically either:

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

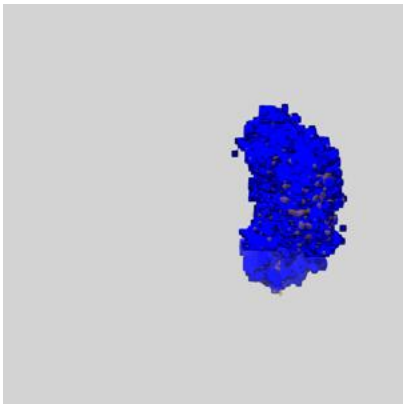
6.6.1 emd_61270_msk_1.map (i)



X



Y

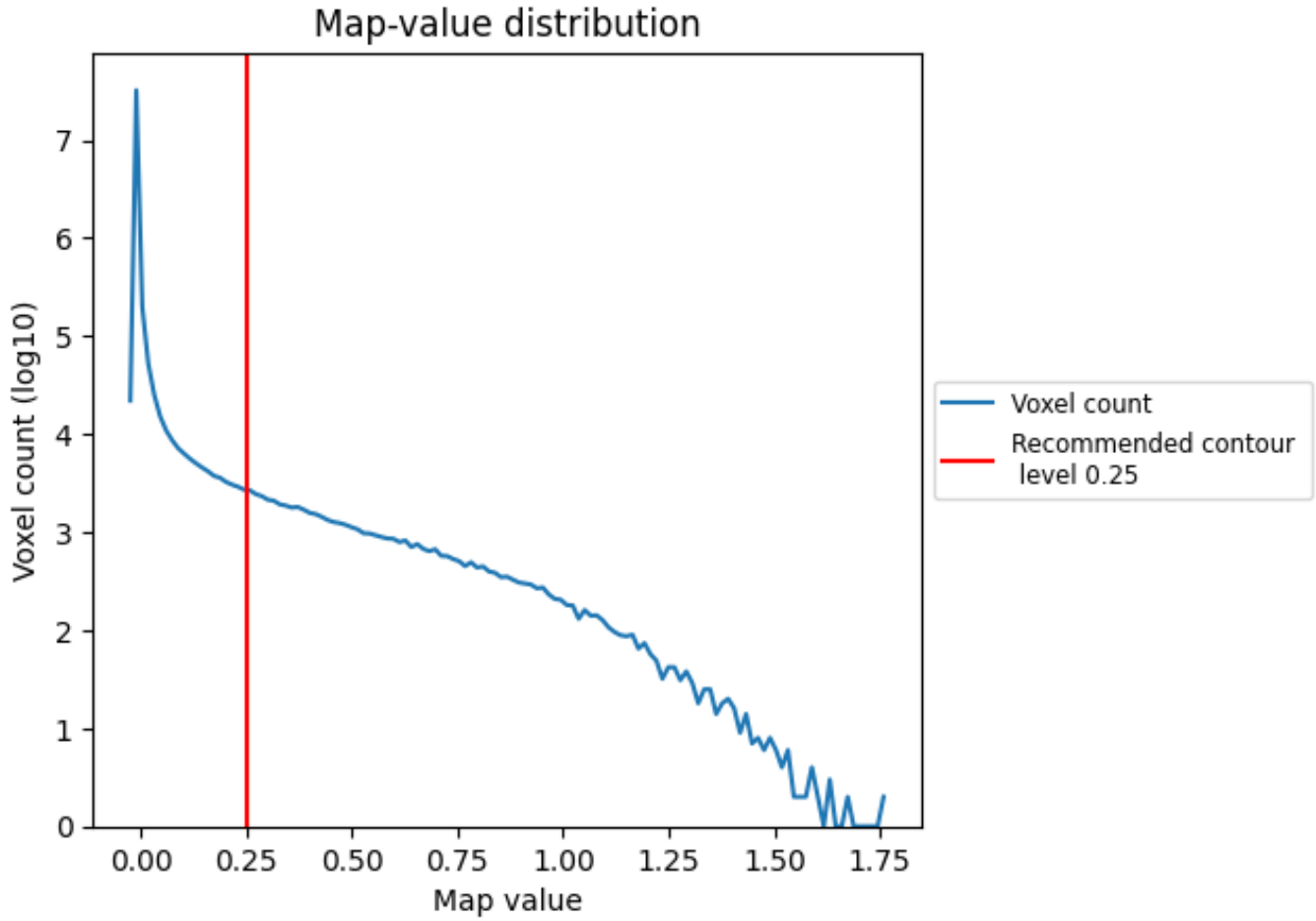


Z

7 Map analysis

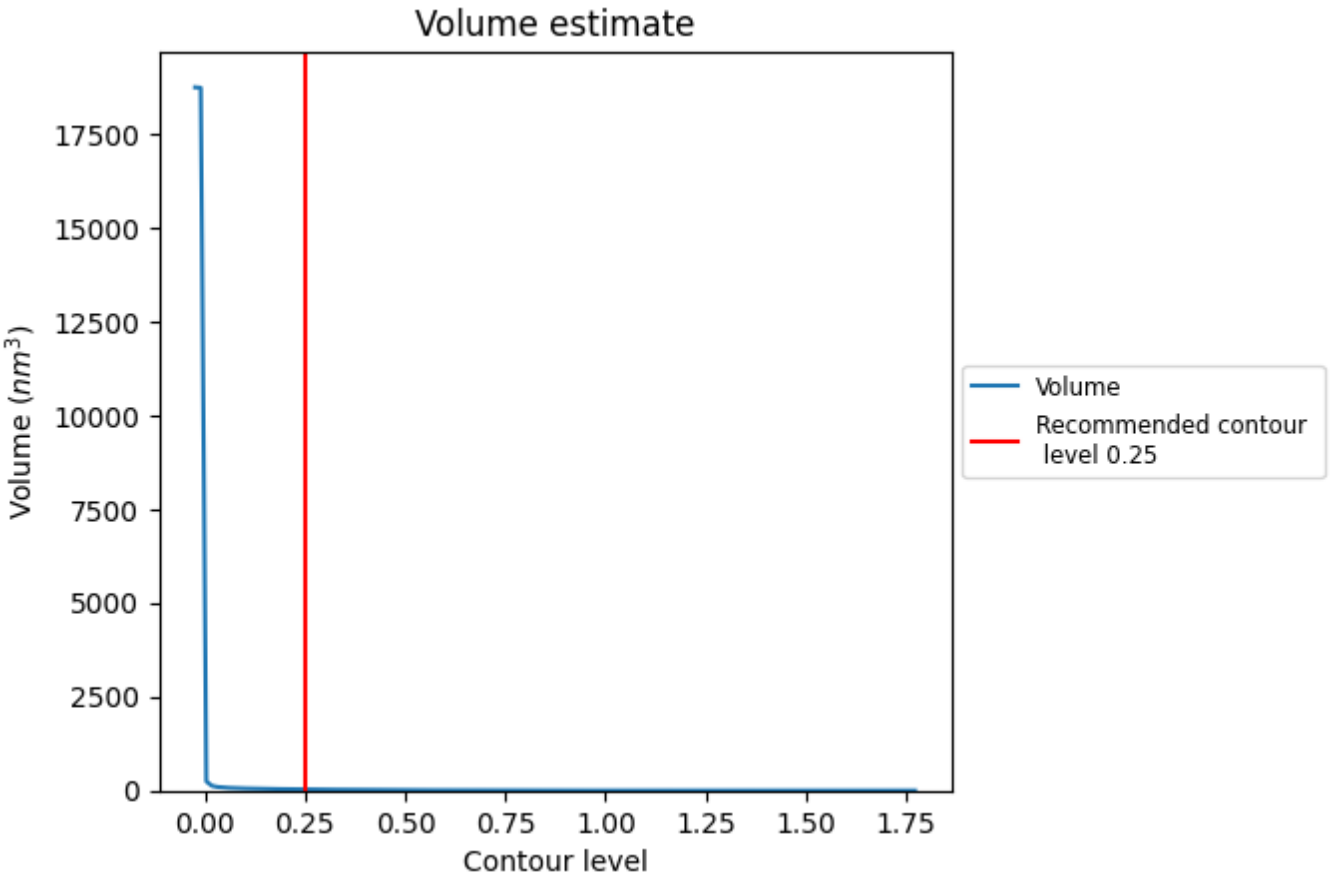
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

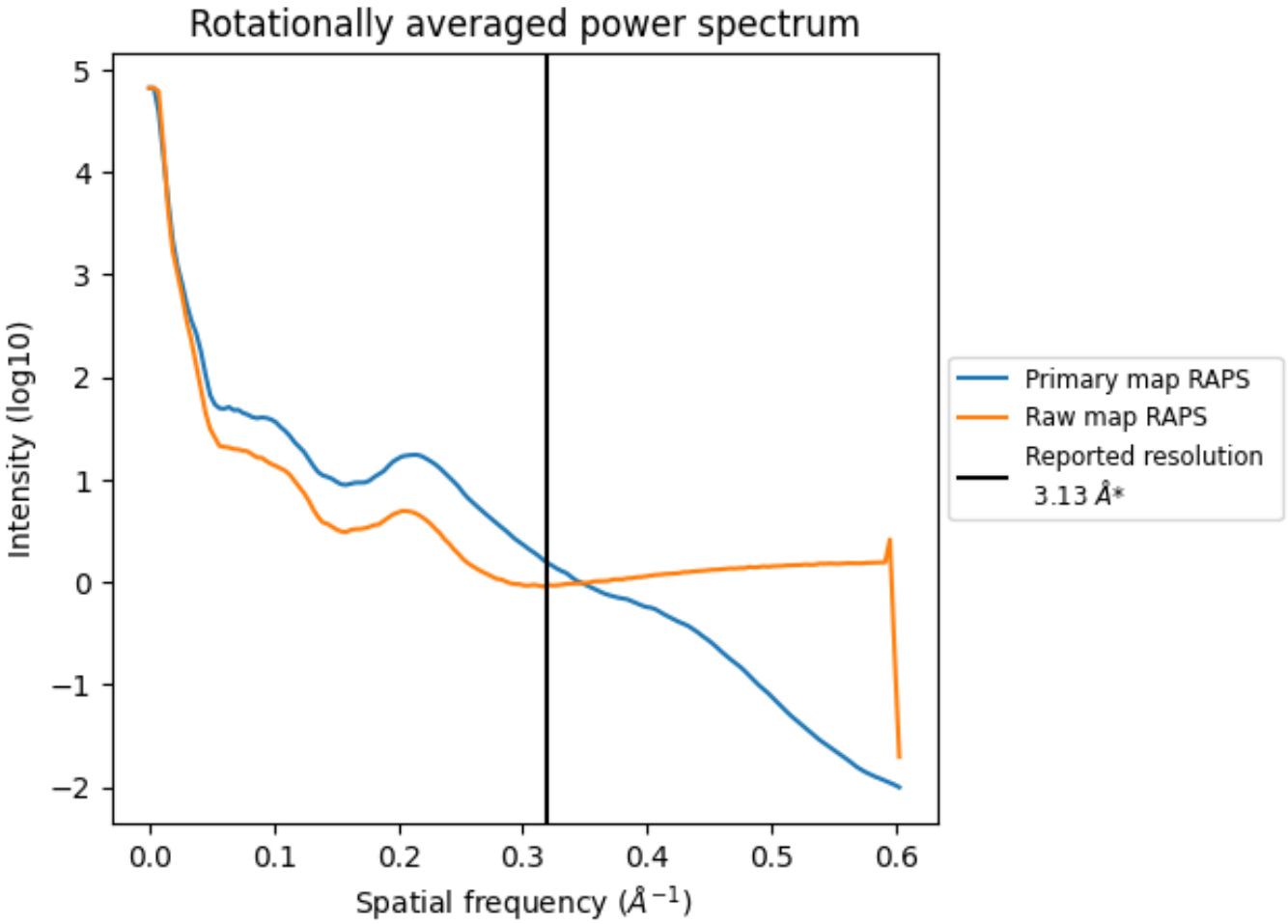
7.2 Volume estimate



The volume at the recommended contour level is 31 nm^3; this corresponds to an approximate mass of 28 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)

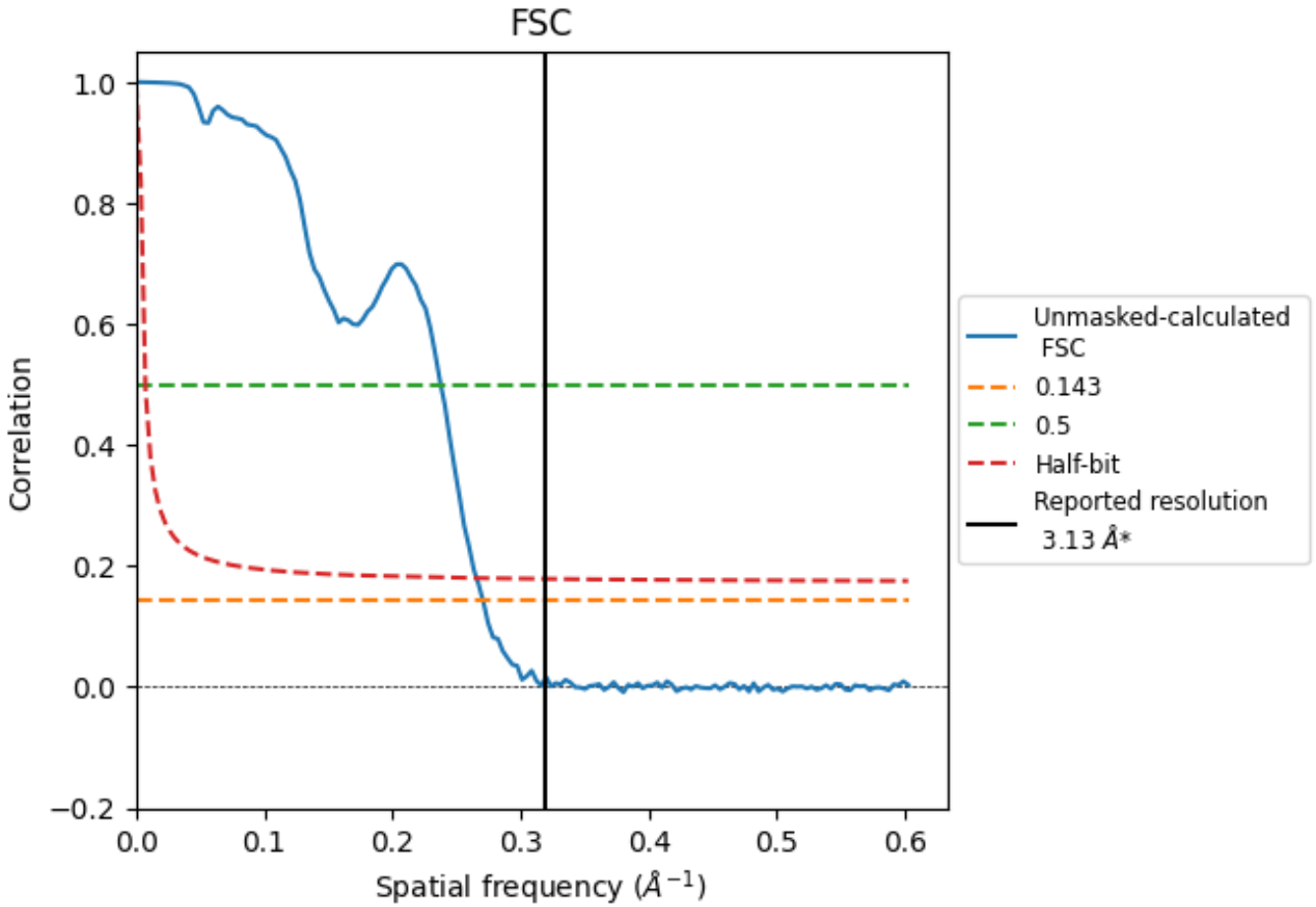


*Reported resolution corresponds to spatial frequency of 0.319 Å^{-1}

8 Fourier-Shell correlation

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

8.1 FSC



*Reported resolution corresponds to spatial frequency of 0.319 Å^{-1}

8.2 Resolution estimates (i)

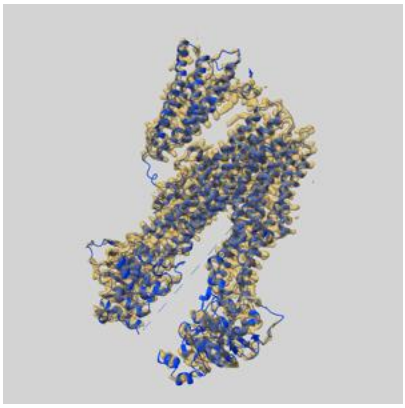
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.13	-	-
Author-provided FSC curve	-	-	-
Unmasked-calculated*	3.69	4.21	3.76

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps. The value from deposited half-maps intersecting FSC 0.143 CUT-OFF 3.69 differs from the reported value 3.13 by more than 10 %

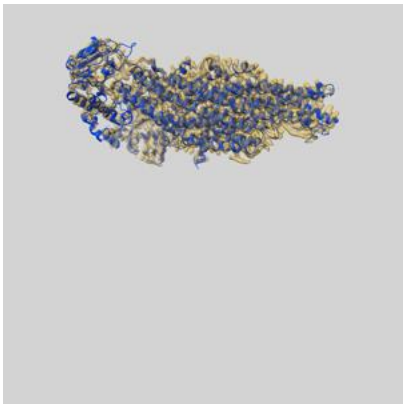
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-61270 and PDB model 9J9F. Per-residue inclusion information can be found in section 3 on page 4.

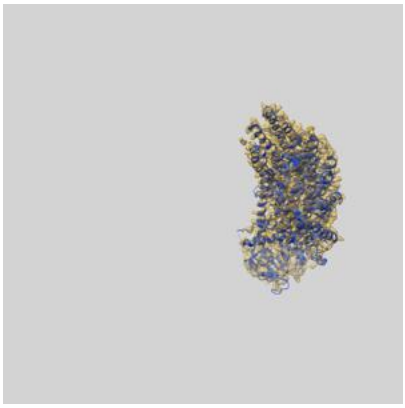
9.1 Map-model overlay



X



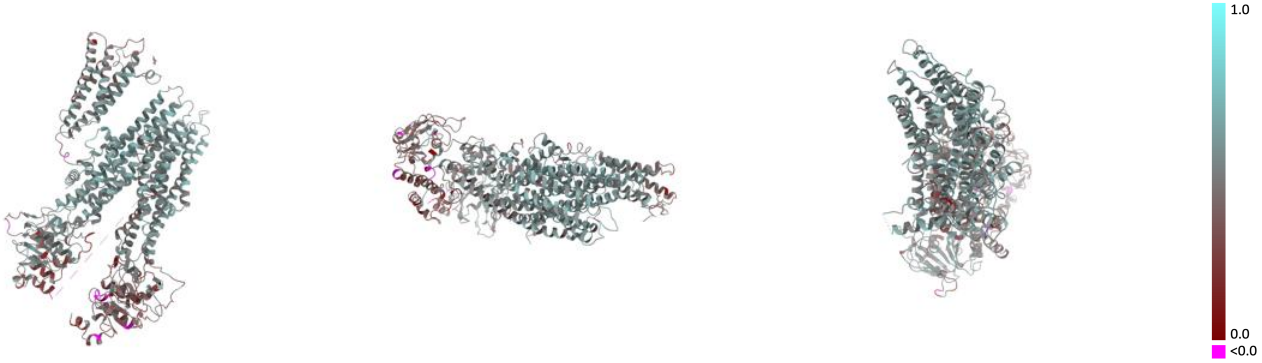
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.25 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.

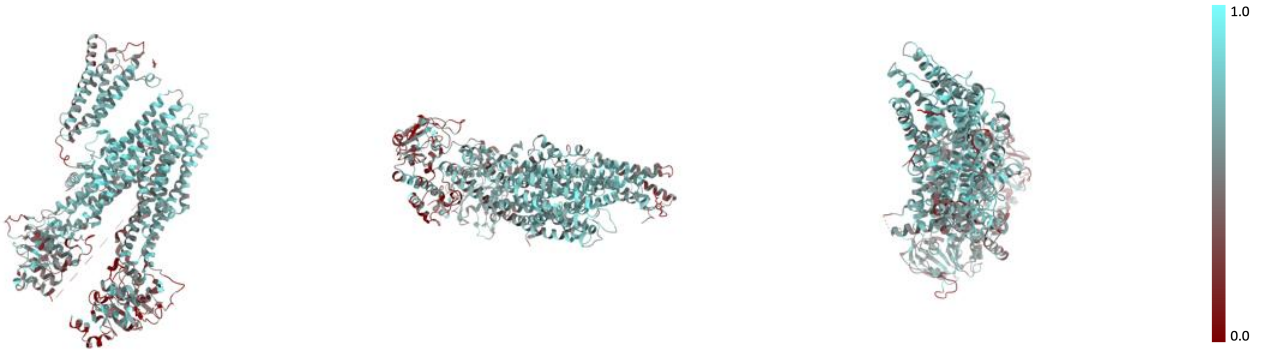
9.2 Q-score mapped to coordinate model (i)



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.

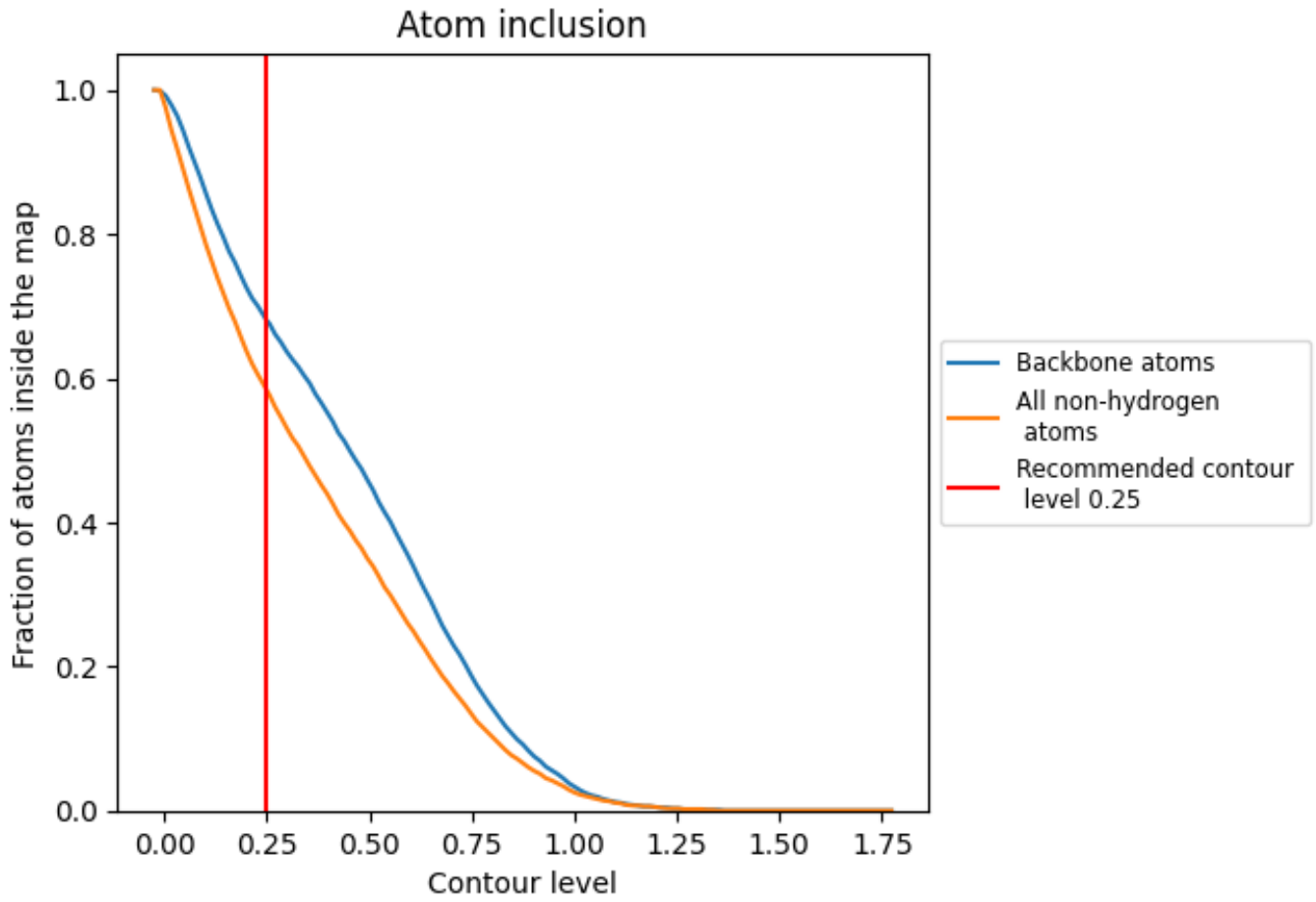
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.25).

9.4 Atom inclusion (i)



At the recommended contour level, 68% of all backbone atoms, 58% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary (i)

The table lists the average atom inclusion at the recommended contour level (0.25) and Q-score for the entire model and for each chain.



Chain	Atom inclusion	Q-score
All	0.5830	0.4930
A	0.5830	0.4930