Full wwPDB EM Validation Report ⓘ

Jun 3, 2025 – 10:27 AM EDT

PDB ID	:	9NWD / pdb_00009nwd
EMDB ID	:	EMD-46688
Title	:	Human E3 ligase UBR4-KCMF1-calmodulin complex (N-terminal)
Authors	:	Yang, Z.; Haakonsen, D.L.; Heider, M.; Witus, S.R.; Zelter, A.; Beschauner, T.; MacCoss, M.J.; Rape, M.
Deposited on	:	2025-03-22
Resolution	:	3.40 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:

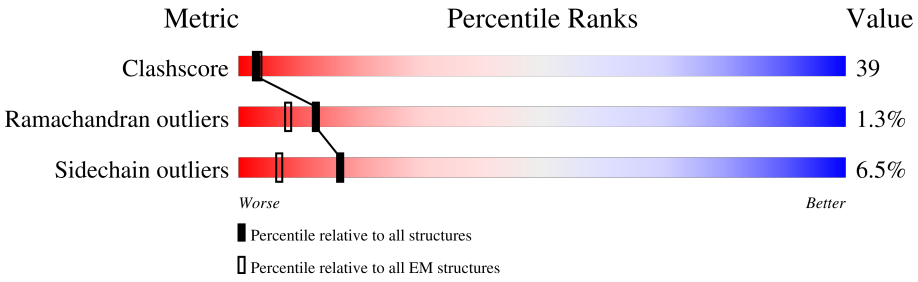
EMDB validation analysis	:	0.0.1.dev118
MolProbity	:	4-5-2 with Phenix2.0rc1
Percentile statistics	:	20231227.v01 (using entries in the PDB archive December 27th 2023)
MapQ	:	1.9.13
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.43.1

1 Overall quality at a glance (i)

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

The reported resolution of this entry is 3.40 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	210492	15764
Ramachandran outliers	207382	16835
Sidechain outliers	206894	16415

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	5183	11% 14% · 73%
1	B	5183	12% 12% · 73%

2 Entry composition (i)

There is only 1 type of molecule in this entry. The entry contains 21667 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 E3 ubiquitin-protein ligase UBR4.

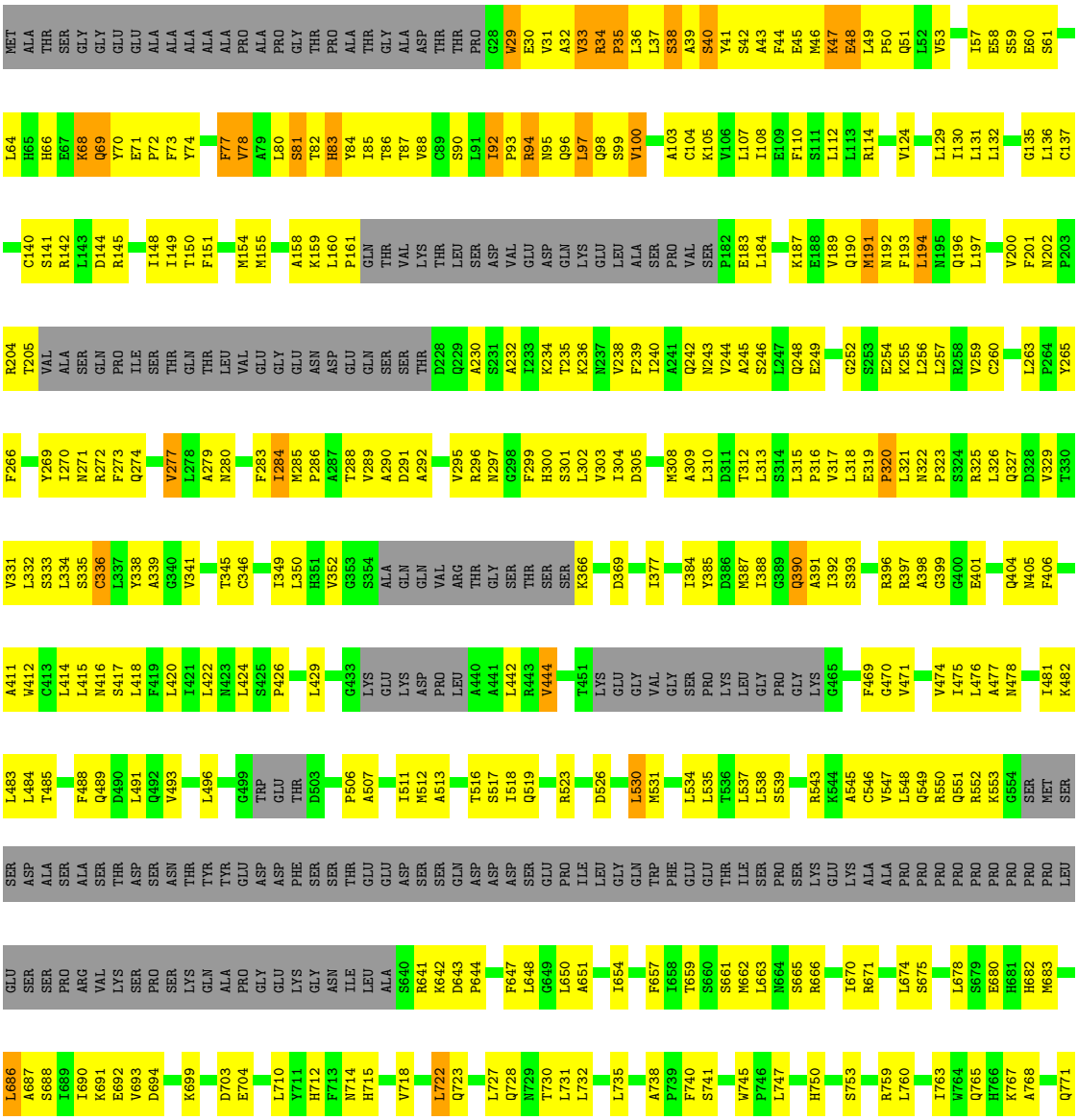
Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	1396	Total	C	N	O	S	0	0
			10853	6909	1833	2049	62		
1	B	1387	Total	C	N	O	S	0	0
			10814	6883	1831	2038	62		

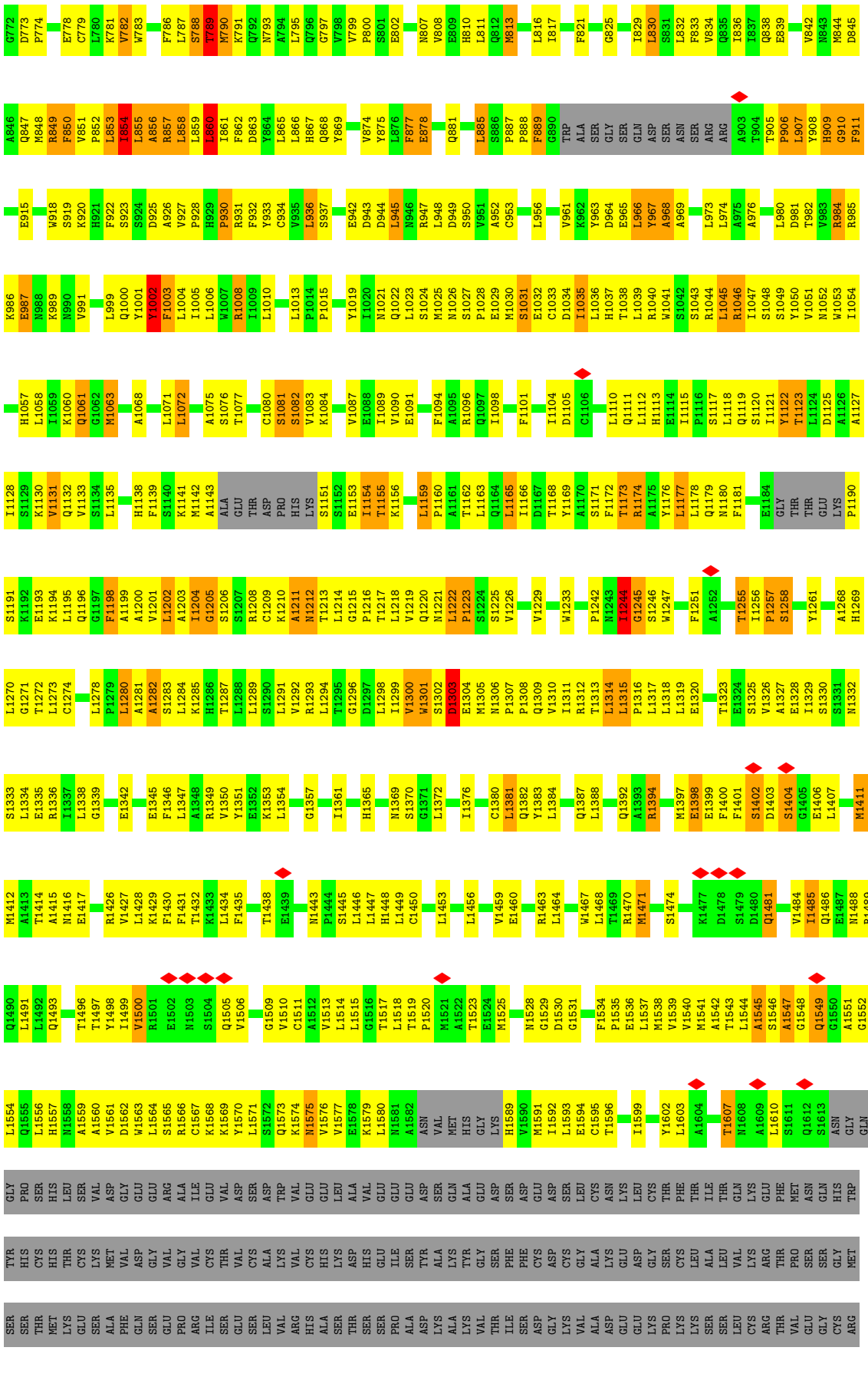
3 Residue-property plots (i)

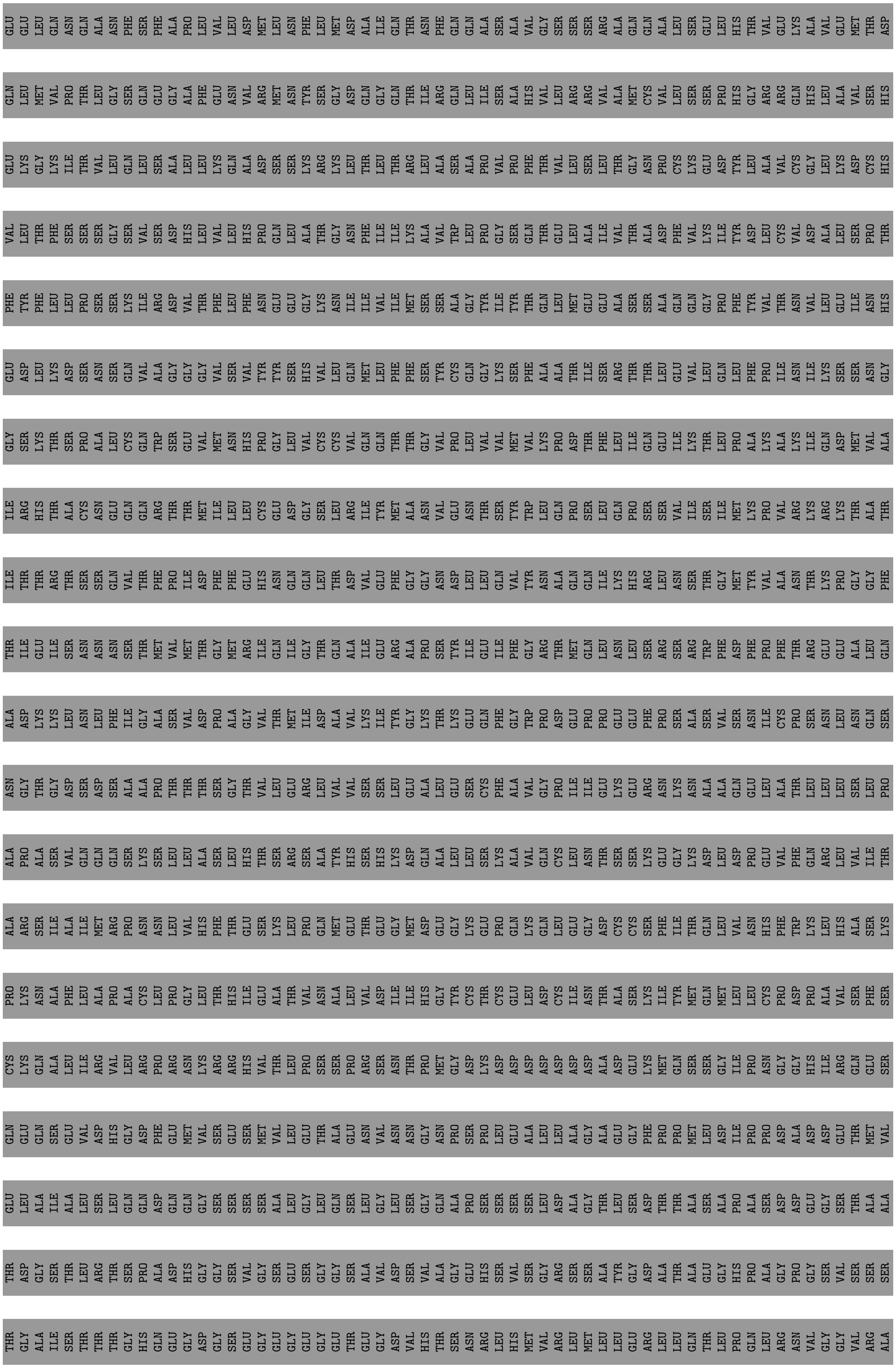
These plots are drawn for all protein, RNA, DNA and oligosaccharide chains in the entry. The first graphic for a chain summarises the proportions of the various outlier classes displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and atom inclusion 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: E3 ubiquitin-protein ligase UBR4

Chain A:






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

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

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

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

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

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

ASP ASP SER VAL LEU TYR PHE LEU LEU GLN VAL SER PHE LEU VAL ASP GLU GLY VAL SER PRO VAL LEU LEU GLN LEU LEU SER CYS ALA LEU CYS GLY SER LYS VAL LEU ALA ALA LEU ALA ALA SER SER GLY SER SER ALA SER SER SER SER ALA PRO VAL ALA ALA SER SER

GLY GLN ALA THR THR GLN SER LYS SER SER THR LYS LYS SER LYS LYS GLU GLU LYS GLU LYS GLU LYS ASP GLY GLU THR SER GLY SER GLN GLU ASP GLN LEU CYS THR ALA LEU VAL ASN GLN LEU ASN LYS PHE ALA ASP LYS GLU THR LEU ILE GLN PHE LEU ARG CYS PHE LEU

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

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

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

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

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

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

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

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

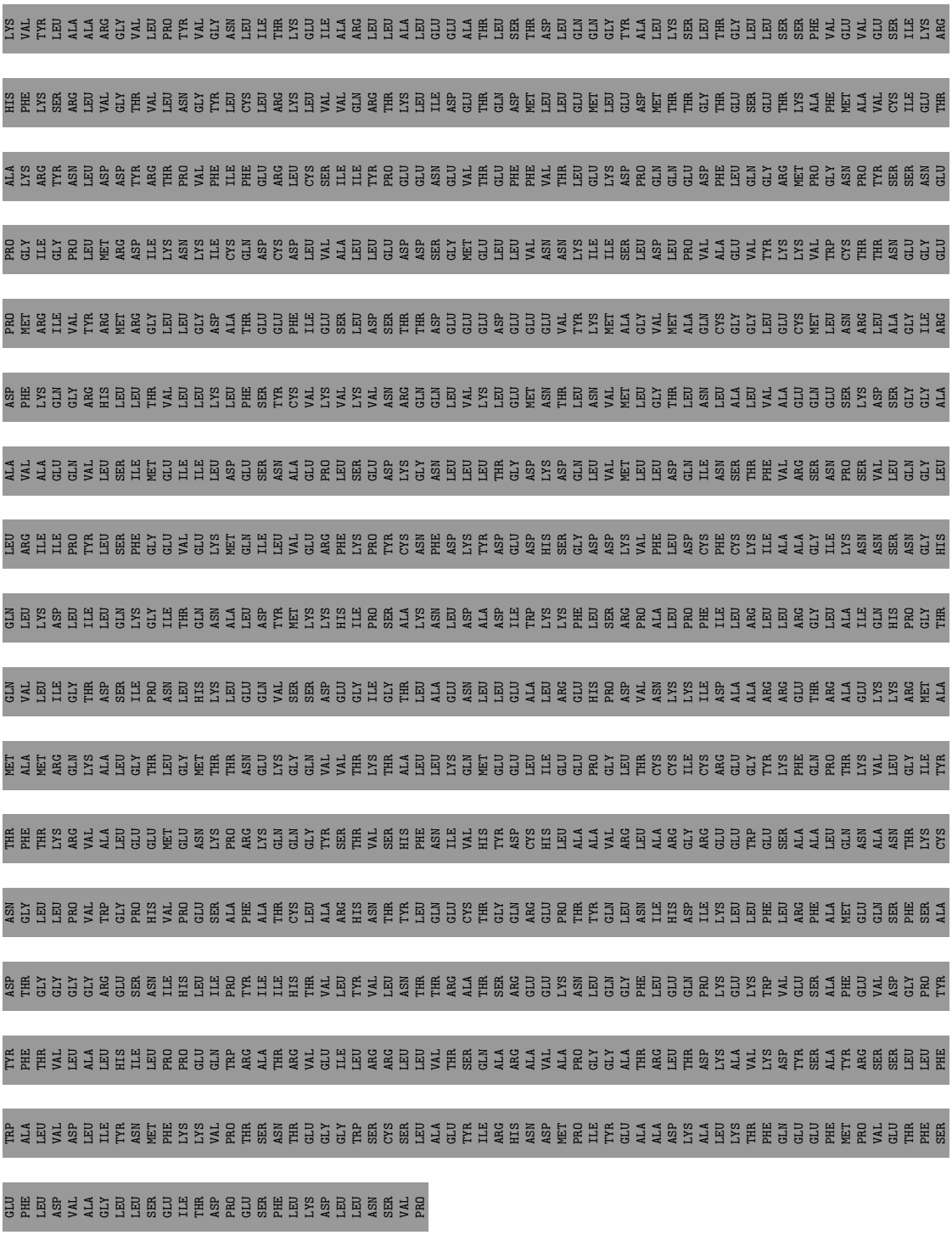
ARG HIS ILE LEU VAL SER GLN GLY LEU ILE ARG GLU LEU PHE ASP TYR ASN LEU ARG ARG GLY ALA ALA ALA MET ARG GLU GLU VAL ARG GLN LEU MET CYS LEU LEU THR ARG ASP ASN PRO GLU ALA THR GLN GLN MET ASN ASP LEU ILE ILE GLY LYS VAL SER THR ALA LEU LYS

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

LEU ARG ILE LEU GLN LYS LEU ILE LYS PRO PRO ALA PRO THR SER LYS LYS ASN LYS ASP VAL PRO VAL GLU ALA LEU THR THR VAL LYS PRO TYR CYS ASN GLU ILE HIS ALA GLN ALA GLN LEU TRP LEU LYS ARG ASP PRO LYS ALA SER TYR ASP ALA TRP LYS LYS CYS LEU PRO

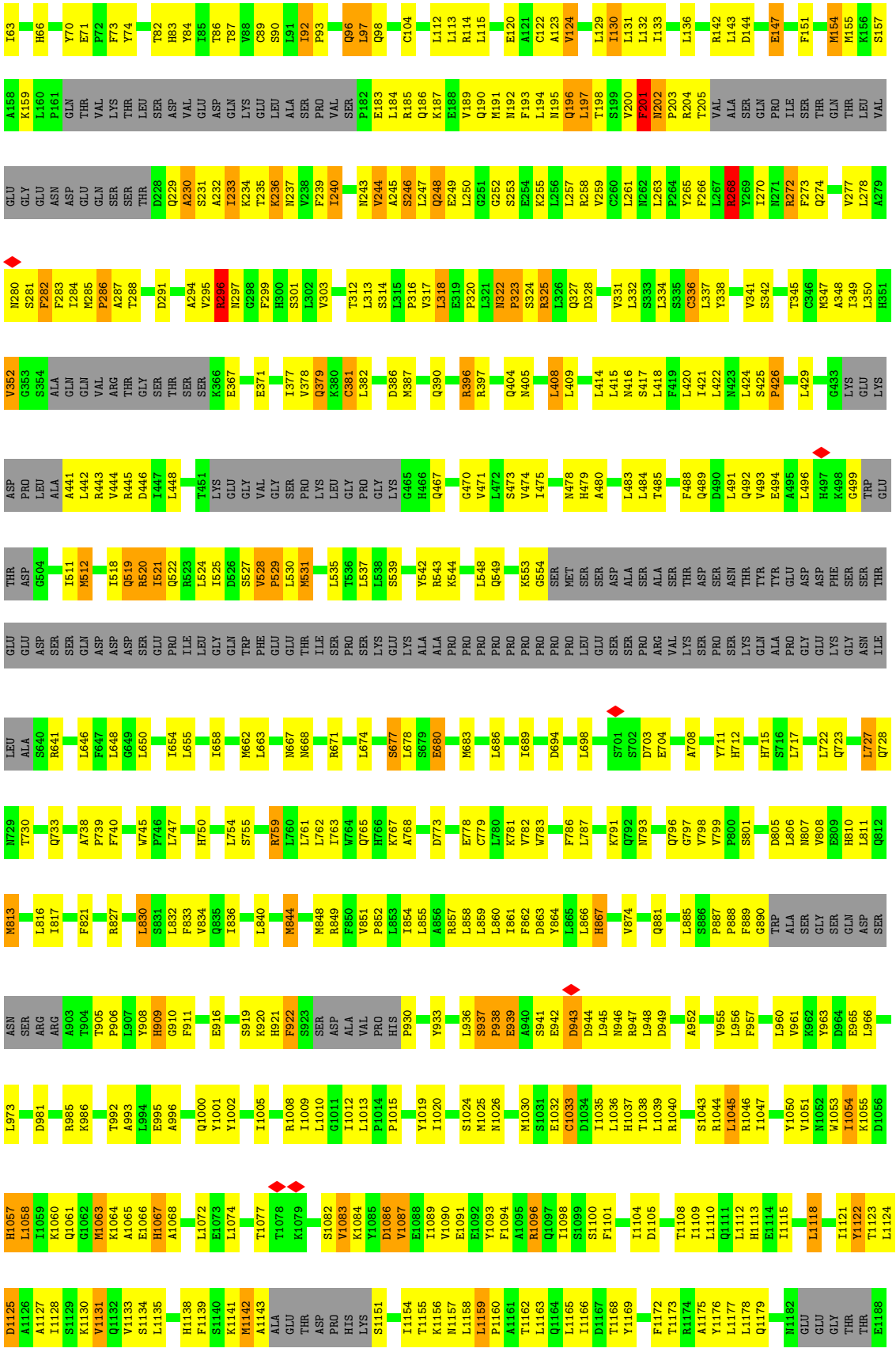
ILE ARG GLY ILE ASP GLY ASN GLY LYS ALA PRO SER LYS SER GLU LEU ARG HIS LEU TYR LEU THR GLU LYS TYR VAL TRP ARG TRP LYS GLN PHE LEU SER ARG ARG GLY LYS ARG THR SER PRO LEU ASP LEU LYS LEU GLY HIS ASN ASN TRP LEU ARG GLN VAL LEU PHE THR PRO

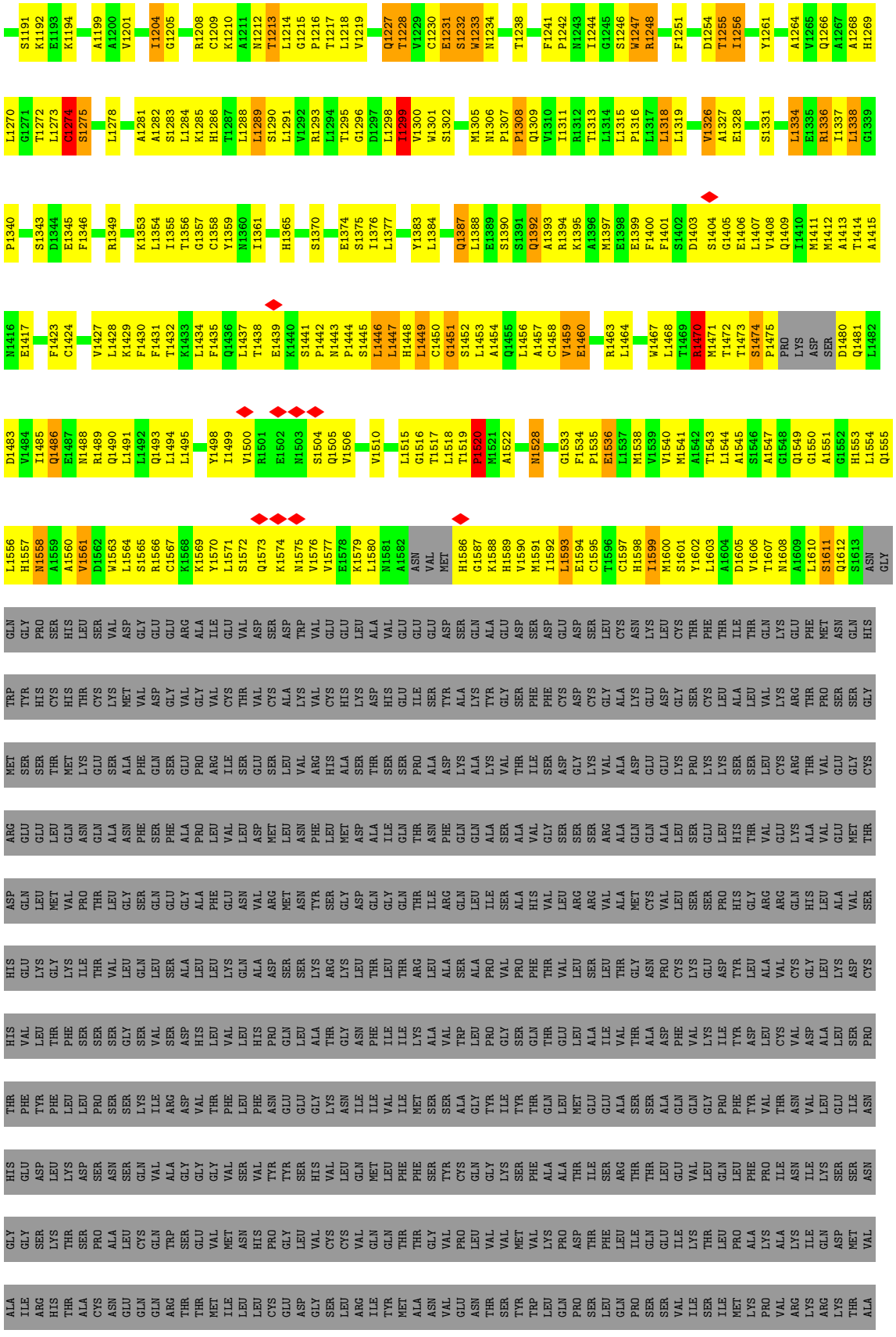
ALA THR GLN ALA ALA ARG GLN ALA ALA CYS THR ILE VAL GLU GLN ALA LEU ALA THR ILE PRO SER ARG LYS GLN GLN VAL LEU ASP LEU LEU THR SER TYR LEU ASP GLU LEU SER ILE ALA GLY GLU CYS ALA ALA GLU TYR LEU ALA LEU TYR GLN LYS LEU ILE THR SER ALA HIS TRP



• Molecule 1: E3 ubiquitin-protein ligase UBR4

Chain B:

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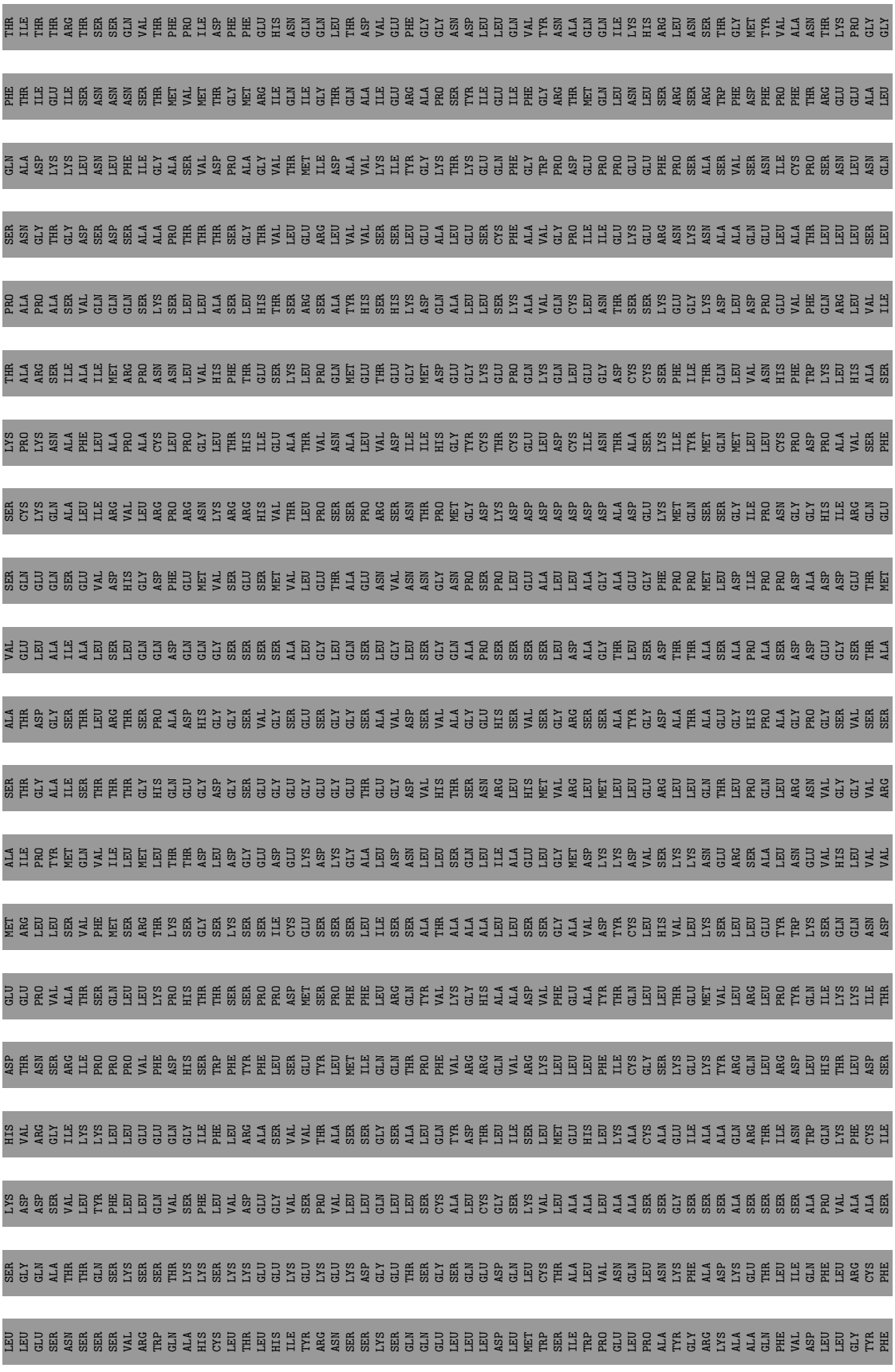
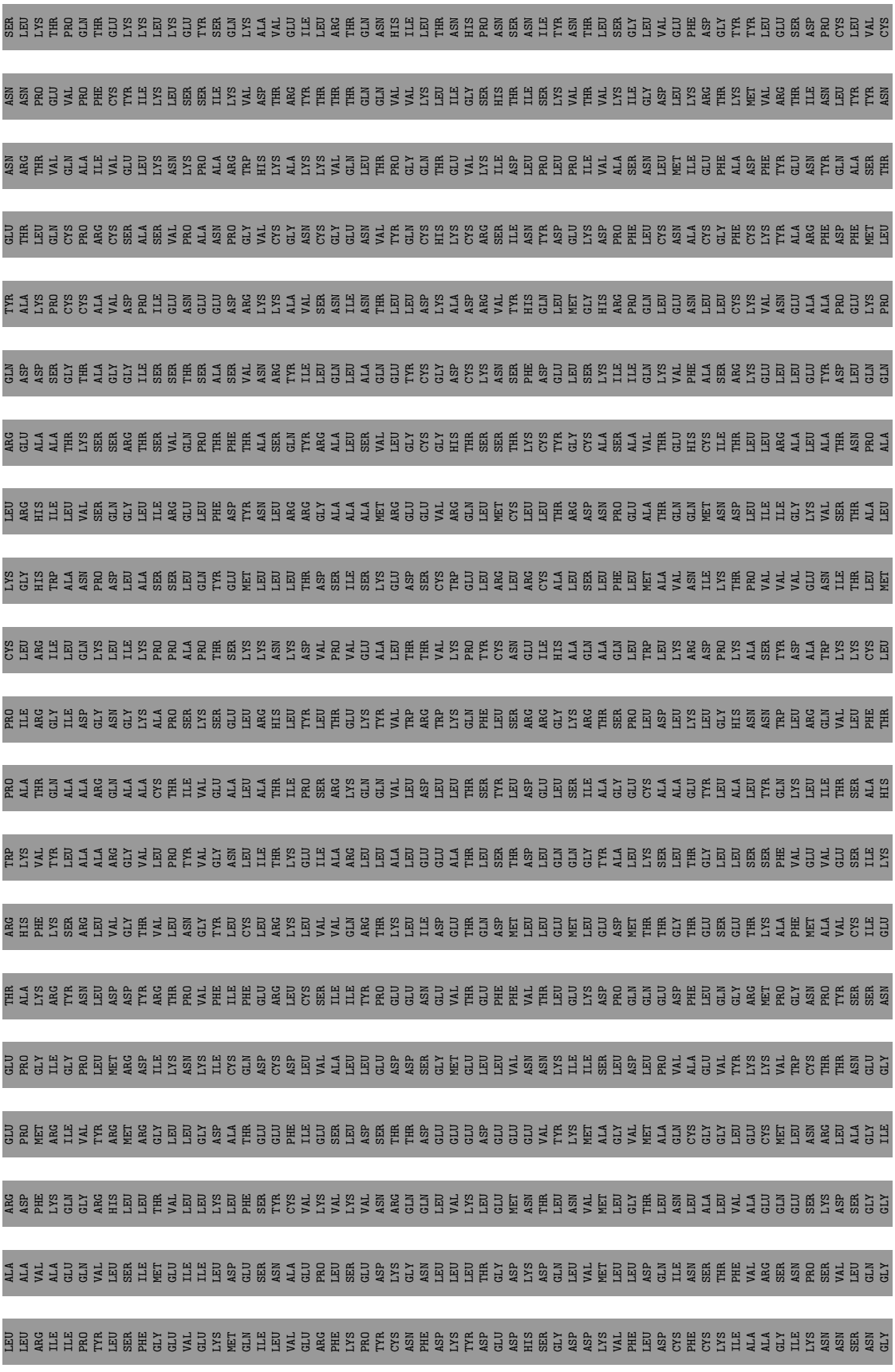
L1270 G1271 T1272 L1273 C1274 S1275 L1278 A1281 A1282 S1283 L1284 K1285 H1286 T1287 L1288 L1289 S1290 L1291 V1292 R1293 L1294 T1295 G1296 D1297 L1298 I1299 V1300 W1301 S1302 M1305 N1306 P1307 P1308 Q1309 V1310 I1311 R1312 T1313 L1314 L1315 P1316 L1317 L1318 L1319 V1326 A1327 E1328 S1331 L1334 E1335 R1336 I1337 L1338 G1339
P1340 S1343 D1344 E1345 F1346 R1349 K1353 L1354 I1355 T1356 G1357 C1358 Y1359 N1360 I1361 H1365 S1370 E1374 S1375 I1376 L1377 Y1383 L1384 Q1387 L1388 E1389 S1390 S1391 Q1392 A1393 R1394 K1395 A1396 M1397 E1398 E1399 F1400 F1401 S1402 D1403 S1404 G1405 E1406 L1407 V1408 Q1409 I1410 M1411 M1412 A1413 T1414 A1415
N1416 E1417 F1423 C1424 V1427 L1428 K1429 F1430 F1431 T1432 K1433 L1434 F1435 Q1436 L1437 T1438 E1439 K1440 S1441 P1442 N1443 P1444 S1445 L1446 L1447 H1448 L1449 C1450 G1451 S1452 L1453 A1454 Q1455 L1456 A1457 C1458 V1459 E1460 R1463 L1464 W1467 L1468 T1469 R1470 M1471 T1472 T1473 S1474 P1475 PRO LYS ASP SER D1480 Q1481 L1482
D1483 V1484 I1485 Q1486 E1487 N1488 R1489 Q1490 L1491 L1492 Q1493 L1494 L1495 Y1498 I1499 V1500 R1501 E1502 N1503 S1504 Q1505 V1506 V1510 L1515 G1516 T1517 L1518 T1519 P1520 M1521 A1522 N1528 G1533 F1534 P1535 E1536 L1537 M1538 Y1539 V1540 M1541 A1542 T1543 L1544 A1545 S1546 A1547 G1548 Q1549 G1550 A1551 G1552 H1553 L1554 Q1555
L1556 H1557 N1558 A1559 A1560 V1561 D1562 W1563 L1564 S1565 R1566 C1567 K1568 K1569 Y1570 L1571 S1572 Q1573 K1574 N1575 V1576 V1577 E1578 K1579 L1580 N1581 A1582 ASN VAL MET H1586 G1587 K1588 H1589 V1590 M1591 I1592 L1593 E1594 C1595 T1596 C1597 H1598 T1599 M1600 S1601 Y1602 L1603 A1604 D1605 V1606 T1607 N1608 A1609 L1610 S1611 Q1612 S1613 ASN GLY
GLN GLY PRO SER HIS LEU SER VAL ASP GLY GLU GLU ARG ALA ILE GLU VAL ASP SER ASP TRP VAL GLU GLU LEU ALA VAL GLU GLU GLU ASP SER GLN ALA GLU ASP SER ASP GLU ASP SER LEU CYS ASN LYS LEU CYS THR PHE THR ILE LEU ALA LYS GLU ASP GLY SER CYS LEU LEU ALA LEU VAL LYS ARG THR PRO SER GLY
TRP TYR HIS CYS HIS THR CYS CYS LYS MET VAL ASP GLY VAL GLY VAL CYS THR VAL CYS ALA LYS VAL CYS HIS LYS ASP HIS GLU ILE SER TYR ALA LYS TYR GLY GLY SER PHE PHE CYS ASP CYS GLY ALA LYS GLU ASP GLY SER CYS LEU LEU ALA LEU VAL LYS ARG THR PRO SER GLY
MET SER SER THR MET LYS GLU SER ALA PHE GLN SER GLU PRO ARG ILE SER GLU SER LEU VAL ARG HIS ALA SER THR SER SER PRO ALA ASP LYS GLY LYS VAL ALA ASP GLU GLU LYS PRO LYS LYS SER LEU CYS ARG THR PRO VAL GLU GLY
ARG GLU GLU LEU GLN ASN GLN ALA ASN PHE SER PHE ALA PRO LEU VAL LEU ASP MET LEU ASN PHE LEU MET ASP ALA ILE GLN THR ASN PHE GLN GLN GLN ALA SER ALA VAL GLY SER SER SER ARG ALA ALA GLN GLN ALA LEU SER GLU LEU HIS THR VAL GLU LYS ALA ARG GLN HIS LEU ALA VAL GLU MET THR
ASP GLN LEU MET VAL PRO THR LEU GLY SER GLN GLU GLY ALA PHE GLU ASN VAL ARG MET ASN TYR SER GLY ASP GLN GLY GLN THR THR ILE ARG GLN LEU ILE SER ALA HIS VAL LEU ARG SER ARG VAL ALA MET CYS VAL LEU SER SER PRO HIS GLY ARG ARG GLN HIS LEU VAL ALA ARG
HIS GLU LYS GLY LYS ILE THR LEU GLN LEU SER ALA LEU LEU LYS GLN ALA ASP SER SER LYS ARG LYS LEU THR LEU THR ARG LEU ALA SER ARG ALA PRO VAL PRO PHE THR VAL LEU SER SER LEU THR GLY ASN PRO CYS LYS GLU ASP TYR LEU ALA VAL ASP CYS
HIS VAL LEU THR PHE SER SER VAL SER GLY SER VAL SER ASP HIS LEU VAL LEU HIS PRO GLN LEU ALA THR GLY ASN PHE ILE ILE LYS ALA VAL PRO GLY SER GLN THR GLU LEU ALA ILE VAL THR ALA ASP PHE VAL LYS ILE TYR ASP LEU CYS VAL ASP SER
THR PHE TYR PHE LEU LEU PRO SER SER LYS ILE ARG ASP VAL THR PHE LEU PHE ASN GLU GLU GLY LYS ASN ILE ILE VAL ILE MET SER SER ALA GLY TYR GLN THR GLN LEU MET GLU GLU GLN GLY PRO PHE TYR VAL THR ASN VAL LEU ASN
HIS GLU ASP LEU LYS ASP SER GLN VAL ALA GLY GLY GLY VAL SER VAL LEU GLN MET LEU PHE PHE SER TYR CYS GLN GLY LYS SER PHE ALA ALA THR ILE SER ARG THR THR GLY VAL LEU GLN LEU PHE PRO ILE ASN ILE LYS SER SER ASN
GLY GLY SER LYS THR SER PRO ALA CYS GLN GLN TRP SER GLU VAL MET ASN HIS PRO GLY LEU GLN ILE TYR MET ALA ASN VAL GLU GLN THR THR GLY VAL PRO LEU VAL VAL LYS GLN ARG THR THR MET ILE LEU LEU CYS GLN ASP GLY SER LEU ARG ILE TYR TRP LEU GLN PRO SER LEU GLN PHE LEU ILE LYS THR LEU PRO ALA LYS PRO VAL ALA ARG LYS ARG LYS THR ALA
ALA ILE ARG HIS THR ALA CYS ASN GLU GLN GLN ARG THR THR MET ILE LEU LEU CYS GLY GLU ASP GLY SER LEU ARG ILE TYR TRP LEU GLN PRO SER LEU GLN PHE LEU ILE LYS THR LEU PRO ALA LYS PRO VAL ALA ARG LYS ARG LYS THR ALA





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

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

ALA MET ALA MET ARG GLN LYS ALA LEU GLY THR LEU GLY MET THR THR ASN GLU LYS GLY GLN VAL VAL THR LYS THR ALA LEU LEU LYS GLN MET GLU GLU LEU ILE GLU GLU PRO GLY LEU THR CYS CYS ILE CYS ARG GLU GLY TYR LYS PHE GLN PRO THR LYS VAL LEU GLY ILE

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

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

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

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

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

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

4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	126259	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING ONLY	Depositor
Microscope	TFS KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	50	Depositor
Minimum defocus (nm)	1000	Depositor
Maximum defocus (nm)	2200	Depositor
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.801	Depositor
Minimum map value	-0.495	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.014	Depositor
Recommended contour level	0.068	Depositor
Map size (Å)	432.64, 432.64, 432.64	wwPDB
Map dimensions	520, 520, 520	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.832, 0.832, 0.832	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	0.89	21/11051 (0.2%)	1.14	66/15000 (0.4%)
1	B	0.99	22/11008 (0.2%)	1.26	65/14932 (0.4%)
All	All	0.95	43/22059 (0.2%)	1.20	131/29932 (0.4%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	4
1	B	0	12
All	All	0	16

All (43) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	878	GLU	CA-C	-8.95	1.41	1.52
1	A	789	THR	CA-C	-8.80	1.41	1.52
1	A	855	LEU	CA-C	-8.66	1.40	1.52
1	A	858	LEU	CA-C	-8.53	1.41	1.52
1	A	782	VAL	CA-C	-8.30	1.42	1.52
1	A	877	PHE	N-CA	-7.87	1.36	1.46
1	A	78	VAL	C-O	-7.66	1.15	1.24
1	B	244	VAL	CA-C	-7.50	1.43	1.52
1	B	1441	SER	C-N	7.38	1.42	1.33
1	A	877	PHE	CA-C	-7.35	1.43	1.52
1	A	782	VAL	CA-CB	-6.99	1.46	1.54
1	A	789	THR	CA-CB	-6.89	1.42	1.53
1	B	518	ILE	C-O	-6.72	1.16	1.24
1	B	1439	GLU	C-N	-6.58	1.25	1.33
1	B	248	GLN	N-CA	-6.03	1.39	1.46
1	B	1213	THR	C-O	5.88	1.32	1.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	850	PHE	C-N	5.86	1.40	1.33
1	B	1442	PRO	C-N	-5.85	1.25	1.32
1	A	858	LEU	C-N	-5.73	1.25	1.33
1	A	789	THR	N-CA	-5.73	1.39	1.46
1	B	1446	LEU	C-O	5.72	1.30	1.24
1	A	857	ARG	CA-CB	-5.70	1.44	1.53
1	A	968	ALA	CA-C	-5.69	1.45	1.52
1	B	246	SER	CA-C	-5.64	1.45	1.52
1	A	856	ALA	CA-CB	-5.57	1.44	1.53
1	B	1460	GLU	CA-C	-5.47	1.46	1.52
1	A	878	GLU	CA-CB	-5.44	1.44	1.53
1	B	529	PRO	N-CA	-5.43	1.40	1.47
1	B	236	LYS	CA-C	-5.43	1.45	1.52
1	B	196	GLN	CA-CB	-5.40	1.45	1.53
1	B	240	ILE	CA-C	-5.40	1.46	1.52
1	A	782	VAL	C-O	-5.38	1.18	1.24
1	B	519	GLN	C-N	-5.33	1.26	1.33
1	A	860	LEU	CA-CB	-5.27	1.45	1.53
1	B	520	ARG	N-CA	-5.20	1.40	1.46
1	B	519	GLN	CA-C	-5.13	1.45	1.52
1	A	855	LEU	C-O	-5.12	1.17	1.24
1	B	1232	SER	C-O	-5.12	1.18	1.24
1	A	967	TYR	CA-CB	-5.11	1.45	1.53
1	B	1233	TRP	CA-C	-5.08	1.45	1.52
1	B	1033	CYS	C-O	5.06	1.29	1.24
1	B	519	GLN	N-CA	-5.03	1.39	1.46
1	B	202	ASN	CA-C	-5.02	1.50	1.53

All (131) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	855	LEU	N-CA-C	-13.01	96.76	112.89
1	B	1451	GLY	N-CA-C	-12.54	98.98	114.16
1	A	789	THR	N-CA-C	-12.48	97.67	111.28
1	B	1083	VAL	N-CA-C	-12.02	96.91	110.62
1	A	860	LEU	N-CA-C	-11.29	98.99	111.07
1	A	34	ARG	CA-C-N	-10.40	108.17	119.19
1	A	34	ARG	C-N-CA	-10.40	108.17	119.19
1	B	1460	GLU	N-CA-C	-10.21	96.78	109.65
1	B	34	ARG	CA-C-N	-10.04	108.24	119.28
1	B	34	ARG	C-N-CA	-10.04	108.24	119.28
1	A	851	VAL	CA-C-N	-9.87	107.51	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	851	VAL	C-N-CA	-9.87	107.51	119.84
1	A	930	PRO	CB-CA-C	-9.71	103.71	111.87
1	A	1123	THR	N-CA-C	-9.26	101.19	111.28
1	B	236	LYS	N-CA-C	-8.79	101.62	111.82
1	A	877	PHE	CA-C-N	-8.66	108.68	120.28
1	A	877	PHE	C-N-CA	-8.66	108.68	120.28
1	A	968	ALA	CA-C-N	-8.58	108.78	120.28
1	A	968	ALA	C-N-CA	-8.58	108.78	120.28
1	B	282	PHE	N-CA-C	-8.45	96.85	110.20
1	A	782	VAL	N-CA-C	-8.15	102.60	110.42
1	A	853	LEU	N-CA-C	-8.14	102.36	111.07
1	B	528	VAL	CA-C-N	-8.09	109.73	119.84
1	B	528	VAL	C-N-CA	-8.09	109.73	119.84
1	B	1520	PRO	CA-N-CD	-7.94	100.89	112.00
1	A	1282	ALA	N-CA-C	-7.83	102.99	112.54
1	B	248	GLN	N-CA-C	-7.79	101.91	111.33
1	A	1404	SER	N-CA-C	7.77	122.86	112.30
1	B	1299	ILE	N-CA-C	-7.55	103.58	111.58
1	A	966	LEU	N-CA-C	-7.48	103.41	112.54
1	A	782	VAL	CB-CA-C	-7.38	102.53	111.97
1	B	229	GLN	N-CA-C	-7.31	102.13	113.02
1	A	38	SER	N-CA-C	-7.24	103.42	111.82
1	A	33	VAL	N-CA-C	-7.23	101.47	111.89
1	B	1123	THR	N-CA-C	-7.18	103.46	111.28
1	A	35	PRO	N-CA-C	-7.17	104.18	113.57
1	B	33	VAL	N-CA-C	-7.13	101.62	111.89
1	A	789	THR	CB-CA-C	-7.12	98.96	110.79
1	A	1402	SER	N-CA-C	-7.09	103.59	111.82
1	B	1447	LEU	N-CA-C	-7.05	103.60	111.28
1	B	1561	VAL	CB-CA-C	-7.00	103.01	111.97
1	B	1449	LEU	CA-C-N	-6.89	109.53	121.66
1	B	1449	LEU	C-N-CA	-6.89	109.53	121.66
1	B	1441	SER	O-C-N	6.85	126.46	121.12
1	B	1057	HIS	CA-CB-CG	-6.76	107.04	113.80
1	A	1303	ASP	CB-CA-C	-6.63	108.92	116.54
1	A	1198	PHE	N-CA-C	-6.62	104.10	111.71
1	B	1058	LEU	N-CA-C	-6.61	104.00	111.07
1	A	1244	ILE	N-CA-C	6.59	123.05	109.34
1	A	29	TRP	N-CA-C	-6.58	104.11	111.28
1	A	967	TYR	N-CA-C	-6.52	104.25	111.36
1	A	47	LYS	N-CA-C	-6.34	105.70	113.50
1	A	81	SER	N-CA-C	-6.33	104.30	111.14

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	788	SER	N-CA-C	6.33	120.21	112.23
1	A	790	MET	N-CA-C	6.25	119.02	111.40
1	A	40	SER	N-CA-C	-6.19	104.53	111.28
1	B	35	PRO	N-CA-C	-6.19	105.30	113.65
1	B	231	SER	N-CA-C	-6.17	105.23	112.89
1	B	520	ARG	N-CA-C	-6.17	104.56	111.28
1	A	877	PHE	N-CA-C	-6.15	103.90	111.40
1	B	887	PRO	N-CA-C	6.15	118.20	110.70
1	A	390	GLN	N-CA-C	-6.13	104.59	111.28
1	A	854	ILE	N-CA-C	6.12	120.60	112.04
1	B	296	ARG	N-CA-C	-6.11	104.63	111.28
1	A	1255	THR	CB-CA-C	-6.10	109.52	116.54
1	A	1125	ASP	N-CA-C	-6.07	104.67	111.28
1	B	1227	GLN	N-CA-C	-6.06	104.30	111.03
1	A	1545	ALA	N-CA-C	-6.05	105.16	112.54
1	A	1082	SER	CA-C-N	-6.05	112.80	120.60
1	A	1082	SER	C-N-CA	-6.05	112.80	120.60
1	B	233	ILE	CB-CA-C	-5.98	104.31	111.97
1	A	194	LEU	N-CA-C	-5.95	105.12	112.38
1	B	531	MET	N-CA-C	-5.81	104.86	111.07
1	B	1248	ARG	CB-CA-C	-5.81	109.86	116.54
1	B	244	VAL	CB-CA-C	-5.77	104.26	112.22
1	A	1575	ASN	N-CA-C	-5.77	104.91	111.14
1	A	1381	LEU	N-CA-C	-5.74	105.02	111.28
1	B	1446	LEU	N-CA-C	-5.70	104.45	111.40
1	B	352	VAL	CA-C-N	-5.69	112.99	120.22
1	B	352	VAL	C-N-CA	-5.69	112.99	120.22
1	B	1125	ASP	N-CA-C	-5.69	105.08	111.28
1	A	77	PHE	N-CA-C	-5.65	104.81	110.97
1	A	991	VAL	O-C-N	-5.64	115.53	122.57
1	A	968	ALA	N-CA-C	5.57	117.35	111.28
1	B	1599	ILE	N-CA-C	-5.54	105.10	110.42
1	B	1413	ALA	N-CA-C	-5.54	105.33	111.36
1	B	336	CYS	N-CA-CB	5.53	118.74	110.22
1	A	46	MET	N-CA-C	-5.53	106.91	113.38
1	B	525	ILE	CB-CA-C	-5.53	103.15	112.16
1	B	230	ALA	N-CA-C	-5.52	105.53	114.09
1	A	1003	PHE	N-CA-C	-5.52	105.16	111.07
1	A	1155	THR	N-CA-C	-5.51	105.36	111.36
1	B	1100	SER	CA-C-N	-5.50	114.36	122.83
1	B	1100	SER	C-N-CA	-5.50	114.36	122.83
1	A	1081	SER	N-CA-C	-5.48	105.20	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	854	ILE	O-C-N	-5.46	114.90	122.05
1	B	965	GLU	N-CA-C	-5.46	106.56	113.43
1	B	519	GLN	CA-C-N	-5.46	112.97	120.28
1	B	519	GLN	C-N-CA	-5.46	112.97	120.28
1	B	1233	TRP	N-CA-C	-5.40	106.39	112.87
1	A	1002	TYR	CA-C-N	-5.39	113.43	120.44
1	A	1002	TYR	C-N-CA	-5.39	113.43	120.44
1	A	1547	ALA	N-CA-C	-5.32	105.88	112.38
1	B	1087	VAL	CA-C-O	-5.32	115.88	121.41
1	A	1315	LEU	CA-C-N	-5.32	113.15	119.05
1	A	1315	LEU	C-N-CA	-5.32	113.15	119.05
1	A	496	LEU	N-CA-C	5.31	117.57	110.35
1	A	853	LEU	CA-C-O	-5.31	115.25	120.82
1	B	192	ASN	N-CA-C	-5.31	105.91	112.38
1	B	314	SER	N-CA-C	-5.25	106.72	113.23
1	B	1444	PRO	N-CA-C	5.22	123.22	112.47
1	B	202	ASN	N-CA-C	-5.20	101.64	112.40
1	B	1065	ALA	N-CA-C	5.20	117.35	111.11
1	B	1449	LEU	CA-C-O	5.19	125.77	119.38
1	B	1086	ASP	N-CA-C	-5.18	105.32	110.97
1	A	48	GLU	N-CA-C	-5.18	107.01	113.38
1	B	201	PHE	CA-C-N	-5.17	118.13	123.10
1	B	201	PHE	C-N-CA	-5.17	118.13	123.10
1	B	268	ARG	CA-C-N	-5.17	113.35	120.28
1	B	268	ARG	C-N-CA	-5.17	113.35	120.28
1	A	83	HIS	CB-CA-C	-5.13	102.61	110.81
1	A	782	VAL	CA-C-N	-5.11	113.80	120.44
1	A	782	VAL	C-N-CA	-5.11	113.80	120.44
1	B	1611	SER	N-CA-C	-5.10	105.72	111.28
1	B	1157	ASN	N-CA-C	-5.09	105.73	111.28
1	A	887	PRO	N-CA-C	5.08	116.89	110.70
1	B	1558	ASN	N-CA-C	-5.05	105.85	111.36
1	B	1054	ILE	CA-C-O	-5.04	115.82	121.17
1	B	426	PRO	N-CA-C	-5.04	106.52	113.53
1	A	782	VAL	N-CA-CB	5.04	116.45	110.55
1	B	244	VAL	N-CA-C	-5.00	105.67	110.72

There are no chirality outliers.

All (16) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	1008	ARG	Sidechain

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Mol	Chain	Res	Type	Group
1	A	1174	ARG	Sidechain
1	A	1394	ARG	Sidechain
1	A	849	ARG	Sidechain
1	B	1008	ARG	Sidechain
1	B	1096	ARG	Sidechain
1	B	1336	ARG	Sidechain
1	B	1470	ARG	Sidechain
1	B	272	ARG	Sidechain
1	B	296	ARG	Sidechain
1	B	325	ARG	Sidechain
1	B	396	ARG	Sidechain
1	B	397	ARG	Sidechain
1	B	759	ARG	Sidechain
1	B	849	ARG	Sidechain
1	B	985	ARG	Sidechain

5.2 Too-close contacts (i)

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	10853	0	10929	945	0
1	B	10814	0	10915	803	0
All	All	21667	0	21844	1708	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 39.

All (1708) 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:B:313:LEU:HD11	1:B:332:LEU:CD2	1.51	1.36
1:B:89:CYS:SG	1:B:239:PHE:HD2	1.54	1.30
1:A:1399:GLU:O	1:A:1403:ASP:OD1	1.56	1.20
1:B:89:CYS:SG	1:B:239:PHE:CD2	2.32	1.20
1:A:73:PHE:CD1	1:A:159:LYS:HA	1.80	1.17
1:B:1205:GLY:HA3	1:B:1215:GLY:HA2	1.25	1.17

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:HIS:O	1:A:949:ASP:OD1	1.66	1.11
1:B:31:VAL:O	1:B:35:PRO:HD3	1.49	1.10
1:A:908:TYR:CE2	1:A:930:PRO:HB3	1.87	1.09
1:A:1450:CYS:HB2	1:A:1505:GLN:HB2	1.33	1.08
1:B:313:LEU:HD11	1:B:332:LEU:HD23	1.31	1.08
1:B:1205:GLY:HA3	1:B:1215:GLY:CA	1.83	1.07
1:B:313:LEU:HD11	1:B:332:LEU:HD21	1.31	1.05
1:B:910:GLY:HA2	1:B:933:TYR:HA	1.37	1.05
1:A:808:VAL:HG11	1:A:908:TYR:HB3	1.38	1.01
1:A:881:GLN:NE2	1:B:193:PHE:HA	1.75	1.01
1:B:1138:HIS:CD2	1:B:1143:ALA:HB3	1.96	0.99
1:A:32:ALA:O	1:A:35:PRO:HD2	1.63	0.98
1:B:352:VAL:HG22	1:B:467:GLN:HG2	1.43	0.98
1:A:349:ILE:HD12	1:A:429:LEU:HD11	1.42	0.98
1:B:263:LEU:HB2	1:B:266:PHE:HB2	1.45	0.97
1:B:313:LEU:CD1	1:B:332:LEU:CD2	2.41	0.97
1:A:53:VAL:HG11	1:A:99:SER:HB3	1.47	0.97
1:A:1087:VAL:HG21	1:A:1154:ILE:HD13	1.45	0.97
1:B:1090:VAL:HG13	1:B:1127:ALA:HB1	1.47	0.96
1:A:1500:VAL:HG22	1:A:1547:ALA:HB2	1.45	0.96
1:A:1438:THR:HA	1:A:1446:LEU:HD13	1.47	0.95
1:B:1159:LEU:HA	1:B:1298:LEU:HD13	1.48	0.95
1:A:1314:LEU:HG	1:A:1333:SER:HB2	1.47	0.94
1:B:1438:THR:OG1	1:B:1446:LEU:HB3	1.67	0.94
1:A:855:LEU:HD23	1:A:1002:TYR:HE2	1.32	0.94
1:A:868:GLN:HA	1:A:949:ASP:OD2	1.68	0.94
1:A:690:ILE:HA	1:A:710:LEU:HD21	1.51	0.92
1:A:1570:TYR:CD2	1:A:1592:ILE:HG21	2.05	0.92
1:B:318:LEU:HA	1:B:325:ARG:HH22	1.35	0.91
1:B:1486:GLN:HA	1:B:1489:ARG:HD2	1.52	0.91
1:B:313:LEU:CD1	1:B:332:LEU:HD21	1.99	0.90
1:B:1449:LEU:O	1:B:1452:SER:HB3	1.72	0.90
1:A:1541:MET:HA	1:A:1544:LEU:HD12	1.53	0.89
1:A:1417:GLU:HA	1:A:1470:ARG:HD2	1.54	0.89
1:B:1394:ARG:HA	1:B:1397:MET:HE2	1.53	0.89
1:A:1105:ASP:H	1:A:1110:LEU:HD21	1.37	0.88
1:B:32:ALA:O	1:B:35:PRO:HD2	1.74	0.88
1:A:193:PHE:HB2	1:B:881:GLN:HE21	1.38	0.88
1:A:910:GLY:HA2	1:A:933:TYR:HA	1.55	0.88
1:B:31:VAL:O	1:B:34:ARG:HB3	1.73	0.88
1:A:31:VAL:O	1:A:35:PRO:HD3	1.72	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:908:TYR:CZ	1:A:930:PRO:HB3	2.09	0.87
1:A:329:VAL:HG12	1:A:388:ILE:HG23	1.57	0.87
1:B:1205:GLY:CA	1:B:1215:GLY:CA	2.53	0.87
1:A:1453:LEU:HB3	1:A:1506:VAL:HG13	1.58	0.86
1:B:1493:GLN:HG2	1:B:1540:VAL:HG22	1.54	0.86
1:B:1205:GLY:CA	1:B:1215:GLY:HA3	2.06	0.86
1:A:1112:LEU:HD13	1:A:1179:GLN:HB2	1.57	0.86
1:A:1338:LEU:HD13	1:A:1346:PHE:HA	1.56	0.85
1:A:867:HIS:O	1:A:949:ASP:CG	2.18	0.85
1:A:687:ALA:HB2	1:A:731:LEU:HD12	1.58	0.84
1:A:1312:ARG:O	1:A:1316:PRO:HD2	1.77	0.84
1:B:1603:LEU:HA	1:B:1606:VAL:HB	1.58	0.84
1:A:31:VAL:O	1:A:34:ARG:HB3	1.77	0.83
1:B:1173:THR:HG22	1:B:1284:LEU:HD13	1.59	0.83
1:B:1414:THR:HG1	1:B:1423:PHE:HE2	1.26	0.83
1:A:193:PHE:HB2	1:B:881:GLN:NE2	1.93	0.82
1:B:910:GLY:CA	1:B:933:TYR:HA	2.09	0.82
1:A:420:LEU:HD22	1:A:442:LEU:HG	1.61	0.82
1:B:1138:HIS:NE2	1:B:1143:ALA:HB3	1.94	0.82
1:A:712:HIS:HA	1:A:715:HIS:CD2	2.15	0.82
1:B:1499:ILE:HG23	1:B:1506:VAL:HB	1.61	0.82
1:B:1407:LEU:HB3	1:B:1431:PHE:CE1	2.15	0.82
1:B:1412:MET:HB3	1:B:1463:ARG:NE	1.94	0.82
1:A:1546:SER:O	1:A:1549:GLN:HG3	1.79	0.81
1:A:73:PHE:HD1	1:A:159:LYS:HA	1.37	0.81
1:A:802:GLU:HG2	1:A:931:ARG:HD2	1.62	0.81
1:B:1407:LEU:HB3	1:B:1431:PHE:HE1	1.45	0.81
1:B:1475:PRO:HD3	1:B:1485:ILE:HD12	1.61	0.81
1:A:32:ALA:C	1:A:35:PRO:HD2	2.05	0.81
1:A:881:GLN:HE21	1:B:193:PHE:HA	1.42	0.81
1:A:124:VAL:HG12	1:A:129:LEU:HG	1.63	0.81
1:A:1545:ALA:HB2	1:A:1556:LEU:CB	2.12	0.80
1:A:868:GLN:CA	1:A:949:ASP:OD2	2.29	0.80
1:B:1077:THR:HG23	1:B:1082:SER:H	1.45	0.80
1:A:1191:SER:HB3	1:A:1194:LYS:HG3	1.62	0.80
1:A:1047:ILE:HD11	1:A:1256:ILE:CD1	2.11	0.79
1:A:131:LEU:HD11	1:A:142:ARG:HD2	1.64	0.79
1:A:659:THR:HA	1:A:663:LEU:HD12	1.63	0.79
1:A:1450:CYS:CB	1:A:1505:GLN:HB2	2.11	0.78
1:A:1515:LEU:HA	1:A:1544:LEU:HD13	1.66	0.78
1:A:68:LYS:HB3	1:A:70:TYR:HD2	1.48	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1451:GLY:O	1:B:1454:ALA:HB3	1.84	0.77
1:A:325:ARG:HH22	1:B:496:LEU:HD23	1.48	0.77
1:A:392:ILE:O	1:A:399:GLY:HA2	1.83	0.77
1:B:247:LEU:O	1:B:248:GLN:C	2.21	0.77
1:B:1438:THR:HA	1:B:1446:LEU:HD13	1.66	0.77
1:B:1046:ARG:HH22	1:B:1130:LYS:HZ1	1.31	0.77
1:A:787:LEU:HD12	1:A:832:LEU:HD23	1.67	0.77
1:A:1047:ILE:HD11	1:A:1256:ILE:HG12	1.67	0.77
1:B:910:GLY:HA2	1:B:933:TYR:CA	2.13	0.77
1:B:1453:LEU:O	1:B:1456:LEU:HB3	1.84	0.77
1:B:867:HIS:CD2	1:B:936:LEU:HD21	2.20	0.76
1:A:349:ILE:HG23	1:A:429:LEU:HD11	1.68	0.76
1:A:984:ARG:HH11	1:A:984:ARG:HB2	1.51	0.76
1:A:1190:PRO:HG2	1:A:1195:LEU:HD21	1.67	0.76
1:A:1567:CYS:SG	1:A:1596:THR:HG23	2.26	0.76
1:A:415:LEU:HD11	1:A:484:LEU:HD21	1.67	0.76
1:A:922:PHE:CZ	1:A:928:PRO:HD2	2.20	0.76
1:B:1407:LEU:H	1:B:1407:LEU:HD12	1.50	0.76
1:B:1414:THR:HG23	1:B:1423:PHE:HD2	1.50	0.76
1:B:1516:GLY:O	1:B:1520:PRO:HD2	1.84	0.76
1:A:909:HIS:O	1:A:934:CYS:HB3	1.85	0.76
1:B:1489:ARG:NH2	1:B:1533:GLY:HA2	2.01	0.75
1:B:1600:MET:HA	1:B:1603:LEU:HG	1.68	0.75
1:A:1315:LEU:HD22	1:A:1349:ARG:HB3	1.69	0.75
1:B:313:LEU:CD1	1:B:332:LEU:HD23	2.10	0.75
1:B:1238:THR:HG21	1:B:1286:HIS:N	2.02	0.75
1:A:1159:LEU:HB3	1:A:1160:PRO:HD3	1.67	0.75
1:B:1218:LEU:HD22	1:B:1376:ILE:HG23	1.68	0.75
1:A:1242:PRO:HB2	1:A:1261:TYR:CE1	2.21	0.74
1:B:425:SER:O	1:B:429:LEU:HG	1.86	0.74
1:B:860:LEU:HB2	1:B:1005:ILE:HD13	1.69	0.74
1:B:1408:VAL:HA	1:B:1411:MET:HE2	1.66	0.74
1:A:1548:GLY:HA3	1:A:1553:HIS:N	2.01	0.74
1:B:1550:GLY:O	1:B:1553:HIS:HB3	1.88	0.74
1:A:1398:GLU:HA	1:A:1449:LEU:HD21	1.67	0.74
1:A:1401:PHE:HB3	1:A:1407:LEU:HD12	1.68	0.74
1:B:1445:SER:HA	1:B:1448:HIS:ND1	2.03	0.74
1:B:1554:LEU:HA	1:B:1557:HIS:CD2	2.22	0.74
1:B:1557:HIS:O	1:B:1561:VAL:HG23	1.86	0.74
1:B:272:ARG:HD3	1:B:285:MET:HG3	1.70	0.74
1:A:1401:PHE:CD1	1:A:1407:LEU:HG	2.22	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1570:TYR:CG	1:A:1592:ILE:HG21	2.22	0.74
1:B:112:LEU:HD12	1:B:250:LEU:HD12	1.68	0.73
1:B:248:GLN:HE22	1:B:316:PRO:HB2	1.53	0.73
1:B:1201:VAL:HG13	1:B:1218:LEU:HB3	1.67	0.73
1:A:333:SER:HG	1:A:406:PHE:HZ	1.34	0.73
1:A:326:LEU:HG	1:A:511:ILE:HD12	1.70	0.73
1:A:1567:CYS:HB2	1:A:1596:THR:OG1	1.87	0.73
1:A:816:LEU:HD21	1:B:193:PHE:CZ	2.23	0.73
1:B:1039:LEU:HD22	1:B:1130:LYS:HD3	1.70	0.73
1:A:200:VAL:HB	1:B:715:HIS:CE1	2.23	0.73
1:A:1201:VAL:CG1	1:A:1222:LEU:HD11	2.17	0.73
1:A:874:VAL:HG13	1:B:189:VAL:HG21	1.69	0.73
1:A:284:ILE:HD12	1:A:442:LEU:HD23	1.70	0.73
1:A:1047:ILE:CG1	1:A:1256:ILE:HG12	2.19	0.73
1:A:945:LEU:HB3	1:A:1053:TRP:CD1	2.23	0.72
1:B:1515:LEU:HD12	1:B:1541:MET:HG3	1.71	0.72
1:A:73:PHE:CE1	1:A:159:LYS:HA	2.24	0.72
1:B:1204:ILE:HG21	1:B:1357:GLY:HA3	1.70	0.72
1:B:1299:ILE:HG13	1:B:1337:ILE:HD11	1.70	0.72
1:A:1201:VAL:HG11	1:A:1222:LEU:HD21	1.72	0.72
1:A:1047:ILE:HD11	1:A:1256:ILE:CG1	2.20	0.72
1:A:1500:VAL:HG21	1:A:1543:THR:O	1.90	0.72
1:A:420:LEU:HD21	1:A:444:VAL:HA	1.71	0.72
1:A:1518:LEU:HB3	1:A:1537:LEU:HD11	1.71	0.72
1:B:1415:ALA:HB2	1:B:1467:TRP:HB2	1.72	0.72
1:B:272:ARG:HD3	1:B:285:MET:CG	2.20	0.72
1:A:790:MET:HE3	1:A:858:LEU:CD2	2.20	0.71
1:A:881:GLN:HE21	1:B:193:PHE:HD2	1.38	0.71
1:A:97:LEU:HD12	1:A:235:THR:HG23	1.72	0.71
1:A:471:VAL:HG21	1:A:641:ARG:H	1.55	0.71
1:A:985:ARG:HH11	1:A:1280:LEU:HD13	1.54	0.71
1:A:816:LEU:HD21	1:B:193:PHE:HZ	1.53	0.71
1:A:869:TYR:N	1:A:949:ASP:OD2	2.23	0.71
1:A:881:GLN:NE2	1:B:193:PHE:HD2	1.89	0.71
1:B:97:LEU:HB3	1:B:201:PHE:HE2	1.56	0.71
1:B:273:PHE:CE1	1:B:334:LEU:HB3	2.25	0.71
1:A:31:VAL:O	1:A:35:PRO:CD	2.39	0.71
1:B:921:HIS:CD2	1:B:993:ALA:HB2	2.25	0.71
1:A:135:GLY:HA2	1:A:140:CYS:O	1.90	0.71
1:A:881:GLN:NE2	1:B:193:PHE:CA	2.52	0.70
1:B:1274:CYS:SG	1:B:1275:SER:N	2.64	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:244:VAL:HG22	1:A:316:PRO:HG2	1.74	0.70
1:A:329:VAL:HG12	1:A:388:ILE:CG2	2.20	0.70
1:A:1545:ALA:HB2	1:A:1556:LEU:HB3	1.74	0.70
1:A:1025:MET:HE3	1:A:1028:PRO:HD3	1.74	0.70
1:A:855:LEU:HD23	1:A:1002:TYR:CE2	2.23	0.70
1:A:82:THR:HB	1:A:132:LEU:HD22	1.74	0.70
1:A:926:ALA:O	1:A:928:PRO:HD3	1.92	0.70
1:B:193:PHE:CE1	1:B:197:LEU:HD11	2.26	0.70
1:A:92:ILE:HD12	1:A:97:LEU:HA	1.75	0.69
1:A:273:PHE:HD2	1:A:338:TYR:HB2	1.57	0.69
1:A:945:LEU:HD13	1:A:1053:TRP:HB2	1.73	0.69
1:B:408:LEU:HD22	1:B:520:ARG:HG2	1.73	0.69
1:A:1043:SER:HB3	1:A:1256:ILE:HG21	1.75	0.69
1:B:1247:TRP:CD1	1:B:1248:ARG:H	2.10	0.69
1:A:73:PHE:HD1	1:A:158:ALA:O	1.75	0.69
1:A:1335:GLU:HA	1:A:1339:GLY:O	1.93	0.69
1:A:1177:LEU:HG	1:A:1233:TRP:CD2	2.28	0.69
1:A:853:LEU:O	1:A:856:ALA:HB3	1.93	0.69
1:B:1338:LEU:HD13	1:B:1346:PHE:HA	1.74	0.69
1:B:1515:LEU:HD11	1:B:1556:LEU:HD22	1.74	0.69
1:A:200:VAL:HB	1:B:715:HIS:ND1	2.07	0.69
1:A:1047:ILE:CD1	1:A:1256:ILE:HG12	2.23	0.69
1:A:1245:GLY:HA2	1:A:1247:TRP:CE2	2.28	0.69
1:A:1398:GLU:HG3	1:A:1445:SER:HA	1.73	0.69
1:B:1159:LEU:HB3	1:B:1160:PRO:HD2	1.75	0.69
1:A:1142:MET:O	1:A:1143:ALA:C	2.35	0.69
1:A:800:PRO:HG3	1:A:854:ILE:HD11	1.73	0.69
1:B:763:ILE:HG22	1:B:767:LYS:HE3	1.74	0.69
1:A:273:PHE:CD2	1:A:338:TYR:HB2	2.28	0.68
1:B:1058:LEU:HD12	1:B:1068:ALA:HB1	1.75	0.68
1:A:1047:ILE:HD11	1:A:1256:ILE:HD11	1.75	0.68
1:A:1121:ILE:HG23	1:A:1169:TYR:HE2	1.58	0.68
1:A:1365:HIS:HB3	1:A:1372:LEU:HD12	1.75	0.68
1:A:1138:HIS:O	1:A:1142:MET:HG2	1.94	0.68
1:B:1214:LEU:HD22	1:B:1383:TYR:CZ	2.29	0.68
1:B:1191:SER:HB3	1:B:1194:LYS:HG3	1.75	0.68
1:B:834:VAL:HG13	1:B:966:LEU:HD13	1.74	0.68
1:A:715:HIS:ND1	1:B:200:VAL:HG21	2.09	0.68
1:A:1041:TRP:CZ3	1:A:1044:ARG:HD2	2.28	0.68
1:B:1338:LEU:HB3	1:B:1345:GLU:HB2	1.76	0.68
1:A:1047:ILE:HB	1:A:1050:TYR:HD2	1.59	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1545:ALA:HB1	1:A:1553:HIS:CG	2.28	0.67
1:A:922:PHE:HZ	1:A:928:PRO:HD2	1.60	0.67
1:B:852:PRO:HB2	1:B:855:LEU:HB3	1.76	0.67
1:B:1159:LEU:HD13	1:B:1298:LEU:HB3	1.76	0.67
1:B:1445:SER:HA	1:B:1448:HIS:CG	2.30	0.67
1:A:1090:VAL:HG13	1:A:1127:ALA:HB1	1.74	0.67
1:A:1315:LEU:HD11	1:A:1350:VAL:HA	1.76	0.67
1:A:1402:SER:HB3	1:A:1448:HIS:HB3	1.74	0.67
1:A:288:THR:HB	1:A:291:ASP:CG	2.19	0.67
1:A:1380:CYS:O	1:A:1380:CYS:SG	2.53	0.67
1:B:185:ARG:HA	1:B:185:ARG:HE	1.59	0.67
1:B:1025:MET:HG2	1:B:1026:ASN:N	2.10	0.67
1:B:471:VAL:HG21	1:B:641:ARG:HA	1.76	0.67
1:B:97:LEU:HB3	1:B:201:PHE:CE2	2.30	0.67
1:B:318:LEU:HA	1:B:325:ARG:NH2	2.08	0.67
1:B:1587:GLY:O	1:B:1591:MET:HG3	1.95	0.67
1:A:352:VAL:HG21	1:A:429:LEU:HG	1.77	0.67
1:A:274:GLN:O	1:A:277:VAL:HG22	1.95	0.66
1:A:1545:ALA:HA	1:A:1553:HIS:HA	1.77	0.66
1:B:1387:GLN:HG3	1:B:1393:ALA:HB1	1.74	0.66
1:A:286:PRO:HB3	1:A:295:VAL:HG21	1.76	0.66
1:B:768:ALA:HA	1:B:773:ASP:HB2	1.75	0.66
1:A:1401:PHE:HD1	1:A:1407:LEU:HG	1.61	0.66
1:A:1499:ILE:HG23	1:A:1506:VAL:HB	1.78	0.66
1:B:39:ALA:HB1	1:B:44:PHE:HA	1.76	0.66
1:A:284:ILE:HG13	1:A:442:LEU:HB3	1.77	0.66
1:B:793:ASN:HB2	1:B:854:ILE:HG21	1.78	0.66
1:A:1361:ILE:HA	1:A:1365:HIS:HB2	1.78	0.66
1:B:909:HIS:CE1	1:B:937:SER:H	2.14	0.66
1:B:1094:PHE:O	1:B:1098:ILE:HG13	1.96	0.66
1:A:763:ILE:HG22	1:A:767:LYS:HE3	1.75	0.66
1:A:1416:ASN:O	1:A:1470:ARG:NH1	2.28	0.66
1:A:325:ARG:HH12	1:B:496:LEU:HD22	1.60	0.66
1:B:1214:LEU:HD21	1:B:1354:LEU:HD13	1.76	0.66
1:B:1414:THR:HG23	1:B:1423:PHE:CD2	2.31	0.66
1:A:1350:VAL:O	1:A:1354:LEU:HG	1.96	0.66
1:A:1194:LYS:HA	1:A:1370:SER:C	2.20	0.66
1:B:415:LEU:HD12	1:B:524:LEU:HD22	1.78	0.66
1:A:790:MET:HE3	1:A:858:LEU:HD23	1.76	0.65
1:A:1314:LEU:HD13	1:A:1317:LEU:HD12	1.79	0.65
1:B:336:CYS:O	1:B:381:CYS:SG	2.54	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1300:VAL:HG13	1:B:1336:ARG:HD3	1.78	0.65
1:A:1176:TYR:CD1	1:A:1281:ALA:HB3	2.32	0.65
1:B:322:ASN:O	1:B:323:PRO:C	2.38	0.65
1:B:382:LEU:HD12	1:B:475:ILE:HG22	1.78	0.65
1:B:711:TYR:CD2	1:B:888:PRO:HD3	2.32	0.65
1:B:1238:THR:CG2	1:B:1285:LYS:HB3	2.26	0.65
1:B:787:LEU:HD12	1:B:832:LEU:HD23	1.78	0.65
1:A:352:VAL:CG2	1:A:429:LEU:HG	2.27	0.65
1:B:89:CYS:SG	1:B:239:PHE:HB3	2.36	0.65
1:A:908:TYR:HB2	1:A:933:TYR:HB2	1.79	0.65
1:B:97:LEU:HD22	1:B:201:PHE:HZ	1.62	0.65
1:A:1104:ILE:HG21	1:A:1168:THR:HG23	1.79	0.64
1:A:1415:ALA:HB2	1:A:1467:TRP:HB2	1.77	0.64
1:B:1443:ASN:H	1:B:1446:LEU:HD12	1.61	0.64
1:A:507:ALA:O	1:A:523:ARG:NE	2.30	0.64
1:A:1428:LEU:HB3	1:A:1491:LEU:HB3	1.78	0.64
1:B:1043:SER:HB3	1:B:1256:ILE:HD12	1.80	0.64
1:B:1047:ILE:O	1:B:1051:VAL:HG23	1.96	0.64
1:A:93:PRO:O	1:A:97:LEU:N	2.28	0.64
1:A:98:GLN:HG3	1:A:201:PHE:CE1	2.32	0.64
1:B:349:ILE:HG23	1:B:429:LEU:HD13	1.79	0.64
1:B:1159:LEU:CA	1:B:1298:LEU:HD13	2.24	0.64
1:B:1228:THR:O	1:B:1231:GLU:HB3	1.97	0.64
1:B:1307:PRO:HB3	1:B:1337:ILE:CG2	2.28	0.64
1:A:1054:ILE:O	1:A:1058:LEU:HG	1.98	0.64
1:A:1515:LEU:CA	1:A:1544:LEU:HD13	2.26	0.64
1:A:31:VAL:C	1:A:34:ARG:HB3	2.23	0.63
1:A:94:ARG:O	1:A:97:LEU:HB3	1.98	0.63
1:A:1030:MET:O	1:A:1031:SER:O	2.16	0.63
1:B:1175:ALA:O	1:B:1179:GLN:HG2	1.98	0.63
1:A:1218:LEU:HD22	1:A:1376:ILE:HG23	1.81	0.63
1:B:1118:LEU:HD13	1:B:1273:LEU:HB2	1.81	0.63
1:B:1318:LEU:HD21	1:B:1331:SER:HA	1.81	0.63
1:A:190:GLN:O	1:A:194:LEU:HG	1.97	0.63
1:B:46:MET:O	1:B:50:PRO:HD3	1.99	0.63
1:A:516:THR:HB	1:A:519:GLN:HG3	1.80	0.63
1:A:1201:VAL:HG11	1:A:1222:LEU:HD11	1.79	0.63
1:B:1133:VAL:HG13	1:B:1247:TRP:CZ3	2.33	0.63
1:A:1019:TYR:OH	1:A:1038:THR:HA	1.99	0.63
1:A:1035:ILE:HG12	1:A:1089:ILE:HD11	1.81	0.63
1:A:1203:ALA:O	1:A:1204:ILE:C	2.42	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1474:SER:HA	1:A:1485:ILE:HD12	1.81	0.63
1:A:136:LEU:HD22	1:A:239:PHE:HZ	1.64	0.63
1:A:866:LEU:HD22	1:A:948:LEU:HD13	1.81	0.63
1:B:441:ALA:HB1	1:B:443:ARG:HH22	1.62	0.63
1:B:1138:HIS:NE2	1:B:1143:ALA:CB	2.61	0.63
1:B:1247:TRP:HD1	1:B:1248:ARG:H	1.47	0.63
1:B:1588:LYS:O	1:B:1592:ILE:HG12	1.98	0.63
1:B:963:TYR:OH	1:B:1013:LEU:HB3	1.99	0.63
1:A:184:LEU:HD22	1:A:184:LEU:H	1.64	0.62
1:A:1214:LEU:O	1:A:1218:LEU:HG	1.98	0.62
1:A:1564:LEU:HB2	1:A:1603:LEU:HD11	1.81	0.62
1:A:257:LEU:HD21	1:A:318:LEU:HD23	1.79	0.62
1:B:1560:ALA:HA	1:B:1563:TRP:CE3	2.34	0.62
1:B:708:ALA:HA	1:B:888:PRO:HG2	1.80	0.62
1:B:867:HIS:HE1	1:B:1012:ILE:HG21	1.63	0.62
1:B:1499:ILE:HG12	1:B:1506:VAL:HG21	1.80	0.62
1:B:1138:HIS:CD2	1:B:1143:ALA:CB	2.77	0.62
1:B:1166:ILE:HD11	1:B:1295:THR:OG1	2.00	0.62
1:A:104:CYS:HA	1:A:107:LEU:HD12	1.81	0.62
1:A:808:VAL:HG11	1:A:908:TYR:CB	2.23	0.62
1:A:1244:ILE:HG12	1:A:1293:ARG:NH1	2.15	0.62
1:A:787:LEU:HD21	1:A:833:PHE:CZ	2.34	0.62
1:B:1204:ILE:HG12	1:B:1357:GLY:HA3	1.80	0.62
1:B:1268:ALA:O	1:B:1272:THR:HG23	1.99	0.62
1:A:908:TYR:CD2	1:A:930:PRO:HB3	2.33	0.62
1:A:1212:ASN:O	1:A:1216:PRO:HD2	2.00	0.62
1:A:1087:VAL:HG11	1:A:1154:ILE:HG12	1.82	0.62
1:A:1289:LEU:HA	1:A:1326:VAL:HG12	1.82	0.62
1:B:1159:LEU:HA	1:B:1298:LEU:CD1	2.28	0.62
1:B:1242:PRO:HG2	1:B:1261:TYR:CE1	2.35	0.62
1:B:1427:VAL:HG13	1:B:1431:PHE:HE2	1.65	0.62
1:A:1576:VAL:HA	1:A:1579:LYS:HD2	1.82	0.62
1:A:1104:ILE:HG23	1:A:1110:LEU:HD11	1.82	0.61
1:B:1159:LEU:O	1:B:1160:PRO:C	2.42	0.61
1:A:93:PRO:O	1:A:96:GLN:N	2.33	0.61
1:A:790:MET:CE	1:A:858:LEU:HD23	2.30	0.61
1:B:244:VAL:O	1:B:248:GLN:HG2	2.00	0.61
1:A:1030:MET:C	1:A:1034:ASP:HB3	2.25	0.61
1:A:1047:ILE:CG1	1:A:1256:ILE:CG1	2.77	0.61
1:A:1565:SER:O	1:A:1569:LYS:HG2	2.01	0.61
1:A:333:SER:OG	1:A:406:PHE:HZ	1.84	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:104:CYS:HB3	1:A:136:LEU:HD13	1.82	0.61
1:A:471:VAL:O	1:A:475:ILE:HG12	1.99	0.61
1:A:1203:ALA:O	1:A:1320:GLU:HA	2.00	0.61
1:A:1538:MET:HA	1:A:1538:MET:HE3	1.82	0.61
1:B:190:GLN:O	1:B:193:PHE:HB3	2.00	0.61
1:B:1595:CYS:O	1:B:1599:ILE:HG13	2.00	0.61
1:A:265:TYR:CZ	1:A:301:SER:HB2	2.36	0.61
1:A:1347:LEU:HB3	1:A:1351:TYR:CE2	2.35	0.61
1:A:1214:LEU:HD21	1:A:1380:CYS:HB2	1.82	0.61
1:B:867:HIS:CG	1:B:936:LEU:HD21	2.35	0.61
1:A:877:PHE:O	1:A:878:GLU:C	2.38	0.61
1:A:1515:LEU:CD1	1:A:1541:MET:HG3	2.31	0.61
1:A:35:PRO:HB2	1:A:48:GLU:HB3	1.82	0.61
1:A:881:GLN:HE22	1:B:193:PHE:HA	1.63	0.61
1:A:1314:LEU:HG	1:A:1333:SER:CB	2.25	0.61
1:A:1534:PHE:N	1:A:1535:PRO:HD2	2.16	0.61
1:B:754:LEU:HD22	1:B:807:ASN:HD21	1.65	0.61
1:B:1151:SER:HB3	1:B:1154:ILE:HG12	1.83	0.61
1:B:1554:LEU:HD11	1:B:1610:LEU:HD11	1.82	0.61
1:A:810:HIS:O	1:A:813:MET:HG3	2.01	0.61
1:A:885:LEU:HD13	1:B:197:LEU:HD23	1.80	0.61
1:A:1201:VAL:HG12	1:A:1222:LEU:HD11	1.81	0.61
1:A:1285:LYS:CG	1:A:1325:SER:HB3	2.31	0.61
1:A:1427:VAL:HG13	1:A:1431:PHE:HE2	1.64	0.61
1:B:806:LEU:HD21	1:B:811:LEU:HB2	1.82	0.61
1:A:263:LEU:HB2	1:A:266:PHE:HB2	1.83	0.60
1:B:273:PHE:CD2	1:B:338:TYR:HB2	2.34	0.60
1:A:93:PRO:O	1:A:94:ARG:C	2.43	0.60
1:A:1315:LEU:HB3	1:A:1316:PRO:HD2	1.83	0.60
1:B:230:ALA:HA	1:B:233:ILE:HG13	1.83	0.60
1:B:246:SER:OG	1:B:247:LEU:N	2.31	0.60
1:B:1519:THR:HG23	1:B:1563:TRP:CZ2	2.35	0.60
1:A:105:LYS:HG3	1:A:246:SER:HB2	1.83	0.60
1:A:1307:PRO:HB2	1:A:1308:PRO:HD3	1.83	0.60
1:A:1574:LYS:HA	1:A:1577:VAL:HB	1.83	0.60
1:B:834:VAL:HG11	1:B:961:VAL:HG13	1.83	0.60
1:A:918:TRP:O	1:A:922:PHE:HB2	2.02	0.60
1:A:1545:ALA:HB2	1:A:1556:LEU:HB2	1.82	0.60
1:B:1340:PRO:HD2	1:B:1343:SER:HB3	1.84	0.60
1:A:1519:THR:HB	1:A:1520:PRO:HD3	1.82	0.60
1:A:1052:ASN:O	1:A:1053:TRP:C	2.45	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1523:THR:HG23	1:A:1566:ARG:HH11	1.67	0.60
1:A:1607:THR:HA	1:A:1610:LEU:HD12	1.82	0.60
1:B:1500:VAL:HG21	1:B:1543:THR:O	2.02	0.60
1:B:1579:LYS:HB3	1:B:1589:HIS:CE1	2.37	0.60
1:A:49:LEU:HB3	1:A:50:PRO:HD3	1.83	0.60
1:A:130:ILE:HD12	1:A:308:MET:HG3	1.84	0.60
1:B:740:PHE:HD1	1:B:778:GLU:HG3	1.66	0.60
1:B:1151:SER:HB3	1:B:1154:ILE:CD1	2.32	0.60
1:B:1356:THR:HA	1:B:1400:PHE:CZ	2.36	0.60
1:A:73:PHE:CD1	1:A:159:LYS:CA	2.70	0.60
1:A:202:ASN:HB3	1:A:204:ARG:NE	2.17	0.60
1:A:252:GLY:HA2	1:A:255:LYS:HD2	1.83	0.60
1:A:85:ILE:HD12	1:A:107:LEU:HD11	1.83	0.60
1:B:851:VAL:HG11	1:B:995:GLU:HG2	1.84	0.60
1:B:1274:CYS:O	1:B:1275:SER:C	2.45	0.60
1:A:1575:ASN:O	1:A:1579:LYS:HG3	2.02	0.59
1:B:921:HIS:HD2	1:B:993:ALA:HB2	1.66	0.59
1:B:996:ALA:HB1	1:B:1274:CYS:HA	1.84	0.59
1:A:43:ALA:O	1:A:44:PHE:C	2.44	0.59
1:A:58:GLU:C	1:A:60:GLU:H	2.11	0.59
1:A:318:LEU:HD13	1:A:321:LEU:HD21	1.84	0.59
1:A:320:PRO:HG3	1:B:493:VAL:HG12	1.85	0.59
1:A:670:ILE:O	1:A:674:LEU:HG	2.02	0.59
1:B:996:ALA:CB	1:B:1274:CYS:HA	2.32	0.59
1:B:1468:LEU:HA	1:B:1471:MET:HE2	1.84	0.59
1:A:349:ILE:HG23	1:A:429:LEU:CD1	2.32	0.59
1:A:1122:TYR:HB2	1:A:1269:HIS:CD2	2.37	0.59
1:A:1204:ILE:HD11	1:A:1357:GLY:HA3	1.84	0.59
1:B:1305:MET:O	1:B:1307:PRO:HD3	2.03	0.59
1:B:1598:HIS:O	1:B:1602:TYR:N	2.34	0.59
1:A:1568:LYS:HD3	1:A:1569:LYS:HD3	1.83	0.59
1:B:151:PHE:HA	1:B:154:MET:HE2	1.84	0.59
1:B:1515:LEU:CD1	1:B:1541:MET:HG3	2.32	0.59
1:A:1171:SER:HA	1:A:1174:ARG:HD2	1.83	0.59
1:B:889:PHE:O	1:B:890:GLY:C	2.44	0.59
1:B:1084:LYS:HD2	1:B:1151:SER:HB2	1.83	0.59
1:A:1047:ILE:HG13	1:A:1256:ILE:HG12	1.83	0.59
1:A:1548:GLY:HA3	1:A:1552:GLY:C	2.28	0.59
1:B:1015:PRO:HB2	1:B:1020:ILE:HD11	1.85	0.59
1:A:84:TYR:O	1:A:88:VAL:HG22	2.03	0.59
1:A:1051:VAL:HG22	1:A:1072:LEU:HD11	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1428:LEU:HD13	1:A:1491:LEU:HB2	1.85	0.59
1:A:1542:ALA:HA	1:A:1556:LEU:CD2	2.33	0.59
1:A:1560:ALA:HA	1:A:1563:TRP:HE3	1.67	0.59
1:B:104:CYS:SG	1:B:239:PHE:HE1	2.26	0.59
1:B:1412:MET:HB3	1:B:1463:ARG:HE	1.67	0.59
1:B:1571:LEU:HA	1:B:1576:VAL:HG11	1.85	0.59
1:A:30:GLU:O	1:A:33:VAL:HG22	2.03	0.59
1:B:247:LEU:C	1:B:249:GLU:N	2.56	0.59
1:B:937:SER:O	1:B:939:GLU:N	2.36	0.59
1:B:1063:MET:HE2	1:B:1067:HIS:NE2	2.17	0.59
1:B:1208:ARG:HD3	1:B:1328:GLU:HB2	1.84	0.59
1:B:1429:LYS:O	1:B:1430:PHE:C	2.45	0.59
1:A:1311:ILE:HG21	1:A:1338:LEU:HD21	1.85	0.58
1:B:93:PRO:HB2	1:B:96:GLN:HB2	1.85	0.58
1:A:888:PRO:O	1:A:889:PHE:C	2.45	0.58
1:A:74:TYR:O	1:A:77:PHE:HB3	2.03	0.58
1:A:857:ARG:NH2	1:A:931:ARG:O	2.36	0.58
1:A:1045:LEU:HD12	1:A:1072:LEU:HD11	1.83	0.58
1:A:1222:LEU:O	1:A:1226:VAL:HB	2.03	0.58
1:A:1591:MET:O	1:A:1594:GLU:HG2	2.03	0.58
1:B:1045:LEU:O	1:B:1051:VAL:HG22	2.04	0.58
1:A:1213:THR:O	1:A:1217:THR:HG23	2.04	0.58
1:B:284:ILE:HD12	1:B:420:LEU:HD12	1.86	0.58
1:A:1514:LEU:O	1:A:1518:LEU:HG	2.03	0.58
1:B:31:VAL:C	1:B:34:ARG:HB3	2.29	0.58
1:A:906:PRO:O	1:A:907:LEU:HB2	2.03	0.58
1:A:1309:GLN:HA	1:A:1312:ARG:HD2	1.85	0.58
1:B:810:HIS:O	1:B:813:MET:HG3	2.04	0.58
1:A:93:PRO:HB2	1:A:96:GLN:HB2	1.86	0.58
1:A:396:ARG:HH21	1:B:404:GLN:NE2	2.02	0.58
1:A:908:TYR:O	1:A:910:GLY:N	2.37	0.58
1:A:1312:ARG:O	1:A:1316:PRO:CD	2.49	0.58
1:B:527:SER:O	1:B:528:VAL:HG13	2.04	0.58
1:B:1563:TRP:HA	1:B:1566:ARG:HD2	1.86	0.58
1:B:680:GLU:HB3	1:B:730:THR:HG21	1.84	0.58
1:B:1214:LEU:O	1:B:1218:LEU:HG	2.04	0.58
1:B:1300:VAL:CG1	1:B:1336:ARG:HD3	2.33	0.58
1:A:53:VAL:O	1:A:57:ILE:HG13	2.03	0.58
1:A:189:VAL:HG21	1:B:874:VAL:HG13	1.85	0.58
1:A:1298:LEU:HA	1:A:1301:TRP:NE1	2.19	0.58
1:B:1296:GLY:O	1:B:1300:VAL:HG22	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:256:LEU:HB3	1:A:312:THR:CG2	2.34	0.57
1:A:284:ILE:H	1:A:442:LEU:H	1.52	0.57
1:A:1218:LEU:HD13	1:A:1376:ILE:HG23	1.85	0.57
1:A:1429:LYS:O	1:A:1430:PHE:C	2.45	0.57
1:A:319:GLU:HB2	1:A:320:PRO:HD3	1.85	0.57
1:A:688:SER:O	1:A:692:GLU:HG3	2.04	0.57
1:A:1571:LEU:HD21	1:A:1593:LEU:HA	1.86	0.57
1:B:844:MET:HB3	1:B:848:MET:HE3	1.85	0.57
1:B:1083:VAL:O	1:B:1084:LYS:C	2.47	0.57
1:A:833:PHE:CZ	1:A:861:ILE:HG21	2.40	0.57
1:A:1210:LYS:O	1:A:1211:ALA:C	2.47	0.57
1:A:1576:VAL:O	1:A:1580:LEU:HG	2.04	0.57
1:B:282:PHE:CZ	1:B:341:VAL:HG21	2.38	0.57
1:B:1044:ARG:C	1:B:1046:ARG:N	2.60	0.57
1:B:1361:ILE:HA	1:B:1365:HIS:HB2	1.85	0.57
1:A:1204:ILE:HD11	1:A:1357:GLY:CA	2.35	0.57
1:B:1456:LEU:C	1:B:1458:CYS:N	2.60	0.57
1:B:89:CYS:SG	1:B:239:PHE:CB	2.92	0.57
1:B:284:ILE:HD13	1:B:345:THR:OG1	2.03	0.57
1:B:422:LEU:HD11	1:B:537:LEU:HG	1.87	0.57
1:B:528:VAL:O	1:B:530:LEU:N	2.38	0.57
1:B:909:HIS:CE1	1:B:937:SER:N	2.72	0.57
1:A:333:SER:OG	1:A:385:TYR:HA	2.04	0.57
1:A:1203:ALA:HA	1:A:1320:GLU:HG3	1.86	0.57
1:A:1481:GLN:HA	1:A:1481:GLN:HE21	1.70	0.57
1:B:39:ALA:CB	1:B:44:PHE:HA	2.35	0.57
1:A:867:HIS:O	1:A:949:ASP:OD2	2.21	0.57
1:A:1118:LEU:HD21	1:A:1269:HIS:HB3	1.86	0.57
1:B:1151:SER:O	1:B:1154:ILE:HG12	2.04	0.57
1:B:1545:ALA:HB2	1:B:1556:LEU:CD2	2.34	0.57
1:B:1579:LYS:HB3	1:B:1589:HIS:NE2	2.19	0.57
1:A:82:THR:HA	1:A:107:LEU:HD13	1.86	0.57
1:A:1029:GLU:HB3	1:A:1096:ARG:HH12	1.69	0.57
1:A:1517:THR:O	1:A:1520:PRO:HD2	2.04	0.57
1:B:1571:LEU:HA	1:B:1576:VAL:CG1	2.35	0.57
1:A:1035:ILE:O	1:A:1039:LEU:HG	2.05	0.57
1:B:58:GLU:C	1:B:60:GLU:H	2.13	0.57
1:B:1159:LEU:HG	1:B:1160:PRO:HD3	1.86	0.57
1:A:908:TYR:CD1	1:A:933:TYR:HB3	2.39	0.57
1:A:1305:MET:O	1:A:1307:PRO:HD3	2.05	0.57
1:B:82:THR:HG23	1:B:136:LEU:HG	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:TRP:HD1	1:B:821:PHE:HE2	1.53	0.57
1:B:1047:ILE:HB	1:B:1050:TYR:HD2	1.70	0.57
1:B:1178:LEU:HD11	1:B:1199:ALA:HB2	1.86	0.57
1:A:310:LEU:HD13	1:A:384:ILE:HG12	1.87	0.56
1:A:745:TRP:HE1	1:A:810:HIS:CE1	2.22	0.56
1:B:1110:LEU:H	1:B:1175:ALA:CB	2.17	0.56
1:A:1543:THR:O	1:A:1546:SER:HB2	2.04	0.56
1:B:1242:PRO:HG2	1:B:1261:TYR:HE1	1.70	0.56
1:A:70:TYR:HD1	1:A:160:LEU:HA	1.70	0.56
1:A:70:TYR:O	1:A:71:GLU:C	2.49	0.56
1:A:788:SER:O	1:A:789:THR:C	2.44	0.56
1:A:1101:PHE:CD2	1:A:1168:THR:HG21	2.40	0.56
1:A:1215:GLY:O	1:A:1216:PRO:C	2.47	0.56
1:A:1556:LEU:HD23	1:A:1602:TYR:OH	2.05	0.56
1:B:683:MET:HE3	1:B:727:LEU:HD23	1.87	0.56
1:B:1058:LEU:CD1	1:B:1068:ALA:HB1	2.35	0.56
1:B:1295:THR:O	1:B:1299:ILE:HD13	2.05	0.56
1:A:299:PHE:O	1:A:303:VAL:HG23	2.05	0.56
1:A:984:ARG:HG2	1:A:989:LYS:C	2.30	0.56
1:B:470:GLY:H	1:B:473:SER:HB2	1.71	0.56
1:B:1401:PHE:HD2	1:B:1449:LEU:HD22	1.70	0.56
1:A:60:GLU:O	1:A:64:LEU:HG	2.05	0.56
1:A:948:LEU:HG	1:A:953:CYS:SG	2.46	0.56
1:A:1037:HIS:CE1	1:A:1041:TRP:HE1	2.22	0.56
1:A:1169:TYR:HA	1:A:1172:PHE:HD2	1.70	0.56
1:B:1495:LEU:HA	1:B:1498:TYR:CD2	2.40	0.56
1:A:93:PRO:HD2	1:A:96:GLN:HB2	1.86	0.56
1:B:246:SER:O	1:B:249:GLU:HB2	2.05	0.56
1:B:663:LEU:HD23	1:B:674:LEU:CD1	2.36	0.56
1:B:1567:CYS:HB3	1:B:1592:ILE:CG2	2.36	0.56
1:A:834:VAL:HG13	1:A:966:LEU:HD13	1.87	0.56
1:A:1176:TYR:CZ	1:A:1280:LEU:HB2	2.41	0.56
1:A:1299:ILE:HG22	1:A:1336:ARG:HH11	1.70	0.56
1:B:1566:ARG:HA	1:B:1569:LYS:HD2	1.88	0.56
1:B:1603:LEU:CA	1:B:1606:VAL:HB	2.34	0.56
1:A:1058:LEU:HB3	1:A:1063:MET:SD	2.46	0.56
1:B:1166:ILE:HG12	1:B:1291:LEU:HB3	1.86	0.56
1:B:1395:LYS:O	1:B:1399:GLU:HG2	2.06	0.56
1:A:317:VAL:O	1:A:318:LEU:HG	2.06	0.56
1:A:1119:GLN:NE2	1:A:1122:TYR:OH	2.39	0.56
1:A:1178:LEU:CD2	1:A:1202:LEU:HD21	2.36	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1138:HIS:NE2	1:B:1143:ALA:O	2.39	0.56
1:A:273:PHE:O	1:A:277:VAL:HG13	2.06	0.55
1:A:491:LEU:HD21	1:A:518:ILE:HA	1.88	0.55
1:B:35:PRO:HB3	1:B:48:GLU:HB3	1.88	0.55
1:B:1307:PRO:O	1:B:1311:ILE:HG13	2.06	0.55
1:A:145:ARG:O	1:A:149:ILE:HG13	2.06	0.55
1:A:183:GLU:H	1:A:183:GLU:CD	2.13	0.55
1:A:329:VAL:CG1	1:A:388:ILE:HG23	2.30	0.55
1:A:982:THR:OG1	1:A:1117:SER:HB3	2.05	0.55
1:A:1281:ALA:HA	1:A:1284:LEU:HB2	1.87	0.55
1:A:1529:GLY:HA2	1:A:1592:ILE:HD11	1.88	0.55
1:B:1453:LEU:H	1:B:1453:LEU:HD12	1.71	0.55
1:A:683:MET:SD	1:A:727:LEU:HD23	2.46	0.55
1:A:781:LYS:HG3	1:A:781:LYS:O	2.04	0.55
1:B:31:VAL:O	1:B:35:PRO:CD	2.39	0.55
1:B:32:ALA:C	1:B:34:ARG:N	2.60	0.55
1:A:404:GLN:HE21	1:B:396:ARG:HB2	1.72	0.55
1:B:1408:VAL:O	1:B:1412:MET:HG2	2.06	0.55
1:A:183:GLU:O	1:A:187:LYS:HD3	2.06	0.55
1:A:193:PHE:HD2	1:B:881:GLN:CG	2.19	0.55
1:A:204:ARG:O	1:A:205:THR:C	2.50	0.55
1:A:352:VAL:HB	1:A:426:PRO:HG3	1.88	0.55
1:A:759:ARG:HG2	1:A:885:LEU:HD23	1.89	0.55
1:B:90:SER:HB3	1:B:232:ALA:HB1	1.88	0.55
1:B:347:MET:HE1	1:B:371:GLU:HG3	1.88	0.55
1:B:1087:VAL:HG12	1:B:1091:GLU:OE1	2.06	0.55
1:A:85:ILE:CG2	1:A:100:VAL:HG13	2.36	0.55
1:A:291:ASP:O	1:A:295:VAL:HG23	2.06	0.55
1:A:674:LEU:O	1:A:678:LEU:HG	2.06	0.55
1:B:553:LYS:O	1:B:554:GLY:C	2.48	0.55
1:B:1299:ILE:HG21	1:B:1336:ARG:HD2	1.87	0.55
1:A:83:HIS:O	1:A:87:THR:HG23	2.06	0.55
1:A:1156:LYS:HG2	1:A:1304:GLU:CD	2.32	0.55
1:B:282:PHE:CB	1:B:416:ASN:HB3	2.37	0.55
1:A:1122:TYR:HD1	1:A:1122:TYR:C	2.15	0.55
1:A:1292:VAL:HG11	1:A:1329:ILE:HB	1.88	0.55
1:A:1306:ASN:OD1	1:A:1308:PRO:HD2	2.06	0.55
1:A:1474:SER:HB2	1:A:1485:ILE:HG21	1.89	0.55
1:B:193:PHE:O	1:B:194:LEU:C	2.49	0.55
1:B:943:ASP:O	1:B:944:ASP:C	2.49	0.55
1:B:973:LEU:HB3	1:B:1002:TYR:OH	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1101:PHE:HA	1:B:1104:ILE:HD13	1.89	0.55
1:A:1127:ALA:O	1:A:1131:VAL:HG22	2.07	0.54
1:B:1168:THR:HG22	1:B:1172:PHE:CE2	2.42	0.54
1:A:270:ILE:HG12	1:A:335:SER:OG	2.07	0.54
1:A:715:HIS:NE2	1:B:200:VAL:HG11	2.22	0.54
1:B:1133:VAL:HG13	1:B:1247:TRP:CE3	2.41	0.54
1:A:393:SER:HA	1:A:399:GLY:O	2.06	0.54
1:A:1094:PHE:HZ	1:A:1128:ILE:HD13	1.73	0.54
1:A:1122:TYR:C	1:A:1122:TYR:CD1	2.85	0.54
1:B:48:GLU:O	1:B:51:GLN:HB3	2.06	0.54
1:B:1159:LEU:HB3	1:B:1160:PRO:CD	2.36	0.54
1:B:1387:GLN:CG	1:B:1393:ALA:HB1	2.37	0.54
1:A:420:LEU:HD21	1:A:444:VAL:CA	2.35	0.54
1:A:881:GLN:NE2	1:B:193:PHE:CD2	2.72	0.54
1:B:195:ASN:O	1:B:196:GLN:C	2.47	0.54
1:B:827:ARG:HG3	1:B:955:VAL:HG13	1.88	0.54
1:A:881:GLN:HA	1:A:885:LEU:HD12	1.89	0.54
1:A:1159:LEU:HB3	1:A:1160:PRO:CD	2.37	0.54
1:A:1177:LEU:HG	1:A:1233:TRP:CE3	2.42	0.54
1:B:783:TRP:CD1	1:B:821:PHE:HE2	2.26	0.54
1:B:1063:MET:SD	1:B:1068:ALA:HB2	2.48	0.54
1:B:1083:VAL:HG21	1:B:1138:HIS:HB2	1.88	0.54
1:B:1456:LEU:O	1:B:1459:VAL:HG13	2.08	0.54
1:A:691:LYS:HD3	1:A:735:LEU:HA	1.88	0.54
1:A:1209:CYS:SG	1:A:1318:LEU:HD11	2.48	0.54
1:B:184:LEU:H	1:B:184:LEU:HD22	1.73	0.54
1:B:827:ARG:HG2	1:B:960:LEU:HD12	1.90	0.54
1:B:1570:TYR:HA	1:B:1573:GLN:HE21	1.72	0.54
1:A:32:ALA:CA	1:A:35:PRO:HD2	2.38	0.54
1:A:791:LYS:HD3	1:A:836:ILE:HG12	1.89	0.54
1:A:968:ALA:O	1:A:969:ALA:C	2.46	0.54
1:A:1132:GLN:HE22	1:A:1293:ARG:HH21	1.56	0.54
1:A:1201:VAL:HG21	1:A:1372:LEU:HD22	1.89	0.54
1:B:349:ILE:HD12	1:B:429:LEU:HD22	1.90	0.54
1:B:1445:SER:HA	1:B:1448:HIS:HB2	1.90	0.54
1:B:1570:TYR:OH	1:B:1588:LYS:HD2	2.07	0.54
1:B:1572:SER:O	1:B:1573:GLN:C	2.49	0.54
1:B:1603:LEU:HA	1:B:1606:VAL:CB	2.35	0.54
1:B:1384:LEU:HD13	1:B:1397:MET:SD	2.48	0.54
1:A:32:ALA:C	1:A:34:ARG:N	2.57	0.54
1:A:881:GLN:HE22	1:B:193:PHE:CA	2.21	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1404:SER:HB2	1:A:1406:GLU:HG3	1.90	0.54
1:B:49:LEU:C	1:B:51:GLN:N	2.63	0.54
1:B:282:PHE:HZ	1:B:341:VAL:HG21	1.71	0.54
1:B:1025:MET:HG2	1:B:1026:ASN:H	1.72	0.54
1:A:322:ASN:O	1:A:323:PRO:C	2.51	0.53
1:A:1552:GLY:C	1:A:1554:LEU:H	2.16	0.53
1:B:1230:CYS:SG	1:B:1234:ASN:ND2	2.81	0.53
1:B:1238:THR:HG22	1:B:1282:ALA:O	2.08	0.53
1:A:39:ALA:HA	1:A:42:SER:O	2.08	0.53
1:A:90:SER:HB3	1:A:232:ALA:HB1	1.89	0.53
1:B:30:GLU:O	1:B:33:VAL:HG22	2.08	0.53
1:B:44:PHE:CD1	1:B:84:TYR:HB3	2.43	0.53
1:B:49:LEU:HB3	1:B:50:PRO:HD3	1.89	0.53
1:B:941:SER:C	1:B:943:ASP:H	2.16	0.53
1:A:1162:THR:HG23	1:A:1291:LEU:HD22	1.89	0.53
1:B:1247:TRP:HA	1:B:1251:PHE:HB2	1.91	0.53
1:B:1518:LEU:HD12	1:B:1544:LEU:HD12	1.90	0.53
1:B:1560:ALA:HA	1:B:1563:TRP:HE3	1.71	0.53
1:A:103:ALA:O	1:A:107:LEU:HG	2.09	0.53
1:A:478:ASN:OD1	1:A:650:LEU:HD13	2.08	0.53
1:A:1394:ARG:HH11	1:A:1443:ASN:HD21	1.56	0.53
1:A:1435:PHE:CD1	1:A:1498:TYR:HB3	2.43	0.53
1:B:183:GLU:O	1:B:187:LYS:HG2	2.09	0.53
1:B:1554:LEU:HD11	1:B:1610:LEU:CD1	2.38	0.53
1:A:715:HIS:CE1	1:B:200:VAL:HB	2.44	0.53
1:A:942:GLU:HG2	1:A:943:ASP:N	2.23	0.53
1:A:1015:PRO:HG3	1:A:1041:TRP:CD2	2.44	0.53
1:B:1460:GLU:OE1	1:B:1463:ARG:HB2	2.09	0.53
1:A:254:GLU:HA	1:A:257:LEU:HD12	1.90	0.53
1:B:1110:LEU:O	1:B:1175:ALA:HB1	2.07	0.53
1:B:1522:ALA:HB1	1:B:1534:PHE:HE1	1.73	0.53
1:A:545:ALA:O	1:A:644:PRO:HB3	2.07	0.53
1:A:552:ARG:NH2	1:A:643:ASP:HA	2.23	0.53
1:A:1080:CYS:HB3	1:A:1084:LYS:HE3	1.91	0.53
1:B:1394:ARG:NH2	1:B:1437:LEU:HD13	2.23	0.53
1:B:1394:ARG:HD3	1:B:1446:LEU:HD21	1.89	0.53
1:A:239:PHE:HA	1:A:242:GLN:OE1	2.08	0.53
1:A:985:ARG:NH1	1:A:1280:LEU:HD22	2.24	0.53
1:A:1155:THR:HG21	1:A:1301:TRP:CD1	2.44	0.53
1:A:1210:LYS:N	1:A:1210:LYS:HD2	2.24	0.53
1:A:1515:LEU:HB2	1:A:1544:LEU:HD13	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:844:MET:HE2	1:B:844:MET:HA	1.90	0.53
1:B:1030:MET:O	1:B:1096:ARG:NH1	2.42	0.53
1:B:1191:SER:H	1:B:1194:LYS:HD3	1.73	0.53
1:B:1435:PHE:CD1	1:B:1498:TYR:HB3	2.43	0.53
1:A:1299:ILE:HD11	1:A:1310:VAL:HG11	1.90	0.53
1:A:1545:ALA:HB1	1:A:1553:HIS:CD2	2.44	0.53
1:B:144:ASP:HB2	1:B:147:GLU:HG3	1.91	0.53
1:B:261:LEU:HD11	1:B:328:ASP:HB3	1.90	0.53
1:B:420:LEU:HD13	1:B:442:LEU:HB2	1.91	0.53
1:B:859:LEU:O	1:B:1009:ILE:HD11	2.09	0.53
1:B:1464:LEU:HD23	1:B:1517:THR:HG21	1.90	0.53
1:A:1525:MET:HA	1:A:1530:ASP:HB2	1.91	0.52
1:B:382:LEU:CD1	1:B:475:ILE:HG22	2.39	0.52
1:B:864:TYR:HD1	1:B:936:LEU:HD13	1.74	0.52
1:A:885:LEU:HD13	1:B:197:LEU:CD2	2.39	0.52
1:A:1000:GLN:HG3	1:A:1270:LEU:HD13	1.91	0.52
1:A:1122:TYR:HD1	1:A:1123:THR:N	2.07	0.52
1:A:1315:LEU:HD21	1:A:1353:LYS:HB2	1.91	0.52
1:A:1383:TYR:O	1:A:1387:GLN:HG2	2.08	0.52
1:B:1084:LYS:HE3	1:B:1151:SER:N	2.23	0.52
1:B:1232:SER:C	1:B:1234:ASN:N	2.64	0.52
1:A:95:ASN:HB3	1:A:192:ASN:HD21	1.74	0.52
1:A:230:ALA:O	1:A:234:LYS:HG3	2.09	0.52
1:A:1094:PHE:O	1:A:1098:ILE:HG13	2.10	0.52
1:A:1315:LEU:HB3	1:A:1316:PRO:CD	2.39	0.52
1:B:32:ALA:O	1:B:35:PRO:CD	2.50	0.52
1:B:265:TYR:CE2	1:B:301:SER:HB2	2.44	0.52
1:B:443:ARG:HB2	1:B:446:ASP:CG	2.33	0.52
1:B:1489:ARG:NH2	1:B:1533:GLY:CA	2.71	0.52
1:A:839:GLU:O	1:A:842:VAL:HG12	2.09	0.52
1:A:1000:GLN:HA	1:A:1270:LEU:HD13	1.91	0.52
1:A:1294:LEU:O	1:A:1298:LEU:HG	2.10	0.52
1:B:759:ARG:HG2	1:B:885:LEU:CD2	2.40	0.52
1:B:1044:ARG:C	1:B:1046:ARG:H	2.17	0.52
1:A:193:PHE:HD2	1:B:881:GLN:HG2	1.75	0.52
1:A:245:ALA:O	1:A:249:GLU:HG3	2.09	0.52
1:A:545:ALA:HB2	1:A:647:PHE:HB2	1.92	0.52
1:A:549:GLN:O	1:A:553:LYS:HG2	2.09	0.52
1:A:1196:GLN:O	1:A:1199:ALA:HB3	2.09	0.52
1:B:1046:ARG:HH22	1:B:1130:LYS:NZ	2.06	0.52
1:A:491:LEU:HD23	1:A:517:SER:OG	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:844:MET:HA	1:A:844:MET:HE2	1.90	0.52
1:A:1225:SER:O	1:A:1229:VAL:HG23	2.10	0.52
1:B:272:ARG:HD3	1:B:285:MET:HG2	1.91	0.52
1:B:712:HIS:HA	1:B:715:HIS:CD2	2.44	0.52
1:B:1063:MET:CG	1:B:1068:ALA:HB2	2.39	0.52
1:B:1163:LEU:HA	1:B:1166:ILE:HD12	1.92	0.52
1:B:1412:MET:O	1:B:1415:ALA:HB3	2.09	0.52
1:B:1414:THR:HG22	1:B:1424:CYS:SG	2.50	0.52
1:A:786:PHE:O	1:A:787:LEU:C	2.48	0.52
1:A:1010:LEU:HB3	1:A:1037:HIS:HE1	1.75	0.52
1:A:1169:TYR:HA	1:A:1172:PHE:CD2	2.44	0.52
1:A:1208:ARG:HG3	1:A:1209:CYS:N	2.25	0.52
1:A:1546:SER:C	1:A:1548:GLY:N	2.65	0.52
1:B:1010:LEU:HD22	1:B:1037:HIS:CE1	2.44	0.52
1:B:1449:LEU:O	1:B:1453:LEU:HD12	2.10	0.52
1:B:123:ALA:HB1	1:B:154:MET:SD	2.50	0.52
1:B:712:HIS:HA	1:B:715:HIS:NE2	2.25	0.52
1:B:1127:ALA:O	1:B:1131:VAL:HG22	2.10	0.52
1:B:1162:THR:HG23	1:B:1291:LEU:HD22	1.91	0.52
1:A:1048:SER:HA	1:A:1051:VAL:HB	1.91	0.52
1:A:1571:LEU:C	1:A:1573:GLN:N	2.65	0.52
1:B:187:LYS:O	1:B:191:MET:HG2	2.09	0.52
1:B:1449:LEU:C	1:B:1452:SER:HB3	2.34	0.52
1:A:193:PHE:HZ	1:B:762:LEU:HD13	1.74	0.52
1:A:396:ARG:HH21	1:B:404:GLN:CD	2.18	0.52
1:A:1010:LEU:HB3	1:A:1037:HIS:CE1	2.45	0.52
1:B:531:MET:HG3	1:B:677:SER:HB2	1.92	0.52
1:B:1064:LYS:HB3	1:B:1067:HIS:HD2	1.75	0.52
1:A:37:LEU:O	1:A:40:SER:HB3	2.09	0.51
1:A:1210:LYS:HE3	1:A:1342:GLU:HG2	1.91	0.51
1:B:740:PHE:HA	1:B:781:LYS:HG2	1.91	0.51
1:B:1058:LEU:HB3	1:B:1063:MET:SD	2.50	0.51
1:A:73:PHE:HB2	1:A:161:PRO:HD3	1.92	0.51
1:A:299:PHE:HZ	1:A:346:CYS:SG	2.34	0.51
1:A:1211:ALA:HA	1:A:1350:VAL:CG1	2.41	0.51
1:B:281:SER:OG	1:B:445:ARG:HB2	2.10	0.51
1:B:723:GLN:HG2	1:B:728:GLN:HG3	1.92	0.51
1:B:1247:TRP:HB2	1:B:1251:PHE:O	2.11	0.51
1:A:302:LEU:HD23	1:A:377:ILE:HD13	1.91	0.51
1:A:317:VAL:C	1:A:318:LEU:HG	2.35	0.51
1:A:546:CYS:O	1:A:550:ARG:HG3	2.11	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:661:SER:O	1:A:665:SER:HB2	2.09	0.51
1:A:963:TYR:HE1	1:A:1013:LEU:HD13	1.75	0.51
1:B:282:PHE:HB2	1:B:416:ASN:OD1	2.10	0.51
1:B:1101:PHE:HB3	1:B:1104:ILE:HB	1.91	0.51
1:A:44:PHE:HD1	1:A:84:TYR:HB3	1.76	0.51
1:A:723:GLN:HG2	1:A:728:GLN:HG3	1.92	0.51
1:A:985:ARG:HH12	1:A:1280:LEU:HD22	1.75	0.51
1:B:282:PHE:CZ	1:B:338:TYR:HD2	2.28	0.51
1:B:479:HIS:O	1:B:483:LEU:HG	2.10	0.51
1:B:1159:LEU:HD13	1:B:1298:LEU:CB	2.39	0.51
1:A:80:LEU:HD22	1:A:148:ILE:HG23	1.92	0.51
1:A:1563:TRP:CD1	1:A:1566:ARG:CZ	2.94	0.51
1:B:1082:SER:C	1:B:1084:LYS:N	2.59	0.51
1:B:1516:GLY:O	1:B:1520:PRO:CD	2.57	0.51
1:A:159:LYS:O	1:A:160:LEU:C	2.52	0.51
1:A:202:ASN:HB3	1:A:204:ARG:CZ	2.41	0.51
1:A:470:GLY:O	1:A:474:VAL:HG23	2.10	0.51
1:A:548:LEU:HD11	1:A:647:PHE:CE2	2.46	0.51
1:A:1019:TYR:CZ	1:A:1023:LEU:HD21	2.45	0.51
1:B:291:ASP:O	1:B:295:VAL:HG23	2.10	0.51
1:B:1151:SER:HB3	1:B:1154:ILE:CG1	2.40	0.51
1:B:1403:ASP:OD2	1:B:1404:SER:N	2.44	0.51
1:B:1473:THR:O	1:B:1485:ILE:HD13	2.10	0.51
1:B:1490:GLN:O	1:B:1494:LEU:HD13	2.09	0.51
1:B:1558:ASN:O	1:B:1561:VAL:HB	2.10	0.51
1:B:1598:HIS:HA	1:B:1601:SER:HB3	1.92	0.51
1:B:1607:THR:O	1:B:1611:SER:N	2.40	0.51
1:A:985:ARG:O	1:A:986:LYS:C	2.53	0.51
1:A:1156:LYS:C	1:A:1156:LYS:HD3	2.36	0.51
1:B:89:CYS:SG	1:B:239:PHE:CG	2.97	0.51
1:B:852:PRO:CB	1:B:855:LEU:HB3	2.41	0.51
1:B:1082:SER:O	1:B:1083:VAL:C	2.54	0.51
1:A:943:ASP:O	1:A:944:ASP:C	2.54	0.51
1:A:1204:ILE:HG22	1:A:1215:GLY:HA2	1.93	0.51
1:A:1206:SER:HB2	1:A:1319:LEU:HA	1.93	0.51
1:A:1417:GLU:HA	1:A:1470:ARG:CD	2.33	0.51
1:A:1568:LYS:HD3	1:A:1569:LYS:N	2.26	0.51
1:B:71:GLU:OE1	1:B:122:CYS:HA	2.11	0.51
1:B:247:LEU:O	1:B:250:LEU:N	2.43	0.51
1:A:61:SER:HA	1:A:64:LEU:HD12	1.92	0.51
1:A:491:LEU:HD22	1:A:518:ILE:HG12	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1306:ASN:O	1:A:1310:VAL:HG23	2.11	0.51
1:B:37:LEU:HD12	1:B:38:SER:N	2.26	0.51
1:B:1214:LEU:HD22	1:B:1383:TYR:CE2	2.45	0.51
1:A:405:ASN:HB2	1:A:511:ILE:HA	1.92	0.51
1:A:418:LEU:HD21	1:A:476:LEU:HB2	1.93	0.51
1:A:1272:THR:HB	1:A:1282:ALA:HB3	1.93	0.51
1:A:1400:PHE:HB3	1:A:1401:PHE:HD2	1.76	0.51
1:B:539:SER:O	1:B:543:ARG:HD3	2.11	0.51
1:B:1156:LYS:O	1:B:1156:LYS:HD3	2.11	0.51
1:B:1414:THR:HG21	1:B:1424:CYS:HA	1.93	0.51
1:B:1545:ALA:HB2	1:B:1556:LEU:HD22	1.92	0.51
1:A:788:SER:C	1:A:790:MET:N	2.59	0.50
1:A:1030:MET:O	1:A:1035:ILE:HG13	2.11	0.50
1:A:1058:LEU:HD23	1:A:1061:GLN:HE22	1.76	0.50
1:B:303:VAL:HG22	1:B:377:ILE:HG13	1.92	0.50
1:B:1238:THR:HB	1:B:1286:HIS:HB2	1.93	0.50
1:A:985:ARG:NH2	1:A:1115:ILE:O	2.44	0.50
1:A:1022:GLN:C	1:A:1024:SER:N	2.67	0.50
1:A:1468:LEU:HD22	1:A:1518:LEU:HD21	1.92	0.50
1:B:341:VAL:HB	1:B:417:SER:HB2	1.94	0.50
1:B:1278:LEU:HB3	1:B:1281:ALA:HB2	1.93	0.50
1:A:93:PRO:CD	1:A:96:GLN:HB2	2.41	0.50
1:A:491:LEU:CD1	1:A:670:ILE:HD11	2.40	0.50
1:A:1162:THR:O	1:A:1166:ILE:HG13	2.11	0.50
1:A:1198:PHE:O	1:A:1202:LEU:HG	2.11	0.50
1:B:1254:ASP:O	1:B:1255:THR:C	2.55	0.50
1:B:1318:LEU:HD11	1:B:1331:SER:HA	1.92	0.50
1:B:1456:LEU:HD22	1:B:1510:VAL:HG13	1.93	0.50
1:A:535:LEU:HD12	1:A:682:HIS:CD2	2.46	0.50
1:A:539:SER:HB2	1:A:543:ARG:NH1	2.25	0.50
1:A:547:VAL:O	1:A:551:GLN:HG3	2.11	0.50
1:A:650:LEU:O	1:A:654:ILE:HG13	2.11	0.50
1:A:1001:TYR:CE2	1:A:1005:ILE:HD11	2.46	0.50
1:A:1233:TRP:HE3	1:A:1278:LEU:HD13	1.76	0.50
1:A:1270:LEU:O	1:A:1273:LEU:HB2	2.10	0.50
1:B:243:ASN:O	1:B:246:SER:OG	2.28	0.50
1:B:247:LEU:O	1:B:249:GLU:N	2.44	0.50
1:B:808:VAL:HG11	1:B:908:TYR:HB3	1.94	0.50
1:A:1087:VAL:HG11	1:A:1154:ILE:HG23	1.93	0.50
1:B:1290:SER:HA	1:B:1293:ARG:HD3	1.93	0.50
1:B:1554:LEU:HD13	1:B:1557:HIS:CD2	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1388:LEU:O	1:A:1394:ARG:NE	2.44	0.50
1:A:1407:LEU:HD11	1:A:1449:LEU:HD22	1.94	0.50
1:A:1269:HIS:ND1	1:A:1283:SER:HB3	2.26	0.50
1:A:1499:ILE:HG12	1:A:1506:VAL:HG21	1.92	0.50
1:B:34:ARG:O	1:B:35:PRO:C	2.51	0.50
1:B:283:PHE:HB3	1:B:443:ARG:HD3	1.94	0.50
1:B:1054:ILE:O	1:B:1058:LEU:HG	2.11	0.50
1:A:130:ILE:HD13	1:A:312:THR:OG1	2.12	0.50
1:A:266:PHE:O	1:A:270:ILE:HG13	2.10	0.50
1:A:974:LEU:HD22	1:A:1003:PHE:CE1	2.46	0.50
1:A:1094:PHE:CZ	1:A:1128:ILE:HD13	2.47	0.50
1:A:1399:GLU:C	1:A:1403:ASP:OD1	2.48	0.50
1:B:83:HIS:O	1:B:87:THR:HG23	2.11	0.50
1:B:765:GLN:NE2	1:B:817:ILE:HG23	2.25	0.50
1:B:941:SER:C	1:B:943:ASP:N	2.70	0.50
1:B:1315:LEU:N	1:B:1316:PRO:HD2	2.27	0.50
1:B:1384:LEU:HB3	1:B:1430:PHE:CE1	2.47	0.50
1:B:1427:VAL:HG13	1:B:1431:PHE:CE2	2.47	0.50
1:A:289:VAL:HA	1:A:349:ILE:HG22	1.93	0.50
1:A:909:HIS:CG	1:A:937:SER:HA	2.47	0.50
1:A:973:LEU:HB3	1:A:1002:TYR:OH	2.12	0.50
1:A:1309:GLN:O	1:A:1313:THR:HG23	2.11	0.50
1:B:39:ALA:CB	1:B:44:PHE:CD1	2.95	0.50
1:B:280:ASN:O	1:B:281:SER:O	2.30	0.50
1:B:443:ARG:HB2	1:B:446:ASP:HB2	1.93	0.50
1:A:296:ARG:HD2	1:A:350:LEU:HD22	1.94	0.49
1:A:949:ASP:O	1:A:950:SER:C	2.54	0.49
1:B:193:PHE:C	1:B:195:ASN:N	2.67	0.49
1:B:528:VAL:O	1:B:529:PRO:C	2.51	0.49
1:B:759:ARG:HG2	1:B:885:LEU:HD22	1.93	0.49
1:B:1553:HIS:CD2	1:B:1602:TYR:OH	2.65	0.49
1:B:1553:HIS:CG	1:B:1553:HIS:O	2.65	0.49
1:A:129:LEU:HA	1:A:132:LEU:HD12	1.94	0.49
1:A:303:VAL:HG22	1:A:377:ILE:HG13	1.93	0.49
1:A:396:ARG:HH21	1:B:404:GLN:HE22	1.61	0.49
1:A:875:TYR:CD2	1:A:909:HIS:HE1	2.31	0.49
1:A:980:LEU:HD23	1:A:999:LEU:HD11	1.93	0.49
1:A:1032:GLU:OE2	1:A:1120:SER:HA	2.11	0.49
1:A:1302:SER:O	1:A:1305:MET:HG2	2.13	0.49
1:A:1347:LEU:HD22	1:A:1351:TYR:OH	2.13	0.49
1:A:1515:LEU:CB	1:A:1544:LEU:HD13	2.42	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:283:PHE:HD2	1:B:285:MET:HE2	1.75	0.49
1:B:485:THR:O	1:B:489:GLN:HG2	2.12	0.49
1:B:745:TRP:HE1	1:B:810:HIS:CE1	2.30	0.49
1:B:1355:ILE:HD13	1:B:1397:MET:HG2	1.94	0.49
1:B:1428:LEU:CD1	1:B:1488:ASN:HA	2.42	0.49
1:A:531:MET:HE1	1:A:535:LEU:HD11	1.94	0.49
1:A:683:MET:HE2	1:A:683:MET:HA	1.93	0.49
1:A:1299:ILE:HG22	1:A:1336:ARG:HE	1.76	0.49
1:A:48:GLU:O	1:A:51:GLN:HB3	2.12	0.49
1:B:49:LEU:C	1:B:51:GLN:H	2.19	0.49
1:B:112:LEU:HD11	1:B:247:LEU:CD1	2.42	0.49
1:B:143:LEU:HD13	1:B:151:PHE:CE2	2.47	0.49
1:B:201:PHE:O	1:B:202:ASN:C	2.53	0.49
1:B:663:LEU:HD23	1:B:674:LEU:HD13	1.93	0.49
1:B:704:GLU:HB3	1:B:889:PHE:CE2	2.47	0.49
1:B:739:PRO:HB3	1:B:782:VAL:HG23	1.94	0.49
1:B:1538:MET:HG2	1:B:1598:HIS:HD2	1.76	0.49
1:A:73:PHE:CD1	1:A:158:ALA:O	2.60	0.49
1:A:397:ARG:O	1:A:398:ALA:HB3	2.12	0.49
1:A:1047:ILE:HB	1:A:1050:TYR:CD2	2.42	0.49
1:A:313:LEU:HD21	1:A:332:LEU:HD23	1.94	0.49
1:A:686:LEU:O	1:A:690:ILE:HG13	2.12	0.49
1:A:949:ASP:O	1:A:952:ALA:N	2.45	0.49
1:A:1233:TRP:CE3	1:A:1278:LEU:HD13	2.48	0.49
1:A:1244:ILE:O	1:A:1246:SER:N	2.45	0.49
1:B:1244:ILE:HG13	1:B:1248:ARG:HB2	1.93	0.49
1:B:1251:PHE:N	1:B:1251:PHE:CD1	2.80	0.49
1:B:1388:LEU:HG	1:B:1397:MET:HE1	1.95	0.49
1:A:1047:ILE:CD1	1:A:1256:ILE:CG1	2.87	0.49
1:A:1101:PHE:HA	1:A:1104:ILE:HD13	1.95	0.49
1:A:1493:GLN:HG2	1:A:1540:VAL:HG22	1.94	0.49
1:A:1515:LEU:HD12	1:A:1541:MET:SD	2.53	0.49
1:A:1548:GLY:HA2	1:A:1552:GLY:HA3	1.93	0.49
1:B:491:LEU:HD21	1:B:667:ASN:CB	2.43	0.49
1:B:867:HIS:O	1:B:949:ASP:HB2	2.13	0.49
1:B:1214:LEU:HD23	1:B:1214:LEU:H	1.77	0.49
1:A:244:VAL:O	1:A:248:GLN:HG2	2.12	0.49
1:A:740:PHE:CD1	1:A:778:GLU:HG3	2.48	0.49
1:A:922:PHE:CG	1:A:923:SER:N	2.80	0.49
1:A:1281:ALA:CA	1:A:1284:LEU:HB2	2.43	0.49
1:A:1510:VAL:O	1:A:1514:LEU:HG	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:ASN:OD1	1:B:650:LEU:HD13	2.12	0.49
1:B:786:PHE:HZ	1:B:806:LEU:HD22	1.77	0.49
1:B:1000:GLN:HA	1:B:1270:LEU:HD13	1.94	0.49
1:A:341:VAL:HB	1:A:417:SER:HB2	1.95	0.49
1:A:1382:GLN:N	1:A:1426:ARG:HH21	2.10	0.49
1:A:1557:HIS:O	1:A:1561:VAL:HG23	2.12	0.49
1:B:1394:ARG:HH11	1:B:1446:LEU:HD21	1.78	0.49
1:A:662:MET:HB3	1:A:674:LEU:HD11	1.94	0.49
1:A:802:GLU:CG	1:A:931:ARG:HD2	2.38	0.49
1:B:857:ARG:O	1:B:861:ILE:HG13	2.13	0.49
1:B:908:TYR:CD2	1:B:908:TYR:N	2.81	0.49
1:B:942:GLU:CG	1:B:947:ARG:HD2	2.43	0.49
1:B:1043:SER:HA	1:B:1046:ARG:NE	2.28	0.49
1:B:1359:TYR:CD1	1:B:1406:GLU:HB3	2.47	0.49
1:B:1428:LEU:HD13	1:B:1491:LEU:HB2	1.94	0.49
1:B:1428:LEU:HB3	1:B:1491:LEU:HB3	1.95	0.49
1:B:1485:ILE:O	1:B:1489:ARG:HG3	2.12	0.49
1:A:317:VAL:HG12	1:A:318:LEU:N	2.28	0.48
1:A:1030:MET:HA	1:A:1034:ASP:CG	2.38	0.48
1:A:1210:LYS:HD2	1:A:1210:LYS:H	1.78	0.48
1:A:1251:PHE:CD2	1:A:1261:TYR:HD1	2.31	0.48
1:A:1300:VAL:HA	1:A:1336:ARG:NH1	2.28	0.48
1:A:1400:PHE:HB3	1:A:1401:PHE:CD2	2.48	0.48
1:B:957:PHE:CD1	1:B:1061:GLN:HG2	2.48	0.48
1:B:1486:GLN:HG3	1:B:1489:ARG:HH11	1.78	0.48
1:A:318:LEU:HD22	1:A:329:VAL:HG22	1.94	0.48
1:A:675:SER:HB3	1:A:722:LEU:HD12	1.95	0.48
1:A:1002:TYR:O	1:A:1003:PHE:C	2.53	0.48
1:A:1208:ARG:CD	1:A:1328:GLU:HA	2.43	0.48
1:A:1459:VAL:HG21	1:A:1464:LEU:HD13	1.95	0.48
1:B:1415:ALA:O	1:B:1470:ARG:HD3	2.13	0.48
1:B:1594:GLU:O	1:B:1598:HIS:N	2.42	0.48
1:A:284:ILE:HG22	1:A:286:PRO:HD2	1.96	0.48
1:A:422:LEU:HD11	1:A:537:LEU:HD23	1.96	0.48
1:A:860:LEU:HD12	1:A:860:LEU:O	2.12	0.48
1:A:1515:LEU:HB2	1:A:1544:LEU:HB3	1.94	0.48
1:B:89:CYS:SG	1:B:236:LYS:HG3	2.53	0.48
1:B:266:PHE:O	1:B:270:ILE:HG13	2.14	0.48
1:B:1024:SER:HB3	1:B:1074:LEU:HD23	1.95	0.48
1:B:1110:LEU:H	1:B:1175:ALA:HB2	1.77	0.48
1:B:1586:HIS:CD2	1:B:1589:HIS:CE1	3.01	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:813:MET:HB2	1:B:813:MET:HE3	1.68	0.48
1:B:946:ASN:O	1:B:947:ARG:C	2.56	0.48
1:B:1032:GLU:O	1:B:1035:ILE:HB	2.13	0.48
1:B:1087:VAL:O	1:B:1091:GLU:HG3	2.14	0.48
1:B:1151:SER:HB3	1:B:1154:ILE:HD13	1.95	0.48
1:B:1600:MET:CA	1:B:1603:LEU:HG	2.42	0.48
1:A:69:GLN:O	1:A:72:PRO:HD2	2.12	0.48
1:A:336:CYS:SG	1:A:384:ILE:HD12	2.53	0.48
1:A:738:ALA:HB3	1:A:741:SER:HB3	1.96	0.48
1:A:1460:GLU:HB2	1:A:1463:ARG:HB3	1.94	0.48
1:B:1599:ILE:O	1:B:1603:LEU:HG	2.13	0.48
1:A:45:GLU:C	1:A:47:LYS:N	2.70	0.48
1:A:548:LEU:HD13	1:A:642:LYS:C	2.38	0.48
1:A:866:LEU:HD22	1:A:948:LEU:CD1	2.44	0.48
1:A:1135:LEU:O	1:A:1139:PHE:HD2	1.96	0.48
1:A:1351:TYR:HA	1:A:1354:LEU:HD12	1.95	0.48
1:A:1560:ALA:HA	1:A:1563:TRP:CE3	2.49	0.48
1:B:32:ALA:O	1:B:33:VAL:C	2.56	0.48
1:B:245:ALA:O	1:B:249:GLU:HG3	2.14	0.48
1:B:1194:LYS:HA	1:B:1370:SER:C	2.38	0.48
1:B:1374:GLU:O	1:B:1375:SER:C	2.56	0.48
1:A:1023:LEU:HD22	1:A:1038:THR:HG23	1.96	0.48
1:A:1434:LEU:CD1	1:A:1449:LEU:HD12	2.44	0.48
1:A:1453:LEU:HB3	1:A:1506:VAL:CG1	2.37	0.48
1:B:285:MET:O	1:B:287:ALA:N	2.46	0.48
1:B:740:PHE:CD1	1:B:778:GLU:HG3	2.48	0.48
1:B:863:ASP:HB2	1:B:1009:ILE:HG12	1.95	0.48
1:B:1009:ILE:O	1:B:1013:LEU:HG	2.14	0.48
1:B:1094:PHE:CE1	1:B:1162:THR:HA	2.49	0.48
1:B:1113:HIS:H	1:B:1113:HIS:CD2	2.31	0.48
1:B:1156:LYS:O	1:B:1160:PRO:HD2	2.13	0.48
1:B:1500:VAL:HG13	1:B:1547:ALA:HA	1.95	0.48
1:A:85:ILE:HG21	1:A:104:CYS:SG	2.54	0.48
1:A:1314:LEU:HD12	1:A:1330:SER:CB	2.44	0.48
1:A:1314:LEU:HB2	1:A:1334:LEU:HD21	1.96	0.48
1:A:1562:ASP:HB3	1:A:1566:ARG:NH2	2.29	0.48
1:B:836:ILE:O	1:B:840:LEU:HG	2.14	0.48
1:A:200:VAL:CB	1:B:715:HIS:ND1	2.77	0.48
1:A:1427:VAL:HG13	1:A:1431:PHE:CE2	2.47	0.48
1:B:239:PHE:O	1:B:243:ASN:ND2	2.47	0.48
1:B:1394:ARG:HD3	1:B:1446:LEU:CD2	2.42	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1536:GLU:O	1:B:1540:VAL:HG23	2.13	0.48
1:A:45:GLU:C	1:A:47:LYS:H	2.20	0.48
1:A:1497:THR:HA	1:A:1543:THR:HG21	1.95	0.48
1:B:255:LYS:HG2	1:B:258:ARG:NH2	2.29	0.48
1:B:274:GLN:O	1:B:277:VAL:HG22	2.13	0.48
1:B:755:SER:O	1:B:759:ARG:HG3	2.14	0.48
1:B:909:HIS:HB2	1:B:938:PRO:HD3	1.95	0.48
1:B:1244:ILE:CG1	1:B:1248:ARG:HB2	2.44	0.48
1:B:1289:LEU:HD12	1:B:1326:VAL:HB	1.96	0.48
1:A:1401:PHE:CD1	1:A:1406:GLU:HB2	2.49	0.47
1:B:253:SER:O	1:B:317:VAL:HG13	2.14	0.47
1:B:549:GLN:O	1:B:553:LYS:HG2	2.14	0.47
1:A:327:GLN:NE2	1:A:512:MET:SD	2.87	0.47
1:A:735:LEU:HD13	1:A:753:SER:HA	1.96	0.47
1:A:1058:LEU:HD23	1:A:1061:GLN:NE2	2.29	0.47
1:A:1208:ARG:HH11	1:A:1327:ALA:HB3	1.79	0.47
1:B:337:LEU:O	1:B:341:VAL:HG13	2.14	0.47
1:B:418:LEU:HD13	1:B:537:LEU:HD11	1.96	0.47
1:B:544:LYS:O	1:B:548:LEU:HG	2.14	0.47
1:B:1169:TYR:O	1:B:1173:THR:HG23	2.14	0.47
1:B:1319:LEU:HD22	1:B:1354:LEU:HD21	1.97	0.47
1:B:1445:SER:O	1:B:1448:HIS:HB2	2.14	0.47
1:A:327:GLN:O	1:A:331:VAL:HG23	2.14	0.47
1:B:733:GLN:HA	1:B:738:ALA:HB2	1.96	0.47
1:B:1121:ILE:HG22	1:B:1269:HIS:CE1	2.49	0.47
1:B:1414:THR:HA	1:B:1423:PHE:CD2	2.49	0.47
1:A:1002:TYR:CD1	1:A:1002:TYR:C	2.93	0.47
1:A:1203:ALA:C	1:A:1205:GLY:N	2.70	0.47
1:A:130:ILE:CD1	1:A:308:MET:HG3	2.43	0.47
1:A:266:PHE:CE1	1:A:305:ASP:HB3	2.50	0.47
1:A:506:PRO:HB2	1:A:523:ARG:NH2	2.29	0.47
1:A:811:LEU:HD11	1:A:861:ILE:HG12	1.95	0.47
1:A:1541:MET:O	1:A:1556:LEU:HD22	2.14	0.47
1:A:1571:LEU:C	1:A:1573:GLN:H	2.23	0.47
1:A:66:HIS:HE1	1:A:71:GLU:HA	1.80	0.47
1:A:922:PHE:HE1	1:A:927:VAL:HA	1.80	0.47
1:A:1570:TYR:CD2	1:A:1570:TYR:C	2.93	0.47
1:A:1570:TYR:CE1	1:A:1592:ILE:HG13	2.50	0.47
1:B:1242:PRO:HG3	1:B:1264:ALA:CB	2.45	0.47
1:A:260:CYS:O	1:A:263:LEU:HG	2.15	0.47
1:A:485:THR:O	1:A:489:GLN:HG2	2.15	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:718:VAL:HG12	1:A:763:ILE:HD12	1.97	0.47
1:A:852:PRO:O	1:A:853:LEU:C	2.56	0.47
1:A:942:GLU:OE2	1:A:947:ARG:HD3	2.14	0.47
1:A:1046:ARG:NH1	1:A:1075:ALA:O	2.43	0.47
1:A:1414:THR:OG1	1:A:1427:VAL:HG21	2.15	0.47
1:A:1552:GLY:O	1:A:1553:HIS:HB3	2.14	0.47
1:B:53:VAL:O	1:B:57:ILE:HG13	2.15	0.47
1:B:338:TYR:O	1:B:341:VAL:HG22	2.14	0.47
1:B:387:MET:O	1:B:390:GLN:HG2	2.15	0.47
1:B:470:GLY:O	1:B:474:VAL:HG23	2.15	0.47
1:B:519:GLN:O	1:B:520:ARG:C	2.51	0.47
1:B:765:GLN:HE22	1:B:817:ILE:HG23	1.79	0.47
1:B:1047:ILE:HB	1:B:1050:TYR:CD2	2.49	0.47
1:B:1093:TYR:HA	1:B:1096:ARG:HG2	1.97	0.47
1:A:506:PRO:HG3	1:A:526:ASP:OD2	2.14	0.47
1:A:932:PHE:HD1	1:A:1001:TYR:CD1	2.33	0.47
1:A:1299:ILE:CG2	1:A:1336:ARG:HE	2.28	0.47
1:B:202:ASN:N	1:B:203:PRO:HD3	2.30	0.47
1:B:1159:LEU:CB	1:B:1160:PRO:CD	2.92	0.47
1:B:1356:THR:HA	1:B:1400:PHE:CE2	2.50	0.47
1:A:191:MET:N	1:A:191:MET:SD	2.88	0.47
1:A:985:ARG:NH1	1:A:1280:LEU:HD13	2.27	0.47
1:B:283:PHE:HB3	1:B:443:ARG:CD	2.44	0.47
1:A:137:CYS:O	1:A:240:ILE:HG23	2.13	0.47
1:A:411:ALA:O	1:A:412:TRP:C	2.56	0.47
1:A:1015:PRO:HG3	1:A:1041:TRP:CE2	2.50	0.47
1:A:1535:PRO:O	1:A:1539:VAL:HG23	2.15	0.47
1:B:45:GLU:O	1:B:46:MET:C	2.58	0.47
1:B:1177:LEU:HD21	1:B:1233:TRP:CD2	2.49	0.47
1:B:1411:MET:O	1:B:1414:THR:HB	2.15	0.47
1:B:1551:ALA:O	1:B:1554:LEU:HD23	2.15	0.47
1:B:1586:HIS:HD2	1:B:1589:HIS:CE1	2.32	0.47
1:B:1592:ILE:HA	1:B:1595:CYS:SG	2.54	0.47
1:A:1101:PHE:HE2	1:A:1165:LEU:HD22	1.80	0.46
1:A:1548:GLY:CA	1:A:1552:GLY:C	2.89	0.46
1:A:1564:LEU:HD22	1:A:1603:LEU:CD1	2.45	0.46
1:B:246:SER:HA	1:B:249:GLU:OE2	2.15	0.46
1:B:694:ASP:CG	1:B:750:HIS:HB3	2.40	0.46
1:B:761:LEU:HB3	1:B:779:CYS:SG	2.56	0.46
1:B:1266:GLN:O	1:B:1270:LEU:HG	2.14	0.46
1:A:833:PHE:HZ	1:A:861:ILE:HG21	1.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:867:HIS:CG	1:A:936:LEU:HD11	2.50	0.46
1:A:1022:GLN:C	1:A:1024:SER:H	2.22	0.46
1:A:1180:ASN:O	1:A:1181:PHE:C	2.58	0.46
1:B:49:LEU:O	1:B:51:GLN:N	2.48	0.46
1:B:341:VAL:HB	1:B:417:SER:CB	2.45	0.46
1:B:1394:ARG:NH1	1:B:1446:LEU:HD21	2.30	0.46
1:B:1431:PHE:O	1:B:1435:PHE:HD2	1.98	0.46
1:A:270:ILE:O	1:A:274:GLN:HG3	2.14	0.46
1:A:710:LEU:HG	1:A:714:ASN:HD21	1.80	0.46
1:A:808:VAL:HG22	1:A:933:TYR:CD2	2.51	0.46
1:A:945:LEU:HD22	1:A:1053:TRP:CG	2.50	0.46
1:A:1101:PHE:O	1:A:1104:ILE:HB	2.14	0.46
1:B:1090:VAL:CG1	1:B:1127:ALA:HB1	2.33	0.46
1:B:1288:LEU:HD23	1:B:1326:VAL:HG11	1.97	0.46
1:B:1572:SER:O	1:B:1577:VAL:HG23	2.15	0.46
1:A:325:ARG:HH12	1:B:496:LEU:CD2	2.28	0.46
1:A:847:GLN:HG3	1:A:976:ALA:HB2	1.98	0.46
1:A:1281:ALA:HB2	1:A:1284:LEU:HD12	1.96	0.46
1:A:1381:LEU:HB3	1:A:1426:ARG:NH2	2.29	0.46
1:B:658:ILE:O	1:B:662:MET:HB2	2.16	0.46
1:B:858:LEU:HD23	1:B:858:LEU:HA	1.80	0.46
1:B:1162:THR:O	1:B:1166:ILE:HG13	2.16	0.46
1:B:1301:TRP:O	1:B:1302:SER:HB2	2.15	0.46
1:B:1600:MET:HA	1:B:1603:LEU:CG	2.41	0.46
1:A:283:PHE:HA	1:A:442:LEU:O	2.16	0.46
1:A:471:VAL:HG21	1:A:641:ARG:HG2	1.98	0.46
1:B:414:LEU:HB3	1:B:480:ALA:HB2	1.98	0.46
1:B:484:LEU:HD22	1:B:488:PHE:HE1	1.81	0.46
1:B:909:HIS:CB	1:B:938:PRO:HD3	2.46	0.46
1:B:1121:ILE:HG22	1:B:1269:HIS:HE1	1.80	0.46
1:B:1305:MET:HE1	1:B:1337:ILE:HG23	1.97	0.46
1:B:1456:LEU:O	1:B:1458:CYS:N	2.48	0.46
1:A:110:PHE:CZ	1:A:114:ARG:HD2	2.51	0.46
1:A:135:GLY:CA	1:A:140:CYS:O	2.63	0.46
1:A:271:ASN:HD22	1:A:271:ASN:N	2.13	0.46
1:A:280:ASN:HD22	1:A:523:ARG:HH11	1.64	0.46
1:A:1036:LEU:HD21	1:A:1123:THR:HA	1.97	0.46
1:A:1412:MET:HB3	1:A:1463:ARG:CZ	2.46	0.46
1:B:668:ASN:HA	1:B:671:ARG:HB2	1.98	0.46
1:B:1019:TYR:OH	1:B:1038:THR:HA	2.15	0.46
1:B:1118:LEU:HD23	1:B:1122:TYR:CD2	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:477:ALA:O	1:A:481:ILE:HG12	2.15	0.46
1:A:1039:LEU:CD2	1:A:1089:ILE:HD13	2.44	0.46
1:A:1431:PHE:O	1:A:1435:PHE:HD2	1.98	0.46
1:B:58:GLU:C	1:B:60:GLU:N	2.74	0.46
1:B:272:ARG:HB3	1:B:338:TYR:CE1	2.51	0.46
1:B:521:ILE:HA	1:B:521:ILE:HD13	1.55	0.46
1:B:827:ARG:NE	1:B:955:VAL:HG22	2.31	0.46
1:B:1047:ILE:C	1:B:1051:VAL:HG23	2.41	0.46
1:B:1247:TRP:CD1	1:B:1248:ARG:N	2.82	0.46
1:B:1318:LEU:HD21	1:B:1331:SER:CB	2.45	0.46
1:A:530:LEU:O	1:A:534:LEU:HG	2.15	0.46
1:A:847:GLN:HG3	1:A:976:ALA:CB	2.46	0.46
1:A:1428:LEU:CD1	1:A:1488:ASN:HA	2.46	0.46
1:B:255:LYS:HG2	1:B:258:ARG:HH21	1.80	0.46
1:B:1105:ASP:HB3	1:B:1108:THR:HB	1.98	0.46
1:A:32:ALA:O	1:A:33:VAL:C	2.54	0.46
1:A:811:LEU:HD23	1:A:933:TYR:HE1	1.80	0.46
1:B:257:LEU:HD23	1:B:257:LEU:HA	1.59	0.46
1:B:1272:THR:OG1	1:B:1283:SER:OG	2.32	0.46
1:A:285:MET:N	1:A:286:PRO:CD	2.79	0.46
1:A:844:MET:HB3	1:A:848:MET:HE3	1.98	0.46
1:A:1122:TYR:CD1	1:A:1123:THR:N	2.84	0.46
1:A:1201:VAL:HG11	1:A:1222:LEU:CD2	2.43	0.46
1:A:1220:GLN:C	1:A:1222:LEU:H	2.24	0.46
1:A:1456:LEU:HD22	1:A:1510:VAL:HG13	1.98	0.46
1:A:1525:MET:SD	1:A:1534:PHE:HA	2.56	0.46
1:B:327:GLN:O	1:B:331:VAL:HG23	2.16	0.46
1:B:348:ALA:CB	1:B:421:ILE:HG23	2.46	0.46
1:B:1553:HIS:CE1	1:B:1606:VAL:HG22	2.50	0.46
1:A:32:ALA:HA	1:A:35:PRO:HD2	1.98	0.45
1:A:325:ARG:O	1:A:329:VAL:HG23	2.16	0.45
1:A:659:THR:HA	1:A:663:LEU:CD1	2.40	0.45
1:A:1213:THR:HA	1:A:1216:PRO:HG2	1.97	0.45
1:A:1299:ILE:O	1:A:1300:VAL:C	2.59	0.45
1:B:747:LEU:HB3	1:B:806:LEU:N	2.31	0.45
1:B:1158:LEU:O	1:B:1159:LEU:C	2.57	0.45
1:B:1377:LEU:HD12	1:B:1377:LEU:H	1.81	0.45
1:A:310:LEU:HD13	1:A:384:ILE:CG1	2.46	0.45
1:A:715:HIS:CG	1:B:200:VAL:HG21	2.50	0.45
1:A:787:LEU:HA	1:A:787:LEU:HD23	1.53	0.45
1:A:911:PHE:O	1:A:915:GLU:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1411:MET:HE3	1:A:1411:MET:HB2	1.78	0.45
1:A:1564:LEU:HA	1:A:1599:ILE:HG21	1.98	0.45
1:B:1299:ILE:HG22	1:B:1300:VAL:HG13	1.99	0.45
1:B:1407:LEU:H	1:B:1407:LEU:CD1	2.25	0.45
1:B:1586:HIS:HD2	1:B:1589:HIS:HE1	1.64	0.45
1:B:1590:VAL:HA	1:B:1593:LEU:HD23	1.97	0.45
1:A:68:LYS:C	1:A:70:TYR:N	2.74	0.45
1:A:948:LEU:HD21	1:A:956:LEU:HD12	1.98	0.45
1:A:1039:LEU:HD22	1:A:1130:LYS:HE2	1.98	0.45
1:A:1176:TYR:CD1	1:A:1281:ALA:CB	2.99	0.45
1:A:1311:ILE:HG23	1:A:1338:LEU:HD11	1.99	0.45
1:B:408:LEU:HD13	1:B:520:ARG:HB3	1.99	0.45
1:B:535:LEU:HD23	1:B:535:LEU:HA	1.81	0.45
1:B:1115:ILE:HD13	1:B:1176:TYR:HB2	1.98	0.45
1:A:104:CYS:SG	1:A:136:LEU:HD22	2.56	0.45
1:A:136:LEU:O	1:A:243:ASN:ND2	2.49	0.45
1:A:309:ALA:O	1:A:313:LEU:HG	2.16	0.45
1:A:1039:LEU:HD21	1:A:1089:ILE:HD13	1.98	0.45
1:A:1087:VAL:O	1:A:1091:GLU:HG3	2.17	0.45
1:A:1346:PHE:O	1:A:1350:VAL:HG23	2.17	0.45
1:B:247:LEU:HD12	1:B:252:GLY:HA3	1.97	0.45
1:B:1213:THR:O	1:B:1216:PRO:HD2	2.16	0.45
1:B:1456:LEU:O	1:B:1457:ALA:C	2.59	0.45
1:B:1489:ARG:O	1:B:1493:GLN:HG3	2.16	0.45
1:B:1570:TYR:CE2	1:B:1592:ILE:HG13	2.52	0.45
1:A:93:PRO:CB	1:A:96:GLN:HB2	2.45	0.45
1:A:471:VAL:CG2	1:A:641:ARG:H	2.26	0.45
1:A:543:ARG:O	1:A:547:VAL:HG23	2.16	0.45
1:A:863:ASP:OD2	1:A:1008:ARG:NH2	2.45	0.45
1:A:984:ARG:HH11	1:A:984:ARG:CB	2.24	0.45
1:A:1417:GLU:CA	1:A:1470:ARG:HD2	2.35	0.45
1:B:197:LEU:O	1:B:198:THR:C	2.59	0.45
1:B:240:ILE:O	1:B:244:VAL:HG23	2.16	0.45
1:B:1308:PRO:O	1:B:1309:GLN:C	2.57	0.45
1:A:49:LEU:C	1:A:51:GLN:N	2.74	0.45
1:A:144:ASP:O	1:A:148:ILE:HG13	2.17	0.45
1:A:718:VAL:HG13	1:A:760:LEU:HD23	1.98	0.45
1:B:114:ARG:HD3	1:B:114:ARG:HA	1.68	0.45
1:A:68:LYS:HD2	1:A:69:GLN:HG3	1.98	0.45
1:A:97:LEU:HD23	1:A:98:GLN:N	2.32	0.45
1:A:919:SER:O	1:A:920:LYS:C	2.57	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:LEU:CD2	1:A:1038:THR:HG23	2.46	0.45
1:A:1048:SER:O	1:A:1049:SER:C	2.55	0.45
1:A:1090:VAL:HG11	1:A:1131:VAL:HG22	1.99	0.45
1:B:678:LEU:HB3	1:B:727:LEU:CD2	2.46	0.45
1:B:722:LEU:H	1:B:722:LEU:HD12	1.82	0.45
1:B:1063:MET:HG2	1:B:1068:ALA:HB2	1.99	0.45
1:B:1231:GLU:OE2	1:B:1232:SER:N	2.49	0.45
1:A:85:ILE:CG2	1:A:104:CYS:SG	3.05	0.45
1:A:256:LEU:HB3	1:A:312:THR:HG22	1.97	0.45
1:A:485:THR:HG22	1:A:657:PHE:HD1	1.81	0.45
1:A:790:MET:O	1:A:791:LYS:C	2.59	0.45
1:A:862:PHE:CE1	1:A:866:LEU:HD21	2.51	0.45
1:A:868:GLN:C	1:A:949:ASP:OD2	2.59	0.45
1:A:1047:ILE:CD1	1:A:1256:ILE:HD11	2.44	0.45
1:A:1156:LYS:O	1:A:1160:PRO:HD2	2.16	0.45
1:A:1511:CYS:O	1:A:1544:LEU:HD22	2.17	0.45
1:B:286:PRO:HD2	1:B:342:SER:HB3	1.97	0.45
1:B:808:VAL:HG22	1:B:933:TYR:CD2	2.51	0.45
1:B:830:LEU:HA	1:B:830:LEU:HD23	1.77	0.45
1:B:1315:LEU:HD21	1:B:1353:LYS:HB2	1.98	0.45
1:A:38:SER:O	1:A:41:TYR:HB3	2.17	0.45
1:A:341:VAL:HB	1:A:417:SER:CB	2.47	0.45
1:A:1046:ARG:NH2	1:A:1077:THR:OG1	2.50	0.45
1:A:1268:ALA:O	1:A:1272:THR:HG23	2.17	0.45
1:A:1509:GLY:O	1:A:1513:VAL:HG23	2.17	0.45
1:B:56:VAL:O	1:B:57:ILE:C	2.60	0.45
1:B:414:LEU:O	1:B:418:LEU:HG	2.17	0.45
1:B:1345:GLU:CD	1:B:1345:GLU:H	2.24	0.45
1:B:1355:ILE:HD13	1:B:1397:MET:CG	2.47	0.45
1:B:1412:MET:HB3	1:B:1463:ARG:CZ	2.46	0.45
1:A:1019:TYR:CE2	1:A:1023:LEU:HD11	2.52	0.45
1:A:1025:MET:O	1:A:1026:ASN:HB2	2.17	0.45
1:A:1563:TRP:N	1:A:1566:ARG:HH21	2.15	0.45
1:B:1053:TRP:CD1	1:B:1053:TRP:C	2.95	0.45
1:B:1110:LEU:H	1:B:1175:ALA:HB1	1.81	0.45
1:B:1151:SER:O	1:B:1155:THR:HG23	2.16	0.45
1:B:1162:THR:HG22	1:B:1166:ILE:HD11	1.98	0.45
1:B:1468:LEU:O	1:B:1472:THR:HG23	2.17	0.45
1:A:349:ILE:CD1	1:A:429:LEU:HD11	2.31	0.44
1:A:680:GLU:HB3	1:A:730:THR:HG21	1.99	0.44
1:A:1030:MET:HG2	1:A:1035:ILE:HG13	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:246:SER:O	1:B:250:LEU:HG	2.17	0.44
1:B:253:SER:HB2	1:B:317:VAL:HA	2.00	0.44
1:B:253:SER:HB2	1:B:317:VAL:O	2.17	0.44
1:B:348:ALA:HB2	1:B:421:ILE:HG23	1.99	0.44
1:B:986:LYS:HG3	1:B:1113:HIS:CE1	2.51	0.44
1:B:1050:TYR:O	1:B:1054:ILE:HG13	2.17	0.44
1:B:1453:LEU:O	1:B:1456:LEU:CB	2.60	0.44
1:A:345:THR:HG23	1:A:424:LEU:HD11	1.99	0.44
1:A:773:ASP:HB3	1:A:774:PRO:HD2	1.99	0.44
1:A:1208:ARG:HD3	1:A:1328:GLU:HA	1.99	0.44
1:A:1284:LEU:HD23	1:A:1284:LEU:HA	1.89	0.44
1:A:1398:GLU:CG	1:A:1445:SER:HA	2.43	0.44
1:B:943:ASP:N	1:B:943:ASP:OD2	2.50	0.44
1:B:1450:CYS:C	1:B:1452:SER:N	2.70	0.44
1:B:1498:TYR:O	1:B:1504:SER:HB2	2.17	0.44
1:B:1570:TYR:CZ	1:B:1588:LYS:HD2	2.52	0.44
1:A:29:TRP:CG	1:A:160:LEU:HD21	2.53	0.44
1:A:297:ASN:O	1:A:300:HIS:NE2	2.50	0.44
1:A:859:LEU:O	1:A:860:LEU:C	2.53	0.44
1:A:1468:LEU:HA	1:A:1471:MET:HE2	1.99	0.44
1:B:379:GLN:HE21	1:B:379:GLN:HB3	1.52	0.44
1:B:414:LEU:CD1	1:B:479:HIS:HB3	2.48	0.44
1:B:443:ARG:HB2	1:B:446:ASP:CB	2.47	0.44
1:A:78:VAL:HG21	1:A:110:PHE:CD2	2.52	0.44
1:A:202:ASN:CG	1:A:204:ARG:HG3	2.43	0.44
1:A:288:THR:HG22	1:A:290:ALA:H	1.81	0.44
1:A:416:ASN:HD22	1:A:416:ASN:N	2.15	0.44
1:A:765:GLN:NE2	1:A:817:ILE:HG23	2.33	0.44
1:A:1030:MET:HA	1:A:1034:ASP:OD2	2.18	0.44
1:A:1077:THR:O	1:A:1081:SER:HB2	2.16	0.44
1:A:1118:LEU:HD23	1:A:1122:TYR:CD2	2.53	0.44
1:B:154:MET:O	1:B:157:SER:OG	2.34	0.44
1:B:493:VAL:O	1:B:496:LEU:N	2.50	0.44
1:B:531:MET:CG	1:B:677:SER:HB2	2.47	0.44
1:B:655:LEU:HD23	1:B:655:LEU:HA	1.75	0.44
1:B:674:LEU:O	1:B:678:LEU:HG	2.18	0.44
1:B:1055:LYS:HA	1:B:1058:LEU:HG	1.98	0.44
1:B:1242:PRO:HG3	1:B:1264:ALA:HB3	2.00	0.44
1:B:1306:ASN:O	1:B:1307:PRO:C	2.60	0.44
1:A:196:GLN:O	1:B:759:ARG:NH2	2.50	0.44
1:A:279:ALA:O	1:A:280:ASN:C	2.59	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:284:ILE:HG22	1:A:286:PRO:CD	2.47	0.44
1:A:1039:LEU:HD22	1:A:1130:LYS:CD	2.48	0.44
1:A:1098:ILE:HG12	1:A:1165:LEU:HD21	2.00	0.44
1:A:1194:LYS:NZ	1:A:1198:PHE:HZ	2.15	0.44
1:A:1212:ASN:O	1:A:1212:ASN:ND2	2.48	0.44
1:A:1296:GLY:O	1:A:1300:VAL:HG23	2.18	0.44
1:A:1564:LEU:HA	1:A:1567:CYS:SG	2.56	0.44
1:B:1191:SER:N	1:B:1194:LYS:HD3	2.32	0.44
1:B:1307:PRO:O	1:B:1308:PRO:C	2.61	0.44
1:B:1538:MET:HE2	1:B:1602:TYR:CG	2.53	0.44
1:A:252:GLY:O	1:A:256:LEU:HG	2.18	0.44
1:A:349:ILE:CD1	1:A:424:LEU:HD13	2.47	0.44
1:A:1489:ARG:O	1:A:1493:GLN:HG3	2.18	0.44
1:B:115:LEU:HD13	1:B:130:ILE:HG13	2.00	0.44
1:B:855:LEU:HD23	1:B:1002:TYR:HE2	1.82	0.44
1:B:862:PHE:CE1	1:B:866:LEU:HD11	2.53	0.44
1:B:908:TYR:O	1:B:908:TYR:CG	2.70	0.44
1:B:1204:ILE:CG2	1:B:1357:GLY:HA3	2.43	0.44
1:B:1445:SER:HA	1:B:1448:HIS:CB	2.47	0.44
1:A:284:ILE:O	1:A:442:LEU:N	2.50	0.44
1:A:511:ILE:HG13	1:A:512:MET:N	2.31	0.44
1:A:539:SER:O	1:A:543:ARG:HD3	2.18	0.44
1:A:715:HIS:CE1	1:B:200:VAL:CB	3.00	0.44
1:A:817:ILE:HG22	1:A:821:PHE:CE2	2.53	0.44
1:A:860:LEU:HD21	1:A:934:CYS:HA	2.00	0.44
1:A:945:LEU:HB3	1:A:1053:TRP:CG	2.52	0.44
1:A:1025:MET:HG2	1:A:1027:SER:H	1.82	0.44
1:A:1515:LEU:HB2	1:A:1544:LEU:CB	2.47	0.44
1:A:1545:ALA:C	1:A:1548:GLY:H	2.24	0.44
1:B:115:LEU:HD12	1:B:133:ILE:HD12	1.99	0.44
1:A:197:LEU:HD23	1:B:885:LEU:HD13	1.99	0.44
1:A:974:LEU:HD23	1:A:1006:LEU:HD23	1.99	0.44
1:A:1118:LEU:HA	1:A:1121:ILE:HD12	1.99	0.44
1:A:1200:ALA:O	1:A:1204:ILE:HD13	2.18	0.44
1:B:98:GLN:HE22	1:B:201:PHE:N	2.16	0.44
1:B:155:MET:C	1:B:157:SER:N	2.74	0.44
1:B:268:ARG:H	1:B:268:ARG:HG3	1.42	0.44
1:B:811:LEU:HD23	1:B:933:TYR:HE1	1.83	0.44
1:B:1109:ILE:HG23	1:B:1178:LEU:HD12	2.00	0.44
1:B:1273:LEU:O	1:B:1274:CYS:C	2.61	0.44
1:B:1557:HIS:C	1:B:1557:HIS:ND1	2.76	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1048:SER:O	1:A:1051:VAL:HB	2.18	0.44
1:A:1313:THR:OG1	1:A:1314:LEU:HD22	2.18	0.44
1:A:1429:LYS:O	1:A:1432:THR:N	2.51	0.44
1:B:97:LEU:HD13	1:B:201:PHE:CZ	2.52	0.44
1:B:204:ARG:O	1:B:205:THR:HB	2.17	0.44
1:B:796:GLN:HB2	1:B:798:VAL:HG23	2.00	0.44
1:B:1094:PHE:CZ	1:B:1128:ILE:HD11	2.52	0.44
1:A:37:LEU:HA	1:A:40:SER:CB	2.47	0.43
1:A:760:LEU:HD23	1:A:760:LEU:HA	1.90	0.43
1:A:932:PHE:HA	1:A:1001:TYR:HE1	1.82	0.43
1:A:1213:THR:O	1:A:1214:LEU:C	2.59	0.43
1:A:1214:LEU:C	1:A:1214:LEU:HD13	2.43	0.43
1:A:1281:ALA:HB1	1:A:1284:LEU:HB2	1.99	0.43
1:A:1314:LEU:HD12	1:A:1330:SER:HB3	2.00	0.43
1:B:1083:VAL:HG11	1:B:1135:LEU:HD23	1.99	0.43
1:B:1205:GLY:HA2	1:B:1215:GLY:HA3	1.94	0.43
1:B:1208:ARG:HD2	1:B:1327:ALA:HB3	2.00	0.43
1:B:1576:VAL:HA	1:B:1579:LYS:HD2	1.99	0.43
1:A:1098:ILE:HG12	1:A:1165:LEU:CD2	2.48	0.43
1:B:66:HIS:NE2	1:B:71:GLU:HG2	2.33	0.43
1:B:124:VAL:HG21	1:B:129:LEU:HD21	2.00	0.43
1:B:527:SER:O	1:B:528:VAL:CG1	2.66	0.43
1:B:648:LEU:HD23	1:B:648:LEU:HA	1.69	0.43
1:B:957:PHE:HE2	1:B:1057:HIS:CE1	2.36	0.43
1:B:1429:LYS:O	1:B:1432:THR:N	2.51	0.43
1:A:124:VAL:HG11	1:A:129:LEU:CD2	2.48	0.43
1:A:861:ILE:O	1:A:865:LEU:HG	2.17	0.43
1:A:1121:ILE:HG22	1:A:1287:THR:OG1	2.18	0.43
1:A:1222:LEU:O	1:A:1223:PRO:O	2.36	0.43
1:A:1548:GLY:HA2	1:A:1551:ALA:O	2.18	0.43
1:B:1407:LEU:HB3	1:B:1431:PHE:CZ	2.51	0.43
1:B:1480:ASP:HB3	1:B:1483:ASP:HB2	2.00	0.43
1:B:1534:PHE:N	1:B:1535:PRO:HD2	2.33	0.43
1:A:80:LEU:HD21	1:A:151:PHE:HB2	1.99	0.43
1:A:296:ARG:HA	1:A:299:PHE:CE2	2.54	0.43
1:A:782:VAL:O	1:A:783:TRP:C	2.56	0.43
1:A:1032:GLU:O	1:A:1036:LEU:HG	2.19	0.43
1:A:1434:LEU:HD11	1:A:1449:LEU:HD12	1.99	0.43
1:B:29:TRP:CE3	1:B:73:PHE:HZ	2.37	0.43
1:B:30:GLU:H	1:B:30:GLU:HG3	1.66	0.43
1:B:864:TYR:CD1	1:B:936:LEU:HD13	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1191:SER:O	1:B:1192:LYS:C	2.61	0.43
1:B:1345:GLU:O	1:B:1349:ARG:HG2	2.18	0.43
1:B:1417:GLU:HA	1:B:1470:ARG:HD2	2.00	0.43
1:B:1608:ASN:O	1:B:1612:GLN:HG2	2.17	0.43
1:A:272:ARG:HD2	1:A:338:TYR:HE1	1.83	0.43
1:A:488:PHE:HE2	1:A:670:ILE:HD12	1.82	0.43
1:A:547:VAL:HA	1:A:550:ARG:HH11	1.83	0.43
1:A:874:VAL:HG22	1:B:186:GLN:HA	2.00	0.43
1:A:1200:ALA:HB2	1:A:1365:HIS:NE2	2.33	0.43
1:A:1317:LEU:O	1:A:1323:THR:HG23	2.19	0.43
1:A:1318:LEU:HD22	1:A:1319:LEU:HD23	1.99	0.43
1:B:104:CYS:SG	1:B:239:PHE:CE1	3.10	0.43
1:B:112:LEU:HD11	1:B:247:LEU:HD12	1.99	0.43
1:B:474:VAL:HG11	1:B:646:LEU:HG	1.99	0.43
1:B:1405:GLY:O	1:B:1409:GLN:HG2	2.18	0.43
1:A:405:ASN:ND2	1:A:513:ALA:O	2.51	0.43
1:A:699:LYS:O	1:A:703:ASP:HB2	2.19	0.43
1:B:190:GLN:OE1	1:B:194:LEU:HD23	2.17	0.43
1:B:793:ASN:O	1:B:797:GLY:N	2.52	0.43
1:B:1285:LYS:HE3	1:B:1285:LYS:HB2	1.88	0.43
1:A:1094:PHE:CZ	1:A:1128:ILE:CD1	3.01	0.43
1:A:1546:SER:C	1:A:1548:GLY:H	2.27	0.43
1:B:247:LEU:CD1	1:B:252:GLY:HA3	2.48	0.43
1:B:801:SER:HA	1:B:930:PRO:HD3	1.99	0.43
1:B:1141:LYS:O	1:B:1142:MET:CB	2.67	0.43
1:B:1238:THR:HG23	1:B:1285:LYS:HB3	1.98	0.43
1:B:1456:LEU:C	1:B:1458:CYS:H	2.27	0.43
1:A:98:GLN:HG3	1:A:201:PHE:CZ	2.54	0.43
1:A:269:TYR:HB3	1:A:338:TYR:HD1	1.83	0.43
1:A:312:THR:O	1:A:315:LEU:HG	2.19	0.43
1:A:387:MET:O	1:A:388:ILE:C	2.60	0.43
1:A:404:GLN:OE1	1:A:404:GLN:HA	2.17	0.43
1:A:420:LEU:O	1:A:424:LEU:HG	2.19	0.43
1:A:1033:CYS:HA	1:A:1036:LEU:HD12	2.01	0.43
1:A:1130:LYS:O	1:A:1131:VAL:C	2.59	0.43
1:A:1576:VAL:HG13	1:A:1589:HIS:HA	2.01	0.43
1:B:493:VAL:O	1:B:494:GLU:C	2.62	0.43
1:B:919:SER:HA	1:B:922:PHE:CD2	2.54	0.43
1:B:1133:VAL:HG22	1:B:1246:SER:CA	2.49	0.43
1:B:1232:SER:C	1:B:1234:ASN:H	2.25	0.43
1:B:1388:LEU:C	1:B:1390:SER:H	2.27	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:93:PRO:CG	1:A:96:GLN:HB2	2.49	0.43
1:A:269:TYR:CD1	1:A:339:ALA:HA	2.54	0.43
1:A:1163:LEU:HA	1:A:1166:ILE:HD12	2.01	0.43
1:A:1214:LEU:HD21	1:A:1380:CYS:CB	2.46	0.43
1:A:1332:ASN:HA	1:A:1335:GLU:CD	2.44	0.43
1:A:1345:GLU:O	1:A:1349:ARG:HG2	2.19	0.43
1:A:1548:GLY:HA2	1:A:1552:GLY:CA	2.49	0.43
1:A:1562:ASP:HB3	1:A:1566:ARG:HH21	1.84	0.43
1:B:1057:HIS:CE1	1:B:1060:LYS:HD2	2.54	0.43
1:B:1063:MET:SD	1:B:1068:ALA:CB	3.07	0.43
1:B:1216:PRO:O	1:B:1217:THR:C	2.61	0.43
1:B:1311:ILE:HA	1:B:1334:LEU:HD21	2.00	0.43
1:A:484:LEU:O	1:A:488:PHE:HD1	2.02	0.43
1:A:732:LEU:HD21	1:A:760:LEU:HD12	2.00	0.43
1:A:838:GLN:NE2	1:A:965:GLU:OE2	2.51	0.43
1:A:947:ARG:O	1:A:948:LEU:C	2.61	0.43
1:A:1173:THR:HG22	1:A:1233:TRP:HZ2	1.84	0.43
1:A:1246:SER:HB3	1:A:1261:TYR:CE1	2.54	0.43
1:B:654:ILE:O	1:B:658:ILE:HG13	2.19	0.43
1:A:32:ALA:C	1:A:34:ARG:H	2.25	0.42
1:A:73:PHE:HD2	1:A:74:TYR:HD1	1.66	0.42
1:A:110:PHE:O	1:A:114:ARG:HG2	2.18	0.42
1:A:845:ASP:HB3	1:A:849:ARG:HH12	1.84	0.42
1:A:1281:ALA:CB	1:A:1284:LEU:HB2	2.49	0.42
1:A:1571:LEU:O	1:A:1573:GLN:N	2.51	0.42
1:A:296:ARG:HA	1:A:299:PHE:CZ	2.54	0.42
1:A:797:GLY:HA3	1:A:850:PHE:HB3	2.01	0.42
1:A:830:LEU:HD23	1:A:830:LEU:HA	1.85	0.42
1:A:1021:ASN:OD1	1:A:1071:LEU:HD21	2.17	0.42
1:A:1076:SER:O	1:A:1077:THR:C	2.62	0.42
1:A:1098:ILE:O	1:A:1101:PHE:HB2	2.18	0.42
1:A:1474:SER:CB	1:A:1485:ILE:HG21	2.48	0.42
1:B:234:LYS:HA	1:B:237:ASN:HD22	1.84	0.42
1:B:303:VAL:HG22	1:B:377:ILE:CG1	2.49	0.42
1:B:1038:THR:O	1:B:1039:LEU:C	2.61	0.42
1:B:1130:LYS:O	1:B:1131:VAL:C	2.62	0.42
1:B:1309:GLN:NE2	1:B:1313:THR:OG1	2.52	0.42
1:A:338:TYR:O	1:A:341:VAL:HG22	2.20	0.42
1:A:1057:HIS:HA	1:A:1060:LYS:HD2	2.01	0.42
1:A:1082:SER:O	1:A:1083:VAL:C	2.60	0.42
1:A:1301:TRP:HD1	1:A:1303:ASP:OD1	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1563:TRP:CD1	1:A:1566:ARG:NH2	2.87	0.42
1:B:386:ASP:OD1	1:B:479:HIS:CE1	2.72	0.42
1:B:527:SER:C	1:B:528:VAL:HG13	2.44	0.42
1:B:801:SER:O	1:B:805:ASP:N	2.52	0.42
1:B:1083:VAL:HG13	1:B:1134:SER:HB3	2.01	0.42
1:A:58:GLU:C	1:A:60:GLU:N	2.73	0.42
1:A:273:PHE:CE1	1:A:334:LEU:HD13	2.54	0.42
1:A:280:ASN:HB2	1:A:412:TRP:HE1	1.84	0.42
1:A:718:VAL:HG13	1:A:760:LEU:CD2	2.49	0.42
1:A:768:ALA:HA	1:A:773:ASP:HB2	2.01	0.42
1:A:963:TYR:O	1:A:964:ASP:C	2.62	0.42
1:A:1400:PHE:O	1:A:1403:ASP:HB2	2.18	0.42
1:A:1531:GLY:HA2	1:A:1595:CYS:SG	2.59	0.42
1:B:184:LEU:HD22	1:B:184:LEU:N	2.33	0.42
1:B:194:LEU:O	1:B:198:THR:HG23	2.20	0.42
1:B:1318:LEU:HD13	1:B:1334:LEU:HD12	2.02	0.42
1:B:1359:TYR:CE1	1:B:1406:GLU:HB3	2.53	0.42
1:B:1434:LEU:HD13	1:B:1449:LEU:HD12	2.01	0.42
1:A:37:LEU:HA	1:A:40:SER:HB2	2.01	0.42
1:A:255:LYS:O	1:A:259:VAL:HG23	2.19	0.42
1:A:908:TYR:CE2	1:A:930:PRO:CB	2.79	0.42
1:A:1281:ALA:C	1:A:1283:SER:N	2.73	0.42
1:A:1438:THR:CA	1:A:1446:LEU:HD13	2.35	0.42
1:A:1538:MET:HE1	1:A:1563:TRP:CZ3	2.53	0.42
1:B:63:ILE:HA	1:B:74:TYR:HD2	1.84	0.42
1:B:294:ALA:O	1:B:297:ASN:HB3	2.19	0.42
1:B:1412:MET:HE1	1:B:1467:TRP:CD2	2.54	0.42
1:B:1571:LEU:HB3	1:B:1580:LEU:HD11	2.02	0.42
1:A:124:VAL:HG11	1:A:129:LEU:HD23	2.02	0.42
1:A:300:HIS:O	1:A:304:ILE:HG13	2.19	0.42
1:A:666:ARG:HA	1:A:671:ARG:HE	1.84	0.42
1:A:860:LEU:HD13	1:A:860:LEU:HA	1.76	0.42
1:A:987:GLU:O	1:A:989:LYS:HG3	2.20	0.42
1:A:1000:GLN:HA	1:A:1270:LEU:HD22	2.01	0.42
1:A:1218:LEU:HD22	1:A:1376:ILE:HA	2.01	0.42
1:A:1306:ASN:HB3	1:A:1309:GLN:HB3	2.01	0.42
1:B:1083:VAL:HG12	1:B:1087:VAL:HG23	2.00	0.42
1:B:1139:PHE:CE2	1:B:1301:TRP:CE2	3.07	0.42
1:A:78:VAL:HG11	1:A:110:PHE:HD2	1.85	0.42
1:A:108:ILE:O	1:A:112:LEU:HG	2.20	0.42
1:A:112:LEU:HD13	1:A:252:GLY:HA3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:150:THR:O	1:A:154:MET:HG3	2.20	0.42
1:A:329:VAL:CG1	1:A:388:ILE:HD12	2.50	0.42
1:A:1090:VAL:HG21	1:A:1131:VAL:HG13	2.02	0.42
1:A:1251:PHE:CE1	1:A:1261:TYR:HA	2.55	0.42
1:A:1345:GLU:H	1:A:1345:GLU:CD	2.27	0.42
1:B:255:LYS:O	1:B:259:VAL:HG23	2.20	0.42
1:B:704:GLU:HB3	1:B:889:PHE:CD2	2.55	0.42
1:B:1064:LYS:HE3	1:B:1066:GLU:H	1.85	0.42
1:B:1233:TRP:O	1:B:1233:TRP:CD1	2.72	0.42
1:B:1556:LEU:HD23	1:B:1602:TYR:OH	2.20	0.42
1:A:193:PHE:CZ	1:B:816:LEU:HD21	2.54	0.42
1:A:516:THR:HG22	1:A:518:ILE:H	1.84	0.42
1:A:1138:HIS:HA	1:A:1141:LYS:HD3	2.02	0.42
1:B:1118:LEU:HD23	1:B:1122:TYR:HD2	1.83	0.42
1:B:1387:GLN:HB3	1:B:1397:MET:SD	2.59	0.42
1:B:1456:LEU:C	1:B:1456:LEU:HD23	2.44	0.42
1:B:1553:HIS:CD2	1:B:1553:HIS:O	2.73	0.42
1:B:1598:HIS:HA	1:B:1601:SER:CB	2.49	0.42
1:A:71:GLU:O	1:A:72:PRO:C	2.63	0.42
1:A:191:MET:C	1:A:193:PHE:N	2.77	0.42
1:A:366:LYS:HA	1:A:369:ASP:CG	2.45	0.42
1:A:418:LEU:HD11	1:A:477:ALA:HA	2.01	0.42
1:A:694:ASP:CB	1:A:750:HIS:HB3	2.50	0.42
1:A:1046:ARG:HD2	1:A:1046:ARG:HA	1.88	0.42
1:A:1453:LEU:CB	1:A:1506:VAL:HG13	2.38	0.42
1:B:131:LEU:HD11	1:B:142:ARG:HG3	2.01	0.42
1:B:405:ASN:O	1:B:409:LEU:HG	2.19	0.42
1:B:866:LEU:HD13	1:B:1013:LEU:HD21	2.01	0.42
1:B:916:GLU:O	1:B:920:LYS:HG3	2.20	0.42
1:A:292:ALA:O	1:A:296:ARG:HG3	2.19	0.42
1:A:548:LEU:HD22	1:A:642:LYS:HA	2.02	0.42
1:A:867:HIS:C	1:A:949:ASP:OD2	2.62	0.42
1:A:945:LEU:N	1:A:945:LEU:HD23	2.35	0.42
1:A:1133:VAL:HG22	1:A:1247:TRP:CE2	2.54	0.42
1:A:1562:ASP:C	1:A:1566:ARG:HE	2.28	0.42
1:B:115:LEU:CD1	1:B:130:ILE:HG13	2.50	0.42
1:B:191:MET:C	1:B:193:PHE:N	2.75	0.42
1:B:296:ARG:HA	1:B:299:PHE:CD2	2.55	0.42
1:B:1443:ASN:OD1	1:B:1446:LEU:HG	2.20	0.42
1:B:1573:GLN:O	1:B:1574:LYS:C	2.60	0.42
1:A:693:VAL:HG21	1:A:710:LEU:HD22	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1195:LEU:HD23	1:A:1198:PHE:HD2	1.85	0.41
1:A:1219:VAL:O	1:A:1222:LEU:HD12	2.20	0.41
1:A:1398:GLU:CG	1:A:1399:GLU:N	2.83	0.41
1:A:1428:LEU:HD12	1:A:1488:ASN:HA	2.01	0.41
1:B:1063:MET:HE2	1:B:1067:HIS:CE1	2.54	0.41
1:B:1209:CYS:SG	1:B:1210:LYS:N	2.93	0.41
1:B:1241:PHE:HB3	1:B:1242:PRO:CD	2.50	0.41
1:B:1599:ILE:O	1:B:1602:TYR:HB3	2.19	0.41
1:A:699:LYS:O	1:A:704:GLU:HG3	2.20	0.41
1:A:1030:MET:SD	1:A:1038:THR:HG21	2.60	0.41
1:A:1047:ILE:HG12	1:A:1256:ILE:HG13	2.02	0.41
1:A:1174:ARG:NE	1:A:1320:GLU:OE2	2.53	0.41
1:A:1194:LYS:NZ	1:A:1194:LYS:HB3	2.35	0.41
1:A:1201:VAL:HG11	1:A:1222:LEU:CD1	2.49	0.41
1:A:1536:GLU:O	1:A:1540:VAL:HG23	2.19	0.41
1:A:1545:ALA:CA	1:A:1553:HIS:HA	2.45	0.41
1:B:338:TYR:HA	1:B:341:VAL:HG22	2.01	0.41
1:B:512:MET:H	1:B:512:MET:HG2	1.62	0.41
1:B:694:ASP:OD2	1:B:750:HIS:HB3	2.21	0.41
1:B:1053:TRP:CD1	1:B:1057:HIS:HD2	2.38	0.41
1:B:1122:TYR:CD1	1:B:1122:TYR:C	2.99	0.41
1:B:1133:VAL:HG22	1:B:1246:SER:HA	2.00	0.41
1:B:1565:SER:O	1:B:1569:LYS:HG3	2.20	0.41
1:A:240:ILE:O	1:A:244:VAL:HG23	2.19	0.41
1:A:1315:LEU:CB	1:A:1316:PRO:CD	2.98	0.41
1:B:1447:LEU:HB3	1:B:1505:GLN:HG3	2.02	0.41
1:B:1473:THR:O	1:B:1485:ILE:HG21	2.19	0.41
1:B:1486:GLN:O	1:B:1490:GLN:HG3	2.20	0.41
1:A:834:VAL:HG11	1:A:961:VAL:HG13	2.03	0.41
1:A:966:LEU:O	1:A:967:TYR:C	2.59	0.41
1:A:1319:LEU:HD11	1:A:1350:VAL:HA	2.02	0.41
1:A:1388:LEU:HD23	1:A:1388:LEU:HA	1.92	0.41
1:A:1568:LYS:CD	1:A:1569:LYS:HD3	2.49	0.41
1:B:248:GLN:O	1:B:249:GLU:C	2.61	0.41
1:B:426:PRO:HD3	1:B:467:GLN:NE2	2.35	0.41
1:B:496:LEU:C	1:B:499:GLY:H	2.28	0.41
1:B:808:VAL:HG11	1:B:908:TYR:CB	2.50	0.41
1:B:860:LEU:HB2	1:B:1005:ILE:CD1	2.47	0.41
1:B:1414:THR:CG2	1:B:1424:CYS:HA	2.50	0.41
1:B:1449:LEU:N	1:B:1449:LEU:HD23	2.35	0.41
1:B:1519:THR:HB	1:B:1520:PRO:HD2	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:PRO:HD2	1:A:999:LEU:HD23	2.01	0.41
1:A:963:TYR:OH	1:A:1013:LEU:HB3	2.20	0.41
1:A:1060:LYS:O	1:A:1061:GLN:C	2.63	0.41
1:A:1292:VAL:HG12	1:A:1329:ILE:CG2	2.51	0.41
1:B:678:LEU:HD23	1:B:678:LEU:HA	1.84	0.41
1:B:1216:PRO:HA	1:B:1219:VAL:HG12	2.02	0.41
1:B:1424:CYS:O	1:B:1428:LEU:HG	2.20	0.41
1:A:1151:SER:N	1:A:1154:ILE:HD12	2.36	0.41
1:A:1153:GLU:HA	1:A:1156:LYS:CB	2.50	0.41
1:A:1244:ILE:HG12	1:A:1293:ARG:CZ	2.50	0.41
1:A:1307:PRO:CB	1:A:1308:PRO:HD3	2.50	0.41
1:A:1308:PRO:O	1:A:1312:ARG:HG3	2.20	0.41
1:A:1312:ARG:O	1:A:1313:THR:C	2.60	0.41
1:A:1499:ILE:HG22	1:A:1511:CYS:SG	2.60	0.41
1:B:905:THR:HG22	1:B:906:PRO:O	2.21	0.41
1:B:1124:LEU:O	1:B:1125:ASP:C	2.63	0.41
1:B:1238:THR:HG21	1:B:1286:HIS:CA	2.50	0.41
1:B:1475:PRO:HG2	1:B:1481:GLN:HB2	2.01	0.41
1:A:73:PHE:CE1	1:A:155:MET:SD	3.14	0.41
1:A:313:LEU:CD1	1:A:384:ILE:HG23	2.50	0.41
1:A:418:LEU:O	1:A:422:LEU:HG	2.21	0.41
1:A:793:ASN:O	1:A:797:GLY:N	2.53	0.41
1:A:813:MET:HE3	1:A:813:MET:HB2	1.70	0.41
1:A:1151:SER:N	1:A:1154:ILE:HB	2.35	0.41
1:A:1151:SER:HB3	1:A:1154:ILE:HG13	2.01	0.41
1:B:132:LEU:HD21	1:B:143:LEU:CD1	2.50	0.41
1:B:1142:MET:HE3	1:B:1142:MET:HB2	1.93	0.41
1:B:1318:LEU:HD21	1:B:1331:SER:CA	2.47	0.41
1:A:493:VAL:HG12	1:B:320:PRO:HB3	2.03	0.41
1:A:1003:PHE:O	1:A:1004:LEU:C	2.62	0.41
1:A:1101:PHE:CE2	1:A:1165:LEU:HD22	2.56	0.41
1:A:1105:ASP:N	1:A:1110:LEU:HD21	2.18	0.41
1:A:1194:LYS:HZ3	1:A:1198:PHE:HZ	1.69	0.41
1:A:1212:ASN:N	1:A:1212:ASN:HD22	2.18	0.41
1:A:1245:GLY:C	1:A:1247:TRP:N	2.75	0.41
1:A:1535:PRO:HG2	1:A:1536:GLU:OE2	2.21	0.41
1:B:115:LEU:HD12	1:B:133:ILE:CD1	2.51	0.41
1:B:120:GLU:H	1:B:120:GLU:HG3	1.59	0.41
1:B:711:TYR:CD2	1:B:888:PRO:CD	3.03	0.41
1:B:945:LEU:HG	1:B:946:ASN:OD1	2.21	0.41
1:B:952:ALA:O	1:B:956:LEU:HG	2.21	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1063:MET:HE3	1:B:1063:MET:HB2	1.78	0.41
1:B:1486:GLN:HG3	1:B:1489:ARG:NH1	2.35	0.41
1:B:1595:CYS:O	1:B:1599:ILE:N	2.51	0.41
1:A:236:LYS:HE3	1:A:236:LYS:HB3	1.90	0.41
1:A:390:GLN:O	1:A:391:ALA:C	2.61	0.41
1:A:415:LEU:HD21	1:A:484:LEU:HD11	2.01	0.41
1:A:478:ASN:O	1:A:482:LYS:HG3	2.20	0.41
1:A:795:LEU:HD23	1:A:795:LEU:HA	1.94	0.41
1:A:825:GLY:O	1:A:829:ILE:HG12	2.21	0.41
1:A:981:ASP:OD2	1:A:1280:LEU:HG	2.21	0.41
1:A:1166:ILE:HG13	1:A:1166:ILE:H	1.68	0.41
1:A:1245:GLY:HA2	1:A:1247:TRP:CZ2	2.55	0.41
1:A:1257:PRO:O	1:A:1258:SER:C	2.64	0.41
1:A:1271:GLY:O	1:A:1274:CYS:HB3	2.21	0.41
1:A:1493:GLN:HG2	1:A:1540:VAL:CG2	2.49	0.41
1:B:159:LYS:HA	1:B:159:LYS:HD2	1.85	0.41
1:B:336:CYS:O	1:B:337:LEU:C	2.62	0.41
1:B:382:LEU:HD12	1:B:475:ILE:CG2	2.50	0.41
1:B:512:MET:HE3	1:B:512:MET:HB3	1.83	0.41
1:B:704:GLU:H	1:B:704:GLU:HG3	1.76	0.41
1:B:791:LYS:HD3	1:B:836:ILE:HG12	2.03	0.41
1:B:973:LEU:HD23	1:B:973:LEU:HA	1.86	0.41
1:B:1233:TRP:O	1:B:1233:TRP:CG	2.73	0.41
1:B:1528:ASN:HD22	1:B:1528:ASN:H	1.68	0.41
1:B:1575:ASN:O	1:B:1579:LYS:HG3	2.21	0.41
1:B:1593:LEU:HG	1:B:1594:GLU:N	2.34	0.41
1:A:86:THR:CG2	1:A:141:SER:HB3	2.51	0.41
1:A:414:LEU:HD12	1:A:483:LEU:HD12	2.01	0.41
1:A:469:PHE:CZ	1:A:474:VAL:HG22	2.55	0.41
1:A:659:THR:O	1:A:663:LEU:HB2	2.21	0.41
1:A:1027:SER:N	1:A:1028:PRO:CD	2.84	0.41
1:A:1041:TRP:HA	1:A:1044:ARG:HG3	2.03	0.41
1:A:1151:SER:HB3	1:A:1154:ILE:CG1	2.51	0.41
1:B:471:VAL:O	1:B:475:ILE:HG12	2.21	0.41
1:B:1001:TYR:CE2	1:B:1005:ILE:HD11	2.56	0.41
1:B:1445:SER:O	1:B:1449:LEU:HG	2.21	0.41
1:B:1587:GLY:O	1:B:1588:LYS:C	2.61	0.41
1:A:108:ILE:HD11	1:A:243:ASN:HB3	2.03	0.40
1:A:422:LEU:HD11	1:A:537:LEU:CD2	2.51	0.40
1:A:671:ARG:HB3	1:A:722:LEU:HD11	2.03	0.40
1:A:1552:GLY:C	1:A:1554:LEU:N	2.78	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:92:ILE:O	1:B:93:PRO:C	2.64	0.40
1:B:281:SER:HB3	1:B:444:VAL:HG12	2.03	0.40
1:B:299:PHE:O	1:B:303:VAL:HG23	2.20	0.40
1:B:441:ALA:HB1	1:B:443:ARG:NH2	2.33	0.40
1:B:1104:ILE:HG23	1:B:1110:LEU:CD1	2.51	0.40
1:B:1388:LEU:HD23	1:B:1394:ARG:HG3	2.02	0.40
1:B:1555:GLN:HA	1:B:1558:ASN:HD22	1.85	0.40
1:B:1573:GLN:HB2	1:B:1576:VAL:HG23	2.03	0.40
1:B:1603:LEU:O	1:B:1607:THR:N	2.54	0.40
1:A:35:PRO:CB	1:A:48:GLU:HB3	2.49	0.40
1:A:184:LEU:HD22	1:A:184:LEU:N	2.32	0.40
1:A:234:LYS:O	1:A:238:VAL:HG23	2.21	0.40
1:A:538:LEU:HD12	1:A:651:ALA:HB1	2.02	0.40
1:A:545:ALA:HB1	1:A:648:LEU:HG	2.04	0.40
1:A:659:THR:HA	1:A:663:LEU:HB2	2.02	0.40
1:A:866:LEU:HB3	1:A:948:LEU:HD13	2.03	0.40
1:A:1051:VAL:HG13	1:A:1072:LEU:HG	2.02	0.40
1:A:1077:THR:C	1:A:1081:SER:HB2	2.46	0.40
1:A:1193:GLU:OE1	1:A:1369:ASN:HB3	2.21	0.40
1:A:1534:PHE:N	1:A:1535:PRO:CD	2.83	0.40
1:B:1493:GLN:CG	1:B:1540:VAL:HG22	2.37	0.40
1:B:1605:ASP:C	1:B:1607:THR:N	2.78	0.40
1:A:303:VAL:HG22	1:A:377:ILE:CG1	2.51	0.40
1:A:484:LEU:HD22	1:A:530:LEU:HD11	2.03	0.40
1:A:779:CYS:HB3	1:A:817:ILE:HG21	2.03	0.40
1:A:1029:GLU:O	1:A:1096:ARG:NH1	2.54	0.40
1:A:1063:MET:SD	1:A:1068:ALA:HB2	2.62	0.40
1:A:1094:PHE:CE1	1:A:1128:ILE:HD11	2.56	0.40
1:A:1255:THR:O	1:A:1256:ILE:C	2.64	0.40
1:A:1292:VAL:CG1	1:A:1329:ILE:HB	2.52	0.40
1:A:1447:LEU:HA	1:A:1505:GLN:HG3	2.04	0.40
1:A:1559:ALA:HB1	1:A:1563:TRP:CH2	2.56	0.40
1:B:855:LEU:CD2	1:B:1002:TYR:HE2	2.34	0.40
1:B:1165:LEU:HD23	1:B:1165:LEU:HA	1.81	0.40
1:B:1244:ILE:HG23	1:B:1244:ILE:O	2.22	0.40
1:B:1392:GLN:CD	1:B:1392:GLN:H	2.28	0.40
1:B:1445:SER:HA	1:B:1448:HIS:HD1	1.83	0.40
1:B:1515:LEU:HD11	1:B:1556:LEU:CD2	2.46	0.40
1:A:81:SER:O	1:A:82:THR:C	2.65	0.40
1:A:481:ILE:O	1:A:485:THR:HG23	2.20	0.40
1:A:925:ASP:OD1	1:A:925:ASP:N	2.54	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1039:LEU:HB3	1:A:1130:LYS:HD2	2.03	0.40
1:A:1111:GLN:HB3	1:A:1113:HIS:ND1	2.36	0.40
1:A:1564:LEU:O	1:A:1565:SER:C	2.64	0.40
1:B:282:PHE:HB2	1:B:416:ASN:CB	2.52	0.40
1:B:833:PHE:HE1	1:B:858:LEU:HD22	1.87	0.40
1:B:1055:LYS:HB2	1:B:1072:LEU:HD12	2.03	0.40
1:B:1299:ILE:CG2	1:B:1336:ARG:HD2	2.49	0.40
1:B:1328:GLU:O	1:B:1331:SER:OG	2.34	0.40
1:A:69:GLN:C	1:A:71:GLU:H	2.29	0.40
1:A:317:VAL:CG1	1:A:318:LEU:N	2.85	0.40
1:A:547:VAL:HG12	1:A:551:GLN:NE2	2.37	0.40
1:A:932:PHE:HA	1:A:1001:TYR:CE1	2.56	0.40
1:A:1128:ILE:O	1:A:1131:VAL:HG23	2.21	0.40
1:A:1203:ALA:O	1:A:1205:GLY:N	2.54	0.40
1:A:1381:LEU:HA	1:A:1381:LEU:HD23	1.88	0.40
1:B:542:TYR:CE2	1:B:689:ILE:HG23	2.57	0.40
1:B:747:LEU:HD11	1:B:793:ASN:ND2	2.37	0.40
1:B:1194:LYS:HA	1:B:1370:SER:O	2.21	0.40
1:B:1374:GLU:OE1	1:B:1423:PHE:HB2	2.21	0.40
1:B:1474:SER:HA	1:B:1485:ILE:CD1	2.51	0.40
1:B:1586:HIS:HB2	1:B:1589:HIS:CE1	2.57	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	1372/5183 (26%)	1288 (94%)	63 (5%)	21 (2%)	8 30
1	B	1359/5183 (26%)	1262 (93%)	82 (6%)	15 (1%)	12 37
All	All	2731/10366 (26%)	2550 (93%)	145 (5%)	36 (1%)	13 33

All (36) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	889	PHE
1	A	906	PRO
1	A	907	LEU
1	A	909	HIS
1	A	1031	SER
1	A	1223	PRO
1	A	1244	ILE
1	B	1159	LEU
1	A	910	GLY
1	A	1245	GLY
1	A	1549	GLN
1	B	197	LEU
1	B	1247	TRP
1	A	59	SER
1	A	94	ARG
1	A	1211	ALA
1	A	1221	ASN
1	A	1257	PRO
1	B	59	SER
1	B	324	SER
1	B	1142	MET
1	B	1274	CYS
1	B	1275	SER
1	B	323	PRO
1	B	492	GLN
1	A	1205	GLY
1	A	1258	SER
1	B	1255	THR
1	B	1308	PRO
1	A	1222	LEU
1	A	1300	VAL
1	B	286	PRO
1	B	937	SER
1	B	938	PRO
1	A	320	PRO
1	A	1204	ILE

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	1218/4521 (27%)	1151 (94%)	67 (6%)	18	44
1	B	1217/4521 (27%)	1126 (92%)	91 (8%)	11	35
All	All	2435/9042 (27%)	2277 (94%)	158 (6%)	17	39

All (158) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	36	LEU
1	A	68	LYS
1	A	69	GLN
1	A	92	ILE
1	A	97	LEU
1	A	100	VAL
1	A	191	MET
1	A	277	VAL
1	A	284	ILE
1	A	336	CYS
1	A	401	GLU
1	A	444	VAL
1	A	530	LEU
1	A	686	LEU
1	A	722	LEU
1	A	747	LEU
1	A	771	GLN
1	A	789	THR
1	A	799	VAL
1	A	807	ASN
1	A	813	MET
1	A	830	LEU
1	A	854	ILE
1	A	860	LEU
1	A	885	LEU
1	A	905	THR
1	A	911	PHE
1	A	936	LEU
1	A	945	LEU
1	A	984	ARG
1	A	987	GLU
1	A	1002	TYR
1	A	1035	ILE

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Mol	Chain	Res	Type
1	A	1040	ARG
1	A	1045	LEU
1	A	1046	ARG
1	A	1061	GLN
1	A	1063	MET
1	A	1072	LEU
1	A	1122	TYR
1	A	1131	VAL
1	A	1154	ILE
1	A	1159	LEU
1	A	1165	LEU
1	A	1173	THR
1	A	1177	LEU
1	A	1202	LEU
1	A	1212	ASN
1	A	1244	ILE
1	A	1280	LEU
1	A	1301	TRP
1	A	1303	ASP
1	A	1314	LEU
1	A	1384	LEU
1	A	1392	GLN
1	A	1397	MET
1	A	1398	GLU
1	A	1411	MET
1	A	1471	MET
1	A	1481	GLN
1	A	1484	VAL
1	A	1485	ILE
1	A	1486	GLN
1	A	1496	THR
1	A	1500	VAL
1	A	1528	ASN
1	A	1607	THR
1	B	33	VAL
1	B	37	LEU
1	B	70	TYR
1	B	86	THR
1	B	92	ILE
1	B	96	GLN
1	B	97	LEU
1	B	113	LEU

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Mol	Chain	Res	Type
1	B	124	VAL
1	B	130	ILE
1	B	147	GLU
1	B	154	MET
1	B	201	PHE
1	B	235	THR
1	B	268	ARG
1	B	278	LEU
1	B	288	THR
1	B	312	THR
1	B	318	LEU
1	B	322	ASN
1	B	350	LEU
1	B	367	GLU
1	B	378	VAL
1	B	379	GLN
1	B	381	CYS
1	B	408	LEU
1	B	424	LEU
1	B	448	LEU
1	B	511	ILE
1	B	512	MET
1	B	521	ILE
1	B	522	GLN
1	B	677	SER
1	B	680	GLU
1	B	686	LEU
1	B	698	LEU
1	B	703	ASP
1	B	717	LEU
1	B	727	LEU
1	B	799	VAL
1	B	813	MET
1	B	830	LEU
1	B	844	MET
1	B	867	HIS
1	B	909	HIS
1	B	911	PHE
1	B	922	PHE
1	B	939	GLU
1	B	943	ASP
1	B	948	LEU

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Mol	Chain	Res	Type
1	B	981	ASP
1	B	992	THR
1	B	1033	CYS
1	B	1036	LEU
1	B	1040	ARG
1	B	1045	LEU
1	B	1063	MET
1	B	1067	HIS
1	B	1086	ASP
1	B	1089	ILE
1	B	1112	LEU
1	B	1118	LEU
1	B	1122	TYR
1	B	1131	VAL
1	B	1204	ILE
1	B	1212	ASN
1	B	1227	GLN
1	B	1228	THR
1	B	1231	GLU
1	B	1256	ILE
1	B	1274	CYS
1	B	1289	LEU
1	B	1299	ILE
1	B	1318	LEU
1	B	1326	VAL
1	B	1334	LEU
1	B	1338	LEU
1	B	1358	CYS
1	B	1387	GLN
1	B	1392	GLN
1	B	1459	VAL
1	B	1470	ARG
1	B	1474	SER
1	B	1486	GLN
1	B	1520	PRO
1	B	1528	ASN
1	B	1536	GLU
1	B	1549	GLN
1	B	1564	LEU
1	B	1593	LEU
1	B	1597	CYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (78)

such sidechains are listed below:

Mol	Chain	Res	Type
1	A	66	HIS
1	A	69	GLN
1	A	96	GLN
1	A	192	ASN
1	A	229	GLN
1	A	243	ASN
1	A	271	ASN
1	A	274	GLN
1	A	402	HIS
1	A	407	GLN
1	A	423	ASN
1	A	466	HIS
1	A	479	HIS
1	A	712	HIS
1	A	714	ASN
1	A	729	ASN
1	A	766	HIS
1	A	867	HIS
1	A	879	GLN
1	A	881	GLN
1	A	909	HIS
1	A	929	HIS
1	A	1026	ASN
1	A	1067	HIS
1	A	1119	GLN
1	A	1132	GLN
1	A	1182	ASN
1	A	1227	GLN
1	A	1253	ASN
1	A	1364	ASN
1	A	1387	GLN
1	A	1392	GLN
1	A	1418	ASN
1	A	1481	GLN
1	A	1493	GLN
1	A	1558	ASN
1	A	1589	HIS
1	B	69	GLN
1	B	83	HIS
1	B	96	GLN
1	B	98	GLN
1	B	192	ASN

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Mol	Chain	Res	Type
1	B	229	GLN
1	B	237	ASN
1	B	243	ASN
1	B	248	GLN
1	B	262	ASN
1	B	379	GLN
1	B	423	ASN
1	B	467	GLN
1	B	656	ASN
1	B	729	ASN
1	B	867	HIS
1	B	881	GLN
1	B	882	HIS
1	B	909	HIS
1	B	921	HIS
1	B	979	GLN
1	B	1037	HIS
1	B	1057	HIS
1	B	1097	GLN
1	B	1111	GLN
1	B	1113	HIS
1	B	1227	GLN
1	B	1234	ASN
1	B	1249	ASN
1	B	1266	GLN
1	B	1364	ASN
1	B	1387	GLN
1	B	1486	GLN
1	B	1493	GLN
1	B	1528	ASN
1	B	1557	HIS
1	B	1573	GLN
1	B	1586	HIS
1	B	1589	HIS
1	B	1598	HIS
1	B	1612	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 oligosaccharides 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.

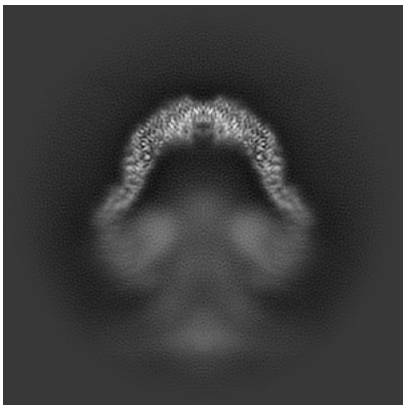
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-46688. These allow visual inspection of the internal detail of the map and identification of artifacts.

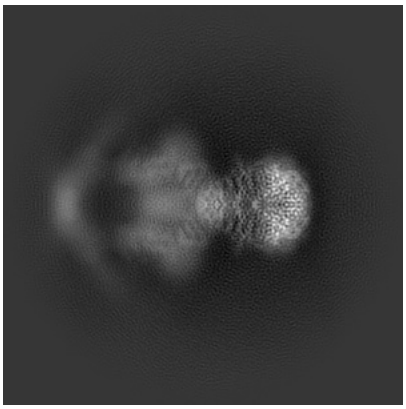
Images derived from a raw map, generated by summing the deposited half-maps, are presented below the corresponding image components of the primary map to allow further visual inspection and comparison with those of the primary map.

6.1 Orthogonal projections

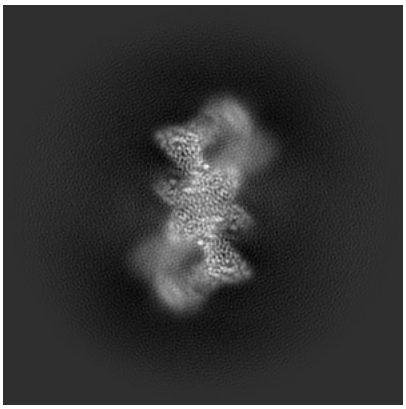
6.1.1 Primary map



X

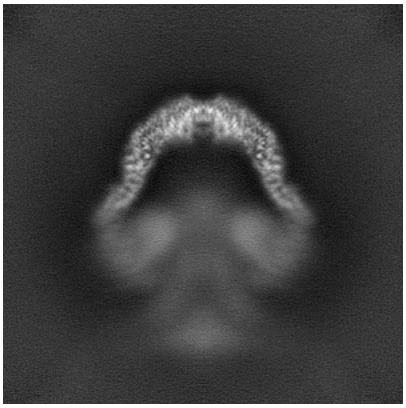


Y

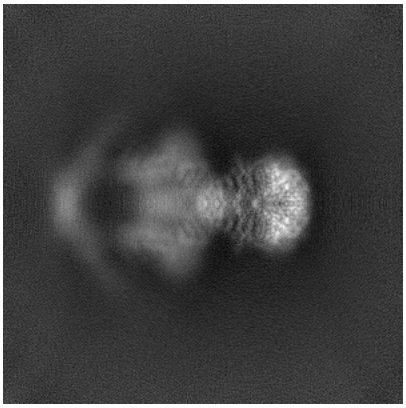


Z

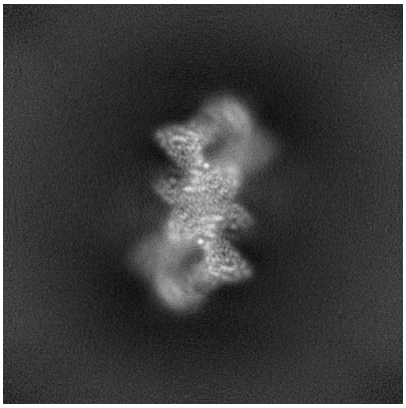
6.1.2 Raw map



X



Y

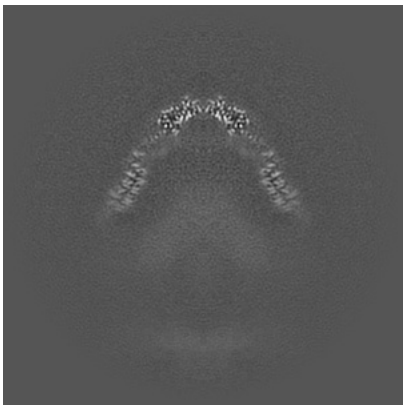


Z

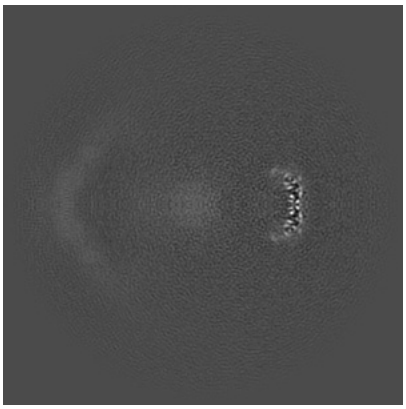
The images above show the map projected in three orthogonal directions.

6.2 Central slices (i)

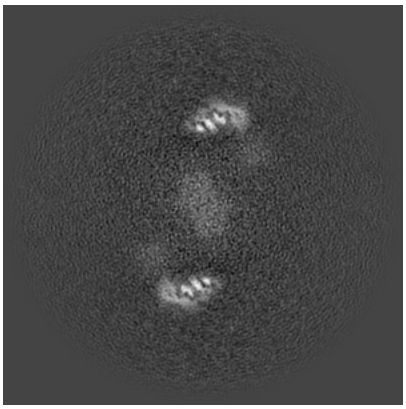
6.2.1 Primary map



X Index: 260

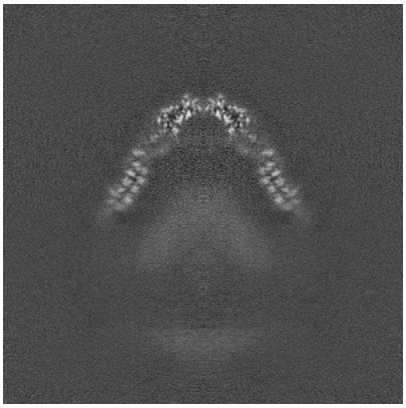


Y Index: 260

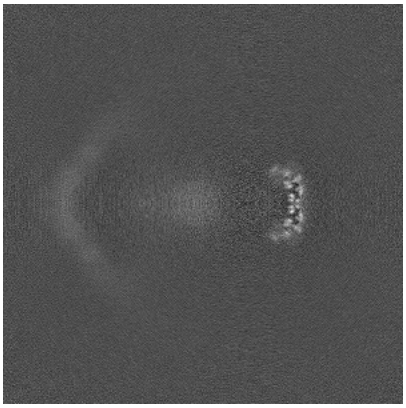


Z Index: 260

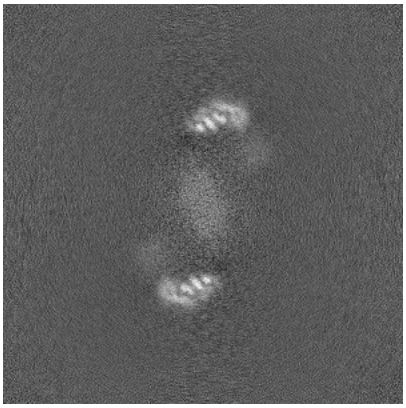
6.2.2 Raw map



X Index: 260



Y Index: 260

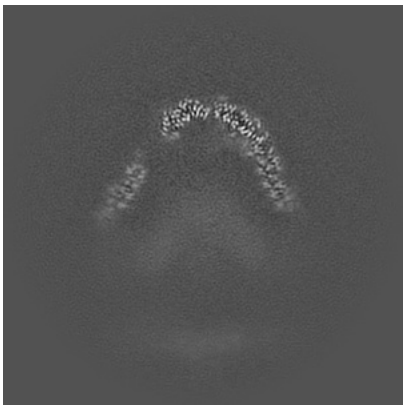


Z Index: 260

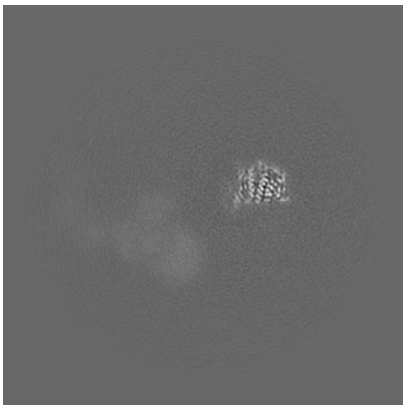
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

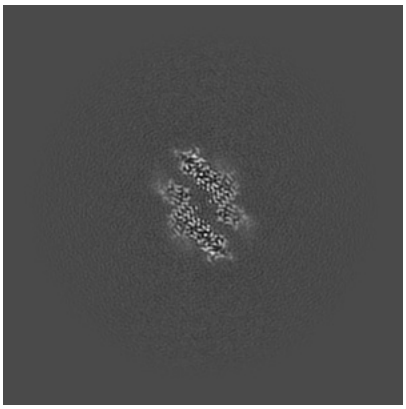
6.3.1 Primary map



X Index: 254

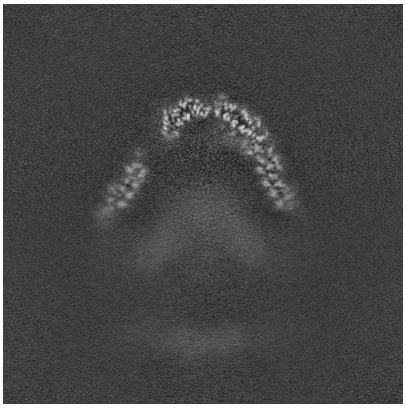


Y Index: 187

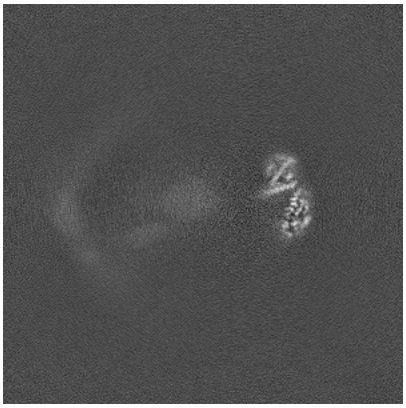


Z Index: 370

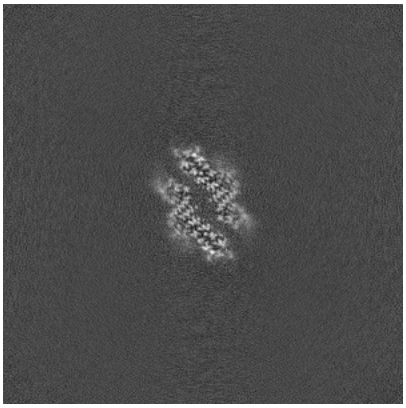
6.3.2 Raw map



X Index: 254



Y Index: 242

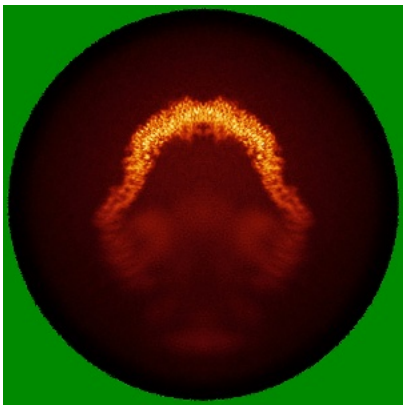


Z Index: 370

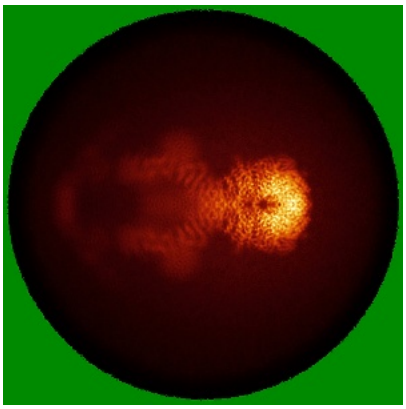
The images above show the largest variance slices of the map in three orthogonal directions.

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

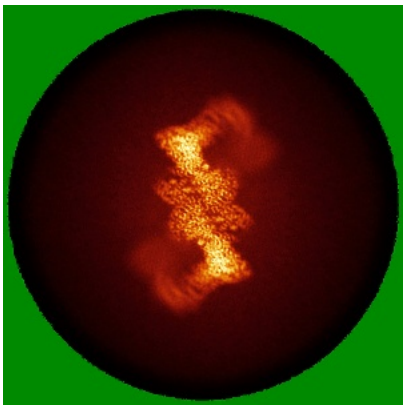
6.4.1 Primary map



X

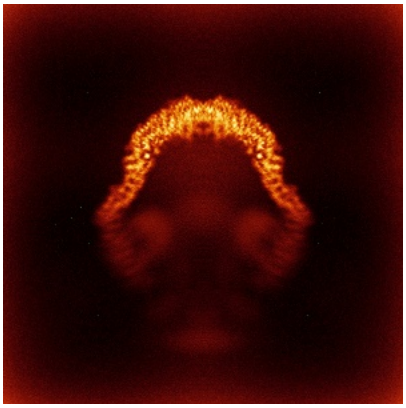


Y

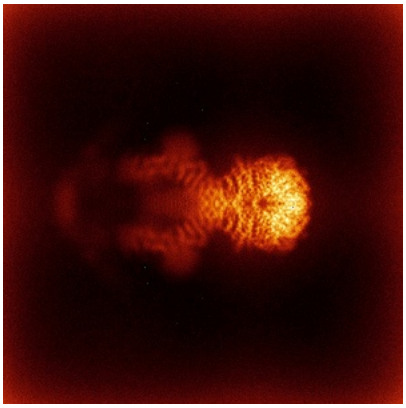


Z

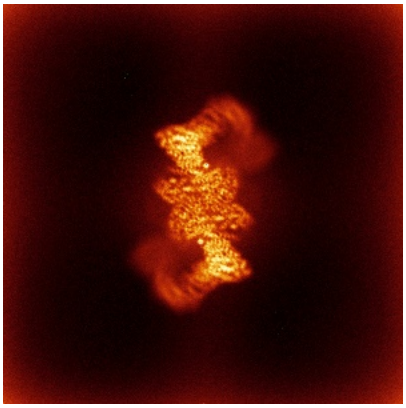
6.4.2 Raw map



X



Y

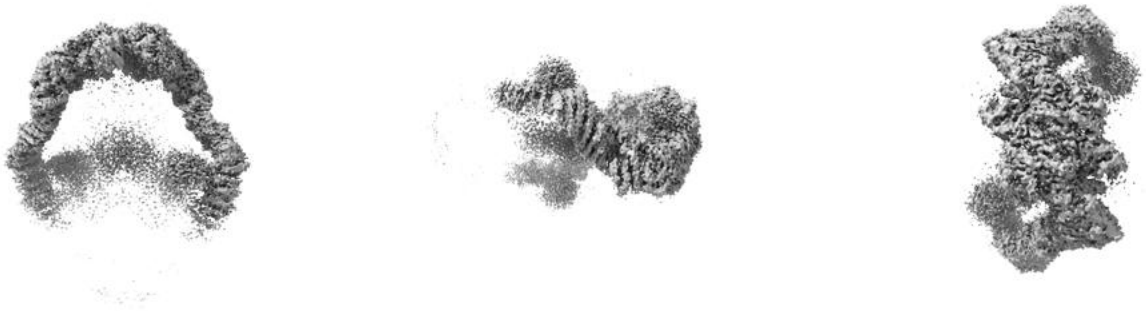


Z

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)

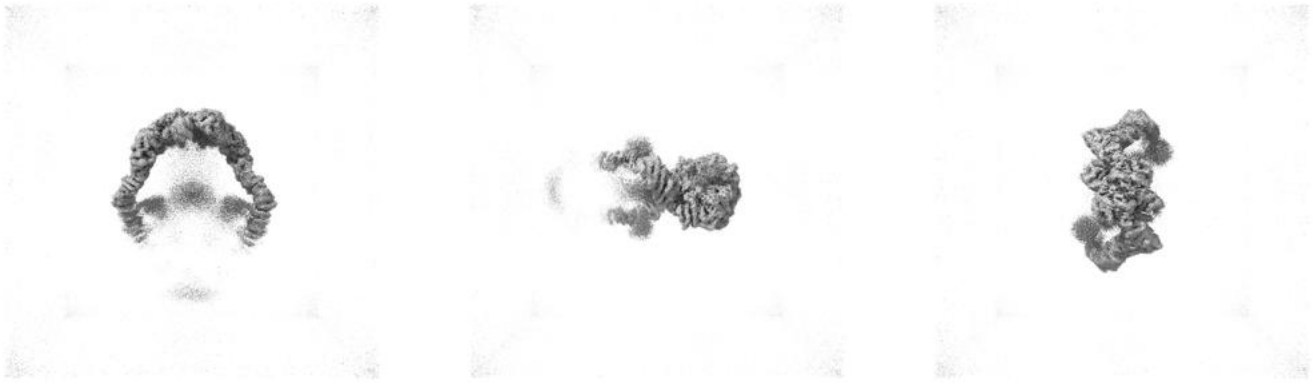
6.5.1 Primary map



X Y Z

The images above show the 3D surface view of the map at the recommended contour level 0.068. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

6.5.2 Raw map



X Y Z

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

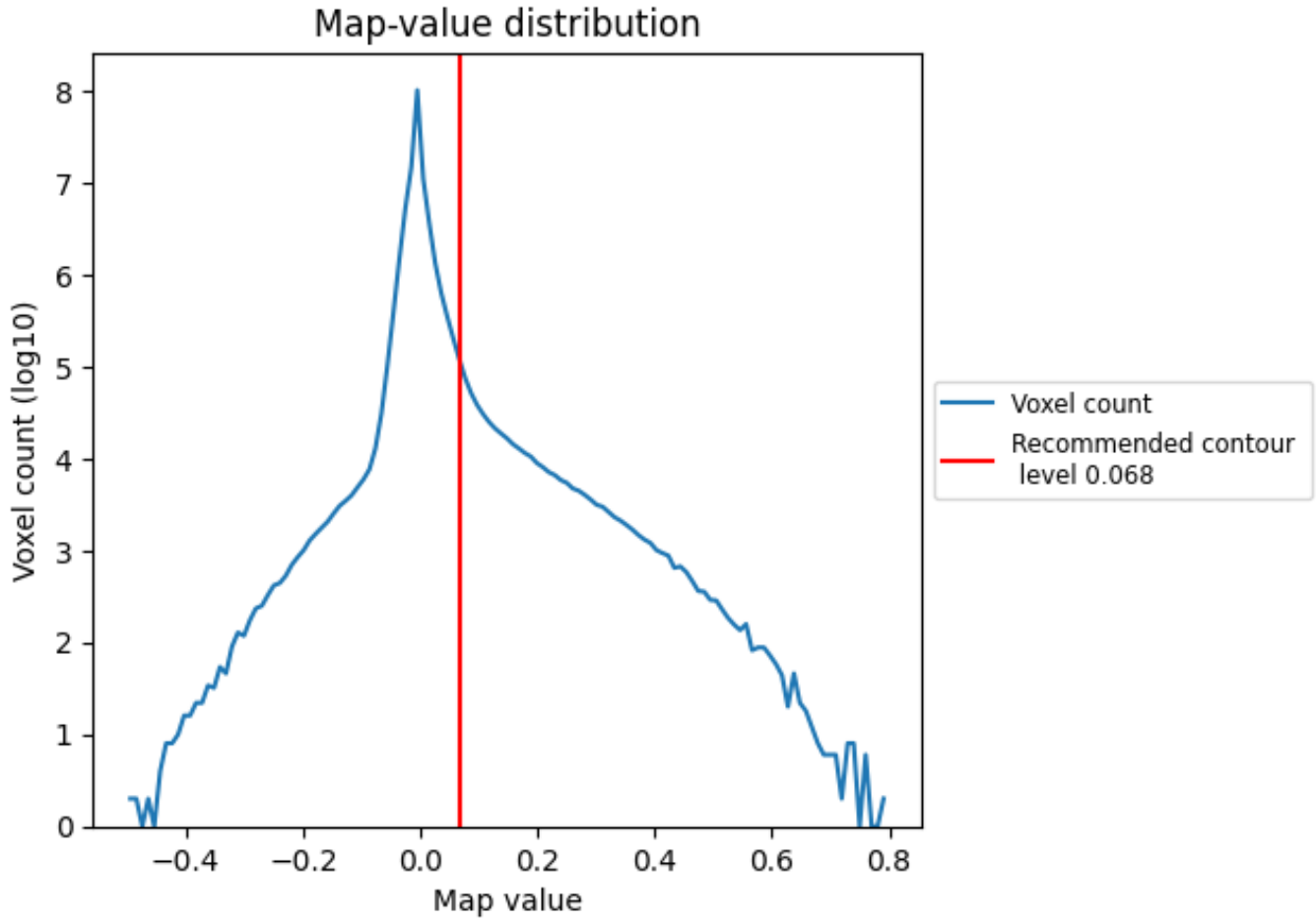
6.6 Mask visualisation (i)

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

7 Map analysis

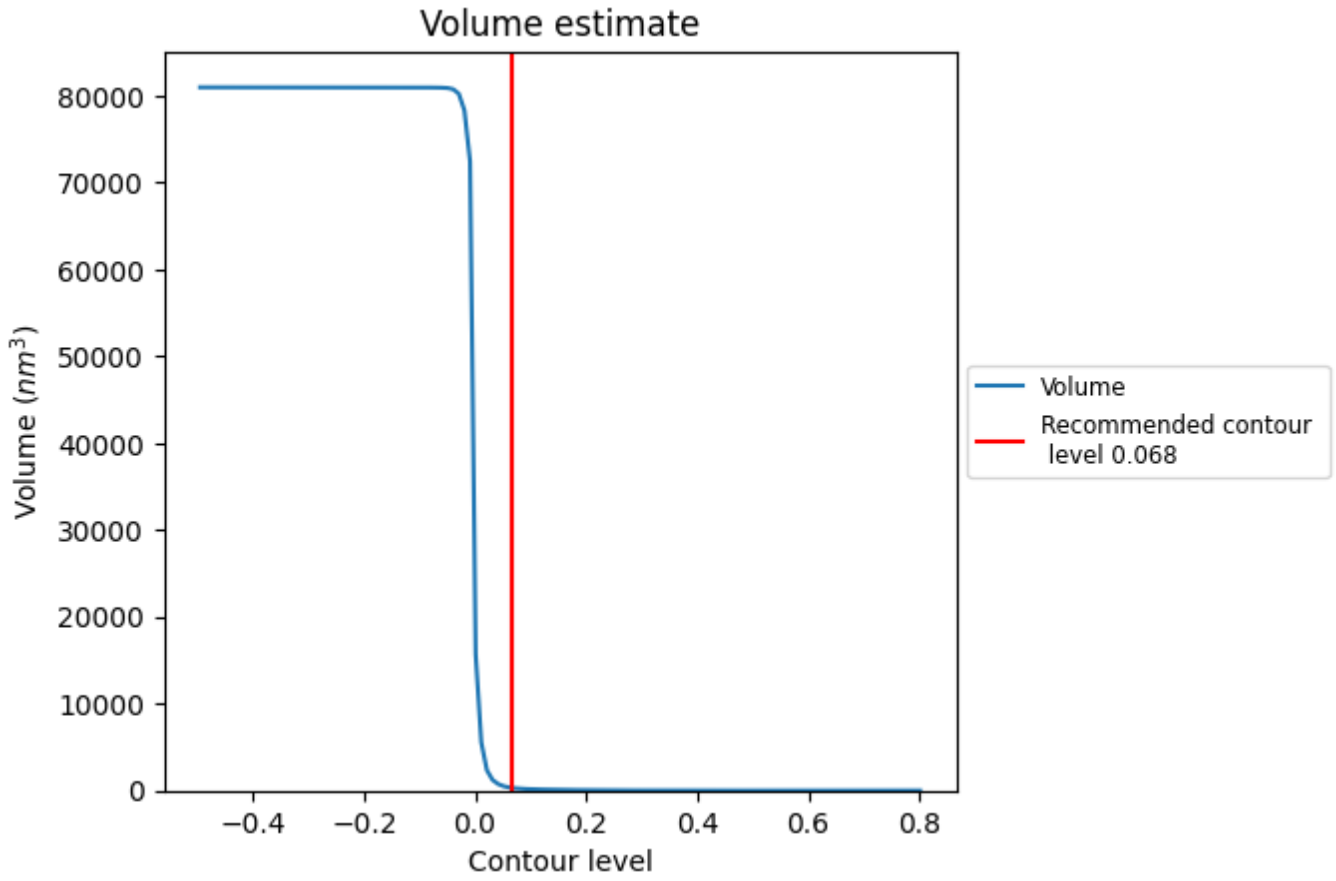
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



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

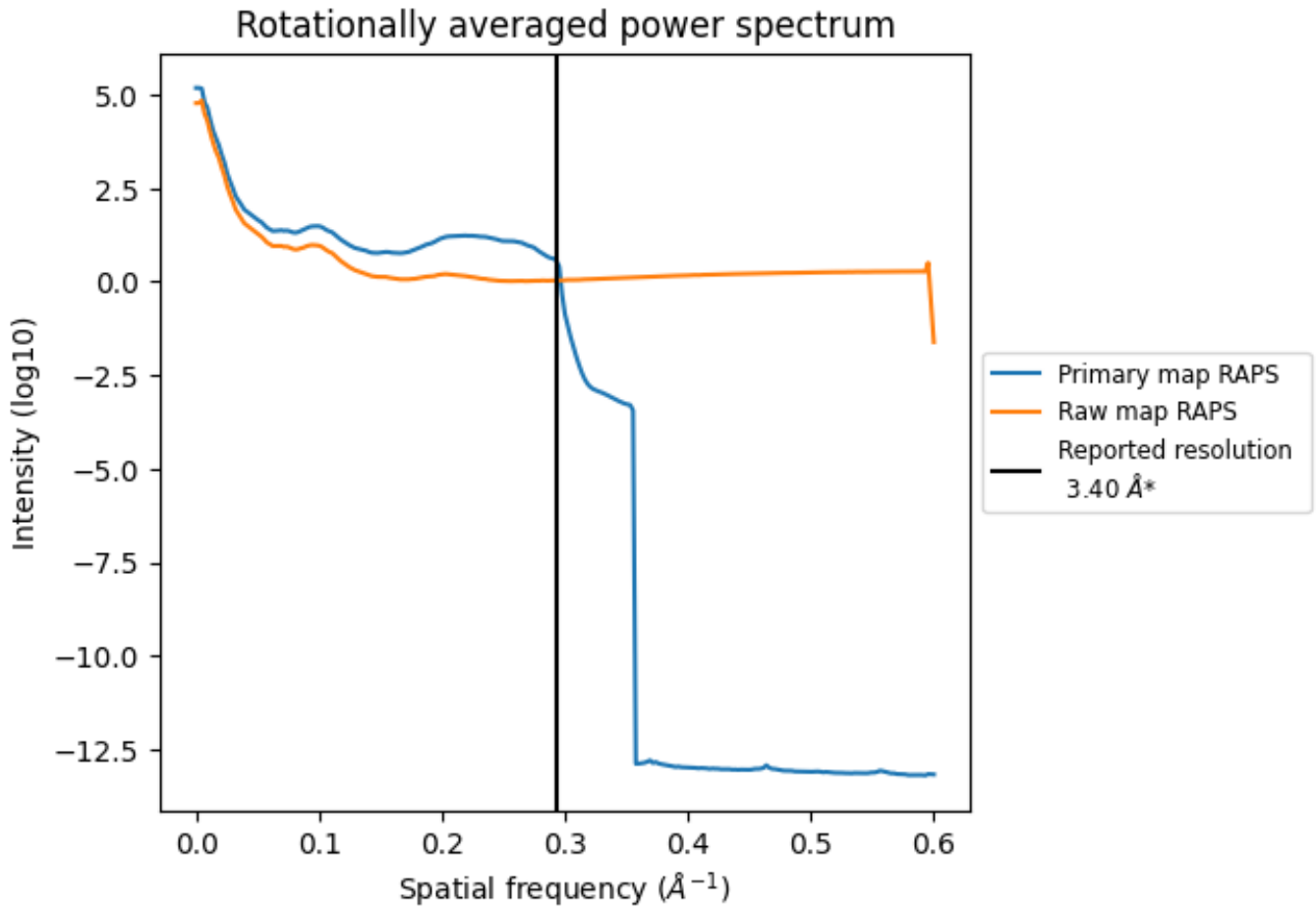
7.2 Volume estimate



The volume at the recommended contour level is 300 nm^3; this corresponds to an approximate mass of 271 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)

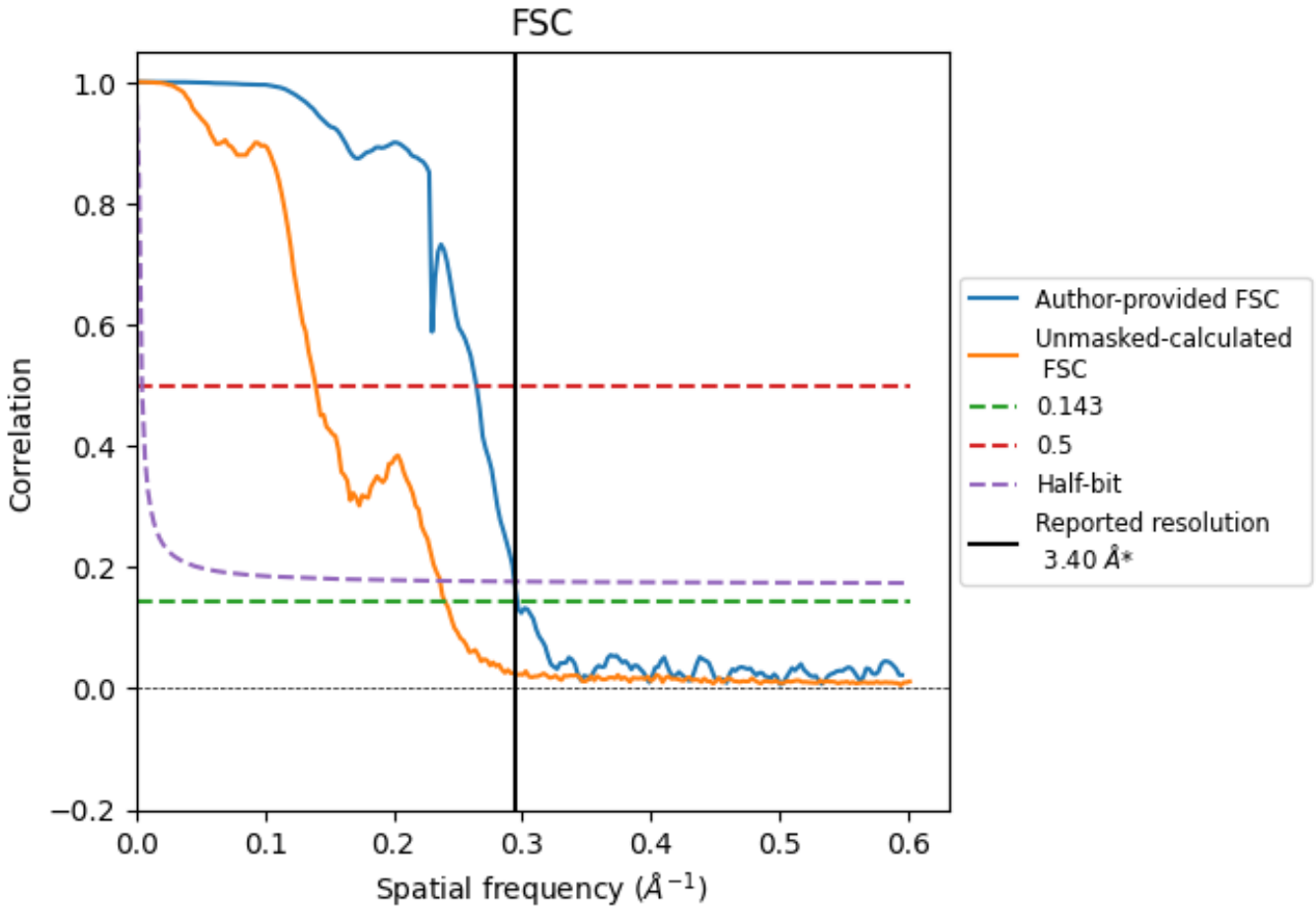


*Reported resolution corresponds to spatial frequency of 0.294 $Å^{-1}$

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 0.294 Å^{-1}

8.2 Resolution estimates (i)

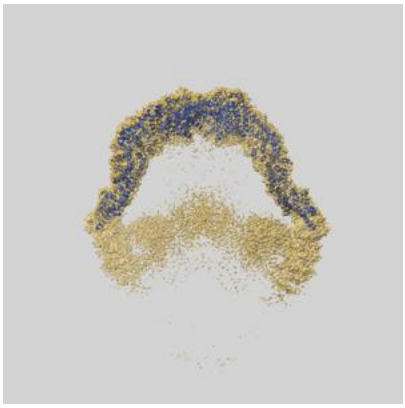
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.38	3.78	3.40
Unmasked-calculated*	4.16	7.17	4.24

*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 4.16 differs from the reported value 3.4 by more than 10 %

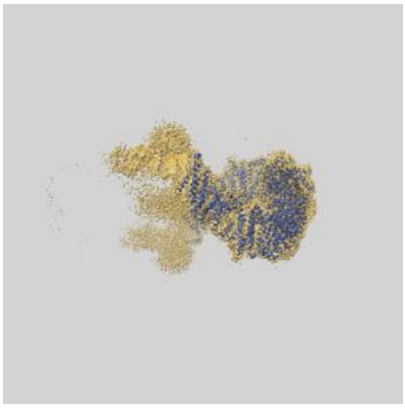
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-46688 and PDB model 9NWD. Per-residue inclusion information can be found in section 3 on page 4.

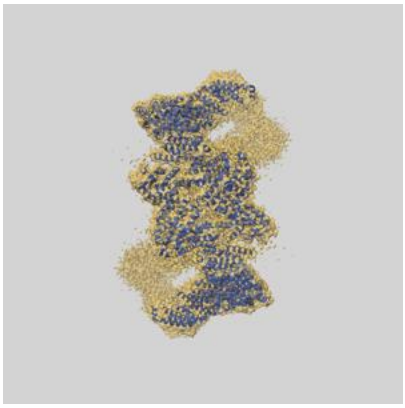
9.1 Map-model overlay



X



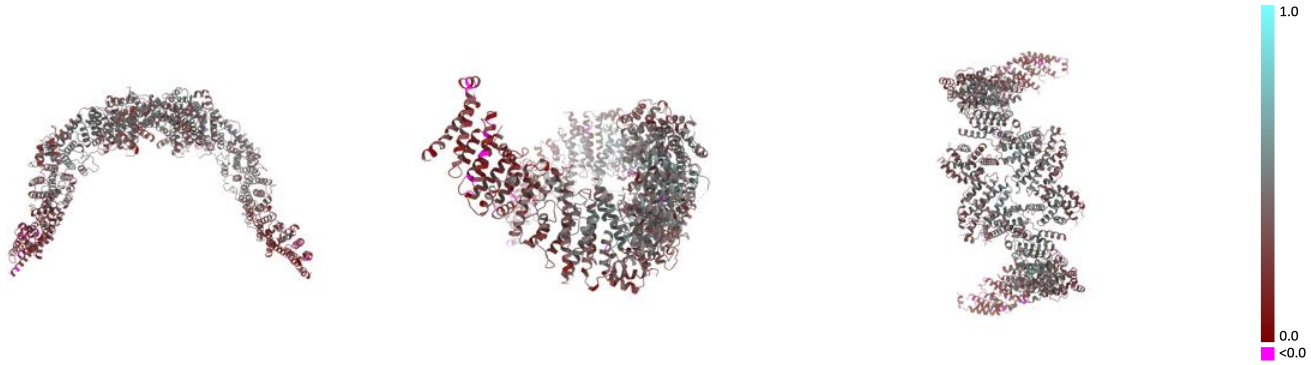
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.068 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.

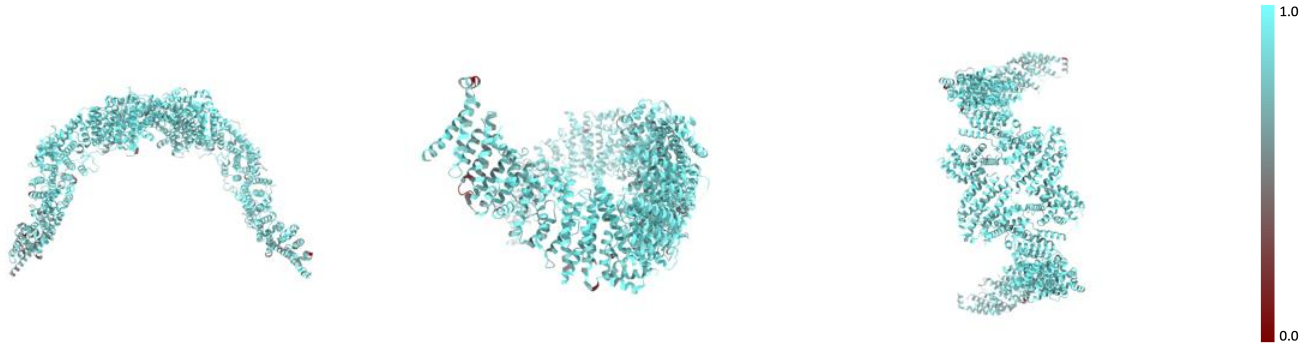
9.2 Q-score mapped to coordinate model (i)



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.

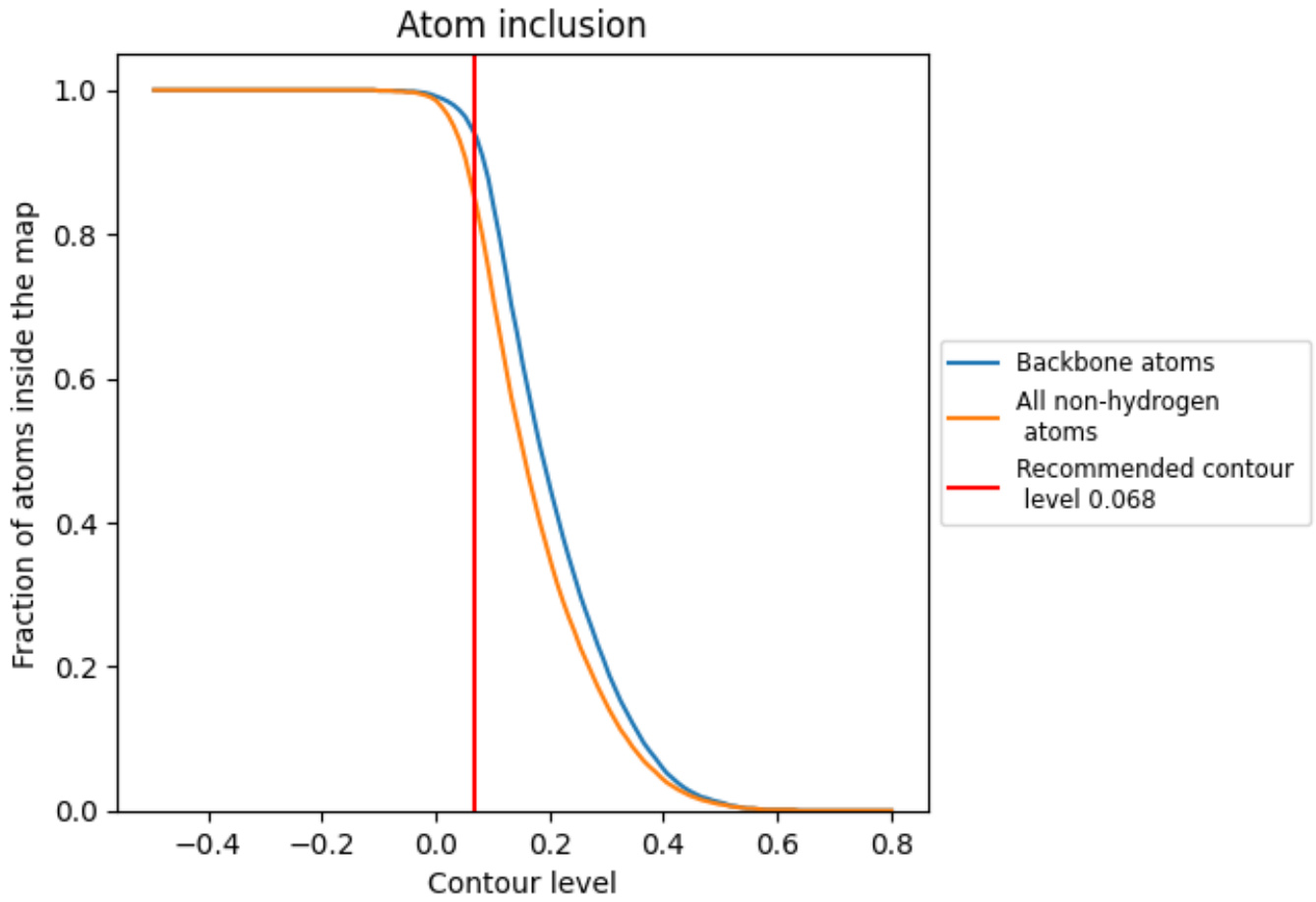
9.3 Atom inclusion mapped to coordinate model (i)



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 (0.068).

9.4 Atom inclusion (i)



At the recommended contour level, 94% of all backbone atoms, 85% 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 (0.068) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.8510	0.3640
A	0.8470	0.3600
B	0.8550	0.3680