Full wwPDB X-ray Structure Validation Report ⓘ

Feb 1, 2016 – 12:38 AM GMT

PDB ID	:	2B39
Title	:	Structure of mammalian C3 with an intact thioester at 3A resolution
Authors	:	Fredslund, F.; Jenner, L.; Husted, L.B.; Nyborg, J.; Andersen, G.R.; Sottrup-Jensen, L.
Deposited on	:	2005-09-20
Resolution	:	3.00 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.
We welcome your comments at validation@mail.wwpdb.org
A user guide is available at
http://wwpdb.org/validation/2016/XrayValidationReportHelp
with specific help available everywhere you see the ⓘ symbol.

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

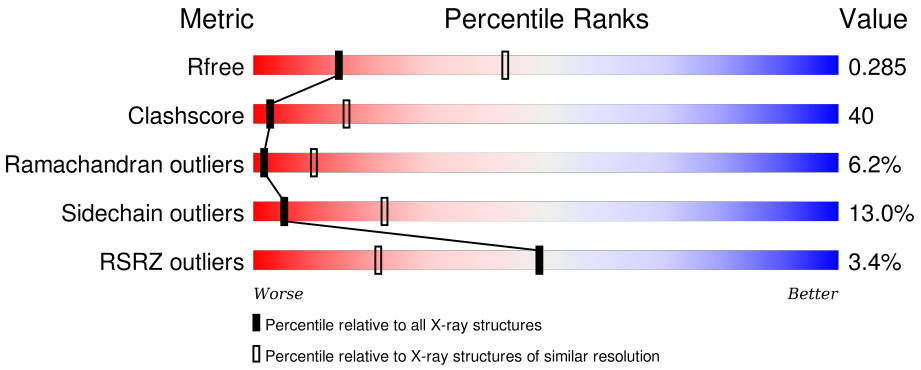
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	trunk26865

1 Overall quality at a glance (i)

The following experimental techniques were used to determine the structure:
X-RAY DIFFRACTION

The reported resolution of this entry is 3.00 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)	Similar resolution (#Entries, resolution range(Å))
R_{free}	91344	1578 (3.00-3.00)
Clashscore	102246	1912 (3.00-3.00)
Ramachandran outliers	100387	1853 (3.00-3.00)
Sidechain outliers	100360	1856 (3.00-3.00)
RSRZ outliers	91569	1592 (3.00-3.00)

The table below summarises the geometric issues observed across the polymeric chains and their fit to the electron density. The red, orange, yellow and green segments on the lower bar indicate the fraction of residues that contain outliers for >=3, 2, 1 and 0 types of geometric quality criteria. 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 electron density. The numeric value is given above the bar.

Mol	Chain	Length	Quality of chain
1	A	1661	4% 39% 46% 11%
1	B	1661	3% 38% 48% 10%

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit criteria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
2	NAG	A	2001	X	-	-	-
2	NAG	B	2001	X	-	-	-

2 Entry composition

There are 2 unique types of molecules in this entry. The entry contains 25624 atoms, of which 0 are hydrogens and 0 are deuteriums.

In the tables below, the ZeroOcc column contains the number of atoms modelled with zero occupancy, 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 C3.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1610	Total	C	N	O	S	0	0	0
			12773	8093	2187	2439	54			
1	B	1610	Total	C	N	O	S	0	0	0
			12773	8093	2187	2439	54			

- Molecule 2 is a polymer of unknown type called SUGAR (3-MER).

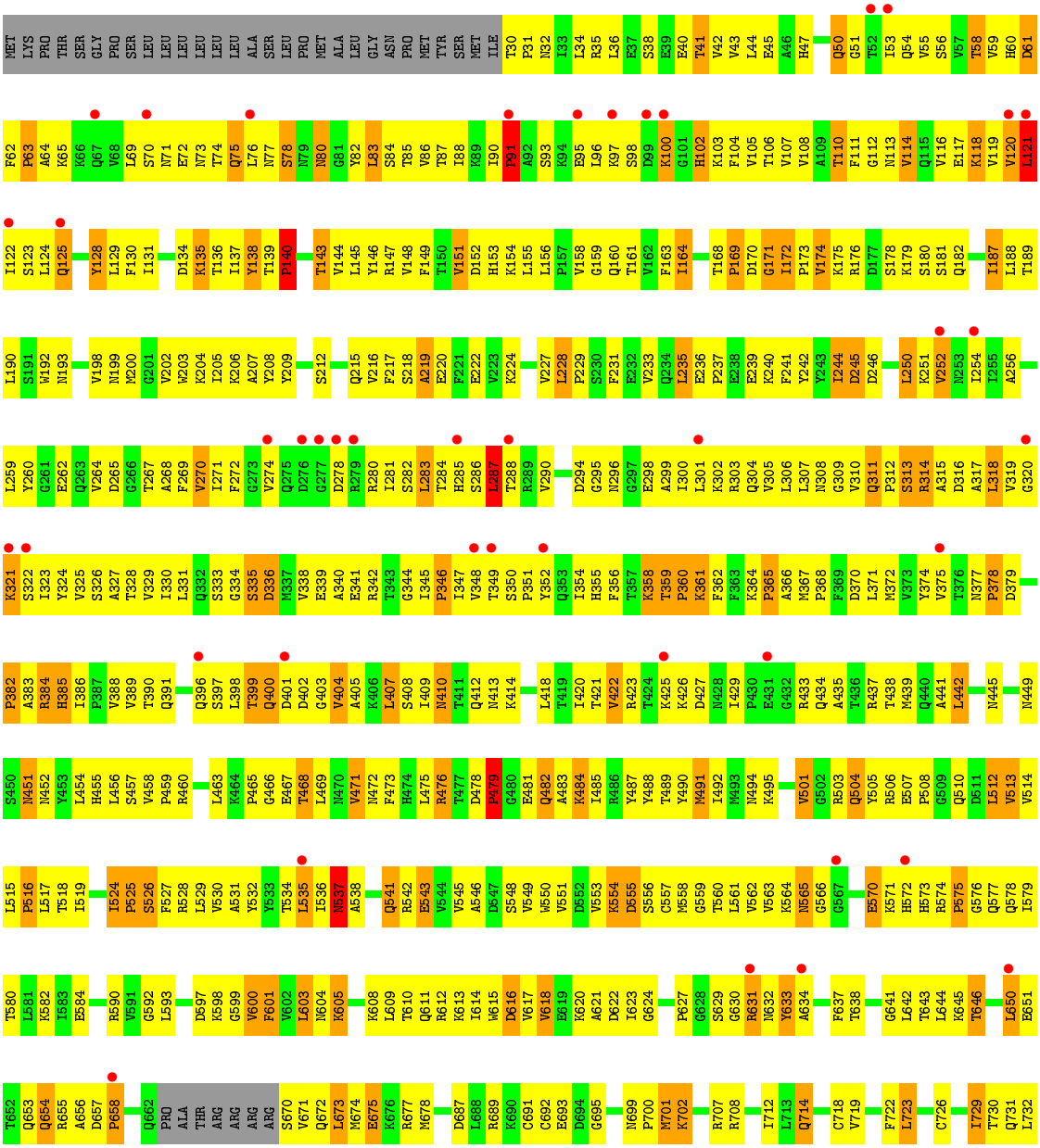
Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
2	A	3	Total	C	N	O	0	0
			39	22	2	15		
2	B	3	Total	C	N	O	0	0
			39	22	2	15		

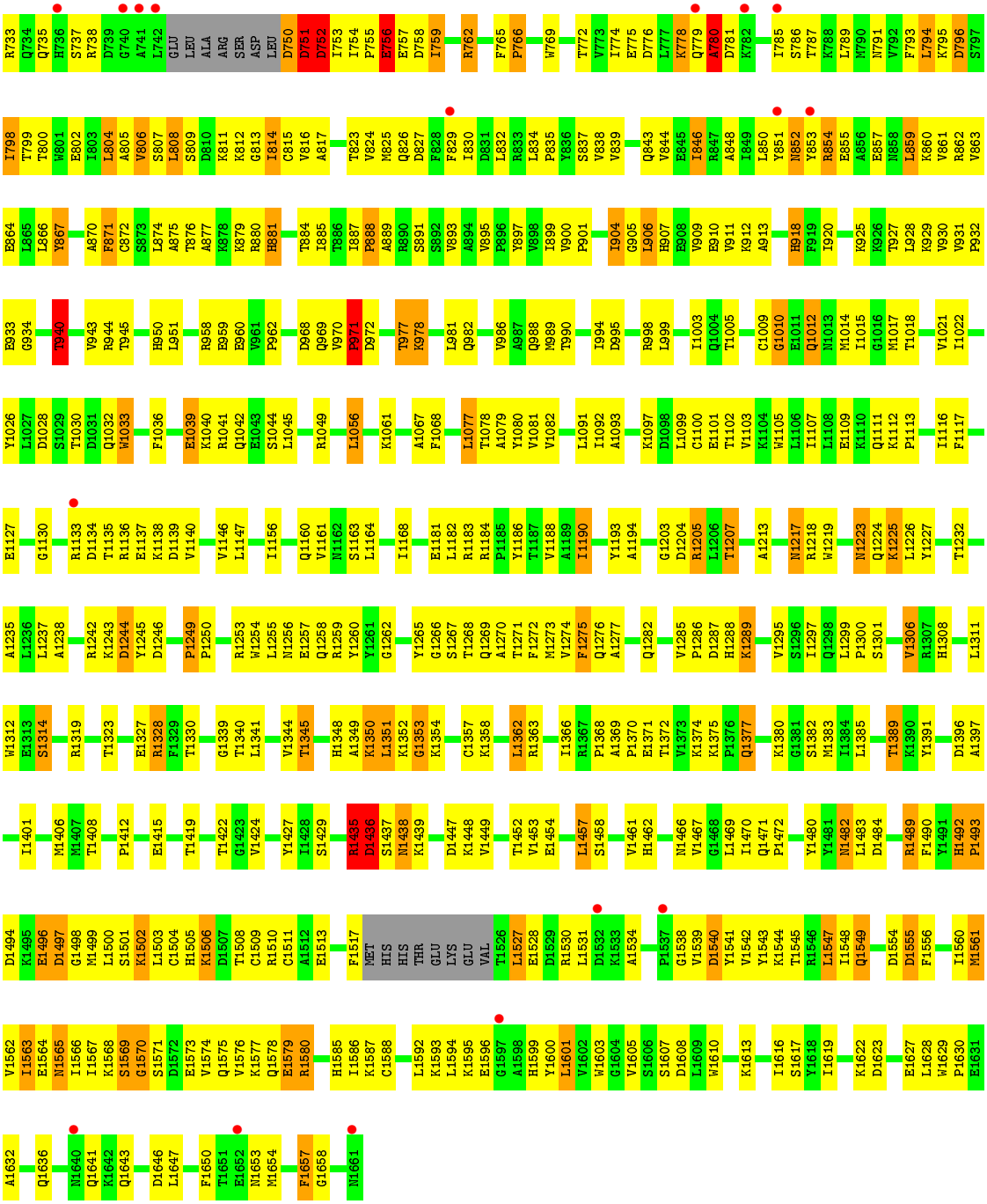
3 Residue-property plots (i)

These plots are drawn for all protein, RNA and DNA chains in the entry. The first graphic for a chain summarises the proportions of errors displayed in the second graphic. The second graphic shows the sequence view annotated by issues in geometry and electron 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 dot above a residue indicates a poor fit to the electron density (RSRZ > 2). 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.

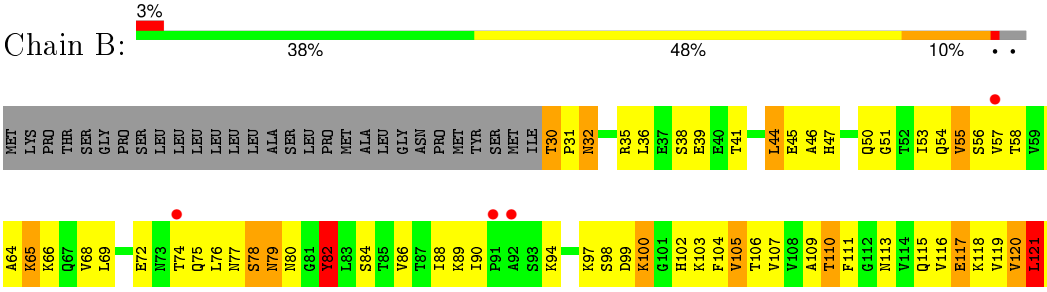
- Molecule 1: C3

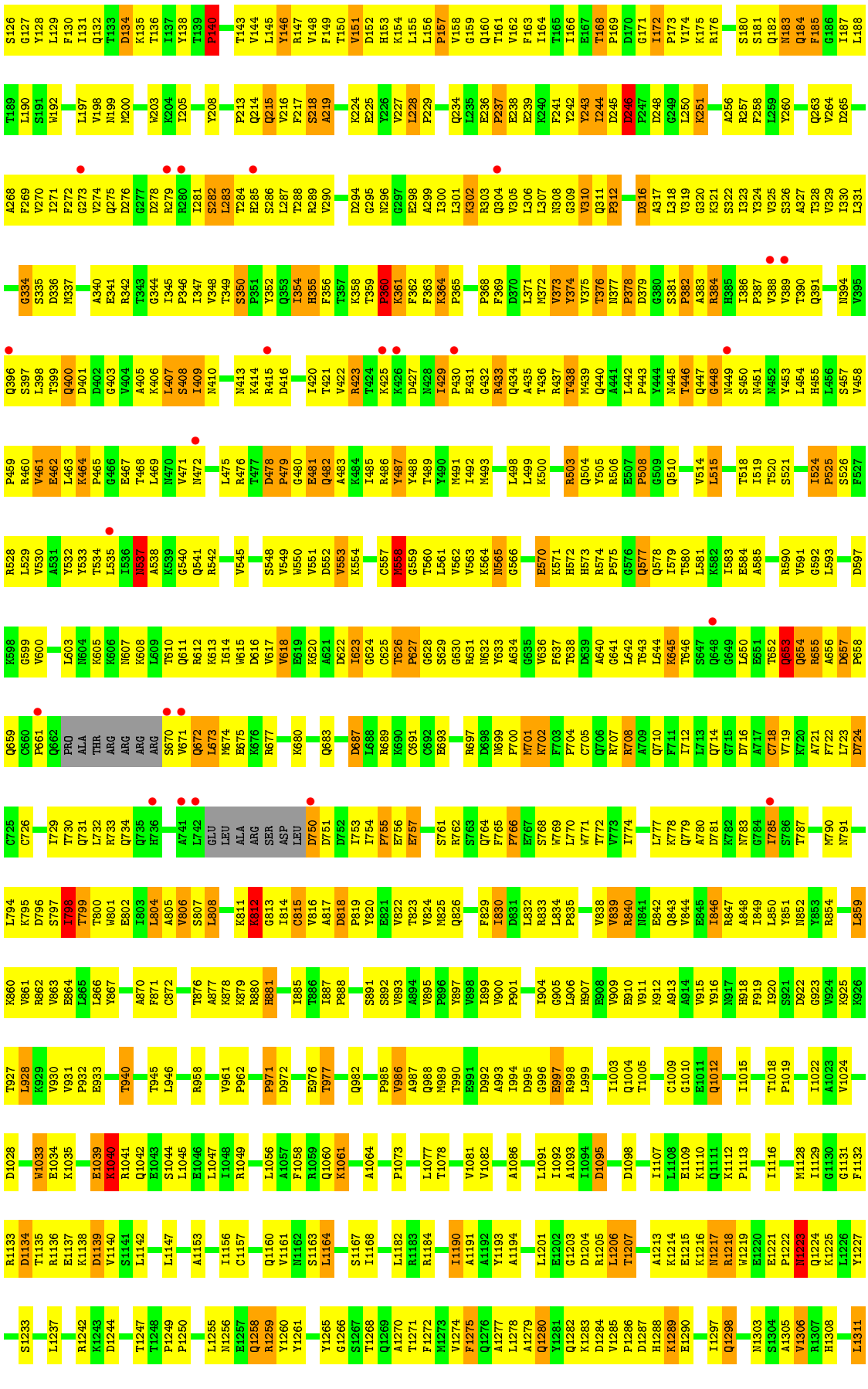
Chain A: 

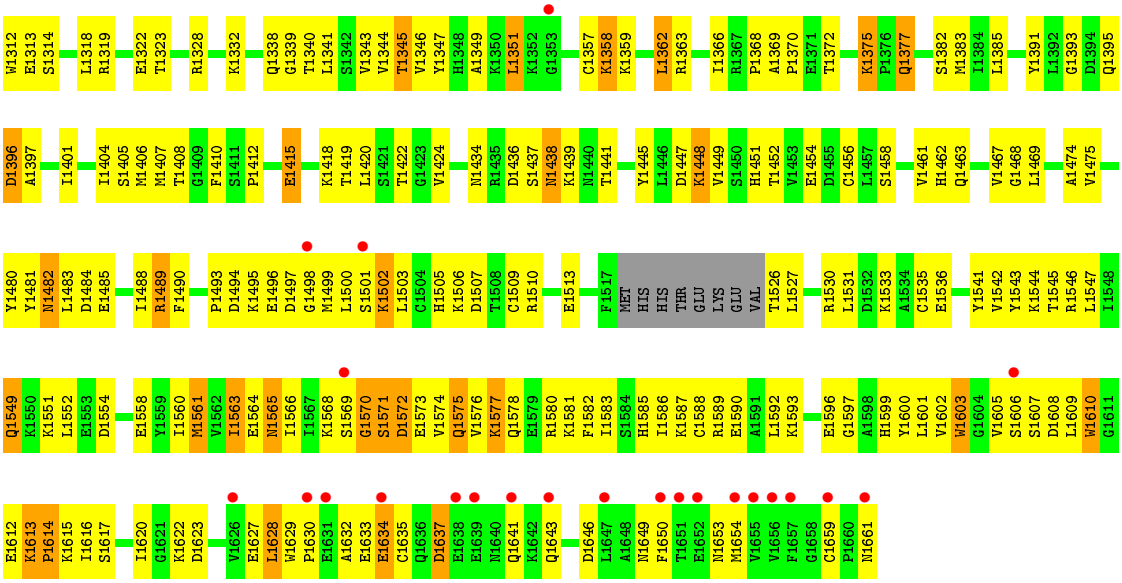




- Molecule 1: C3






W1312 E1313 S1314 L1318 R1319 E1322 T1323 R1328 K1332 Q1338 G1339 T1340 L1341 S1342 V1343 V1344 T1345 V1346 Y1347 H1348 A1349 K1350 L1351 K1352 G1353 C1357 K1358 K1359 L1362 R1363 I1366 R1367 P1368 A1369 P1370 E1371 T1372 K1375 P1376 Q1377 S1382 M1383 I1384 L1385 Y1391 L1392 G1393 D1394 Q1395
D1396 A1397 I1401 I1404 S1405 M1406 M1407 T1408 G1409 F1410 S1411 P1412 E1415 K1418 T1419 L1420 S1421 T1422 G1423 V1424 N1434 R1435 D1436 S1437 N1438 K1439 N1440 T1441 Y1445 L1446 D1447 K1448 V1449 S1450 H1451 T1452 V1453 E1454 D1455 C1456 L1457 S1458 V1461 H1462 Q1463 V1467 G1468 L1469 A1474 V1475
Y1480 Y1481 N1482 L1483 D1484 E1485 I1488 R1489 F1490 P1493 D1494 K1495 E1496 D1497 G1498 M1499 L1500 S1501 K1502 L1503 C1504 H1505 K1506 D1507 T1508 C1509 R1510 E1513 F1517 MET HIS HIS THR GLU LYS GLU VAL T1526 L1527 R1530 L1531 D1532 K1533 A1534 C1535 E1536 Y1541 V1542 Y1543 K1544 T1545 R1546 L1547 I1548
Q1549 K1550 K1551 L1552 E1553 D1554 E1558 Y1559 I1560 M1561 V1562 I1563 E1564 N1565 I1566 I1567 K1568 S1569 G1570 S1571 D1572 E1573 V1574 Q1575 V1576 K1577 Q1578 E1579 R1580 K1581 F1582 I1583 S1584 H1585 I1586 K1587 C1588 R1589 E1590 A1591 L1592 K1593 E1596 G1597 A1598 H1599 Y1600 L1601 V1602 W1603 G1604 V1605 S1606 S1607 D1608 L1609 W1610 G1611
E1612 K1613 P1614 K1615 I1616 S1617 I1620 G1621 K1622 D1623 V1626 E1627 L1628 W1629 P1630 E1631 A1632 E1633 E1634 C1635 Q1636 D1637 E1638 E1639 N1640 Q1641 K1642 Q1643 D1646 L1647 A1648 N1649 F1650 T1651 E1652 N1653 M1654 V1655 V1656 F1657 G1658 C1659 P1660 N1661

4 Data and refinement statistics (i)

Property	Value	Source
Space group	P 21 21 2	Depositor
Cell constants a, b, c, α, β, γ	254.25Å 246.86Å 113.35Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	40.00 – 3.00 37.85 – 3.00	Depositor EDS
% Data completeness (in resolution range)	(Not available) (40.00-3.00) 97.2 (37.85-3.00)	Depositor EDS
R_{merge}	0.10	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	1.73 (at 3.01Å)	Xtriage
Refinement program	CNS 1.1	Depositor
R, R_{free}	0.278 , 0.286 0.273 , 0.285	Depositor DCC
R_{free} test set	1392 reflections (1.00%)	DCC
Wilson B-factor (Å^2)	69.3	Xtriage
Anisotropy	0.479	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.27 , 75.6	EDS
Estimated twinning fraction	0.008 for k,h,-l	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.43$, $< L^2 > = 0.26$	Xtriage
Outliers	2 of 138964 reflections (0.001%)	Xtriage
F_o,F_c correlation	0.91	EDS
Total number of atoms	25624	wwPDB-VP
Average B, all atoms (Å^2)	97.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 18.36% of the height of the origin peak. No significant pseudotranslation is detected.*

[1] Intensities estimated from amplitudes.

[2] Theoretical values of $< |L| >$, $< L^2 >$ for acentric reflections are 0.5, 0.375 respectively for untwinned datasets, and 0.333, 0.2 for perfectly twinned datasets.

5 Model quality

5.1 Standard geometry

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.58	1/13020 (0.0%)	0.82	15/17632 (0.1%)
1	B	0.57	0/13020	0.81	11/17632 (0.1%)
All	All	0.57	1/26040 (0.0%)	0.82	26/35264 (0.1%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	B	0	1
2	A	1	0
2	B	1	0
All	All	2	2

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	102	HIS	CB-CG	6.64	1.61	1.50

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	B	121	LEU	CA-CB-CG	-9.75	92.87	115.30
1	A	91	PRO	N-CA-C	7.91	132.66	112.10
1	B	1362	LEU	CA-CB-CG	6.57	130.40	115.30
1	A	1362	LEU	CA-CB-CG	6.54	130.34	115.30
1	A	1130	GLY	N-CA-C	-6.49	96.87	113.10
1	B	228	LEU	CA-CB-CG	6.41	130.03	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	78	SER	N-CA-C	6.32	128.07	111.00
1	B	1502	LYS	N-CA-C	-6.08	94.59	111.00
1	B	815	CYS	CA-CB-SG	-6.02	103.16	114.00
1	B	82	TYR	CB-CG-CD1	5.92	124.55	121.00
1	A	524	ILE	C-N-CD	5.86	140.70	128.40
1	B	77	ASN	C-N-CA	5.84	136.29	121.70
1	A	780	ALA	N-CA-C	5.74	126.50	111.00
1	A	121	LEU	CA-CB-CG	-5.62	102.38	115.30
1	A	171	GLY	N-CA-C	-5.54	99.24	113.10
1	A	1436	ASP	CB-CG-OD1	5.52	123.27	118.30
1	B	185	PHE	N-CA-C	5.50	125.84	111.00
1	B	558	MET	N-CA-C	5.50	125.84	111.00
1	A	123	SER	N-CA-C	-5.34	96.59	111.00
1	A	860	LYS	N-CA-C	-5.31	96.66	111.00
1	B	80	ASN	CB-CA-C	-5.28	99.84	110.40
1	B	127	GLY	N-CA-C	5.25	126.22	113.10
1	A	940	THR	N-CA-C	-5.21	96.92	111.00
1	A	287	LEU	CA-CB-CG	5.17	127.18	115.30
1	A	525	PRO	N-CA-C	-5.11	98.81	112.10
1	A	245	ASP	N-CA-C	5.06	124.67	111.00

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2001	NAG	C1
2	B	2001	NAG	C1

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	138	TYR	Sidechain
1	B	820	TYR	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	12773	0	12782	1027	0
1	B	12773	0	12782	1002	0
2	A	39	0	34	3	0
2	B	39	0	34	3	0
All	All	25624	0	25632	2029	0

The all-atom clashscore is defined as the number of clashes found per 1000 atoms (including hydrogen atoms). The all-atom clashscore for this structure is 40.

All (2029) 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:117:GLU:O	1:B:118:LYS:HG2	1.47	1.14
1:B:369:PHE:HB3	1:B:409:ILE:HD12	1.32	1.10
1:A:44:LEU:HD13	1:A:55:VAL:HG11	1.34	1.09
1:B:244:ILE:HD11	1:B:319:VAL:CG2	1.84	1.08
1:B:116:VAL:HG13	1:B:645:LYS:HG2	1.28	1.06
1:A:1575:GLN:HB3	1:A:1578:GLN:NE2	1.70	1.05
1:B:116:VAL:CG1	1:B:645:LYS:HG2	1.87	1.04
1:A:55:VAL:HG13	1:A:111:PHE:HB3	1.39	1.04
1:A:651:GLU:HB3	1:A:653:GLN:HE22	1.18	1.04
1:B:558:MET:HB2	1:B:812:LYS:HE2	1.38	1.03
1:B:118:LYS:HD3	1:B:645:LYS:HE2	1.40	1.03
1:B:227:VAL:HG12	1:B:229:PRO:HD3	1.39	1.03
1:A:281:ILE:HD13	1:A:310:VAL:HG22	1.41	1.02
1:A:244:ILE:HD11	1:A:319:VAL:HG22	1.39	1.02
1:A:61:ASP:HB2	1:A:63:PRO:HD2	1.40	1.02
1:A:55:VAL:HG23	1:A:75:GLN:HA	1.39	1.02
1:A:256:ALA:O	1:A:264:VAL:HB	1.61	1.01
1:B:503:ARG:HE	1:B:503:ARG:H	1.05	1.00
1:B:1493:PRO:HB2	1:B:1497:ASP:OD2	1.61	0.99
1:A:359:THR:HG22	1:A:360:PRO:HD2	1.44	0.98
1:A:800:THR:HG23	1:A:823:THR:HG22	1.45	0.97
1:B:244:ILE:HD11	1:B:319:VAL:HG22	1.44	0.96
1:B:272:PHE:HD1	1:B:325:VAL:HG21	1.30	0.96
1:A:272:PHE:HD1	1:A:325:VAL:HG21	1.29	0.94
1:B:442:LEU:HD13	1:B:631:ARG:HH21	1.32	0.94
1:A:700:PRO:HB2	1:A:701:MET:HE3	1.49	0.94
1:B:243:TYR:CZ	1:B:245:ASP:HB2	2.03	0.94
1:A:574:ARG:NH1	1:A:920:ILE:HB	1.82	0.94
1:B:808:LEU:HB2	1:B:814:ILE:HG12	1.47	0.93
1:B:276:ASP:HB2	1:B:279:ARG:HB2	1.51	0.93

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:396:GLN:HE21	1:B:407:LEU:HA	1.30	0.93
1:A:1492:HIS:ND1	1:A:1493:PRO:HD2	1.84	0.93
1:A:904:ILE:HG22	1:A:905:GLY:H	1.31	0.92
1:B:1415:GLU:HA	1:B:1415:GLU:OE1	1.66	0.92
1:A:524:ILE:HG23	1:A:525:PRO:HD3	1.51	0.92
1:B:382:PRO:HB3	1:B:403:GLY:HA3	1.52	0.91
1:A:339:GLU:HG3	1:A:759:ILE:HG23	1.52	0.91
1:B:371:LEU:HD23	1:B:371:LEU:H	1.34	0.91
1:A:118:LYS:NZ	1:A:645:LYS:HD2	1.85	0.90
1:B:1547:LEU:HD22	1:B:1596:GLU:HA	1.53	0.90
1:B:234:GLN:HE22	1:B:257:ARG:NH2	1.67	0.90
1:B:398:LEU:HD11	1:B:403:GLY:O	1.72	0.90
1:A:83:LEU:HD12	1:A:83:LEU:C	1.91	0.90
1:B:1415:GLU:OE1	1:B:1418:LYS:HE2	1.72	0.89
1:A:118:LYS:HZ3	1:A:645:LYS:HD2	1.34	0.89
1:B:1311:LEU:HD12	1:B:1313:GLU:HB3	1.53	0.89
1:B:852:ASN:HD22	1:B:859:LEU:HD23	1.34	0.89
1:B:66:LYS:NZ	1:B:94:LYS:HG2	1.88	0.89
1:A:1147:LEU:HD23	1:A:1194:ALA:HB1	1.55	0.88
1:A:1435:ARG:O	1:A:1436:ASP:OD1	1.91	0.88
1:A:476:ARG:HB3	1:A:476:ARG:HH11	1.36	0.88
1:B:117:GLU:O	1:B:118:LYS:CG	2.21	0.88
1:A:72:GLU:HG2	1:A:86:VAL:HG13	1.56	0.88
1:A:1289:LYS:HD3	1:A:1289:LYS:H	1.36	0.88
1:A:458:VAL:HG13	1:A:469:LEU:HD11	1.56	0.87
1:B:421:THR:HG22	1:B:438:THR:HB	1.53	0.87
1:B:1563:ILE:HD12	1:B:1563:ILE:H	1.40	0.87
1:B:700:PRO:HB2	1:B:701:MET:HE2	1.56	0.87
1:A:290:VAL:HG11	1:A:298:GLU:H	1.39	0.86
1:B:530:VAL:HG21	1:B:642:LEU:HD11	1.56	0.86
1:B:110:THR:HB	1:B:115:GLN:HB3	1.58	0.86
1:B:161:THR:HG22	1:B:180:SER:HB2	1.59	0.85
1:B:60:HIS:HB3	1:B:65:LYS:HB3	1.59	0.85
1:B:129:LEU:HB2	1:B:217:PHE:CD2	2.12	0.85
1:B:573:HIS:ND1	1:B:579:ILE:HD11	1.90	0.85
1:B:1573:GLU:HG2	1:B:1580:ARG:HH21	1.42	0.85
1:B:977:THR:HG23	1:B:1323:THR:HG23	1.58	0.84
1:A:43:VAL:HA	1:A:85:THR:HG22	1.59	0.84
1:B:611:GLN:NE2	1:B:815:CYS:HA	1.91	0.84
1:A:1494:ASP:OD2	1:B:1203:GLY:HA2	1.77	0.84
1:A:812:LYS:O	1:A:812:LYS:HD3	1.77	0.84

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:272:PHE:HD1	1:B:325:VAL:CG2	1.90	0.84
1:A:700:PRO:HB2	1:A:701:MET:CE	2.07	0.84
1:B:633:TYR:O	1:B:637:PHE:HD2	1.60	0.84
1:A:407:LEU:HD23	1:A:408:SER:H	1.42	0.83
1:A:1217:ASN:HD21	1:A:1218:ARG:HD3	1.43	0.83
1:B:398:LEU:HD12	1:B:405:ALA:H	1.44	0.83
1:B:846:ILE:HD12	1:B:899:ILE:HD12	1.58	0.83
1:A:368:PRO:HA	1:A:410:ASN:HA	1.60	0.83
1:A:228:LEU:HG	1:A:228:LEU:O	1.77	0.83
1:B:458:VAL:HG13	1:B:469:LEU:HD11	1.61	0.82
1:B:442:LEU:HD13	1:B:631:ARG:NH2	1.92	0.82
1:A:271:ILE:HG12	1:A:287:LEU:HB3	1.61	0.82
1:B:992:ASP:HB2	1:B:998:ARG:HB3	1.59	0.82
1:B:271:ILE:HG12	1:B:287:LEU:HB3	1.62	0.82
1:A:260:TYR:HB3	1:A:853:TYR:CE1	2.14	0.82
1:A:808:LEU:HD23	1:A:808:LEU:O	1.80	0.82
1:A:242:TYR:CD1	1:A:250:LEU:HD11	2.14	0.81
1:B:398:LEU:HA	1:B:405:ALA:HB2	1.59	0.81
1:A:558:MET:C	1:A:812:LYS:HZ2	1.83	0.81
1:B:374:TYR:HE2	1:B:376:THR:HG23	1.44	0.81
1:B:1217:ASN:ND2	1:B:1218:ARG:HD3	1.96	0.81
1:B:105:VAL:HB	1:B:122:ILE:HD11	1.60	0.81
1:A:1579:GLU:O	1:A:1580:ARG:HG2	1.81	0.81
1:A:1566:ILE:HG13	1:A:1576:VAL:HG22	1.62	0.81
1:A:36:LEU:HD12	1:A:124:LEU:HB3	1.61	0.81
1:A:532:TYR:HB3	1:A:546:ALA:HB2	1.61	0.80
1:B:384:ARG:HA	1:B:400:GLN:HB2	1.64	0.80
1:A:809:SER:OG	1:A:812:LYS:HB3	1.80	0.80
1:A:1573:GLU:CD	1:A:1580:ARG:HE	1.83	0.80
1:A:859:LEU:H	1:A:859:LEU:HD22	1.45	0.80
1:A:846:ILE:HD12	1:A:899:ILE:HD12	1.63	0.80
1:A:83:LEU:O	1:A:83:LEU:HG	1.81	0.80
1:B:1112:LYS:HB3	1:B:1113:PRO:HD2	1.64	0.80
1:B:398:LEU:HD12	1:B:405:ALA:N	1.97	0.80
1:A:272:PHE:HA	1:A:325:VAL:HG22	1.63	0.80
1:A:904:ILE:HG22	1:A:905:GLY:N	1.97	0.80
1:B:1571:SER:O	1:B:1572:ASP:HB2	1.82	0.79
1:A:314:ARG:HA	1:A:314:ARG:HE	1.47	0.79
1:A:314:ARG:O	1:A:318:LEU:HB2	1.82	0.79
1:A:1605:VAL:HG12	1:A:1607:SER:H	1.46	0.79
1:A:346:PRO:HB2	1:A:348:VAL:HG23	1.65	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:846:ILE:CD1	1:A:899:ILE:HD12	2.12	0.79
1:B:593:LEU:HD11	1:B:774:ILE:HD11	1.62	0.79
1:B:888:PRO:HB2	1:B:891:SER:HB2	1.63	0.79
1:A:281:ILE:CD1	1:A:310:VAL:HG22	2.13	0.79
1:A:610:THR:HG22	1:A:613:LYS:HD2	1.65	0.79
1:A:32:ASN:HB2	1:A:641:GLY:HA2	1.64	0.79
1:A:829:PHE:HD2	1:A:853:TYR:HE2	1.29	0.78
1:A:375:VAL:HG11	1:A:386:ILE:HD12	1.62	0.78
1:B:359:THR:HG22	1:B:360:PRO:HD2	1.63	0.78
1:B:389:VAL:HG13	1:B:394:ASN:O	1.82	0.78
1:B:530:VAL:HG13	1:B:548:SER:HB3	1.63	0.78
1:B:369:PHE:HB3	1:B:409:ILE:CD1	2.11	0.78
1:B:396:GLN:HG2	1:B:407:LEU:HG	1.65	0.78
1:A:260:TYR:HB3	1:A:853:TYR:HE1	1.48	0.78
1:B:714:GLN:HE21	1:B:1424:VAL:HG13	1.49	0.78
1:B:44:LEU:HD11	1:B:86:VAL:HG23	1.64	0.78
1:B:234:GLN:HE22	1:B:257:ARG:HH22	1.32	0.78
1:B:1217:ASN:HD21	1:B:1218:ARG:HD3	1.48	0.78
1:B:995:ASP:HB3	1:B:998:ARG:HB2	1.67	0.77
1:A:605:LYS:HB3	1:A:608:LYS:HE2	1.66	0.77
1:B:503:ARG:H	1:B:503:ARG:NE	1.83	0.77
1:A:611:GLN:HG2	1:A:816:VAL:HB	1.67	0.77
1:A:106:THR:HG22	1:A:119:VAL:HG22	1.66	0.77
1:A:271:ILE:HG23	1:A:287:LEU:HD22	1.65	0.77
1:B:270:VAL:HG13	1:B:327:ALA:HB2	1.66	0.77
1:B:208:TYR:HD2	1:B:213:PRO:HA	1.50	0.77
1:B:373:VAL:HG11	1:B:388:VAL:HG11	1.66	0.77
1:B:272:PHE:CE2	1:B:301:LEU:HB2	2.20	0.77
1:A:458:VAL:HG13	1:A:459:PRO:HD2	1.65	0.77
1:B:1498:GLY:O	1:B:1501:SER:HB3	1.84	0.77
1:B:852:ASN:HD22	1:B:859:LEU:CD2	1.97	0.76
1:B:62:PHE:HA	1:B:106:THR:HG23	1.67	0.76
1:B:1285:VAL:N	1:B:1286:PRO:HD3	2.00	0.76
1:A:1204:ASP:HB2	1:A:1205:ARG:HH21	1.49	0.76
1:B:243:TYR:OH	1:B:245:ASP:HB2	1.86	0.76
1:B:700:PRO:HB2	1:B:701:MET:CE	2.14	0.76
1:A:274:VAL:HG23	1:A:283:LEU:HD11	1.68	0.76
1:B:701:MET:O	1:B:702:LYS:HB2	1.86	0.76
1:A:245:ASP:OD1	1:A:246:ASP:N	2.17	0.76
1:B:336:ASP:CG	1:B:1377:GLN:HE22	1.89	0.76
1:A:1237:LEU:HD21	1:A:1277:ALA:HA	1.68	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:ASN:HB2	1:A:859:LEU:HD23	1.67	0.75
1:B:1610:TRP:HB3	1:B:1617:SER:HB2	1.68	0.75
1:B:537:ASN:ND2	1:B:538:ALA:H	1.84	0.75
1:A:651:GLU:HB3	1:A:653:GLN:NE2	2.00	0.75
1:B:301:LEU:HD13	1:B:301:LEU:O	1.86	0.75
1:A:382:PRO:HB3	1:A:403:GLY:HA3	1.67	0.75
1:B:344:GLY:O	1:B:346:PRO:HD3	1.86	0.75
1:B:977:THR:HB	1:B:1345:THR:HB	1.68	0.75
1:A:507:GLU:HB3	1:A:510:GLN:NE2	2.02	0.75
1:A:1630:PRO:HD3	1:A:1643:GLN:HE21	1.52	0.75
1:B:46:ALA:HB2	1:B:76:LEU:HD13	1.67	0.75
1:B:256:ALA:O	1:B:264:VAL:HB	1.86	0.75
1:B:208:TYR:CD2	1:B:213:PRO:HA	2.21	0.74
1:A:359:THR:HG23	1:A:371:LEU:HA	1.69	0.74
1:B:323:ILE:CG1	1:B:347:ILE:HD11	2.17	0.74
1:B:871:PHE:HB3	1:B:901:PRO:HA	1.67	0.74
1:A:691:CYS:HA	1:A:1424:VAL:HG21	1.69	0.74
1:B:611:GLN:HE21	1:B:815:CYS:HA	1.50	0.74
1:A:149:PHE:CZ	1:A:806:VAL:HG11	2.23	0.74
1:A:1492:HIS:ND1	1:A:1493:PRO:CD	2.51	0.74
1:B:1630:PRO:HD3	1:B:1643:GLN:HE21	1.51	0.74
1:B:611:GLN:HE21	1:B:816:VAL:H	1.34	0.74
1:A:1217:ASN:ND2	1:A:1218:ARG:HD3	2.02	0.74
1:A:827:ASP:HB2	1:A:854:ARG:HH21	1.53	0.74
1:B:503:ARG:HE	1:B:503:ARG:N	1.83	0.73
1:A:272:PHE:HD1	1:A:325:VAL:CG2	2.01	0.73
1:A:364:LYS:O	1:A:367:MET:HB2	1.88	0.73
1:B:931:VAL:HG11	1:B:1438:ASN:HB3	1.68	0.73
1:A:1636:GLN:HA	1:A:1641:GLN:HE22	1.54	0.73
1:A:598:LYS:HB2	1:A:800:THR:O	1.89	0.73
1:A:1036:PHE:HB3	1:A:1040:LYS:HG3	1.69	0.72
1:A:131:ILE:HG12	1:A:148:VAL:HG22	1.71	0.72
1:B:915:VAL:HB	1:B:920:ILE:HB	1.71	0.72
1:B:895:VAL:HG23	1:B:895:VAL:O	1.88	0.72
1:A:871:PHE:HB3	1:A:901:PRO:HA	1.70	0.72
1:B:1255:LEU:HD22	1:B:1274:VAL:HG23	1.71	0.72
1:B:1368:PRO:HA	1:B:1383:MET:HG2	1.71	0.72
1:B:319:VAL:HG13	1:B:347:ILE:O	1.89	0.72
1:B:251:LYS:HG2	1:B:300:ILE:HG12	1.71	0.72
1:A:614:ILE:O	1:A:617:VAL:HB	1.89	0.72
1:A:442:LEU:HD22	1:A:631:ARG:HH22	1.54	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:323:ILE:HD11	1:A:347:ILE:HD11	1.70	0.72
1:B:492:ILE:HG22	1:B:499:LEU:HB3	1.70	0.72
1:B:1147:LEU:HD23	1:B:1194:ALA:HB1	1.70	0.72
1:A:830:ILE:HD11	1:A:911:VAL:HG12	1.72	0.72
1:A:1003:ILE:HG12	1:A:1268:THR:HG22	1.70	0.72
1:A:314:ARG:HE	1:A:314:ARG:CA	2.03	0.72
1:B:359:THR:CG2	1:B:360:PRO:HD2	2.20	0.72
1:A:1575:GLN:HB3	1:A:1578:GLN:CD	2.10	0.72
1:B:330:ILE:HG22	1:B:337:MET:HB3	1.70	0.72
1:A:910:GLU:HG3	1:A:925:LYS:HB3	1.70	0.71
1:B:391:GLN:HA	1:B:423:ARG:HH22	1.55	0.71
1:A:876:THR:HB	1:A:879:LYS:HG3	1.71	0.71
1:A:377:ASN:HD21	1:A:383:ALA:HA	1.54	0.71
1:B:904:ILE:HG22	1:B:905:GLY:N	2.03	0.71
1:A:850:LEU:HD12	1:A:885:ILE:HD11	1.73	0.71
1:A:80:ASN:ND2	1:A:83:LEU:H	1.88	0.71
1:A:359:THR:CG2	1:A:360:PRO:HD2	2.20	0.71
1:A:118:LYS:HA	1:A:118:LYS:HE3	1.73	0.71
1:A:274:VAL:O	1:A:281:ILE:HG22	1.91	0.71
1:A:610:THR:CG2	1:A:613:LYS:HG3	2.19	0.71
1:B:228:LEU:O	1:B:228:LEU:HD23	1.89	0.71
1:B:1566:ILE:CD1	1:B:1576:VAL:HG22	2.21	0.71
1:B:611:GLN:HG2	1:B:816:VAL:HB	1.72	0.71
1:A:848:ALA:HB3	1:A:895:VAL:CG2	2.21	0.71
1:A:359:THR:HG22	1:A:360:PRO:CD	2.21	0.71
1:A:580:THR:HB	1:A:791:ASN:ND2	2.05	0.70
1:A:284:THR:HG22	1:A:678:MET:HE2	1.73	0.70
1:A:134:ASP:HB2	1:A:145:LEU:HB2	1.72	0.70
1:B:227:VAL:CG1	1:B:229:PRO:HD3	2.20	0.70
1:A:270:VAL:HG21	1:A:299:ALA:HB2	1.73	0.70
1:A:605:LYS:HE2	1:A:605:LYS:H	1.55	0.70
1:B:1401:ILE:HD12	1:B:1480:TYR:HD1	1.57	0.70
1:A:1156:ILE:HD12	1:A:1156:ILE:H	1.56	0.70
1:A:564:LYS:HG2	1:A:565:ASN:N	2.06	0.70
1:A:339:GLU:HB2	1:A:759:ILE:HD12	1.73	0.70
1:B:806:VAL:HG22	1:B:816:VAL:HA	1.72	0.70
1:A:1354:LYS:HA	1:A:1489:ARG:NH2	2.07	0.70
1:A:835:PRO:HG3	1:A:844:VAL:HG11	1.73	0.70
1:B:62:PHE:CD2	1:B:63:PRO:HD3	2.27	0.70
1:A:386:ILE:H	1:A:398:LEU:HB3	1.55	0.70
1:A:377:ASN:HB3	1:A:378:PRO:HD2	1.73	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1545:THR:HG22	1:B:1563:ILE:HG23	1.74	0.70
1:A:532:TYR:CB	1:A:546:ALA:HB2	2.21	0.70
1:A:1610:TRP:HB3	1:A:1617:SER:HB2	1.74	0.70
1:A:1061:LYS:HD2	1:A:1061:LYS:H	1.56	0.70
1:A:537:ASN:ND2	1:A:538:ALA:H	1.90	0.70
1:B:528:ARG:NH2	1:B:623:ILE:HD11	2.06	0.70
1:A:610:THR:HG22	1:A:613:LYS:CD	2.22	0.70
1:A:418:LEU:HB3	1:A:441:ALA:HB3	1.74	0.70
1:B:1287:ASP:HA	1:B:1290:GLU:OE1	1.91	0.70
1:B:1605:VAL:HG12	1:B:1606:SER:H	1.56	0.70
1:B:407:LEU:HD23	1:B:408:SER:H	1.56	0.69
1:B:134:ASP:HB2	1:B:145:LEU:HB2	1.74	0.69
1:A:491:MET:HG3	1:A:501:VAL:HG12	1.73	0.69
1:B:986:VAL:O	1:B:990:THR:HG23	1.92	0.69
1:B:892:SER:O	1:B:893:VAL:HG23	1.91	0.69
1:B:852:ASN:ND2	1:B:859:LEU:HD23	2.07	0.69
1:B:520:THR:HG22	1:B:521:SER:H	1.57	0.69
1:A:573:HIS:CD2	1:A:579:ILE:HD11	2.28	0.69
1:B:1566:ILE:HD12	1:B:1576:VAL:HG22	1.74	0.69
1:B:504:GLN:HG3	1:B:515:LEU:HB2	1.75	0.69
1:B:118:LYS:CD	1:B:645:LYS:HE2	2.22	0.69
1:A:673:LEU:HD12	1:A:674:MET:H	1.56	0.69
1:A:611:GLN:HE21	1:A:815:CYS:HA	1.58	0.69
1:A:852:ASN:ND2	1:A:859:LEU:CD2	2.56	0.69
1:B:691:CYS:HA	1:B:1424:VAL:HG21	1.74	0.69
1:B:358:LYS:HD2	1:B:550:TRP:CZ3	2.28	0.69
1:A:152:ASP:HB3	1:A:158:VAL:HG21	1.74	0.69
1:A:593:LEU:HD12	1:A:772:THR:HG23	1.73	0.69
1:B:616:ASP:O	1:B:620:LYS:HB2	1.93	0.69
1:A:155:LEU:O	1:A:813:GLY:HA2	1.93	0.69
1:B:524:ILE:HG22	1:B:525:PRO:HD3	1.74	0.69
1:B:63:PRO:HG2	1:B:64:ALA:H	1.57	0.69
1:A:600:VAL:HG22	1:A:765:PHE:CG	2.28	0.69
1:A:616:ASP:O	1:A:620:LYS:HB2	1.93	0.68
1:B:1156:ILE:HD12	1:B:1156:ILE:H	1.58	0.68
1:B:429:ILE:HG22	1:B:430:PRO:HD2	1.73	0.68
1:A:250:LEU:N	1:A:250:LEU:HD12	2.07	0.68
1:B:1498:GLY:O	1:B:1501:SER:CB	2.41	0.68
1:A:83:LEU:CG	1:A:83:LEU:O	2.41	0.68
1:A:904:ILE:CG2	1:A:905:GLY:H	2.05	0.68
1:A:1435:ARG:C	1:A:1436:ASP:OD1	2.32	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:859:LEU:HD22	1:A:859:LEU:N	2.08	0.68
1:B:1613:LYS:HE2	1:B:1614:PRO:HD3	1.74	0.68
1:B:561:LEU:HD13	1:B:807:SER:HB3	1.76	0.68
1:B:128:TYR:HE2	1:B:617:VAL:HG12	1.58	0.68
1:B:753:ILE:C	1:B:754:ILE:HD12	2.14	0.68
1:A:1470:ILE:HG21	1:A:1499:MET:HG2	1.76	0.68
1:B:1585:HIS:HB3	1:B:1587:LYS:HG2	1.76	0.68
1:B:499:LEU:HG	1:B:500:LYS:HG2	1.75	0.68
1:B:940:THR:HB	1:B:1344:VAL:HG22	1.75	0.68
1:A:846:ILE:HD13	1:A:846:ILE:H	1.59	0.68
1:A:336:ASP:CG	1:A:1377:GLN:HE22	1.96	0.68
1:B:996:GLY:HA2	1:B:1047:LEU:HD11	1.75	0.68
1:B:244:ILE:HD11	1:B:319:VAL:HG21	1.73	0.68
1:A:423:ARG:HD2	1:A:425:LYS:HZ1	1.59	0.68
1:A:750:ASP:HB2	1:A:752:ASP:OD1	1.93	0.67
1:A:794:LEU:HD21	1:A:824:VAL:CG2	2.24	0.67
1:A:794:LEU:HG	1:A:795:LYS:H	1.59	0.67
1:A:524:ILE:O	1:A:553:VAL:HG23	1.94	0.67
1:B:241:PHE:HD2	1:B:378:PRO:HG3	1.59	0.67
1:B:62:PHE:CB	1:B:104:PHE:HB2	2.25	0.67
1:B:605:LYS:O	1:B:608:LYS:HG2	1.93	0.67
1:B:1223:ASN:O	1:B:1224:GLN:HG2	1.94	0.67
1:B:237:PRO:HG2	1:B:239:GLU:O	1.93	0.67
1:A:307:LEU:C	1:A:308:ASN:HD22	1.98	0.67
1:B:781:ASP:C	1:B:783:ASN:H	1.96	0.67
1:A:601:PHE:HD2	1:A:802:GLU:HG3	1.58	0.67
1:A:524:ILE:HG23	1:A:525:PRO:CD	2.24	0.67
1:B:1577:LYS:HE2	1:B:1577:LYS:HA	1.77	0.67
1:A:854:ARG:CD	1:A:857:GLU:HB2	2.25	0.67
1:A:876:THR:HG22	1:A:877:ALA:N	2.10	0.67
1:B:116:VAL:HG13	1:B:645:LYS:CG	2.16	0.67
1:B:32:ASN:HD22	1:B:643:THR:HG23	1.60	0.67
1:B:264:VAL:HG13	1:B:331:LEU:HD23	1.76	0.67
1:B:848:ALA:HB3	1:B:895:VAL:CG2	2.24	0.67
1:B:1161:VAL:HG12	1:B:1163:SER:H	1.59	0.67
1:B:1564:GLU:O	1:B:1565:ASN:HB2	1.94	0.67
1:A:74:THR:HG22	1:A:86:VAL:HG23	1.76	0.66
1:B:157:PRO:HB3	1:B:808:LEU:HD21	1.77	0.66
1:B:66:LYS:HZ3	1:B:94:LYS:HG2	1.60	0.66
1:A:271:ILE:CG2	1:A:287:LEU:HD22	2.24	0.66
1:A:561:LEU:HA	1:A:584:GLU:O	1.95	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:701:MET:HE1	1:A:1458:SER:H	1.60	0.66
1:B:808:LEU:HD12	1:B:814:ILE:HD11	1.76	0.66
1:A:848:ALA:O	1:A:895:VAL:HG22	1.95	0.66
1:B:864:GLU:OE2	1:B:880:ARG:HD3	1.96	0.66
1:B:1563:ILE:HD12	1:B:1563:ILE:N	2.11	0.66
1:B:436:THR:HG22	1:B:437:ARG:N	2.10	0.66
1:A:610:THR:HG22	1:A:613:LYS:CG	2.26	0.66
1:A:558:MET:HB3	1:A:812:LYS:NZ	2.10	0.66
1:A:1297:ILE:HB	1:A:1306:VAL:HG13	1.78	0.66
1:A:1391:TYR:CG	1:A:1397:ALA:HB2	2.31	0.66
1:B:208:TYR:HB3	1:B:216:VAL:HG13	1.78	0.66
1:B:1566:ILE:HG13	1:B:1576:VAL:HG13	1.78	0.66
1:B:104:PHE:CE1	1:B:656:ALA:HB2	2.31	0.66
1:B:863:VAL:HG12	1:B:913:ALA:HB2	1.77	0.66
1:B:781:ASP:OD2	1:B:783:ASN:HB3	1.96	0.66
1:A:1368:PRO:HA	1:A:1383:MET:HG2	1.76	0.66
1:B:377:ASN:HB2	1:B:381:SER:OG	1.96	0.65
1:B:330:ILE:HD11	1:B:750:ASP:OD1	1.96	0.65
1:A:1547:LEU:HA	1:A:1561:MET:HG3	1.78	0.65
1:B:323:ILE:HG13	1:B:347:ILE:HD11	1.77	0.65
1:A:637:PHE:CE1	1:A:644:LEU:HD11	2.31	0.65
1:A:318:LEU:HA	1:A:321:LYS:HD3	1.78	0.65
1:A:1213:ALA:HB2	1:A:1219:TRP:CE2	2.32	0.65
1:B:846:ILE:HD13	1:B:897:TYR:O	1.96	0.65
1:B:400:GLN:HG2	1:B:401:ASP:N	2.11	0.65
1:A:331:LEU:HD22	1:A:333:SER:OG	1.96	0.65
1:B:198:VAL:HG22	1:B:199:ASN:N	2.11	0.65
1:A:829:PHE:CD2	1:A:853:TYR:HE2	2.12	0.65
1:A:396:GLN:HG3	1:A:397:SER:H	1.61	0.65
1:B:272:PHE:CD1	1:B:325:VAL:HG21	2.22	0.65
1:B:701:MET:CE	1:B:1420:LEU:HD21	2.26	0.65
1:B:270:VAL:O	1:B:287:LEU:HA	1.97	0.65
1:A:106:THR:HG22	1:A:119:VAL:HG13	1.77	0.65
1:A:58:THR:HA	1:A:70:SER:O	1.95	0.65
1:B:406:LYS:HD2	1:B:460:ARG:HG2	1.78	0.65
1:B:1415:GLU:OE1	1:B:1418:LYS:CE	2.44	0.65
1:B:32:ASN:ND2	1:B:643:THR:HG23	2.12	0.65
1:A:852:ASN:HB3	1:A:887:ILE:CG2	2.26	0.65
1:B:1201:LEU:HD23	1:B:1242:ARG:HD3	1.79	0.65
1:B:1003:ILE:HD12	1:B:1268:THR:HA	1.77	0.65
1:A:1554:ASP:C	1:A:1586:ILE:HD11	2.17	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:44:LEU:HD13	1:A:55:VAL:CG1	2.20	0.65
1:A:354:ILE:O	1:A:437:ARG:HG3	1.97	0.65
1:B:1502:LYS:HE2	1:B:1590:GLU:HG3	1.79	0.65
1:B:128:TYR:HB2	1:B:151:VAL:HG12	1.79	0.65
1:B:350:SER:HB2	1:B:433:ARG:O	1.97	0.65
1:A:490:TYR:CE2	1:A:515:LEU:HD22	2.31	0.65
1:B:287:LEU:HD23	1:B:287:LEU:H	1.62	0.65
1:A:314:ARG:HA	1:A:314:ARG:NE	2.11	0.65
1:B:566:GLY:HA3	1:B:580:THR:HG23	1.79	0.65
1:A:398:LEU:HD11	1:A:403:GLY:C	2.17	0.65
1:A:1397:ALA:HB3	1:A:1449:VAL:HB	1.77	0.65
1:B:117:GLU:C	1:B:118:LYS:HG2	2.15	0.65
1:B:1128:MET:HE3	1:B:1142:LEU:HB2	1.79	0.65
1:B:272:PHE:CD2	1:B:301:LEU:HG	2.31	0.64
1:A:605:LYS:O	1:A:608:LYS:HG2	1.97	0.64
1:A:558:MET:C	1:A:812:LYS:NZ	2.49	0.64
1:A:348:VAL:CG1	1:A:350:SER:C	2.65	0.64
1:A:895:VAL:O	1:A:895:VAL:HG23	1.98	0.64
1:B:689:ARG:O	1:B:693:GLU:HG3	1.97	0.64
1:A:1010:GLY:HA3	1:A:1067:ALA:HA	1.79	0.64
1:B:377:ASN:HD21	1:B:383:ALA:HA	1.62	0.64
1:B:1397:ALA:HB3	1:B:1449:VAL:HB	1.79	0.64
1:B:149:PHE:HD1	1:B:187:ILE:HG12	1.63	0.64
1:A:323:ILE:O	1:A:345:ILE:HB	1.98	0.64
1:B:446:THR:HG21	1:B:450:SER:O	1.98	0.64
1:A:76:LEU:HB3	1:A:82:TYR:HB3	1.80	0.64
1:B:839:VAL:HG13	1:B:842:GLU:CD	2.18	0.64
1:B:1270:ALA:O	1:B:1274:VAL:HG12	1.97	0.64
1:A:1223:ASN:O	1:A:1224:GLN:HG2	1.96	0.64
1:B:323:ILE:HD11	1:B:347:ILE:HD11	1.79	0.64
1:A:554:LYS:O	1:A:556:SER:N	2.31	0.64
1:B:840:ARG:NH2	1:B:972:ASP:HB3	2.13	0.64
1:A:176:ARG:HE	1:A:1093:ALA:HB1	1.62	0.64
1:B:1573:GLU:HG2	1:B:1580:ARG:NH2	2.12	0.64
1:A:605:LYS:CE	1:A:605:LYS:H	2.10	0.64
1:A:362:PHE:HA	1:A:442:LEU:O	1.98	0.64
1:B:171:GLY:O	1:B:172:ILE:HB	1.98	0.64
1:B:729:ILE:HA	1:B:732:LEU:HB3	1.80	0.64
1:B:290:VAL:HG11	1:B:298:GLU:H	1.62	0.64
1:B:389:VAL:HG12	1:B:390:THR:H	1.62	0.64
1:A:1504:CYS:HB2	1:A:1508:THR:OG1	1.98	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:429:ILE:HG21	1:B:433:ARG:HD2	1.79	0.64
1:B:1012:GLN:HG2	1:B:1480:TYR:CZ	2.32	0.64
1:B:778:LYS:HG3	1:B:779:GLN:HG2	1.80	0.64
1:B:227:VAL:HG12	1:B:229:PRO:CD	2.20	0.63
1:A:290:VAL:HG21	1:A:298:GLU:O	1.98	0.63
1:B:228:LEU:O	1:B:228:LEU:CD2	2.45	0.63
1:A:977:THR:HB	1:A:1345:THR:HB	1.79	0.63
1:B:1493:PRO:CB	1:B:1497:ASP:OD2	2.43	0.63
1:B:57:VAL:HG21	1:B:86:VAL:HG21	1.79	0.63
1:B:303:ARG:HA	1:B:306:LEU:HB2	1.81	0.63
1:A:1369:ALA:HB1	1:A:1370:PRO:HD2	1.80	0.63
1:B:128:TYR:CE2	1:B:617:VAL:HG12	2.33	0.63
1:A:615:TRP:O	1:A:617:VAL:N	2.31	0.63
1:B:610:THR:HG23	1:B:613:LYS:H	1.63	0.63
1:A:530:VAL:HG21	1:A:642:LEU:HD11	1.81	0.63
1:B:1265:TYR:HB2	1:B:1271:THR:OG1	1.99	0.63
1:A:134:ASP:HB3	1:A:138:TYR:OH	1.98	0.63
1:A:240:LYS:O	1:A:240:LYS:HG3	1.99	0.63
1:A:834:LEU:HD22	1:A:846:ILE:HG21	1.78	0.63
1:A:885:ILE:HD12	1:A:893:VAL:HG11	1.80	0.63
2:A:2001:NAG:H61	2:A:2002:NAG:O7	1.98	0.63
1:A:610:THR:HG23	1:A:613:LYS:H	1.64	0.63
1:A:645:LYS:O	1:A:646:THR:HB	1.98	0.63
1:B:389:VAL:HG12	1:B:390:THR:N	2.14	0.63
1:B:1116:ILE:HG23	1:B:1139:ASP:HB3	1.80	0.63
1:B:454:LEU:HB2	1:B:533:TYR:HE2	1.62	0.63
1:A:489:THR:HG22	1:A:503:ARG:NE	2.13	0.63
1:A:605:LYS:N	1:A:605:LYS:HE2	2.14	0.63
1:A:838:VAL:HA	1:A:1408:THR:HG21	1.81	0.63
1:B:458:VAL:HG11	1:B:469:LEU:HD21	1.80	0.62
1:B:359:THR:HG22	1:B:360:PRO:CD	2.29	0.62
1:A:995:ASP:HB3	1:A:998:ARG:HB2	1.81	0.62
1:A:287:LEU:H	1:A:287:LEU:HD23	1.63	0.62
1:A:354:ILE:O	1:A:354:ILE:HD12	1.99	0.62
1:A:61:ASP:CB	1:A:63:PRO:HD2	2.21	0.62
1:B:134:ASP:OD2	1:B:768:SER:HB2	1.99	0.62
1:B:1391:TYR:CG	1:B:1397:ALA:HB2	2.34	0.62
1:B:135:LYS:HB3	1:B:600:VAL:HG11	1.82	0.62
1:B:997:GLU:OE2	2:B:2003:BMA:H4	1.99	0.62
1:B:36:LEU:HD12	1:B:124:LEU:HD13	1.80	0.62
1:A:653:GLN:HB3	1:A:655:ARG:HG2	1.80	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:362:PHE:CE2	1:A:631:ARG:NH1	2.67	0.62
1:B:268:ALA:HB2	1:B:329:VAL:HG22	1.81	0.62
1:B:319:VAL:C	1:B:321:LYS:H	2.03	0.62
1:A:633:TYR:O	1:A:637:PHE:HD2	1.83	0.62
1:B:272:PHE:CZ	1:B:301:LEU:HB2	2.34	0.62
1:A:674:MET:CG	1:A:751:ASP:HA	2.30	0.62
1:B:274:VAL:HG23	1:B:283:LEU:HD11	1.79	0.62
1:A:239:GLU:HB3	1:A:241:PHE:CZ	2.35	0.62
1:A:1012:GLN:HG2	1:A:1480:TYR:CZ	2.34	0.62
1:A:1545:THR:CG2	1:A:1563:ILE:HG23	2.29	0.62
1:B:448:GLY:O	1:B:450:SER:N	2.33	0.62
1:B:904:ILE:CG2	1:B:905:GLY:N	2.61	0.62
1:B:35:ARG:HB3	1:B:38:SER:OG	2.00	0.62
1:A:451:ASN:HB2	1:A:478:ASP:OD2	2.00	0.62
1:B:460:ARG:HH21	1:B:462:GLU:HB2	1.64	0.62
1:A:348:VAL:HG11	1:A:350:SER:O	2.00	0.62
1:B:44:LEU:HD12	1:B:84:SER:O	2.00	0.62
1:B:839:VAL:HG13	1:B:842:GLU:OE1	2.00	0.62
1:B:316:ASP:O	1:B:318:LEU:N	2.32	0.62
1:A:1549:GLN:HB3	1:A:1560:ILE:HD12	1.81	0.62
1:A:574:ARG:HH12	1:A:920:ILE:HB	1.62	0.62
1:B:269:PHE:CE1	1:B:289:ARG:HD3	2.34	0.62
1:A:348:VAL:CG1	1:A:350:SER:O	2.48	0.62
1:A:800:THR:CG2	1:A:823:THR:HG22	2.27	0.61
1:B:241:PHE:CD2	1:B:378:PRO:HG3	2.35	0.61
1:B:673:LEU:HG	1:B:674:MET:N	2.14	0.61
1:A:97:LYS:HE2	1:A:124:LEU:HD21	1.81	0.61
1:A:354:ILE:HG22	1:A:375:VAL:HG22	1.82	0.61
1:B:290:VAL:HG21	1:B:298:GLU:O	2.00	0.61
1:A:62:PHE:N	1:A:63:PRO:CD	2.63	0.61
1:A:1022:ILE:HD11	1:A:1275:PHE:CG	2.35	0.61
1:B:396:GLN:NE2	1:B:407:LEU:HA	2.08	0.61
1:B:32:ASN:HB2	1:B:641:GLY:HA2	1.81	0.61
1:A:1543:TYR:HB3	1:A:1563:ILE:CG2	2.31	0.61
1:A:476:ARG:CB	1:A:476:ARG:HH11	2.12	0.61
1:A:846:ILE:HD13	1:A:897:TYR:O	2.00	0.61
1:B:876:THR:HB	1:B:879:LYS:HG3	1.82	0.61
1:A:311:GLN:HB3	1:A:312:PRO:HD3	1.83	0.61
1:A:848:ALA:HB3	1:A:895:VAL:HG21	1.82	0.61
1:B:116:VAL:HG11	1:B:645:LYS:HG2	1.79	0.61
1:A:347:ILE:HG22	1:A:347:ILE:O	1.99	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:VAL:O	1:A:287:LEU:HA	2.00	0.61
1:A:287:LEU:HD21	1:A:678:MET:SD	2.40	0.61
1:A:152:ASP:HB3	1:A:158:VAL:CG2	2.31	0.61
1:A:306:LEU:C	1:A:308:ASN:H	2.03	0.61
1:A:420:ILE:CD1	1:A:439:MET:HB3	2.30	0.61
1:B:319:VAL:O	1:B:321:LYS:N	2.34	0.61
1:A:794:LEU:HD21	1:A:824:VAL:HG22	1.81	0.61
1:A:611:GLN:OE1	1:A:614:ILE:HD11	2.00	0.61
1:A:829:PHE:HD2	1:A:853:TYR:CE2	2.14	0.61
1:B:309:GLY:O	1:B:311:GLN:N	2.34	0.61
1:B:56:SER:O	1:B:109:ALA:HA	1.99	0.61
1:A:575:PRO:C	1:A:577:GLN:H	2.04	0.61
1:B:436:THR:HG22	1:B:437:ARG:H	1.66	0.61
1:B:798:ILE:HG21	1:B:829:PHE:HZ	1.64	0.61
1:A:610:THR:CG2	1:A:613:LYS:CG	2.79	0.61
1:A:34:LEU:HD22	1:A:40:GLU:HG3	1.83	0.61
1:B:906:LEU:N	1:B:906:LEU:HD23	2.14	0.61
1:A:729:ILE:O	1:A:733:ARG:HB2	2.01	0.61
1:A:268:ALA:HB2	1:A:329:VAL:HG22	1.82	0.61
1:B:407:LEU:CD2	1:B:408:SER:H	2.14	0.60
1:A:1563:ILE:HD12	1:A:1578:GLN:O	2.02	0.60
1:A:1289:LYS:HD3	1:A:1289:LYS:N	2.12	0.60
1:B:1575:GLN:HB3	1:B:1578:GLN:CD	2.21	0.60
1:B:373:VAL:HG11	1:B:388:VAL:CG1	2.31	0.60
1:A:111:PHE:CD1	1:A:111:PHE:C	2.75	0.60
1:B:129:LEU:HB2	1:B:217:PHE:HD2	1.63	0.60
1:B:269:PHE:O	1:B:327:ALA:HB1	2.01	0.60
1:B:430:PRO:C	1:B:432:GLY:H	2.04	0.60
1:B:1545:THR:HB	1:B:1561:MET:HG2	1.84	0.60
1:B:904:ILE:HD13	1:B:932:PRO:HB3	1.84	0.60
1:A:871:PHE:CZ	1:A:909:VAL:HG22	2.36	0.60
1:B:128:TYR:OH	1:B:618:VAL:HA	2.02	0.60
1:A:359:THR:O	1:A:627:PRO:HG2	2.00	0.60
1:A:171:GLY:O	1:A:172:ILE:HB	2.01	0.60
1:A:252:VAL:HG23	1:A:252:VAL:O	2.01	0.60
1:B:1297:ILE:HB	1:B:1306:VAL:HG13	1.84	0.60
1:A:575:PRO:O	1:A:577:GLN:N	2.33	0.60
1:A:615:TRP:C	1:A:617:VAL:N	2.54	0.60
1:B:562:VAL:HG12	1:B:563:VAL:N	2.17	0.60
1:A:612:ARG:HH11	1:A:612:ARG:HG2	1.65	0.60
1:B:323:ILE:CD1	1:B:347:ILE:HD11	2.31	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:653:GLN:O	1:A:654:GLN:HG2	2.02	0.60
1:B:389:VAL:HG21	1:B:425:LYS:HD2	1.83	0.60
1:A:876:THR:HB	1:A:879:LYS:CG	2.30	0.60
1:B:781:ASP:C	1:B:783:ASN:N	2.55	0.60
1:A:1112:LYS:HB3	1:A:1113:PRO:HD2	1.84	0.60
1:B:859:LEU:N	1:B:859:LEU:HD22	2.17	0.60
1:B:1377:GLN:N	1:B:1377:GLN:CD	2.54	0.60
1:B:398:LEU:CD1	1:B:405:ALA:H	2.12	0.60
1:B:872:CYS:HB2	1:B:900:VAL:HB	1.84	0.60
1:B:107:VAL:O	1:B:117:GLU:HA	2.00	0.60
1:A:116:VAL:HG11	1:A:645:LYS:HB3	1.84	0.60
1:B:1563:ILE:HD13	1:B:1578:GLN:H	1.66	0.60
1:B:994:ILE:HG23	1:B:1044:SER:HB3	1.84	0.60
1:B:653:GLN:H	1:B:653:GLN:NE2	1.99	0.60
1:A:137:ILE:HB	1:A:603:LEU:HD23	1.84	0.60
1:A:407:LEU:HD22	1:A:409:ILE:HG23	1.84	0.60
1:A:830:ILE:O	1:A:830:ILE:HG23	2.02	0.60
1:A:147:ARG:HE	1:A:189:THR:HG22	1.66	0.60
1:A:1496:GLU:O	1:A:1498:GLY:N	2.34	0.60
1:B:931:VAL:HG13	1:B:932:PRO:HD2	1.84	0.59
1:B:1237:LEU:HD21	1:B:1277:ALA:HA	1.82	0.59
1:A:530:VAL:HG12	1:A:548:SER:CB	2.32	0.59
1:B:580:THR:HA	1:B:791:ASN:HA	1.84	0.59
1:A:272:PHE:CD2	1:A:301:LEU:HG	2.37	0.59
1:A:250:LEU:HD12	1:A:250:LEU:H	1.65	0.59
1:A:712:ILE:HG21	1:A:719:VAL:HG22	1.85	0.59
1:A:58:THR:OG1	1:A:108:VAL:HB	2.02	0.59
1:B:1045:LEU:O	1:B:1049:ARG:HG3	2.02	0.59
1:A:530:VAL:HG12	1:A:548:SER:HB3	1.84	0.59
1:B:852:ASN:O	1:B:852:ASN:CG	2.40	0.59
1:B:843:GLN:HG3	1:B:900:VAL:HG22	1.83	0.59
1:A:507:GLU:OE1	1:A:508:PRO:HD2	2.01	0.59
1:B:323:ILE:HG22	1:B:324:TYR:N	2.16	0.59
1:A:1545:THR:HG22	1:A:1563:ILE:HG23	1.84	0.59
1:B:272:PHE:CD1	1:B:325:VAL:CG2	2.80	0.59
1:A:1654:MET:HA	1:A:1657:PHE:HB3	1.84	0.59
1:A:566:GLY:HA3	1:A:580:THR:HG23	1.84	0.59
1:A:271:ILE:HG23	1:A:287:LEU:CD2	2.32	0.59
1:A:1354:LYS:HA	1:A:1489:ARG:HH21	1.65	0.59
1:A:1270:ALA:O	1:A:1274:VAL:HG12	2.03	0.59
1:A:1542:VAL:HG22	1:A:1603:TRP:HB2	1.82	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1544:LYS:HB3	1:A:1565:ASN:HB3	1.84	0.59
1:A:83:LEU:C	1:A:83:LEU:CD1	2.56	0.59
1:B:347:ILE:O	1:B:347:ILE:HG22	2.03	0.59
1:A:311:GLN:HB3	1:A:312:PRO:CD	2.32	0.59
1:B:121:LEU:O	1:B:122:ILE:HD13	2.02	0.59
1:B:977:THR:HB	1:B:1345:THR:CB	2.31	0.59
1:B:850:LEU:HD11	1:B:863:VAL:HG11	1.84	0.59
1:A:1242:ARG:O	1:A:1243:LYS:HB2	2.03	0.59
1:B:218:SER:O	1:B:219:ALA:HB2	2.03	0.59
1:B:273:GLY:O	1:B:324:TYR:CD2	2.56	0.59
1:B:72:GLU:HG3	1:B:86:VAL:HG13	1.85	0.59
1:A:737:SER:O	1:B:1222:PRO:HB3	2.02	0.59
1:B:958:ARG:HG3	1:B:1332:LYS:HG2	1.85	0.59
1:A:843:GLN:HG2	1:A:900:VAL:HG22	1.85	0.59
1:A:590:ARG:NH1	1:A:775:GLU:O	2.36	0.59
1:A:837:SER:HA	1:A:929:LYS:HB2	1.85	0.59
1:A:100:LYS:HD3	1:A:100:LYS:H	1.67	0.59
1:B:66:LYS:HZ1	1:B:94:LYS:HG2	1.64	0.59
1:B:561:LEU:CD1	1:B:807:SER:HB3	2.33	0.59
1:A:670:SER:HA	1:A:673:LEU:HD11	1.84	0.59
1:A:852:ASN:ND2	1:A:888:PRO:O	2.36	0.59
1:B:148:VAL:HG12	1:B:188:LEU:HB2	1.84	0.59
1:A:1014:MET:HG3	1:A:1080:TYR:CE2	2.38	0.59
1:A:541:GLN:HA	1:A:541:GLN:HE21	1.68	0.59
1:A:852:ASN:HB3	1:A:887:ILE:HG21	1.83	0.59
1:B:1498:GLY:C	1:B:1500:LEU:H	2.07	0.59
1:A:1528:GLU:HA	1:A:1531:LEU:HB2	1.85	0.59
1:B:362:PHE:CD1	1:B:631:ARG:HG3	2.38	0.58
1:A:1289:LYS:H	1:A:1289:LYS:CD	2.14	0.58
1:B:1437:SER:O	1:B:1438:ASN:C	2.41	0.58
1:A:1469:LEU:N	1:A:1499:MET:O	2.36	0.58
1:B:802:GLU:O	1:B:804:LEU:HD13	2.03	0.58
1:B:38:SER:O	1:B:39:GLU:HG2	2.03	0.58
1:B:164:ILE:HD13	1:B:190:LEU:HD11	1.85	0.58
1:B:852:ASN:HB2	1:B:859:LEU:HD23	1.85	0.58
1:A:1147:LEU:CD1	1:A:1168:ILE:HG23	2.32	0.58
1:A:169:PRO:HD3	1:A:203:TRP:CD1	2.38	0.58
1:A:575:PRO:CB	1:A:796:ASP:HA	2.33	0.58
1:B:102:HIS:O	1:B:103:LYS:HG3	2.03	0.58
1:A:250:LEU:CD1	1:A:250:LEU:H	2.16	0.58
1:A:584:GLU:HG2	1:A:787:THR:HG22	1.85	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1014:MET:HG3	1:A:1080:TYR:HE2	1.67	0.58
1:B:564:LYS:HG2	1:B:565:ASN:N	2.18	0.58
1:A:1437:SER:O	1:A:1438:ASN:C	2.41	0.58
1:A:1204:ASP:HA	1:A:1207:THR:CG2	2.33	0.58
1:A:876:THR:CG2	1:A:877:ALA:N	2.67	0.58
1:B:850:LEU:HD12	1:B:885:ILE:HD11	1.85	0.58
1:B:460:ARG:HH12	1:B:552:ASP:H	1.50	0.58
1:B:384:ARG:HA	1:B:400:GLN:CB	2.33	0.58
1:B:439:MET:HG2	1:B:440:GLN:N	2.18	0.58
1:A:344:GLY:O	1:A:346:PRO:HD3	2.04	0.58
1:B:1601:LEU:HB3	1:B:1627:GLU:HB2	1.86	0.58
1:A:832:LEU:HD21	1:A:909:VAL:HG12	1.86	0.58
1:A:58:THR:HG22	1:A:71:ASN:HD22	1.67	0.58
1:A:931:VAL:HG11	1:A:1438:ASN:HB3	1.85	0.58
1:B:61:ASP:C	1:B:63:PRO:HD2	2.24	0.58
1:A:854:ARG:CZ	1:A:859:LEU:HD11	2.33	0.58
1:B:570:GLU:C	1:B:572:HIS:H	2.07	0.58
1:A:1184:ARG:HH11	1:A:1184:ARG:HG2	1.67	0.58
1:A:825:MET:HG3	1:A:826:GLN:N	2.18	0.58
1:A:824:VAL:O	1:A:824:VAL:HG12	2.04	0.58
1:B:377:ASN:O	1:B:379:ASP:N	2.32	0.58
1:B:642:LEU:O	1:B:643:THR:CG2	2.52	0.58
1:A:34:LEU:HB2	1:A:121:LEU:O	2.04	0.58
1:A:1138:LYS:HE3	1:A:1139:ASP:OD2	2.04	0.58
1:B:524:ILE:O	1:B:553:VAL:HG22	2.03	0.57
1:A:854:ARG:HD2	1:A:857:GLU:HB2	1.85	0.57
1:B:236:GLU:OE1	1:B:237:PRO:HD2	2.04	0.57
1:B:1600:TYR:HD2	1:B:1628:LEU:HA	1.69	0.57
1:B:1298:GLN:HG2	1:B:1305:ALA:HB2	1.86	0.57
1:B:398:LEU:HA	1:B:405:ALA:CB	2.32	0.57
1:B:1206:LEU:O	1:B:1206:LEU:HD22	2.04	0.57
1:A:529:LEU:HD12	1:A:530:VAL:N	2.19	0.57
1:B:881:HIS:HE1	1:B:897:TYR:HE2	1.51	0.57
1:B:72:GLU:CG	1:B:86:VAL:HG13	2.34	0.57
1:B:348:VAL:HG12	1:B:349:THR:N	2.18	0.57
1:B:348:VAL:HG12	1:B:350:SER:H	1.68	0.57
1:B:163:PHE:HB2	1:B:208:TYR:CE1	2.39	0.57
1:B:1600:TYR:CD2	1:B:1628:LEU:HA	2.40	0.57
1:B:1582:PHE:HB3	1:B:1620:ILE:HD11	1.85	0.57
1:A:41:THR:HB	1:A:87:THR:HG22	1.86	0.57
1:A:1579:GLU:O	1:A:1580:ARG:NH1	2.37	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:74:THR:CG2	1:B:84:SER:HB2	2.33	0.57
1:A:302:LYS:HD2	1:A:304:GLN:OE1	2.03	0.57
1:B:985:PRO:CB	1:B:1256:ASN:ND2	2.68	0.57
1:B:825:MET:CG	1:B:826:GLN:N	2.68	0.57
1:A:149:PHE:HD1	1:A:187:ILE:HG12	1.70	0.57
1:A:384:ARG:HD2	1:A:400:GLN:HB2	1.87	0.57
1:B:839:VAL:HA	1:B:931:VAL:O	2.03	0.57
1:A:235:LEU:HD12	1:A:340:ALA:HB1	1.87	0.57
1:A:1259:ARG:NH1	1:A:1340:THR:HG21	2.19	0.57
1:B:524:ILE:HA	1:B:553:VAL:HG21	1.85	0.57
1:A:615:TRP:C	1:A:617:VAL:H	2.06	0.57
1:A:295:GLY:C	1:A:296:ASN:HD22	2.08	0.57
1:A:611:GLN:NE2	1:A:815:CYS:HA	2.19	0.57
1:B:457:SER:HB3	1:B:472:ASN:HB2	1.86	0.57
1:A:866:LEU:HD11	1:A:910:GLU:OE2	2.04	0.57
1:A:933:GLU:HG2	1:A:970:VAL:HG11	1.86	0.57
1:A:1136:ARG:HD3	1:A:1181:GLU:HB3	1.86	0.57
1:B:55:VAL:HG13	1:B:111:PHE:HB3	1.87	0.57
1:B:272:PHE:HA	1:B:325:VAL:HG22	1.86	0.57
1:A:577:GLN:O	1:A:794:LEU:HB2	2.05	0.57
1:B:60:HIS:O	1:B:105:VAL:HG22	2.04	0.57
1:A:105:VAL:HB	1:A:122:ILE:HD11	1.86	0.57
1:B:904:ILE:CD1	1:B:932:PRO:HB3	2.35	0.57
1:A:885:ILE:CD1	1:A:893:VAL:HG11	2.35	0.57
1:A:473:PHE:HB2	1:A:513:VAL:HG12	1.85	0.57
1:B:269:PHE:HE1	1:B:289:ARG:HD3	1.70	0.57
1:A:159:GLY:HA2	1:A:181:SER:OG	2.05	0.57
1:A:969:GLN:HA	1:A:1348:HIS:O	2.05	0.57
1:B:463:LEU:HD13	1:B:467:GLU:HG2	1.87	0.56
1:A:281:ILE:O	1:A:281:ILE:HG23	2.04	0.56
1:B:35:ARG:CZ	1:B:153:HIS:HB2	2.35	0.56
1:A:235:LEU:HD12	1:A:340:ALA:CB	2.34	0.56
1:B:1022:ILE:HD11	1:B:1275:PHE:CD1	2.39	0.56
1:B:129:LEU:HD23	1:B:150:THR:HA	1.87	0.56
1:A:830:ILE:HD11	1:A:911:VAL:CG1	2.34	0.56
1:A:1268:THR:HB	1:A:1272:PHE:CE2	2.40	0.56
1:A:129:LEU:HG	1:A:209:TYR:CE1	2.40	0.56
1:A:504:GLN:HE21	1:A:504:GLN:HA	1.69	0.56
1:A:613:LYS:O	1:A:617:VAL:HG23	2.05	0.56
1:B:1575:GLN:O	1:B:1578:GLN:HG3	2.04	0.56
1:A:290:VAL:HG11	1:A:298:GLU:N	2.17	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:592:GLY:O	1:B:805:ALA:HA	2.05	0.56
1:B:611:GLN:HE21	1:B:816:VAL:N	2.03	0.56
1:B:876:THR:HG22	1:B:877:ALA:N	2.21	0.56
1:A:198:VAL:HG22	1:A:199:ASN:N	2.21	0.56
1:A:137:ILE:HD12	1:A:603:LEU:HD21	1.86	0.56
1:A:1500:LEU:O	1:A:1500:LEU:HD12	2.05	0.56
1:B:1247:THR:O	1:B:1247:THR:HG22	2.05	0.56
1:A:163:PHE:HE1	1:A:178:SER:HG	1.52	0.56
1:A:525:PRO:O	1:A:526:SER:O	2.24	0.56
1:A:852:ASN:C	1:A:852:ASN:OD1	2.43	0.56
1:B:445:ASN:HB2	1:B:632:ASN:HD21	1.71	0.56
1:B:876:THR:CG2	1:B:877:ALA:N	2.69	0.56
1:A:1593:LYS:HE2	1:A:1595:LYS:NZ	2.20	0.56
1:B:1147:LEU:CD1	1:B:1168:ILE:HG23	2.35	0.56
1:A:1564:GLU:O	1:A:1565:ASN:HB2	2.05	0.56
1:B:506:ARG:NE	1:B:510:GLN:O	2.38	0.56
1:B:946:LEU:O	1:B:1338:GLN:HA	2.05	0.56
1:B:559:GLY:HA3	1:B:812:LYS:HD2	1.87	0.56
1:A:490:TYR:HB2	1:A:529:LEU:HD11	1.86	0.56
1:A:1415:GLU:O	1:A:1419:THR:HG23	2.04	0.56
1:B:1406:MET:SD	1:B:1412:PRO:HD3	2.46	0.56
1:A:994:ILE:HG23	1:A:1044:SER:HB3	1.86	0.56
1:B:396:GLN:HG2	1:B:406:LYS:O	2.05	0.56
1:B:150:THR:HG22	1:B:162:VAL:HG21	1.87	0.56
1:A:827:ASP:HB3	1:A:854:ARG:HB3	1.88	0.56
1:B:168:THR:HG23	1:B:172:ILE:O	2.06	0.56
1:A:779:GLN:O	1:A:781:ASP:N	2.36	0.56
1:A:83:LEU:O	1:A:83:LEU:CD1	2.54	0.56
1:A:321:LYS:O	1:A:347:ILE:N	2.33	0.56
1:B:573:HIS:CE1	1:B:579:ILE:HD11	2.41	0.56
1:B:754:ILE:CG2	1:B:755:PRO:HD2	2.35	0.56
1:A:32:ASN:HB2	1:A:641:GLY:CA	2.35	0.56
1:B:1527:LEU:HG	1:B:1646:ASP:HB3	1.88	0.56
1:A:701:MET:CE	1:A:1458:SER:H	2.19	0.56
1:B:701:MET:HE1	1:B:1420:LEU:HD21	1.88	0.56
1:B:825:MET:HG3	1:B:826:GLN:N	2.20	0.56
1:B:398:LEU:CA	1:B:405:ALA:HB2	2.32	0.55
1:A:1568:LYS:HG3	1:A:1569:SER:N	2.21	0.55
1:B:835:PRO:HG3	1:B:844:VAL:HG11	1.89	0.55
1:A:83:LEU:HD12	1:A:84:SER:N	2.21	0.55
1:B:334:GLY:O	1:B:335:SER:HB2	2.07	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:808:LEU:CB	1:B:814:ILE:HG12	2.30	0.55
1:A:887:ILE:HD12	1:A:887:ILE:N	2.21	0.55
1:A:492:ILE:HD13	1:A:529:LEU:HD13	1.88	0.55
1:A:910:GLU:CG	1:A:925:LYS:HB3	2.36	0.55
1:B:155:LEU:O	1:B:813:GLY:HA2	2.06	0.55
1:A:814:ILE:O	1:A:814:ILE:HG22	2.05	0.55
1:A:400:GLN:HG2	1:A:401:ASP:N	2.20	0.55
1:A:361:LYS:HD3	1:A:362:PHE:CZ	2.40	0.55
1:A:593:LEU:HD12	1:A:772:THR:CG2	2.36	0.55
1:B:306:LEU:C	1:B:308:ASN:N	2.59	0.55
1:A:1190:ILE:O	1:A:1190:ILE:HD13	2.05	0.55
1:A:1300:PRO:HG2	1:A:1301:SER:H	1.71	0.55
1:B:525:PRO:HG2	1:B:526:SER:H	1.71	0.55
1:A:575:PRO:HB2	1:A:796:ASP:HA	1.87	0.55
1:B:578:GLN:OE1	1:B:791:ASN:HB3	2.06	0.55
1:B:915:VAL:CB	1:B:920:ILE:HB	2.35	0.55
1:B:354:ILE:HD12	1:B:355:HIS:N	2.22	0.55
1:A:231:PHE:CE1	1:A:338:VAL:HB	2.42	0.55
1:A:55:VAL:HG13	1:A:111:PHE:CB	2.26	0.55
1:B:1569:SER:O	1:B:1571:SER:N	2.39	0.55
1:B:1576:VAL:O	1:B:1578:GLN:HG2	2.07	0.55
1:B:475:LEU:HB2	1:B:488:TYR:OH	2.06	0.55
1:A:366:ALA:HB2	1:A:413:ASN:CG	2.27	0.55
1:A:1502:LYS:O	1:A:1503:LEU:C	2.44	0.55
1:B:489:THR:HB	1:B:532:TYR:CE2	2.41	0.55
1:A:137:ILE:HD12	1:A:603:LEU:CD2	2.37	0.55
1:B:769:TRP:CD1	1:B:769:TRP:N	2.75	0.55
1:B:785:ILE:HG22	1:B:787:THR:HG22	1.88	0.55
1:A:112:GLY:O	1:A:114:VAL:HG22	2.06	0.55
1:B:1461:VAL:O	1:B:1461:VAL:HG23	2.06	0.55
1:B:1494:ASP:C	1:B:1496:GLU:H	2.10	0.55
1:A:149:PHE:CZ	1:A:806:VAL:CG1	2.89	0.55
1:A:1285:VAL:O	1:A:1285:VAL:HG12	2.07	0.55
1:B:1577:LYS:CE	1:B:1577:LYS:HA	2.37	0.55
1:B:560:THR:O	1:B:561:LEU:HD23	2.06	0.55
1:A:798:ILE:HG21	1:A:829:PHE:CZ	2.42	0.55
1:B:1494:ASP:O	1:B:1496:GLU:N	2.39	0.55
1:A:334:GLY:O	1:A:335:SER:HB2	2.07	0.55
1:B:634:ALA:HA	1:B:652:THR:HG22	1.88	0.55
1:B:68:VAL:O	1:B:68:VAL:HG13	2.06	0.55
1:B:642:LEU:C	1:B:643:THR:HG23	2.28	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:TYR:CG	1:A:250:LEU:HD11	2.42	0.55
1:B:1501:SER:O	1:B:1502:LYS:C	2.44	0.55
1:A:561:LEU:HD13	1:A:807:SER:HB3	1.89	0.55
1:B:1568:LYS:HG3	1:B:1569:SER:N	2.22	0.55
1:B:458:VAL:HG13	1:B:459:PRO:HD2	1.89	0.55
1:B:754:ILE:N	1:B:754:ILE:HD12	2.22	0.55
1:A:1547:LEU:HB3	1:A:1596:GLU:HA	1.89	0.55
1:A:1265:TYR:HB2	1:A:1271:THR:OG1	2.07	0.55
1:B:487:TYR:HB3	1:B:505:TYR:CD1	2.41	0.55
1:B:1284:ASP:C	1:B:1286:PRO:HD3	2.27	0.54
1:B:1405:SER:CB	1:B:1441:THR:HG22	2.37	0.54
1:B:1622:LYS:HG3	1:B:1623:ASP:OD1	2.07	0.54
1:B:701:MET:HE3	1:B:1420:LEU:HD21	1.89	0.54
1:B:577:GLN:HG2	1:B:578:GLN:O	2.07	0.54
1:B:581:LEU:N	1:B:790:MET:O	2.35	0.54
1:A:829:PHE:CD2	1:A:853:TYR:CE2	2.91	0.54
1:A:1566:ILE:HD12	1:A:1576:VAL:HG23	1.89	0.54
1:B:423:ARG:HG2	1:B:434:GLN:HE22	1.72	0.54
1:B:369:PHE:O	1:B:408:SER:HA	2.07	0.54
1:A:578:GLN:HB2	1:A:793:PHE:CD1	2.42	0.54
1:B:156:LEU:HD22	1:B:811:LYS:HA	1.88	0.54
1:B:360:PRO:CB	1:B:628:GLY:HA2	2.38	0.54
1:A:1287:ASP:HA	1:A:1289:LYS:HE2	1.87	0.54
1:B:74:THR:HG21	1:B:84:SER:HB2	1.88	0.54
1:B:1184:ARG:NH1	1:B:1221:GLU:OE1	2.40	0.54
1:A:904:ILE:HG23	1:A:930:VAL:O	2.07	0.54
1:A:1579:GLU:O	1:A:1580:ARG:CG	2.54	0.54
1:A:714:GLN:NE2	1:A:1424:VAL:HG13	2.21	0.54
1:A:487:TYR:HA	1:A:505:TYR:HA	1.88	0.54
1:A:429:ILE:HB	1:A:433:ARG:HB3	1.88	0.54
1:B:578:GLN:HG2	1:B:579:ILE:N	2.22	0.54
1:A:612:ARG:HG2	1:A:612:ARG:NH1	2.22	0.54
1:A:136:THR:OG1	1:A:604:ASN:HB3	2.07	0.54
1:B:105:VAL:O	1:B:120:VAL:HG23	2.06	0.54
1:A:164:ILE:HG23	1:A:207:ALA:HB2	1.90	0.54
1:A:1249:PRO:HB2	1:A:1250:PRO:HD3	1.90	0.54
1:A:861:VAL:HG12	1:A:862:ARG:N	2.23	0.54
1:A:1575:GLN:O	1:A:1578:GLN:HG2	2.07	0.54
1:B:104:PHE:HE1	1:B:656:ALA:HB2	1.72	0.54
1:A:250:LEU:N	1:A:250:LEU:CD1	2.71	0.54
1:B:336:ASP:OD1	1:B:1377:GLN:NE2	2.41	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:ASP:O	1:B:481:GLU:HG2	2.08	0.54
1:B:885:ILE:HD12	1:B:893:VAL:HG11	1.88	0.54
1:B:653:GLN:C	1:B:655:ARG:H	2.11	0.54
1:A:83:LEU:O	1:A:83:LEU:HD12	2.08	0.54
1:B:377:ASN:HB2	1:B:381:SER:HG	1.71	0.54
1:B:1545:THR:CG2	1:B:1563:ILE:HG23	2.37	0.54
1:A:1622:LYS:HG3	1:A:1623:ASP:OD1	2.08	0.54
1:B:726:CYS:O	1:B:729:ILE:HD12	2.07	0.54
1:A:541:GLN:CA	1:A:541:GLN:HE21	2.21	0.54
1:B:825:MET:CG	1:B:826:GLN:H	2.21	0.54
1:A:1078:THR:O	1:A:1082:VAL:HG23	2.08	0.54
1:B:1549:GLN:HB2	1:B:1560:ILE:HB	1.90	0.54
1:B:225:GLU:O	1:B:227:VAL:HG23	2.07	0.54
1:B:270:VAL:HG22	1:B:327:ALA:CB	2.37	0.54
1:B:593:LEU:HD12	1:B:772:THR:HG23	1.90	0.54
1:B:79:ASN:C	1:B:79:ASN:ND2	2.61	0.54
1:A:573:HIS:HB2	1:A:824:VAL:HA	1.90	0.53
1:A:592:GLY:O	1:A:805:ALA:HA	2.08	0.53
1:A:58:THR:HG22	1:A:71:ASN:ND2	2.23	0.53
1:A:1136:ARG:O	1:A:1137:GLU:HB2	2.08	0.53
1:A:504:GLN:O	1:A:504:GLN:HG3	2.09	0.53
2:B:2001:NAG:H61	2:B:2002:NAG:C7	2.38	0.53
1:A:215:GLN:OE1	1:A:215:GLN:N	2.42	0.53
1:A:80:ASN:HD22	1:A:83:LEU:H	1.56	0.53
1:A:524:ILE:HD11	1:A:556:SER:HB3	1.89	0.53
1:A:829:PHE:HB2	1:A:851:TYR:HB2	1.90	0.53
1:A:336:ASP:OD2	1:A:1377:GLN:NE2	2.42	0.53
1:B:605:LYS:HB3	1:B:608:LYS:HE2	1.89	0.53
1:A:70:SER:OG	1:A:88:ILE:HD13	2.09	0.53
1:B:610:THR:HG22	1:B:613:LYS:HD2	1.88	0.53
1:B:876:THR:HB	1:B:879:LYS:CG	2.37	0.53
1:B:45:GLU:HG2	1:B:82:TYR:HB2	1.89	0.53
1:A:906:LEU:HD23	1:A:906:LEU:N	2.23	0.53
1:B:585:ALA:HB3	1:B:777:LEU:HD13	1.89	0.53
1:A:574:ARG:HH11	1:A:918:HIS:CE1	2.26	0.53
1:A:805:ALA:O	1:A:806:VAL:HG23	2.08	0.53
1:A:559:GLY:HA3	1:A:812:LYS:HE3	1.91	0.53
1:A:674:MET:HG2	1:A:751:ASP:HA	1.91	0.53
1:A:977:THR:HA	1:A:1345:THR:HA	1.91	0.53
1:A:735:GLN:HA	1:A:738:ARG:HG2	1.88	0.53
1:B:1543:TYR:HB2	1:B:1545:THR:HG23	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:575:PRO:HB2	1:B:796:ASP:HB2	1.89	0.53
1:A:348:VAL:HG21	1:A:378:PRO:HB3	1.91	0.53
1:A:1610:TRP:O	1:A:1616:ILE:HG23	2.09	0.53
1:A:208:TYR:HB3	1:A:216:VAL:HG13	1.90	0.53
1:A:1300:PRO:HG3	1:A:1327:GLU:HB3	1.90	0.53
1:A:326:SER:HA	1:A:341:GLU:HA	1.90	0.53
1:A:1366:ILE:HD12	1:A:1385:LEU:HD13	1.91	0.53
1:A:1193:TYR:HA	1:A:1238:ALA:HB2	1.91	0.53
1:B:1039:GLU:H	1:B:1039:GLU:CD	2.12	0.53
1:A:650:LEU:HD12	1:A:651:GLU:O	2.08	0.53
1:B:977:THR:HB	1:B:1345:THR:CG2	2.39	0.53
1:A:1573:GLU:OE2	1:A:1580:ARG:NH2	2.41	0.53
1:A:138:TYR:CZ	1:A:144:VAL:HG22	2.43	0.53
1:A:161:THR:HG22	1:A:180:SER:HB2	1.90	0.53
1:B:1004:GLN:OE1	1:B:1261:TYR:HB3	2.08	0.53
1:A:323:ILE:N	1:A:345:ILE:O	2.42	0.53
1:A:118:LYS:HZ2	1:A:645:LYS:HD2	1.71	0.53
1:B:97:LYS:HA	1:B:103:LYS:NZ	2.23	0.53
1:A:346:PRO:CB	1:A:348:VAL:HG23	2.34	0.53
1:A:303:ARG:HA	1:A:306:LEU:HB2	1.90	0.53
1:B:1128:MET:HE3	1:B:1142:LEU:CA	2.39	0.53
1:A:438:THR:HG22	1:A:439:MET:H	1.73	0.53
1:B:396:GLN:CG	1:B:407:LEU:HG	2.36	0.53
1:A:272:PHE:CD1	1:A:325:VAL:CG2	2.88	0.53
1:B:672:GLN:HG2	1:B:673:LEU:N	2.23	0.53
1:B:593:LEU:HD11	1:B:774:ILE:CD1	2.35	0.53
1:B:1507:ASP:HA	1:B:1510:ARG:HB3	1.91	0.53
1:B:468:THR:HG22	1:B:518:THR:HG22	1.90	0.53
1:B:1382:SER:HB3	1:B:1462:HIS:ND1	2.24	0.53
1:A:580:THR:HA	1:A:791:ASN:HA	1.91	0.53
1:A:1472:PRO:HB3	1:A:1492:HIS:CD2	2.43	0.53
1:A:839:VAL:HA	1:A:931:VAL:O	2.09	0.53
1:B:32:ASN:ND2	1:B:643:THR:CG2	2.72	0.53
1:B:574:ARG:O	1:B:577:GLN:HB3	2.09	0.53
1:A:284:THR:O	1:A:287:LEU:HD23	2.08	0.53
1:B:374:TYR:CE2	1:B:376:THR:HG23	2.35	0.53
1:A:846:ILE:HD11	1:A:899:ILE:HD12	1.89	0.53
1:A:1010:GLY:HA3	1:A:1077:LEU:HD11	1.91	0.53
1:A:731:GLN:HG3	1:A:732:LEU:N	2.23	0.53
1:B:131:ILE:HG12	1:B:148:VAL:HG23	1.90	0.53
1:A:618:VAL:HG12	1:A:622:ASP:OD1	2.09	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:55:VAL:HG12	1:A:56:SER:H	1.74	0.53
1:A:1575:GLN:HB3	1:A:1578:GLN:HE22	1.71	0.53
1:B:574:ARG:HG3	1:B:575:PRO:HD2	1.91	0.53
1:A:85:THR:HG21	1:A:501:VAL:HG21	1.90	0.53
1:A:1217:ASN:HD22	1:A:1217:ASN:H	1.57	0.53
1:B:1285:VAL:N	1:B:1286:PRO:CD	2.69	0.53
1:B:904:ILE:CG2	1:B:905:GLY:H	2.20	0.53
1:B:1289:LYS:N	1:B:1289:LYS:HE2	2.24	0.53
1:A:1077:LEU:O	1:A:1081:VAL:HG23	2.07	0.53
1:B:283:LEU:HB2	1:B:286:SER:OG	2.08	0.53
1:A:420:ILE:HD12	1:A:439:MET:HB3	1.89	0.53
1:A:199:ASN:HD21	1:A:1056:LEU:HB3	1.73	0.53
1:A:1255:LEU:HD22	1:A:1274:VAL:HG23	1.91	0.53
1:B:838:VAL:HG21	1:B:928:LEU:HD11	1.90	0.53
1:A:1545:THR:HG22	1:A:1563:ILE:HA	1.91	0.53
1:A:1470:ILE:CG2	1:A:1499:MET:CG	2.87	0.53
1:A:834:LEU:CD2	1:A:846:ILE:HG21	2.39	0.52
1:A:399:THR:OG1	1:A:402:ASP:HB2	2.09	0.52
1:A:1517:PHE:HE2	1:A:1592:LEU:HD22	1.73	0.52
1:B:41:THR:OG1	1:B:498:LEU:HD13	2.09	0.52
1:A:272:PHE:CD1	1:A:325:VAL:HG21	2.22	0.52
1:A:454:LEU:HD12	1:A:455:HIS:H	1.74	0.52
1:A:272:PHE:HD2	1:A:286:SER:HB3	1.74	0.52
1:A:524:ILE:CG2	1:A:525:PRO:HD3	2.33	0.52
1:A:1289:LYS:HA	1:A:1312:TRP:CD1	2.44	0.52
1:B:530:VAL:HG21	1:B:642:LEU:CD1	2.32	0.52
1:B:105:VAL:O	1:B:120:VAL:N	2.40	0.52
1:A:862:ARG:NH1	1:A:884:THR:OG1	2.43	0.52
1:B:800:THR:HG23	1:B:823:THR:HG22	1.90	0.52
1:A:1227:TYR:CE2	1:A:1482:ASN:HB2	2.45	0.52
1:A:578:GLN:HB2	1:A:793:PHE:CE1	2.45	0.52
1:A:580:THR:HB	1:A:791:ASN:HD21	1.75	0.52
1:A:384:ARG:HA	1:A:400:GLN:HB2	1.91	0.52
1:B:549:VAL:HG12	1:B:550:TRP:N	2.25	0.52
1:A:285:HIS:HB2	1:A:305:VAL:HG13	1.90	0.52
1:B:229:PRO:HG3	1:B:762:ARG:HB2	1.90	0.52
1:A:421:THR:HG22	1:A:438:THR:OG1	2.10	0.52
1:A:164:ILE:HD12	1:A:164:ILE:H	1.73	0.52
1:B:976:GLU:OE2	1:B:1322:GLU:HG2	2.10	0.52
1:B:721:ALA:O	1:B:724:ASP:HB3	2.09	0.52
1:A:1039:GLU:CD	1:A:1039:GLU:H	2.10	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:GLN:HE21	1:A:816:VAL:H	1.57	0.52
1:A:852:ASN:CB	1:A:859:LEU:HD23	2.38	0.52
1:A:1362:LEU:O	1:A:1489:ARG:HD3	2.09	0.52
1:A:179:LYS:HD2	1:A:190:LEU:HD21	1.92	0.52
1:B:1570:GLY:O	1:B:1572:ASP:N	2.43	0.52
1:A:374:TYR:CD1	1:A:404:VAL:HG22	2.44	0.52
1:A:385:HIS:HA	1:A:398:LEU:O	2.10	0.52
1:B:336:ASP:CG	1:B:1377:GLN:NE2	2.62	0.52
1:A:712:ILE:HG12	1:A:1424:VAL:HG12	1.92	0.52
1:B:1614:PRO:HG2	1:B:1615:LYS:H	1.75	0.52
1:A:306:LEU:C	1:A:308:ASN:N	2.63	0.52
1:B:1041:ARG:O	1:B:1045:LEU:HD23	2.10	0.52
1:B:1041:ARG:NH1	1:B:1045:LEU:HD21	2.25	0.52
1:B:1533:LYS:HA	1:B:1536:GLU:HG3	1.91	0.52
1:A:637:PHE:HB3	1:A:642:LEU:HB2	1.92	0.52
1:A:321:LYS:HB3	1:A:347:ILE:HB	1.91	0.52
1:B:308:ASN:O	1:B:309:GLY:C	2.48	0.52
1:B:482:GLN:HG2	1:B:506:ARG:HH22	1.75	0.52
1:A:285:HIS:HB2	1:A:305:VAL:CG1	2.40	0.52
1:A:1308:HIS:ND1	1:A:1319:ARG:HD2	2.24	0.52
1:A:62:PHE:HB3	1:A:104:PHE:O	2.08	0.52
1:B:371:LEU:HD23	1:B:371:LEU:N	2.15	0.52
1:A:558:MET:HB3	1:A:812:LYS:HZ3	1.73	0.52
1:A:854:ARG:HD3	1:A:857:GLU:OE1	2.10	0.52
1:B:198:VAL:CG2	1:B:199:ASN:N	2.73	0.52
1:B:1213:ALA:HB2	1:B:1219:TRP:CZ2	2.45	0.52
1:B:762:ARG:HG2	1:B:762:ARG:HH11	1.75	0.52
1:A:931:VAL:HG21	1:A:1438:ASN:HB3	1.92	0.52
1:B:977:THR:HA	1:B:1345:THR:HA	1.92	0.52
1:A:673:LEU:CD1	1:A:674:MET:H	2.23	0.52
1:B:843:GLN:OE1	1:B:1502:LYS:HA	2.10	0.52
1:A:140:PRO:HD3	1:A:224:LYS:O	2.10	0.52
1:A:1017:MET:O	1:A:1021:VAL:HG23	2.10	0.52
1:A:637:PHE:CG	1:A:650:LEU:HD22	2.45	0.51
1:B:158:VAL:HG12	1:B:160:GLN:HG3	1.92	0.51
1:B:852:ASN:CG	1:B:887:ILE:CG2	2.79	0.51
1:A:399:THR:O	1:A:403:GLY:HA2	2.09	0.51
1:B:871:PHE:CZ	1:B:909:VAL:HG22	2.45	0.51
1:B:445:ASN:HB2	1:B:632:ASN:ND2	2.25	0.51
1:A:30:THR:HG22	1:A:42:VAL:HG22	1.91	0.51
1:A:562:VAL:HG12	1:A:563:VAL:N	2.25	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:794:LEU:HD13	1:B:824:VAL:HG22	1.93	0.51
1:B:1280:GLN:HG2	1:B:1283:LYS:HD2	1.90	0.51
1:B:642:LEU:O	1:B:643:THR:HG23	2.09	0.51
1:B:843:GLN:CG	1:B:900:VAL:HG22	2.40	0.51
1:B:358:LYS:HD2	1:B:550:TRP:CH2	2.44	0.51
1:A:176:ARG:HE	1:A:1093:ALA:CB	2.23	0.51
1:A:933:GLU:HG3	1:A:1556:PHE:HE1	1.76	0.51
1:A:800:THR:HA	1:A:823:THR:HA	1.93	0.51
1:B:234:GLN:NE2	1:B:257:ARG:NH2	2.49	0.51
1:B:1498:GLY:O	1:B:1501:SER:N	2.43	0.51
1:B:849:ILE:HA	1:B:893:VAL:O	2.09	0.51
1:A:971:PRO:HD3	1:A:1350:LYS:HE2	1.92	0.51
1:B:808:LEU:O	1:B:808:LEU:HD23	2.10	0.51
1:B:591:VAL:HG13	1:B:807:SER:HB2	1.93	0.51
1:B:670:SER:O	1:B:672:GLN:N	2.44	0.51
1:B:375:VAL:HG12	1:B:376:THR:N	2.26	0.51
1:B:1289:LYS:H	1:B:1289:LYS:HE2	1.75	0.51
1:B:876:THR:HG22	1:B:878:LYS:H	1.76	0.51
1:B:276:ASP:CB	1:B:279:ARG:HB2	2.34	0.51
1:A:362:PHE:CE1	1:A:631:ARG:HD2	2.46	0.51
1:B:492:ILE:HD11	1:B:529:LEU:HD12	1.93	0.51
1:B:885:ILE:CD1	1:B:893:VAL:HG11	2.41	0.51
1:A:390:THR:HG22	1:A:422:VAL:HG13	1.92	0.51
1:A:204:LYS:HA	1:A:220:GLU:HA	1.93	0.51
1:B:119:VAL:HB	1:B:654:GLN:HG3	1.93	0.51
1:A:827:ASP:CB	1:A:854:ARG:HH21	2.22	0.51
1:A:334:GLY:O	1:A:335:SER:CB	2.57	0.51
1:B:1061:LYS:CE	1:B:1061:LYS:H	2.23	0.51
1:B:30:THR:N	1:B:644:LEU:HD21	2.26	0.51
1:A:494:ASN:O	1:A:495:LYS:HB2	2.10	0.51
1:B:350:SER:OG	1:B:435:ALA:HB2	2.11	0.51
1:B:762:ARG:NH1	1:B:764:GLN:O	2.43	0.51
1:A:1147:LEU:HD11	1:A:1168:ILE:HG23	1.93	0.51
1:A:1288:HIS:HB3	1:A:1312:TRP:CE3	2.45	0.51
1:B:421:THR:HG22	1:B:438:THR:CB	2.32	0.51
1:A:1406:MET:SD	1:A:1412:PRO:HD3	2.51	0.51
1:B:132:GLN:O	1:B:146:TYR:HA	2.10	0.51
1:A:1161:VAL:HG12	1:A:1163:SER:H	1.75	0.51
1:B:1366:ILE:HD12	1:B:1385:LEU:HD13	1.92	0.51
1:B:271:ILE:HG23	1:B:287:LEU:HD22	1.92	0.51
1:B:985:PRO:HB3	1:B:1256:ASN:ND2	2.26	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1184:ARG:HH12	1:B:1221:GLU:CD	2.14	0.51
1:B:175:LYS:HD2	1:B:192:TRP:CD1	2.46	0.51
1:A:80:ASN:HD22	1:A:82:TYR:N	2.09	0.51
1:A:839:VAL:HG21	1:A:1471:GLN:HG3	1.93	0.51
1:A:645:LYS:HG2	1:A:646:THR:H	1.75	0.51
1:B:852:ASN:ND2	1:B:888:PRO:O	2.40	0.51
1:A:284:THR:O	1:A:287:LEU:CD2	2.59	0.51
1:B:623:ILE:HG23	1:B:625:CYS:H	1.76	0.51
1:B:365:PRO:HG2	1:B:453:TYR:CE1	2.46	0.51
1:A:1041:ARG:HH11	1:A:1045:LEU:HD11	1.74	0.51
1:B:276:ASP:HB2	1:B:279:ARG:CB	2.33	0.51
1:A:456:LEU:HD21	1:A:473:PHE:CD1	2.46	0.51
1:A:633:TYR:CD1	1:A:634:ALA:N	2.79	0.51
1:B:852:ASN:HB2	1:B:859:LEU:CD2	2.41	0.51
1:A:290:VAL:CG1	1:A:298:GLU:H	2.18	0.51
1:A:384:ARG:O	1:A:386:ILE:HG13	2.11	0.51
1:B:905:GLY:C	1:B:906:LEU:HD23	2.30	0.51
1:A:442:LEU:HB2	1:A:631:ARG:NH2	2.26	0.51
1:B:1606:SER:O	1:B:1609:LEU:HB2	2.10	0.51
1:B:732:LEU:HD13	1:B:732:LEU:O	2.10	0.51
1:B:798:ILE:CG2	1:B:829:PHE:HZ	2.24	0.51
1:B:801:TRP:O	1:B:802:GLU:HG2	2.11	0.51
1:B:638:THR:CG2	1:B:652:THR:HB	2.41	0.51
1:A:472:ASN:HA	1:A:514:VAL:HG22	1.93	0.51
1:B:658:PRO:HG2	1:B:659:GLN:H	1.75	0.51
1:B:461:VAL:O	1:B:463:LEU:HG	2.11	0.50
1:B:1415:GLU:OE1	1:B:1415:GLU:CA	2.50	0.50
1:B:699:ASN:O	1:B:702:LYS:HD2	2.11	0.50
1:B:805:ALA:O	1:B:806:VAL:HG23	2.11	0.50
1:A:377:ASN:ND2	1:A:383:ALA:HA	2.24	0.50
1:B:848:ALA:HB3	1:B:895:VAL:HG22	1.93	0.50
1:A:971:PRO:HD3	1:A:1350:LYS:CE	2.42	0.50
1:A:982:GLN:O	1:A:1339:GLY:HA3	2.11	0.50
1:B:573:HIS:CE1	1:B:579:ILE:CD1	2.94	0.50
1:B:590:ARG:O	1:B:807:SER:OG	2.22	0.50
1:A:1353:GLY:O	1:A:1354:LYS:HB2	2.12	0.50
1:B:1526:THR:O	1:B:1530:ARG:HG2	2.11	0.50
1:A:1505:HIS:O	1:A:1506:LYS:C	2.49	0.50
1:A:458:VAL:CG2	1:A:471:VAL:HG13	2.42	0.50
1:B:374:TYR:HE2	1:B:376:THR:CG2	2.21	0.50
1:B:138:TYR:CZ	1:B:144:VAL:HG22	2.47	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:275:GLN:HB3	1:B:322:SER:O	2.11	0.50
1:A:268:ALA:CB	1:A:329:VAL:HG22	2.41	0.50
1:A:1534:ALA:O	1:A:1539:VAL:HG21	2.11	0.50
1:A:274:VAL:HB	1:A:281:ILE:CG2	2.42	0.50
1:A:62:PHE:N	1:A:63:PRO:HD2	2.27	0.50
1:A:574:ARG:NH1	1:A:918:HIS:ND1	2.60	0.50
1:B:887:ILE:HD12	1:B:887:ILE:N	2.26	0.50
1:A:1288:HIS:O	1:A:1312:TRP:HB2	2.12	0.50
1:A:454:LEU:HD23	1:A:546:ALA:HA	1.93	0.50
1:A:854:ARG:NH1	1:A:859:LEU:CD1	2.74	0.50
1:B:147:ARG:HG3	1:B:771:TRP:CH2	2.47	0.50
1:B:1259:ARG:HH11	1:B:1340:THR:HG21	1.76	0.50
1:B:553:VAL:HG23	1:B:554:LYS:N	2.26	0.50
1:A:315:ALA:O	1:A:319:VAL:HG23	2.11	0.50
1:A:323:ILE:CD1	1:A:347:ILE:HD11	2.39	0.50
1:A:793:PHE:O	1:A:794:LEU:O	2.29	0.50
1:A:454:LEU:HD12	1:A:455:HIS:N	2.27	0.50
1:A:507:GLU:HB3	1:A:510:GLN:HE22	1.76	0.50
1:A:1156:ILE:N	1:A:1156:ILE:HD12	2.24	0.50
1:B:1249:PRO:HB2	1:B:1250:PRO:HD3	1.93	0.50
1:A:358:LYS:HB3	1:A:550:TRP:CZ3	2.47	0.50
1:B:866:LEU:HD21	1:B:912:LYS:NZ	2.26	0.50
1:A:512:LEU:O	1:A:512:LEU:HG	2.12	0.50
1:A:77:ASN:O	1:A:80:ASN:ND2	2.43	0.50
1:B:62:PHE:CG	1:B:63:PRO:HD3	2.46	0.50
1:A:852:ASN:HB3	1:A:887:ILE:HG22	1.92	0.50
1:A:374:TYR:HD1	1:A:404:VAL:HG22	1.76	0.50
1:B:373:VAL:O	1:B:373:VAL:HG12	2.11	0.50
1:A:423:ARG:HD2	1:A:425:LYS:NZ	2.26	0.50
1:B:268:ALA:CB	1:B:329:VAL:HG22	2.41	0.50
1:A:262:GLU:OE2	1:A:891:SER:HA	2.11	0.50
1:B:1552:LEU:HD12	1:B:1552:LEU:H	1.77	0.50
1:B:386:ILE:HB	1:B:398:LEU:HB3	1.94	0.50
1:A:798:ILE:HG21	1:A:829:PHE:HZ	1.76	0.50
1:A:593:LEU:HD11	1:A:774:ILE:HD11	1.93	0.50
1:B:274:VAL:HG12	1:B:275:GLN:N	2.27	0.50
1:A:1540:ASP:OD2	1:A:1571:SER:HB3	2.12	0.50
1:A:236:GLU:OE1	1:A:237:PRO:HD2	2.12	0.50
1:A:251:LYS:CD	1:A:300:ILE:HG12	2.41	0.50
1:A:794:LEU:HD21	1:A:824:VAL:HG21	1.94	0.50
1:B:371:LEU:CD2	1:B:371:LEU:H	2.15	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:290:VAL:HG11	1:A:298:GLU:O	2.11	0.50
1:A:1576:VAL:HG12	1:A:1577:LYS:N	2.27	0.50
1:B:1003:ILE:HG22	1:B:1005:THR:H	1.76	0.50
1:B:597:ASP:OD2	1:B:599:GLY:N	2.45	0.50
1:B:800:THR:HA	1:B:823:THR:HA	1.93	0.50
1:B:1359:LYS:HB3	1:B:1485:GLU:HB3	1.93	0.50
1:A:55:VAL:HG21	1:A:76:LEU:HG	1.94	0.49
1:B:227:VAL:CG1	1:B:762:ARG:HA	2.42	0.49
1:B:580:THR:HA	1:B:790:MET:O	2.11	0.49
1:A:1237:LEU:CD2	1:A:1277:ALA:HA	2.40	0.49
1:A:719:VAL:HG12	1:A:723:LEU:CD2	2.42	0.49
1:A:331:LEU:HD13	1:A:1377:GLN:HE21	1.76	0.49
1:B:1600:TYR:HA	1:B:1629:TRP:H	1.78	0.49
1:B:585:ALA:HB3	1:B:777:LEU:CD1	2.42	0.49
1:A:1592:LEU:HB3	1:A:1594:LEU:HG	1.93	0.49
1:B:1552:LEU:HD23	1:B:1589:ARG:NE	2.27	0.49
1:A:670:SER:N	1:A:673:LEU:HD21	2.27	0.49
1:B:1377:GLN:H	1:B:1377:GLN:CD	2.15	0.49
1:A:362:PHE:HD1	1:A:630:GLY:C	2.15	0.49
1:B:1289:LYS:H	1:B:1289:LYS:CE	2.24	0.49
1:B:1358:LYS:O	1:B:1359:LYS:HB2	2.10	0.49
1:A:485:ILE:HG13	1:A:506:ARG:HH21	1.76	0.49
1:B:117:GLU:O	1:B:118:LYS:CD	2.60	0.49
1:B:156:LEU:O	1:B:158:VAL:HG23	2.13	0.49
1:A:557:CYS:SG	1:A:611:GLN:HG3	2.52	0.49
1:A:117:GLU:O	1:A:118:LYS:HD2	2.12	0.49
1:B:992:ASP:HB2	1:B:998:ARG:CB	2.37	0.49
1:A:1573:GLU:OE2	1:A:1580:ARG:NE	2.45	0.49
1:A:712:ILE:CG2	1:A:719:VAL:HG22	2.42	0.49
1:B:31:PRO:HA	1:B:641:GLY:O	2.12	0.49
1:B:561:LEU:HD12	1:B:815:CYS:HB3	1.95	0.49
1:B:1588:CYS:O	1:B:1592:LEU:HB2	2.13	0.49
1:B:1609:LEU:HG	1:B:1616:ILE:HG21	1.95	0.49
1:B:1156:ILE:HD12	1:B:1156:ILE:N	2.26	0.49
1:B:765:PHE:O	1:B:766:PRO:C	2.51	0.49
1:A:421:THR:HG22	1:A:438:THR:HG23	1.94	0.49
1:B:439:MET:HG2	1:B:440:GLN:H	1.77	0.49
1:B:838:VAL:HA	1:B:1408:THR:HG21	1.93	0.49
1:B:1060:GLN:HB3	1:B:1061:LYS:HE3	1.93	0.49
1:B:862:ARG:HB2	1:B:916:TYR:HE1	1.77	0.49
1:A:1391:TYR:CD1	1:A:1397:ALA:HB2	2.46	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1363:ARG:NH2	1:B:1454:GLU:OE1	2.45	0.49
1:A:229:PRO:O	1:A:259:LEU:HD11	2.13	0.49
1:B:325:VAL:O	1:B:342:ARG:N	2.44	0.49
1:B:32:ASN:N	1:B:641:GLY:O	2.46	0.49
1:B:895:VAL:O	1:B:895:VAL:CG2	2.58	0.49
1:B:528:ARG:HA	1:B:549:VAL:O	2.13	0.49
1:B:830:ILE:HG13	1:B:850:LEU:CD2	2.43	0.49
1:A:1022:ILE:HD12	1:A:1276:GLN:HA	1.95	0.49
1:B:260:TYR:HE1	1:B:798:ILE:HG12	1.77	0.49
1:A:1111:GLN:HB2	1:A:1117:PHE:CE2	2.47	0.49
1:B:302:LYS:HD2	1:B:304:GLN:OE1	2.12	0.49
1:A:574:ARG:O	1:A:575:PRO:C	2.49	0.49
1:B:1541:TYR:O	1:B:1603:TRP:HA	2.12	0.49
1:B:459:PRO:HD2	1:B:469:LEU:HD11	1.94	0.49
1:B:904:ILE:HG23	1:B:930:VAL:O	2.12	0.49
1:B:848:ALA:HB3	1:B:895:VAL:HG21	1.94	0.49
1:B:798:ILE:HG21	1:B:829:PHE:CZ	2.46	0.49
1:B:1531:LEU:HD22	1:B:1654:MET:SD	2.53	0.49
1:A:642:LEU:O	1:A:643:THR:HG23	2.11	0.49
1:A:904:ILE:CD1	1:A:932:PRO:HB3	2.43	0.49
1:A:116:VAL:HG13	1:A:645:LYS:NZ	2.28	0.49
1:B:104:PHE:CZ	1:B:656:ALA:HB2	2.48	0.49
1:A:798:ILE:HG12	1:A:829:PHE:HZ	1.78	0.49
1:A:852:ASN:CG	1:A:859:LEU:CD2	2.81	0.49
1:A:561:LEU:CD1	1:A:807:SER:CB	2.90	0.49
1:A:864:GLU:OE2	1:A:880:ARG:HD3	2.12	0.49
1:B:319:VAL:C	1:B:321:LYS:N	2.66	0.49
1:B:250:LEU:O	1:B:251:LYS:C	2.50	0.49
1:B:1217:ASN:HD21	1:B:1218:ARG:CD	2.22	0.49
1:A:375:VAL:HB	1:A:398:LEU:CD2	2.43	0.49
1:A:863:VAL:HG12	1:A:913:ALA:HB2	1.95	0.49
1:B:342:ARG:HH21	1:B:345:ILE:HG12	1.78	0.49
1:B:359:THR:CG2	1:B:360:PRO:CD	2.88	0.49
1:B:852:ASN:CG	1:B:887:ILE:HG22	2.33	0.49
1:B:110:THR:HB	1:B:115:GLN:CB	2.37	0.49
1:B:580:THR:HB	1:B:791:ASN:ND2	2.28	0.49
1:A:121:LEU:HD23	1:A:122:ILE:H	1.78	0.49
1:B:1003:ILE:CD1	1:B:1268:THR:HA	2.43	0.49
1:A:1496:GLU:HG2	1:B:1204:ASP:OD1	2.13	0.49
1:A:934:GLY:HA3	1:A:970:VAL:HG21	1.93	0.49
1:B:1351:LEU:HD23	1:B:1351:LEU:N	2.28	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1024:VAL:HG13	1:B:1033:TRP:HH2	1.77	0.49
1:A:118:LYS:HA	1:A:118:LYS:CE	2.34	0.48
1:B:1576:VAL:HG12	1:B:1577:LYS:H	1.78	0.48
1:A:355:HIS:HB3	1:A:437:ARG:NH1	2.28	0.48
1:B:303:ARG:CA	1:B:306:LEU:HB2	2.43	0.48
1:A:159:GLY:HA3	1:A:182:GLN:HG3	1.94	0.48
1:A:1045:LEU:O	1:A:1049:ARG:HG3	2.13	0.48
1:A:864:GLU:OE2	1:A:880:ARG:HB2	2.13	0.48
1:B:1541:TYR:HB2	1:B:1543:TYR:CE1	2.48	0.48
1:B:633:TYR:OH	1:B:650:LEU:HA	2.12	0.48
1:B:110:THR:CB	1:B:115:GLN:HB3	2.38	0.48
1:B:436:THR:CG2	1:B:437:ARG:N	2.77	0.48
1:A:1555:ASP:N	1:A:1586:ILE:HD11	2.28	0.48
1:B:159:GLY:HA2	1:B:181:SER:OG	2.13	0.48
1:A:950:HIS:O	1:A:951:LEU:HD23	2.13	0.48
1:A:60:HIS:CG	1:A:65:LYS:HB2	2.48	0.48
1:A:986:VAL:HG22	1:A:990:THR:HG23	1.95	0.48
1:A:529:LEU:O	1:A:548:SER:HA	2.14	0.48
1:A:634:ALA:O	1:A:638:THR:HG23	2.13	0.48
1:B:1575:GLN:HB3	1:B:1578:GLN:NE2	2.28	0.48
1:B:566:GLY:HA3	1:B:580:THR:CG2	2.43	0.48
1:B:915:VAL:CG2	1:B:920:ILE:HB	2.42	0.48
1:B:623:ILE:HG12	1:B:624:GLY:H	1.78	0.48
1:B:729:ILE:O	1:B:733:ARG:HB2	2.13	0.48
1:A:1530:ARG:HG3	1:A:1650:PHE:HZ	1.79	0.48
1:A:358:LYS:HB2	1:A:372:MET:CE	2.44	0.48
1:B:350:SER:HA	1:B:433:ARG:HB2	1.95	0.48
1:A:490:TYR:HB3	1:A:531:ALA:HB2	1.95	0.48
1:B:1605:VAL:HG12	1:B:1606:SER:N	2.26	0.48
1:B:990:THR:O	1:B:994:ILE:HG13	2.13	0.48
1:B:1128:MET:HE3	1:B:1142:LEU:CB	2.44	0.48
1:B:1279:ALA:O	1:B:1283:LYS:HB2	2.13	0.48
1:A:1099:LEU:O	1:A:1102:THR:HB	2.13	0.48
1:B:464:LYS:HZ2	1:B:554:LYS:HE2	1.78	0.48
1:A:72:GLU:HG3	1:A:73:ASN:N	2.27	0.48
1:A:281:ILE:HD13	1:A:310:VAL:CG2	2.28	0.48
1:B:62:PHE:N	1:B:63:PRO:CD	2.76	0.48
1:B:611:GLN:O	1:B:614:ILE:HG12	2.13	0.48
1:A:751:ASP:C	1:A:753:ILE:H	2.17	0.48
1:A:673:LEU:HD22	1:A:751:ASP:OD2	2.13	0.48
1:B:44:LEU:HD11	1:B:86:VAL:CG2	2.39	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:910:GLU:OE1	1:A:925:LYS:HD3	2.13	0.48
1:A:1156:ILE:CD1	1:A:1156:ILE:H	2.25	0.48
1:B:994:ILE:HG22	1:B:1040:LYS:HE2	1.95	0.48
1:B:610:THR:CG2	1:B:613:LYS:HG3	2.43	0.48
1:A:843:GLN:CG	1:A:900:VAL:HG22	2.43	0.48
1:A:1328:ARG:NH2	1:A:1330:THR:HG23	2.28	0.48
1:B:396:GLN:HA	1:B:396:GLN:OE1	2.13	0.48
1:A:644:LEU:H	1:A:650:LEU:CD2	2.26	0.48
1:B:120:VAL:HG12	1:B:121:LEU:H	1.77	0.48
1:B:79:ASN:C	1:B:79:ASN:HD22	2.16	0.48
1:B:1157:CYS:HB2	1:B:1164:LEU:HD12	1.96	0.48
1:A:149:PHE:CD1	1:A:187:ILE:HG12	2.47	0.48
1:B:1542:VAL:HA	1:B:1602:VAL:O	2.14	0.48
1:B:712:ILE:HG21	1:B:719:VAL:HG22	1.96	0.48
1:B:130:PHE:HE1	1:B:617:VAL:HG21	1.79	0.48
1:B:940:THR:HA	1:B:1344:VAL:HG22	1.95	0.48
1:B:1213:ALA:HB2	1:B:1219:TRP:CE2	2.49	0.48
1:A:389:VAL:HG12	1:A:390:THR:N	2.27	0.48
1:B:1024:VAL:HG11	1:B:1091:LEU:HD13	1.96	0.48
1:A:1244:ASP:O	1:A:1246:ASP:N	2.47	0.48
1:B:1509:CYS:O	1:B:1513:GLU:HG2	2.13	0.48
1:A:388:VAL:HG21	1:A:405:ALA:HB2	1.94	0.48
1:A:318:LEU:HD13	1:A:321:LYS:HZ2	1.79	0.48
1:B:362:PHE:HD1	1:B:630:GLY:CA	2.27	0.48
1:B:834:LEU:CD2	1:B:846:ILE:HG21	2.43	0.48
1:A:129:LEU:HB2	1:A:217:PHE:CD2	2.49	0.48
1:B:1227:TYR:CE2	1:B:1482:ASN:HB2	2.49	0.48
1:A:515:LEU:HD12	1:A:516:PRO:HD2	1.96	0.48
1:A:187:ILE:H	1:A:808:LEU:HD13	1.78	0.48
1:A:398:LEU:HG	1:A:399:THR:O	2.14	0.48
1:B:843:GLN:O	1:B:1467:VAL:HG13	2.13	0.48
1:B:481:GLU:OE2	1:B:538:ALA:HB2	2.14	0.48
1:B:863:VAL:HG12	1:B:913:ALA:CB	2.43	0.48
1:A:574:ARG:O	1:A:577:GLN:CB	2.62	0.48
1:B:1566:ILE:HD11	1:B:1576:VAL:HG22	1.93	0.48
1:A:382:PRO:CB	1:A:403:GLY:HA3	2.40	0.48
1:B:1204:ASP:HA	1:B:1207:THR:HG23	1.96	0.48
1:B:487:TYR:HB3	1:B:505:TYR:HD1	1.77	0.48
1:B:468:THR:CG2	1:B:518:THR:HG22	2.44	0.48
1:A:534:THR:O	1:A:534:THR:HG22	2.13	0.48
1:A:672:GLN:O	1:A:675:GLU:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:617:VAL:O	1:A:621:ALA:HB3	2.14	0.47
1:A:977:THR:HB	1:A:1345:THR:CB	2.42	0.47
1:A:1018:THR:O	1:A:1022:ILE:HG23	2.14	0.47
1:A:519:ILE:HG22	1:A:519:ILE:O	2.13	0.47
1:A:319:VAL:C	1:A:321:LYS:H	2.18	0.47
1:B:359:THR:HG23	1:B:371:LEU:HA	1.97	0.47
1:A:271:ILE:CD1	1:A:753:ILE:HD13	2.43	0.47
1:B:271:ILE:CG2	1:B:287:LEU:HD22	2.44	0.47
1:A:402:ASP:HB3	1:A:404:VAL:HG23	1.95	0.47
1:A:1275:PHE:O	1:A:1276:GLN:C	2.53	0.47
1:B:423:ARG:HG2	1:B:434:GLN:NE2	2.30	0.47
1:B:493:MET:HB2	1:B:528:ARG:HB3	1.96	0.47
1:B:138:TYR:CE2	1:B:144:VAL:HG22	2.49	0.47
1:B:731:GLN:HG3	1:B:732:LEU:N	2.28	0.47
1:A:41:THR:HA	1:A:87:THR:HA	1.95	0.47
1:B:818:ASP:OD1	1:B:819:PRO:HD2	2.13	0.47
1:B:1369:ALA:HB1	1:B:1370:PRO:HD2	1.96	0.47
1:B:368:PRO:HA	1:B:409:ILE:O	2.14	0.47
1:B:566:GLY:CA	1:B:580:THR:HG23	2.44	0.47
1:A:798:ILE:HG12	1:A:829:PHE:CZ	2.49	0.47
1:B:1217:ASN:H	1:B:1217:ASN:HD22	1.62	0.47
1:A:1203:GLY:O	1:A:1207:THR:HG22	2.14	0.47
1:B:330:ILE:O	1:B:330:ILE:HG13	2.14	0.47
1:A:158:VAL:HG12	1:A:160:GLN:HG3	1.95	0.47
1:B:840:ARG:HH22	1:B:972:ASP:HB3	1.79	0.47
1:A:173:PRO:HG3	1:A:176:ARG:NH2	2.28	0.47
2:A:2001:NAG:H61	2:A:2002:NAG:C7	2.44	0.47
1:A:1548:ILE:HG22	1:A:1560:ILE:O	2.14	0.47
1:B:88:ILE:HG22	1:B:89:LYS:N	2.29	0.47
1:B:1404:ILE:HG23	1:B:1475:VAL:HG22	1.96	0.47
1:A:1285:VAL:N	1:A:1286:PRO:CD	2.78	0.47
1:A:270:VAL:HA	1:A:327:ALA:HB2	1.95	0.47
1:B:520:THR:HG22	1:B:521:SER:N	2.28	0.47
1:B:36:LEU:HA	1:B:90:ILE:O	2.15	0.47
1:B:99:ASP:HB2	1:B:100:LYS:NZ	2.30	0.47
1:B:361:LYS:HB3	1:B:361:LYS:NZ	2.30	0.47
1:B:305:VAL:O	1:B:305:VAL:HG12	2.14	0.47
1:B:238:GLU:HB3	1:B:251:LYS:O	2.14	0.47
1:B:362:PHE:HD1	1:B:630:GLY:HA2	1.79	0.47
1:B:60:HIS:CD2	1:B:65:LYS:HD3	2.49	0.47
1:B:1468:GLY:HA3	1:B:1501:SER:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:800:THR:CG2	1:B:823:THR:HG22	2.44	0.47
1:A:944:ARG:HG3	1:A:944:ARG:HH11	1.79	0.47
1:A:944:ARG:NH1	1:A:959:GLU:HB3	2.28	0.47
1:A:44:LEU:CD1	1:A:55:VAL:HG11	2.25	0.47
1:A:650:LEU:HD12	1:A:651:GLU:C	2.35	0.47
1:A:104:PHE:CE1	1:A:656:ALA:HB2	2.48	0.47
1:A:354:ILE:C	1:A:354:ILE:HD12	2.34	0.47
1:A:712:ILE:HD11	1:A:722:PHE:CG	2.50	0.47
1:B:528:ARG:HH22	1:B:623:ILE:HD11	1.79	0.47
1:B:528:ARG:CZ	1:B:623:ILE:HD11	2.45	0.47
1:A:601:PHE:CD2	1:A:802:GLU:HG3	2.46	0.47
1:B:1546:ARG:HD2	1:B:1599:HIS:CE1	2.50	0.47
1:A:1136:ARG:HH11	1:A:1183:ARG:NH1	2.12	0.47
1:A:426:LYS:HB3	1:A:429:ILE:HG12	1.97	0.47
1:A:324:TYR:HB2	1:A:342:ARG:O	2.15	0.47
1:B:98:SER:HB2	1:B:100:LYS:HE2	1.96	0.47
1:B:51:GLY:O	1:B:78:SER:HB3	2.13	0.47
1:A:699:ASN:O	1:A:702:LYS:N	2.42	0.47
1:A:528:ARG:HH12	1:A:624:GLY:HA3	1.80	0.47
1:A:780:ALA:HB3	1:A:786:SER:HA	1.97	0.47
1:B:464:LYS:HB3	1:B:465:PRO:HD2	1.95	0.47
1:A:56:SER:HA	1:A:73:ASN:HB2	1.96	0.47
1:B:272:PHE:HZ	1:B:299:ALA:O	1.97	0.47
1:A:577:GLN:HG2	1:A:578:GLN:O	2.15	0.47
1:B:104:PHE:CD1	1:B:121:LEU:HG	2.50	0.47
1:A:348:VAL:HG12	1:A:350:SER:C	2.35	0.47
1:B:451:ASN:HD22	1:B:476:ARG:HH12	1.63	0.47
1:A:561:LEU:HD13	1:A:807:SER:CB	2.45	0.47
1:A:168:THR:O	1:A:170:ASP:N	2.43	0.47
1:B:1362:LEU:O	1:B:1489:ARG:HD3	2.15	0.47
1:B:1109:GLU:O	1:B:1110:LYS:HD3	2.14	0.47
1:B:1318:LEU:O	1:B:1319:ARG:HG2	2.15	0.47
1:A:799:THR:OG1	1:A:800:THR:N	2.48	0.47
1:B:1545:THR:HB	1:B:1561:MET:CG	2.44	0.47
1:B:904:ILE:HG22	1:B:905:GLY:H	1.75	0.47
1:B:431:GLU:O	1:B:434:GLN:HG2	2.14	0.47
1:A:998:ARG:HH11	1:A:998:ARG:HG3	1.80	0.47
1:A:1401:ILE:HD12	1:A:1480:TYR:HD1	1.79	0.47
1:A:1587:LYS:HG3	1:A:1588:CYS:N	2.30	0.47
1:A:459:PRO:HD2	1:A:469:LEU:HD11	1.95	0.47
1:B:119:VAL:HB	1:B:654:GLN:HE21	1.80	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1502:LYS:CE	1:B:1590:GLU:HG3	2.43	0.47
1:A:227:VAL:HG12	1:A:229:PRO:HD3	1.96	0.47
1:B:1131:GLY:O	1:B:1134:ASP:HB2	2.15	0.47
1:B:1347:TYR:CE1	1:B:1349:ALA:HB2	2.50	0.47
1:B:118:LYS:HD3	1:B:645:LYS:CE	2.29	0.46
1:B:852:ASN:C	1:B:854:ARG:H	2.18	0.46
1:B:673:LEU:HD21	1:B:751:ASP:CG	2.36	0.46
1:A:242:TYR:CE1	1:A:246:ASP:OD1	2.68	0.46
1:B:128:TYR:CB	1:B:151:VAL:HG12	2.44	0.46
1:A:423:ARG:HA	1:A:435:ALA:O	2.14	0.46
1:A:1502:LYS:O	1:A:1504:CYS:N	2.48	0.46
1:A:978:LYS:HD2	2:A:2001:NAG:H62	1.97	0.46
1:B:866:LEU:HD21	1:B:912:LYS:HZ3	1.80	0.46
1:A:251:LYS:NZ	1:A:300:ILE:HG12	2.30	0.46
1:A:1030:THR:CB	1:A:1032:GLN:HE21	2.28	0.46
1:B:797:SER:O	1:B:799:THR:HG22	2.15	0.46
1:A:1269:GLN:O	1:A:1273:MET:HB2	2.15	0.46
1:A:689:ARG:O	1:A:693:GLU:HG3	2.15	0.46
1:A:1601:LEU:HD12	1:A:1627:GLU:HG3	1.98	0.46
1:B:62:PHE:HB3	1:B:104:PHE:HB2	1.94	0.46
1:B:63:PRO:CG	1:B:64:ALA:H	2.25	0.46
1:A:242:TYR:CD1	1:A:250:LEU:CD1	2.94	0.46
1:A:859:LEU:H	1:A:859:LEU:CD2	2.21	0.46
1:B:264:VAL:CG1	1:B:265:ASP:N	2.78	0.46
1:A:445:ASN:O	1:A:632:ASN:OD1	2.32	0.46
1:B:1288:HIS:H	1:B:1289:LYS:HZ1	1.62	0.46
1:A:1092:ILE:HG22	1:A:1093:ALA:N	2.30	0.46
1:A:1253:ARG:O	1:A:1256:ASN:HB3	2.14	0.46
1:A:452:ASN:O	1:A:545:VAL:HG21	2.15	0.46
1:A:80:ASN:HB2	1:A:83:LEU:HG	1.98	0.46
1:B:250:LEU:HD12	1:B:301:LEU:HB3	1.96	0.46
1:B:1566:ILE:HD13	1:B:1574:VAL:HG12	1.97	0.46
1:A:1576:VAL:CG1	1:A:1577:LYS:N	2.78	0.46
1:B:446:THR:OG1	1:B:450:SER:HB3	2.15	0.46
1:A:537:ASN:HD22	1:A:538:ALA:H	1.63	0.46
1:A:1470:ILE:CG2	1:A:1499:MET:HG2	2.42	0.46
1:A:1415:GLU:HA	1:A:1415:GLU:OE1	2.15	0.46
1:B:468:THR:HG22	1:B:518:THR:CG2	2.45	0.46
1:A:156:LEU:HD22	1:A:811:LYS:HA	1.96	0.46
1:B:1078:THR:O	1:B:1082:VAL:HG23	2.16	0.46
1:B:719:VAL:HG12	1:B:723:LEU:HD23	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:909:VAL:O	1:A:925:LYS:HA	2.16	0.46
1:B:326:SER:HA	1:B:341:GLU:HA	1.97	0.46
1:B:183:ASN:HB3	1:B:184:GLN:NE2	2.30	0.46
1:A:110:THR:O	1:A:110:THR:OG1	2.33	0.46
1:A:74:THR:HG22	1:A:86:VAL:CG2	2.44	0.46
1:A:644:LEU:H	1:A:650:LEU:HD21	1.80	0.46
1:B:1564:GLU:HG3	1:B:1599:HIS:CD2	2.51	0.46
1:A:151:VAL:H	1:A:209:TYR:HH	1.62	0.46
1:A:60:HIS:CD2	1:A:65:LYS:HD2	2.50	0.46
1:A:475:LEU:HB2	1:A:488:TYR:OH	2.16	0.46
1:A:54:GLN:HA	1:A:75:GLN:HB3	1.97	0.46
1:A:769:TRP:CH2	1:A:794:LEU:HD12	2.50	0.46
1:A:931:VAL:HG13	1:A:932:PRO:HD2	1.96	0.46
1:B:701:MET:O	1:B:702:LYS:CB	2.60	0.46
1:B:833:ARG:O	1:B:846:ILE:HB	2.15	0.46
1:A:355:HIS:N	1:A:355:HIS:ND1	2.64	0.46
1:A:1003:ILE:HD13	1:A:1015:ILE:HD12	1.98	0.46
1:B:147:ARG:HG3	1:B:771:TRP:CZ2	2.51	0.46
1:A:1574:VAL:N	1:A:1575:GLN:OE1	2.48	0.46
1:A:633:TYR:N	1:A:633:TYR:CD1	2.82	0.46
1:A:314:ARG:NE	1:A:314:ARG:CA	2.74	0.46
1:B:386:ILE:HB	1:B:398:LEU:CD2	2.45	0.46
1:B:475:LEU:HG	1:B:476:ARG:N	2.31	0.46
1:A:631:ARG:O	1:A:632:ASN:HB2	2.16	0.46
1:B:1077:LEU:O	1:B:1081:VAL:HG23	2.15	0.46
1:A:50:GLN:HG3	1:A:51:GLY:H	1.81	0.46
1:B:282:SER:O	1:B:284:THR:N	2.49	0.46
1:A:756:GLU:O	1:A:758:ASP:N	2.48	0.46
1:B:485:ILE:HD12	1:B:485:ILE:H	1.80	0.46
1:B:396:GLN:HG3	1:B:397:SER:H	1.81	0.46
1:B:348:VAL:HG12	1:B:349:THR:H	1.81	0.46
1:A:1437:SER:O	1:A:1439:LYS:N	2.49	0.46
1:A:610:THR:HG23	1:A:613:LYS:N	2.29	0.46
1:B:271:ILE:HG23	1:B:287:LEU:CD2	2.46	0.46
1:A:97:LYS:HE2	1:A:124:LEU:CD2	2.45	0.46
1:A:1363:ARG:NH2	1:A:1454:GLU:OE1	2.48	0.46
1:B:1086:ALA:HB2	1:B:1153:ALA:HB2	1.97	0.46
1:A:1563:ILE:CD1	1:A:1578:GLN:O	2.63	0.46
1:A:575:PRO:C	1:A:577:GLN:N	2.70	0.46
1:A:491:MET:HG3	1:A:501:VAL:CG1	2.43	0.46
1:A:827:ASP:HB2	1:A:854:ARG:NH2	2.26	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1288:HIS:HB3	1:B:1312:TRP:CE3	2.51	0.46
1:A:308:ASN:N	1:A:308:ASN:HD22	2.11	0.46
1:B:1351:LEU:HD13	1:B:1490:PHE:CD2	2.51	0.46
1:B:707:ARG:NE	1:B:710:GLN:OE1	2.49	0.46
1:B:1147:LEU:HD11	1:B:1168:ILE:HG23	1.98	0.46
1:B:1288:HIS:N	1:B:1289:LYS:HE2	2.31	0.46
1:B:1156:ILE:CD1	1:B:1156:ILE:H	2.28	0.46
1:B:260:TYR:CE1	1:B:798:ILE:HG12	2.51	0.46
1:A:825:MET:CG	1:A:826:GLN:N	2.79	0.46
1:A:960:GLU:HG2	1:A:1330:THR:HG22	1.98	0.46
1:B:961:VAL:HG11	1:B:1343:VAL:HG21	1.98	0.46
1:B:1659:CYS:C	1:B:1661:ASN:H	2.18	0.46
1:B:654:GLN:O	1:B:654:GLN:HG2	2.16	0.45
1:A:59:VAL:HG11	1:A:90:ILE:HG23	1.98	0.45
1:A:164:ILE:HD13	1:A:190:LEU:HD11	1.98	0.45
1:A:280:ARG:HG2	1:A:324:TYR:CE2	2.51	0.45
1:A:468:THR:HA	1:A:517:LEU:O	2.16	0.45
1:A:202:VAL:HG12	1:A:202:VAL:O	2.16	0.45
1:A:867:TYR:HB2	1:A:875:ALA:O	2.17	0.45
1:B:117:GLU:O	1:B:645:LYS:HE3	2.16	0.45
1:B:1563:ILE:HD12	1:B:1578:GLN:O	2.15	0.45
1:A:124:LEU:N	1:A:124:LEU:HD23	2.31	0.45
1:A:346:PRO:HG3	1:A:378:PRO:HB2	1.97	0.45
1:B:1587:LYS:HG3	1:B:1588:CYS:SG	2.57	0.45
1:A:1267:SER:OG	1:A:1268:THR:N	2.48	0.45
1:B:1289:LYS:HG2	1:B:1290:GLU:OE2	2.16	0.45
1:A:59:VAL:HG11	1:A:90:ILE:CG2	2.46	0.45
1:A:90:ILE:HA	1:A:91:PRO:HD2	1.41	0.45
1:B:260:TYR:OH	1:B:798:ILE:HD11	2.16	0.45
1:B:860:LYS:HB3	1:B:916:TYR:HB2	1.96	0.45
1:A:76:LEU:HD22	1:A:82:TYR:O	2.15	0.45
1:B:430:PRO:C	1:B:432:GLY:N	2.69	0.45
1:A:272:PHE:CD2	1:A:286:SER:HB3	2.51	0.45
1:A:318:LEU:HD22	1:A:321:LYS:HZ2	1.81	0.45
1:A:989:MET:HB3	1:A:1275:PHE:CE1	2.51	0.45
1:B:562:VAL:CG1	1:B:563:VAL:N	2.79	0.45
1:A:1100:CYS:SG	1:A:1160:GLN:HG3	2.56	0.45
1:A:1097:LYS:HE2	1:A:1101:GLU:CG	2.45	0.45
1:B:1558:GLU:HG2	1:B:1583:ILE:HD12	1.98	0.45
1:B:1551:LYS:NZ	1:B:1581:LYS:HE2	2.30	0.45
1:A:80:ASN:ND2	1:A:82:TYR:N	2.64	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:852:ASN:ND2	1:A:859:LEU:HD23	2.31	0.45
1:A:382:PRO:HB3	1:A:403:GLY:CA	2.40	0.45
1:B:1401:ILE:HD12	1:B:1480:TYR:CD1	2.44	0.45
1:A:843:GLN:O	1:A:1467:VAL:HG13	2.17	0.45
1:B:181:SER:HB3	1:B:188:LEU:HD21	1.97	0.45
1:A:1530:ARG:HH12	1:A:1647:LEU:HD21	1.81	0.45
1:A:578:GLN:HG2	1:A:579:ILE:N	2.30	0.45
1:B:156:LEU:HA	1:B:157:PRO:HD2	1.71	0.45
1:B:32:ASN:CB	1:B:641:GLY:HA2	2.46	0.45
1:A:374:TYR:HA	1:A:404:VAL:HG13	1.99	0.45
1:B:1600:TYR:CE2	1:B:1628:LEU:HG	2.52	0.45
1:B:1405:SER:HA	1:B:1441:THR:HA	1.98	0.45
1:A:527:PHE:CE1	1:A:551:VAL:HB	2.52	0.45
1:A:1140:VAL:HG21	1:A:1182:LEU:HD21	1.98	0.45
1:B:534:THR:HG22	1:B:542:ARG:HG2	1.98	0.45
1:A:205:ILE:HG22	1:A:206:LYS:H	1.82	0.45
1:B:1258:GLN:HE21	1:B:1258:GLN:HB3	1.49	0.45
1:B:464:LYS:NZ	1:B:554:LYS:HE2	2.32	0.45
1:A:701:MET:HE2	1:A:1458:SER:HB3	1.98	0.45
1:A:116:VAL:CG1	1:A:645:LYS:HB3	2.46	0.45
1:A:375:VAL:HB	1:A:398:LEU:HD22	1.99	0.45
1:B:57:VAL:CG2	1:B:86:VAL:HG21	2.45	0.45
1:A:507:GLU:HB3	1:A:510:GLN:HE21	1.80	0.45
1:B:492:ILE:HG21	1:B:499:LEU:HD23	1.98	0.45
1:B:600:VAL:CG2	1:B:765:PHE:CG	2.99	0.45
1:A:562:VAL:CG1	1:A:563:VAL:N	2.79	0.45
1:B:1558:GLU:HG2	1:B:1583:ILE:CD1	2.47	0.45
1:A:1254:TRP:CZ2	1:A:1258:GLN:HG3	2.51	0.45
1:A:1382:SER:CB	1:A:1462:HIS:ND1	2.79	0.45
1:A:582:LYS:HD2	1:A:789:LEU:HD21	1.99	0.45
1:B:117:GLU:O	1:B:645:LYS:CE	2.65	0.45
1:A:244:ILE:CD1	1:A:349:THR:CG2	2.95	0.45
1:A:314:ARG:HE	1:A:315:ALA:H	1.64	0.45
1:B:754:ILE:HG23	1:B:755:PRO:HD2	1.97	0.45
1:A:384:ARG:O	1:A:398:LEU:HD23	2.17	0.45
1:B:1501:SER:O	1:B:1503:LEU:N	2.50	0.45
1:B:330:ILE:HD11	1:B:750:ASP:CG	2.35	0.45
1:A:863:VAL:HG12	1:A:913:ALA:CB	2.47	0.45
1:B:1288:HIS:O	1:B:1312:TRP:HB2	2.17	0.45
1:B:1544:LYS:HB3	1:B:1565:ASN:HB3	1.98	0.45
1:A:1012:GLN:HG2	1:A:1480:TYR:CE2	2.52	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1298:GLN:HG2	1:B:1305:ALA:CB	2.46	0.45
1:A:1608:ASP:HB2	1:A:1619:ILE:O	2.16	0.45
1:B:1375:LYS:HD3	1:B:1375:LYS:O	2.17	0.45
1:A:244:ILE:CD1	1:A:349:THR:HG21	2.46	0.45
1:A:904:ILE:HD13	1:A:932:PRO:HB3	1.99	0.45
1:A:611:GLN:O	1:A:614:ILE:HG12	2.17	0.45
1:B:360:PRO:HB3	1:B:628:GLY:HA2	1.98	0.45
1:A:718:CYS:SG	1:A:1424:VAL:HG11	2.56	0.45
1:A:600:VAL:HG22	1:A:765:PHE:CB	2.47	0.45
1:B:480:GLY:O	1:B:482:GLN:N	2.49	0.45
1:A:154:LYS:HB2	1:A:156:LEU:HG	1.99	0.45
1:A:931:VAL:CG1	1:A:1438:ASN:HB3	2.47	0.45
1:B:458:VAL:CG1	1:B:469:LEU:HD21	2.46	0.45
1:B:840:ARG:CZ	1:B:972:ASP:HB3	2.46	0.45
1:A:487:TYR:HB3	1:A:505:TYR:CD1	2.52	0.45
1:A:1570:GLY:O	1:A:1571:SER:C	2.56	0.45
1:B:1134:ASP:C	1:B:1136:ARG:H	2.19	0.45
1:B:933:GLU:CD	1:B:933:GLU:H	2.20	0.45
1:A:566:GLY:HA3	1:A:580:THR:CG2	2.47	0.45
1:B:852:ASN:CB	1:B:859:LEU:HD23	2.46	0.45
1:A:368:PRO:CA	1:A:410:ASN:HA	2.40	0.45
1:B:712:ILE:HG23	1:B:1424:VAL:CG1	2.47	0.45
1:B:356:PHE:HE1	1:B:437:ARG:HG3	1.82	0.45
1:A:1531:LEU:HG	1:A:1650:PHE:CZ	2.52	0.45
1:B:242:TYR:CE1	1:B:246:ASP:HB2	2.51	0.45
1:B:173:PRO:HG3	1:B:176:ARG:NH2	2.32	0.45
1:B:1190:ILE:HD13	1:B:1190:ILE:O	2.17	0.45
1:A:633:TYR:N	1:A:633:TYR:HD1	2.15	0.44
1:B:573:HIS:ND1	1:B:579:ILE:CD1	2.73	0.44
1:B:834:LEU:HD22	1:B:846:ILE:HG21	1.97	0.44
1:A:887:ILE:CD1	1:A:887:ILE:N	2.79	0.44
1:A:386:ILE:O	1:A:398:LEU:N	2.50	0.44
1:B:919:PHE:O	1:B:920:ILE:HD13	2.17	0.44
1:A:910:GLU:CB	1:A:925:LYS:HB3	2.47	0.44
1:A:134:ASP:OD2	1:A:145:LEU:HD12	2.17	0.44
1:B:1064:ALA:HB1	1:B:1073:PRO:HB3	1.99	0.44
1:A:1585:HIS:HD2	1:A:1587:LYS:H	1.65	0.44
1:B:1092:ILE:HG22	1:B:1093:ALA:N	2.32	0.44
1:A:74:THR:OG1	1:A:75:GLN:N	2.50	0.44
1:B:1415:GLU:O	1:B:1419:THR:HG23	2.17	0.44
1:A:673:LEU:HD13	1:A:674:MET:HG3	1.98	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1508:THR:O	1:A:1511:CYS:HB3	2.18	0.44
1:A:147:ARG:NE	1:A:189:THR:HG22	2.29	0.44
1:A:769:TRP:CD1	1:A:769:TRP:N	2.85	0.44
1:B:156:LEU:CD2	1:B:811:LYS:HA	2.47	0.44
1:A:904:ILE:CG2	1:A:905:GLY:N	2.66	0.44
1:B:1498:GLY:C	1:B:1500:LEU:N	2.69	0.44
1:A:134:ASP:OD1	1:A:135:LYS:HG2	2.17	0.44
1:A:561:LEU:CD1	1:A:807:SER:HB3	2.47	0.44
1:A:1256:ASN:ND2	1:A:1259:ARG:HH12	2.16	0.44
1:B:1362:LEU:CD1	1:B:1489:ARG:HB2	2.48	0.44
1:A:1600:TYR:CD2	1:A:1628:LEU:HA	2.52	0.44
1:B:1488:ILE:O	1:B:1488:ILE:HG23	2.17	0.44
1:B:1554:ASP:O	1:B:1586:ILE:HD11	2.18	0.44
1:B:386:ILE:HB	1:B:398:LEU:HD23	1.99	0.44
1:A:355:HIS:HB3	1:A:437:ARG:CZ	2.47	0.44
1:A:366:ALA:HB2	1:A:413:ASN:ND2	2.32	0.44
1:B:520:THR:CG2	1:B:521:SER:H	2.22	0.44
1:B:829:PHE:HB2	1:B:851:TYR:HD2	1.83	0.44
1:B:1646:ASP:HA	1:B:1649:ASN:ND2	2.32	0.44
1:B:146:TYR:CD1	1:B:205:ILE:HD13	2.52	0.44
1:B:861:VAL:HG12	1:B:862:ARG:N	2.33	0.44
1:A:597:ASP:OD2	1:A:599:GLY:N	2.50	0.44
1:B:1019:PRO:HD3	1:B:1272:PHE:CE1	2.52	0.44
1:A:1103:VAL:O	1:A:1107:ILE:HG12	2.17	0.44
1:B:430:PRO:O	1:B:432:GLY:N	2.49	0.44
1:A:63:PRO:HG2	1:A:64:ALA:H	1.82	0.44
1:A:645:LYS:O	1:A:646:THR:CB	2.63	0.44
1:A:269:PHE:O	1:A:327:ALA:HB1	2.17	0.44
1:B:451:ASN:HB2	1:B:478:ASP:OD1	2.17	0.44
1:A:1010:GLY:CA	1:A:1067:ALA:HA	2.46	0.44
1:B:283:LEU:O	1:B:286:SER:HB2	2.18	0.44
1:B:334:GLY:O	1:B:335:SER:CB	2.66	0.44
1:B:227:VAL:HG11	1:B:761:SER:O	2.18	0.44
1:B:97:LYS:HA	1:B:103:LYS:HZ2	1.82	0.44
1:B:387:PRO:HG3	1:B:425:LYS:O	2.17	0.44
1:B:1289:LYS:H	1:B:1289:LYS:CD	2.30	0.44
1:A:765:PHE:O	1:A:766:PRO:C	2.54	0.44
1:A:561:LEU:CD1	1:A:807:SER:HB2	2.47	0.44
1:B:610:THR:HG22	1:B:613:LYS:CD	2.46	0.44
1:A:438:THR:HG22	1:A:439:MET:N	2.32	0.44
1:B:526:SER:HA	1:B:552:ASP:HA	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:62:PHE:CE2	1:A:103:LYS:HD3	2.52	0.44
1:B:398:LEU:HD11	1:B:403:GLY:C	2.36	0.44
1:A:362:PHE:CZ	1:A:631:ARG:HD2	2.52	0.44
1:B:492:ILE:HD13	1:B:492:ILE:HA	1.89	0.44
1:A:482:GLN:O	1:A:484:LYS:N	2.51	0.44
1:B:281:ILE:O	1:B:283:LEU:N	2.51	0.44
1:A:781:ASP:HB3	1:A:785:ILE:O	2.18	0.44
1:B:1434:ASN:HB3	1:B:1441:THR:OG1	2.18	0.44
1:A:1041:ARG:NH1	1:A:1045:LEU:HD11	2.33	0.44
1:B:346:PRO:HG3	1:B:378:PRO:HB2	2.00	0.44
1:B:359:THR:HG23	1:B:372:MET:H	1.83	0.44
1:A:106:THR:HG22	1:A:119:VAL:CG2	2.44	0.44
1:B:1585:HIS:HD2	1:B:1587:LYS:H	1.66	0.44
1:B:446:THR:HG21	1:B:450:SER:C	2.38	0.44
1:B:848:ALA:O	1:B:895:VAL:HG22	2.18	0.44
1:B:830:ILE:O	1:B:830:ILE:HG23	2.17	0.44
1:A:1549:GLN:CB	1:A:1560:ILE:HD12	2.48	0.44
1:A:1510:ARG:HA	1:A:1513:GLU:HG3	2.00	0.44
1:B:870:ALA:HB1	1:B:907:HIS:CD2	2.52	0.44
1:A:370:ASP:HB3	1:A:460:ARG:HE	1.83	0.44
1:A:1105:TRP:CD1	1:A:1109:GLU:HG3	2.53	0.44
1:A:754:ILE:N	1:A:755:PRO:CD	2.81	0.44
1:B:461:VAL:O	1:B:462:GLU:C	2.56	0.44
1:A:1545:THR:HG23	1:A:1563:ILE:HG23	1.98	0.44
1:B:859:LEU:CD2	1:B:859:LEU:N	2.80	0.44
1:A:491:MET:N	1:A:491:MET:SD	2.90	0.44
1:A:753:ILE:HG23	1:A:753:ILE:O	2.18	0.44
1:A:31:PRO:HG2	1:A:34:LEU:HD21	2.00	0.44
1:A:695:GLY:HA2	1:A:722:PHE:CE2	2.53	0.44
1:B:354:ILE:HD11	1:B:437:ARG:HB3	1.99	0.44
1:B:794:LEU:HD13	1:B:824:VAL:CG2	2.47	0.44
1:A:943:VAL:O	1:A:944:ARG:HD3	2.18	0.44
1:A:1453:VAL:HG23	1:A:1454:GLU:N	2.31	0.44
1:B:214:GLN:O	1:B:215:GLN:C	2.57	0.44
1:A:1286:PRO:HB2	1:A:1289:LYS:HZ3	1.82	0.43
1:B:1566:ILE:CG2	1:B:1568:LYS:O	2.66	0.43
1:B:1003:ILE:HG12	1:B:1015:ILE:HD12	1.99	0.43
1:A:47:HIS:HD2	1:A:534:THR:OG1	2.01	0.43
1:A:1461:VAL:O	1:A:1461:VAL:HG23	2.18	0.43
1:A:577:GLN:O	1:A:794:LEU:CB	2.66	0.43
1:A:577:GLN:HG2	1:A:578:GLN:N	2.32	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:62:PHE:HE2	1:B:103:LYS:HG2	1.83	0.43
1:B:561:LEU:CD1	1:B:815:CYS:HB3	2.48	0.43
1:A:270:VAL:O	1:A:287:LEU:CA	2.65	0.43
1:B:271:ILE:HD12	1:B:755:PRO:HG3	1.99	0.43
1:A:1003:ILE:HG23	1:A:1005:THR:H	1.83	0.43
1:A:1500:LEU:C	1:A:1500:LEU:HD12	2.38	0.43
1:B:1494:ASP:C	1:B:1496:GLU:N	2.71	0.43
1:B:1136:ARG:C	1:B:1138:LYS:H	2.22	0.43
1:B:326:SER:HB2	1:B:340:ALA:O	2.18	0.43
1:A:370:ASP:CB	1:A:460:ARG:HE	2.32	0.43
1:B:415:ARG:O	1:B:443:PRO:HG3	2.18	0.43
1:B:263:GLN:HE21	1:B:295:GLY:HA3	1.83	0.43
1:A:318:LEU:CD1	1:A:321:LYS:HZ2	2.31	0.43
1:B:377:ASN:HB3	1:B:378:PRO:HD2	2.00	0.43
1:A:270:VAL:HG13	1:A:327:ALA:HB2	1.99	0.43
1:B:450:SER:OG	1:B:451:ASN:N	2.50	0.43
1:A:364:LYS:HA	1:A:365:PRO:HD2	1.68	0.43
1:B:1609:LEU:HG	1:B:1616:ILE:CG2	2.48	0.43
1:B:145:LEU:HA	1:B:145:LEU:HD23	1.84	0.43
1:A:762:ARG:HG3	1:A:765:PHE:CZ	2.54	0.43
1:B:354:ILE:HD12	1:B:354:ILE:C	2.39	0.43
1:A:1213:ALA:HB2	1:A:1219:TRP:CZ2	2.53	0.43
1:B:1128:MET:HE3	1:B:1142:LEU:HA	2.00	0.43
1:B:306:LEU:HA	1:B:306:LEU:HD23	1.67	0.43
1:A:137:ILE:HG23	1:A:224:LYS:HG3	1.99	0.43
1:B:1184:ARG:HG2	1:B:1184:ARG:HH11	1.83	0.43
1:A:35:ARG:NH1	1:A:153:HIS:HB3	2.33	0.43
1:B:169:PRO:HD3	1:B:203:TRP:CE2	2.53	0.43
1:A:130:PHE:HE1	1:A:617:VAL:HG21	1.84	0.43
1:B:1568:LYS:HG3	1:B:1569:SER:H	1.82	0.43
1:A:96:LEU:O	1:A:97:LYS:C	2.56	0.43
1:A:379:ASP:N	1:A:379:ASP:OD1	2.52	0.43
1:A:31:PRO:HA	1:A:641:GLY:O	2.18	0.43
1:B:264:VAL:HG12	1:B:265:ASP:N	2.32	0.43
1:A:148:VAL:O	1:A:188:LEU:HB2	2.18	0.43
1:A:1470:ILE:HG21	1:A:1499:MET:CG	2.46	0.43
1:A:396:GLN:HG3	1:A:397:SER:N	2.32	0.43
1:B:533:TYR:CE2	1:B:545:VAL:HB	2.53	0.43
1:A:420:ILE:HD12	1:A:420:ILE:O	2.18	0.43
1:A:421:THR:CG2	1:A:438:THR:HG23	2.49	0.43
1:B:258:PHE:C	1:B:260:TYR:H	2.21	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1193:TYR:CE1	1:B:1237:LEU:HB3	2.52	0.43
1:B:1319:ARG:HG2	1:B:1319:ARG:HH11	1.82	0.43
1:A:102:HIS:ND1	1:A:102:HIS:N	2.67	0.43
1:A:968:ASP:OD2	1:A:1349:ALA:HB1	2.18	0.43
1:B:524:ILE:HG21	1:B:558:MET:HG2	1.99	0.43
1:A:359:THR:HG23	1:A:371:LEU:CA	2.44	0.43
1:A:574:ARG:O	1:A:577:GLN:HB3	2.18	0.43
1:B:561:LEU:HA	1:B:584:GLU:O	2.19	0.43
1:A:407:LEU:CD2	1:A:408:SER:H	2.20	0.43
1:A:270:VAL:HG21	1:A:299:ALA:CB	2.47	0.43
1:B:537:ASN:ND2	1:B:538:ALA:N	2.60	0.43
1:A:832:LEU:HD21	1:A:909:VAL:CG1	2.49	0.43
1:A:481:GLU:O	1:A:482:GLN:C	2.57	0.43
1:A:100:LYS:HD3	1:A:100:LYS:N	2.34	0.43
1:B:1405:SER:HB3	1:B:1441:THR:HG22	1.98	0.43
1:B:657:ASP:HB3	1:B:659:GLN:O	2.18	0.43
1:B:989:MET:O	1:B:993:ALA:HB2	2.19	0.43
1:B:1633:GLU:HG3	1:B:1634:GLU:HG3	2.01	0.43
1:B:420:ILE:O	1:B:420:ILE:HD12	2.19	0.43
1:A:244:ILE:HD12	1:A:349:THR:HG21	2.00	0.43
1:A:1493:PRO:HB2	1:A:1494:ASP:H	1.61	0.43
1:B:701:MET:HG2	1:B:701:MET:H	1.44	0.43
1:B:642:LEU:C	1:B:643:THR:CG2	2.87	0.43
1:B:532:TYR:HA	1:B:545:VAL:O	2.18	0.43
1:A:487:TYR:CD1	1:A:503:ARG:HD2	2.54	0.43
1:A:1259:ARG:HH11	1:A:1340:THR:HG21	1.82	0.43
1:B:365:PRO:HG2	1:B:453:TYR:HE1	1.84	0.43
1:B:326:SER:HB3	1:B:341:GLU:CB	2.49	0.43
1:A:870:ALA:HB1	1:A:907:HIS:CD2	2.54	0.43
1:B:465:PRO:O	1:B:519:ILE:O	2.37	0.43
1:B:362:PHE:CE2	1:B:631:ARG:NE	2.86	0.43
1:B:1542:VAL:HG22	1:B:1603:TRP:HB2	2.01	0.43
1:B:1563:ILE:H	1:B:1563:ILE:CD1	2.20	0.43
1:A:346:PRO:CG	1:A:348:VAL:HG23	2.49	0.43
1:A:364:LYS:HB2	1:A:364:LYS:HE3	1.83	0.43
1:B:850:LEU:CD1	1:B:885:ILE:HD11	2.48	0.43
1:B:415:ARG:HB3	1:B:443:PRO:HG3	2.01	0.43
1:A:1186:TYR:C	1:A:1186:TYR:CD2	2.92	0.43
1:B:447:GLN:HG3	1:B:447:GLN:O	2.19	0.43
1:A:653:GLN:HB3	1:A:655:ARG:CG	2.48	0.43
1:B:574:ARG:O	1:B:577:GLN:CB	2.67	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1605:VAL:HB	1:B:1608:ASP:OD1	2.19	0.43
1:A:1470:ILE:CG2	1:A:1499:MET:HG3	2.49	0.43
1:B:172:ILE:HD11	1:B:1098:ASP:OD1	2.19	0.43
1:A:1344:VAL:HG12	1:A:1345:THR:N	2.34	0.43
1:A:729:ILE:HD12	1:A:730:THR:N	2.33	0.43
1:B:1405:SER:HA	1:B:1441:THR:HG22	2.00	0.43
1:A:274:VAL:HG11	1:A:321:LYS:HZ3	1.84	0.43
1:B:630:GLY:CA	1:B:636:VAL:HG22	2.49	0.43
1:A:458:VAL:HG11	1:A:469:LEU:HD21	2.01	0.43
1:B:1545:THR:CB	1:B:1561:MET:HG2	2.48	0.43
1:B:701:MET:CE	1:B:1458:SER:H	2.32	0.43
1:B:977:THR:HB	1:B:1345:THR:HG22	2.01	0.43
1:B:458:VAL:HG23	1:B:471:VAL:HG13	2.01	0.43
1:B:197:LEU:HD21	1:B:1058:PHE:CZ	2.54	0.43
1:B:533:TYR:CZ	1:B:545:VAL:HB	2.53	0.43
1:B:785:ILE:HG22	1:B:787:THR:CG2	2.49	0.43
1:B:1190:ILE:CG2	1:B:1191:ALA:N	2.82	0.43
1:A:274:VAL:HG11	1:A:321:LYS:NZ	2.34	0.43
1:B:251:LYS:HG3	1:B:300:ILE:HG23	1.99	0.43
1:B:852:ASN:HB3	1:B:887:ILE:HG21	2.01	0.43
1:A:559:GLY:N	1:A:812:LYS:NZ	2.66	0.43
1:B:1233:SER:OG	1:B:1274:VAL:HA	2.19	0.43
1:A:59:VAL:HG23	1:A:70:SER:OG	2.18	0.43
1:A:998:ARG:NH1	1:A:998:ARG:HG3	2.34	0.43
1:B:1410:PHE:CE1	1:B:1463:GLN:HB2	2.54	0.43
1:B:460:ARG:HH21	1:B:462:GLU:CB	2.32	0.42
1:A:644:LEU:N	1:A:650:LEU:HD21	2.34	0.42
1:B:345:ILE:O	1:B:345:ILE:HG22	2.19	0.42
1:A:674:MET:O	1:A:678:MET:HG3	2.19	0.42
1:A:377:ASN:O	1:A:379:ASP:N	2.52	0.42
1:A:413:ASN:O	1:A:414:LYS:HG2	2.19	0.42
1:B:612:ARG:HH11	1:B:612:ARG:HG2	1.84	0.42
1:A:59:VAL:HB	1:A:69:LEU:HB2	2.00	0.42
1:A:1554:ASP:HA	1:A:1586:ILE:HD11	2.01	0.42
1:A:1012:GLN:HG3	1:A:1012:GLN:H	1.49	0.42
1:A:172:ILE:HG21	1:A:1056:LEU:HD21	2.00	0.42
1:B:1275:PHE:CD2	1:B:1275:PHE:C	2.92	0.42
1:A:352:TYR:HE2	1:A:429:ILE:HD13	1.82	0.42
1:A:1042:GLN:HA	1:A:1045:LEU:HD12	2.00	0.42
1:A:1026:TYR:CE1	1:A:1030:THR:HG21	2.54	0.42
1:A:1351:LEU:HD13	1:A:1490:PHE:CD2	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:53:ILE:HB	1:A:76:LEU:HB2	2.01	0.42
1:A:62:PHE:CG	1:A:63:PRO:HD3	2.54	0.42
1:B:398:LEU:HG	1:B:399:THR:O	2.19	0.42
1:A:558:MET:CB	1:A:812:LYS:NZ	2.82	0.42
1:B:712:ILE:HD11	1:B:722:PHE:CG	2.53	0.42
1:A:137:ILE:HA	1:A:222:GLU:O	2.19	0.42
1:A:429:ILE:HG22	1:A:433:ARG:HD2	2.01	0.42
1:A:944:ARG:NH1	1:A:944:ARG:HG3	2.33	0.42
1:B:910:GLU:HG3	1:B:925:LYS:HB3	2.00	0.42
1:A:570:GLU:HG2	1:A:571:LYS:H	1.82	0.42
1:B:323:ILE:CG2	1:B:324:TYR:N	2.80	0.42
1:A:391:GLN:OE1	1:A:420:ILE:HA	2.18	0.42
1:A:44:LEU:O	1:A:45:GLU:HG3	2.19	0.42
1:B:243:TYR:HH	1:B:245:ASP:HB2	1.78	0.42
1:A:574:ARG:NH1	1:A:918:HIS:CE1	2.87	0.42
1:B:359:THR:O	1:B:627:PRO:HG2	2.19	0.42
1:A:812:LYS:C	1:A:812:LYS:HD3	2.38	0.42
1:A:1362:LEU:CD1	1:A:1489:ARG:HB2	2.50	0.42
1:A:303:ARG:O	1:A:307:LEU:HG	2.18	0.42
1:A:1541:TYR:O	1:A:1603:TRP:HA	2.19	0.42
1:A:1184:ARG:O	1:A:1188:VAL:HG23	2.19	0.42
1:B:166:ILE:HD12	1:B:175:LYS:HD3	2.02	0.42
1:A:990:THR:HG21	1:A:1026:TYR:CD2	2.54	0.42
1:A:778:LYS:C	1:A:780:ALA:H	2.22	0.42
1:B:1396:ASP:HA	1:B:1451:HIS:HB3	2.00	0.42
1:A:55:VAL:CG2	1:A:76:LEU:HG	2.49	0.42
1:A:530:VAL:HG12	1:A:548:SER:HB2	2.01	0.42
1:A:637:PHE:CE1	1:A:644:LEU:CD1	3.00	0.42
1:A:615:TRP:CE3	1:A:615:TRP:HA	2.54	0.42
1:A:673:LEU:CD1	1:A:674:MET:HG3	2.49	0.42
1:A:854:ARG:NH1	1:A:859:LEU:HD11	2.33	0.42
1:A:354:ILE:CG2	1:A:375:VAL:HG22	2.48	0.42
1:B:134:ASP:HB3	1:B:138:TYR:OH	2.19	0.42
1:B:830:ILE:HD11	1:B:911:VAL:HG12	2.02	0.42
1:B:514:VAL:CG1	1:B:515:LEU:N	2.83	0.42
1:B:355:HIS:N	1:B:355:HIS:ND1	2.66	0.42
1:B:149:PHE:CD1	1:B:187:ILE:HG12	2.50	0.42
1:A:163:PHE:HD2	1:A:208:TYR:CE2	2.37	0.42
1:A:358:LYS:HB2	1:A:372:MET:HE2	2.00	0.42
1:A:143:THR:HB	1:A:193:ASN:ND2	2.34	0.42
1:A:881:HIS:ND1	1:A:881:HIS:O	2.52	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:556:SER:OG	1:A:557:CYS:N	2.51	0.42
1:B:271:ILE:CD1	1:B:755:PRO:HG3	2.50	0.42
1:B:528:ARG:HH12	1:B:623:ILE:HG12	1.85	0.42
1:A:244:ILE:HD11	1:A:319:VAL:CG2	2.26	0.42
1:A:918:HIS:ND1	1:A:918:HIS:O	2.53	0.42
1:B:846:ILE:CD1	1:B:899:ILE:HD12	2.40	0.42
1:B:148:VAL:CG1	1:B:188:LEU:HD12	2.50	0.42
1:A:1116:ILE:HG23	1:A:1139:ASP:HB3	2.01	0.42
1:B:1505:HIS:ND1	1:B:1506:LYS:N	2.57	0.42
1:B:1499:MET:C	1:B:1501:SER:H	2.18	0.42
1:A:876:THR:CG2	1:A:877:ALA:H	2.32	0.42
1:B:504:GLN:HG3	1:B:515:LEU:HD13	2.02	0.42
1:A:1499:MET:C	1:A:1501:SER:H	2.23	0.42
1:A:1265:TYR:CD2	1:A:1274:VAL:HG11	2.55	0.42
1:B:53:ILE:HG22	1:B:111:PHE:HB2	2.01	0.42
1:A:1314:SER:HB2	1:A:1319:ARG:HH22	1.85	0.42
1:B:1650:PHE:O	1:B:1654:MET:HB2	2.20	0.42
1:A:1600:TYR:HE2	1:A:1628:LEU:HG	1.84	0.42
1:B:680:LYS:HD2	1:B:683:GLN:NE2	2.35	0.42
1:A:175:LYS:HD2	1:A:192:TRP:CD1	2.54	0.42
1:A:310:VAL:HG12	1:A:311:GLN:N	2.35	0.42
1:A:578:GLN:OE1	1:A:791:ASN:HB3	2.20	0.42
1:B:888:PRO:CB	1:B:891:SER:HB2	2.43	0.42
1:A:1435:ARG:HG3	1:A:1435:ARG:H	1.36	0.42
1:B:269:PHE:CE1	1:B:289:ARG:CD	3.02	0.42
1:B:287:LEU:HD12	1:B:674:MET:HE2	2.02	0.42
1:A:124:LEU:H	1:A:124:LEU:HD23	1.84	0.42
1:B:1469:LEU:N	1:B:1499:MET:O	2.51	0.42
1:B:1590:GLU:C	1:B:1592:LEU:H	2.23	0.42
1:B:931:VAL:CG1	1:B:932:PRO:HD2	2.49	0.42
1:B:612:ARG:NH1	1:B:616:ASP:OD2	2.53	0.42
1:A:1503:LEU:HD12	1:A:1503:LEU:HA	1.75	0.42
1:B:707:ARG:HD2	1:B:707:ARG:HA	1.93	0.42
1:B:363:PHE:CD1	1:B:364:LYS:N	2.88	0.42
1:B:611:GLN:HG2	1:B:816:VAL:CB	2.46	0.42
1:B:74:THR:HG23	1:B:84:SER:HB2	2.01	0.42
1:A:1204:ASP:HA	1:A:1207:THR:HG22	2.02	0.42
1:B:197:LEU:O	1:B:198:VAL:HB	2.19	0.42
1:B:445:ASN:H	1:B:632:ASN:ND2	2.17	0.42
1:A:215:GLN:O	1:A:215:GLN:HG2	2.20	0.42
1:A:1539:VAL:HG12	1:A:1540:ASP:H	1.85	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:699:ASN:O	1:A:702:LYS:HE2	2.20	0.42
1:A:468:THR:CG2	1:A:518:THR:HG22	2.50	0.42
1:A:570:GLU:C	1:A:572:HIS:H	2.23	0.42
1:A:1527:LEU:HG	1:A:1646:ASP:CB	2.50	0.42
1:A:981:LEU:HD13	1:A:1295:VAL:HG11	2.01	0.42
1:B:1214:LYS:HD3	1:B:1214:LYS:HA	1.94	0.42
1:A:290:VAL:CG2	1:A:298:GLU:O	2.68	0.41
1:A:36:LEU:HD12	1:A:124:LEU:CB	2.40	0.41
1:B:1607:SER:C	1:B:1609:LEU:H	2.22	0.41
1:A:765:PHE:N	1:A:765:PHE:CD1	2.88	0.41
1:A:1265:TYR:CE2	1:A:1274:VAL:HG21	2.55	0.41
1:A:236:GLU:OE2	1:A:342:ARG:HD3	2.20	0.41
1:A:229:PRO:O	1:A:259:LEU:CD1	2.68	0.41
1:B:413:ASN:O	1:B:414:LYS:HG3	2.20	0.41
1:B:1107:ILE:HD12	1:B:1167:SER:CB	2.49	0.41
1:A:283:LEU:O	1:A:286:SER:HB2	2.20	0.41
1:B:629:SER:O	1:B:636:VAL:HG22	2.19	0.41
1:B:852:ASN:CG	1:B:887:ILE:HG21	2.40	0.41
1:A:270:VAL:O	1:A:287:LEU:CB	2.68	0.41
1:B:998:ARG:HA	1:B:998:ARG:NE	2.35	0.41
1:A:895:VAL:O	1:A:895:VAL:CG2	2.67	0.41
1:A:1466:ASN:O	1:A:1503:LEU:CD2	2.68	0.41
1:A:489:THR:HG22	1:A:503:ARG:CD	2.50	0.41
1:A:1599:HIS:O	1:A:1629:TRP:HB3	2.19	0.41
1:A:1138:LYS:O	1:A:1139:ASP:HB2	2.20	0.41
1:A:351:PRO:HG2	1:A:352:TYR:CD2	2.55	0.41
1:B:1061:LYS:HE2	1:B:1061:LYS:H	1.84	0.41
1:B:169:PRO:HD3	1:B:203:TRP:NE1	2.35	0.41
1:A:536:ILE:HG22	1:A:542:ARG:HA	2.03	0.41
1:B:104:PHE:HB3	1:B:119:VAL:HG12	2.02	0.41
1:B:60:HIS:CG	1:B:65:LYS:HD3	2.55	0.41
1:B:1112:LYS:HB3	1:B:1113:PRO:CD	2.42	0.41
1:A:386:ILE:N	1:A:398:LEU:HB3	2.31	0.41
1:B:986:VAL:HB	1:B:1282:GLN:HE22	1.85	0.41
1:A:729:ILE:HA	1:A:732:LEU:HB3	2.02	0.41
1:A:1629:TRP:CE3	1:A:1647:LEU:HD13	2.55	0.41
1:B:769:TRP:HB3	1:B:795:LYS:HE3	2.03	0.41
1:B:1060:GLN:OE1	1:B:1073:PRO:HG3	2.20	0.41
1:A:465:PRO:HA	1:A:519:ILE:HG22	2.02	0.41
1:A:708:ARG:HD2	1:A:1427:TYR:OH	2.20	0.41
1:A:940:THR:HG22	1:A:1262:GLY:H	1.85	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1225:LYS:HG3	1:A:1484:ASP:CG	2.41	0.41
1:B:154:LYS:HB2	1:B:156:LEU:HG	2.01	0.41
1:B:1563:ILE:CD1	1:B:1578:GLN:H	2.33	0.41
1:A:398:LEU:HD11	1:A:403:GLY:O	2.21	0.41
1:A:850:LEU:HD11	1:A:863:VAL:HG11	2.01	0.41
1:B:311:GLN:HA	1:B:312:PRO:HD3	1.56	0.41
1:A:872:CYS:HB2	1:A:900:VAL:HB	2.02	0.41
1:A:233:VAL:HG12	1:A:340:ALA:HB2	2.02	0.41
1:B:634:ALA:O	1:B:638:THR:HG23	2.19	0.41
1:B:1436:ASP:HB2	2:B:2002:NAG:O6	2.20	0.41
1:A:390:THR:CG2	1:A:422:VAL:HG13	2.50	0.41
1:A:457:SER:OG	1:A:472:ASN:HB2	2.20	0.41
1:A:1585:HIS:CD2	1:A:1587:LYS:H	2.38	0.41
1:A:1068:PHE:CD1	1:A:1429:SER:HB3	2.56	0.41
1:B:559:GLY:CA	1:B:812:LYS:HD2	2.50	0.41
1:B:319:VAL:HG11	1:B:349:THR:HG23	2.01	0.41
1:B:106:THR:HA	1:B:119:VAL:HA	2.02	0.41
1:B:457:SER:O	1:B:458:VAL:HG23	2.20	0.41
1:B:270:VAL:HG22	1:B:327:ALA:HB2	2.01	0.41
1:A:754:ILE:O	1:A:754:ILE:HG22	2.20	0.41
1:B:140:PRO:HD3	1:B:224:LYS:O	2.20	0.41
1:A:274:VAL:HG11	1:A:321:LYS:HE2	2.03	0.41
1:A:274:VAL:HG23	1:A:283:LEU:CD1	2.45	0.41
1:A:272:PHE:CA	1:A:325:VAL:HG22	2.43	0.41
1:B:32:ASN:HD22	1:B:32:ASN:HA	1.55	0.41
1:A:409:ILE:HD12	1:A:409:ILE:C	2.41	0.41
1:A:128:TYR:HB2	1:A:151:VAL:HG12	2.03	0.41
1:A:1226:LEU:HD12	1:A:1482:ASN:HA	2.03	0.41
1:B:1481:TYR:O	1:B:1482:ASN:HB2	2.21	0.41
1:A:143:THR:HA	1:A:193:ASN:HA	2.03	0.41
1:A:1374:LYS:HG2	1:A:1374:LYS:H	1.56	0.41
1:A:473:PHE:HE2	1:A:515:LEU:HB3	1.86	0.41
1:A:313:SER:O	1:A:314:ARG:HB2	2.21	0.41
1:A:318:LEU:CD2	1:A:321:LYS:HZ2	2.34	0.41
1:A:615:TRP:O	1:A:616:ASP:C	2.58	0.41
1:B:712:ILE:HG23	1:B:1424:VAL:HG12	2.03	0.41
1:A:365:PRO:HB3	1:A:414:LYS:O	2.20	0.41
1:B:171:GLY:O	1:B:172:ILE:CB	2.68	0.41
1:B:131:ILE:CG1	1:B:148:VAL:HG23	2.50	0.41
1:A:163:PHE:O	1:A:207:ALA:HA	2.21	0.41
1:B:1474:ALA:HB2	1:B:1490:PHE:CD1	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:173:PRO:HD2	1:B:1095:ASP:OD2	2.21	0.41
1:A:1028:ASP:OD1	1:A:1033:TRP:CZ3	2.73	0.41
1:B:525:PRO:HB3	1:B:615:TRP:CE3	2.55	0.41
1:B:646:THR:OG1	1:B:650:LEU:HB2	2.20	0.41
1:B:673:LEU:HG	1:B:674:MET:H	1.82	0.41
1:B:714:GLN:HB2	1:B:718:CYS:SG	2.60	0.41
1:B:537:ASN:HB3	1:B:541:GLN:H	1.86	0.41
1:A:866:LEU:HD21	1:A:912:LYS:NZ	2.35	0.41
1:B:281:ILE:HG21	1:B:310:VAL:HG21	2.02	0.41
1:A:726:CYS:O	1:A:729:ILE:HD12	2.20	0.41
1:B:769:TRP:O	1:B:770:LEU:HB3	2.20	0.41
1:A:205:ILE:HG22	1:A:206:LYS:N	2.34	0.41
1:A:1509:CYS:O	1:A:1513:GLU:HG2	2.20	0.41
1:A:1527:LEU:HG	1:A:1646:ASP:CG	2.41	0.41
1:A:1079:ALA:HB2	1:A:1146:VAL:HG22	2.02	0.41
1:B:553:VAL:O	1:B:554:LYS:C	2.59	0.41
1:B:524:ILE:HG22	1:B:525:PRO:CD	2.45	0.41
1:A:1543:TYR:O	1:A:1601:LEU:HD23	2.20	0.41
1:A:456:LEU:HA	1:A:456:LEU:HD23	1.76	0.41
1:A:654:GLN:HE21	1:A:654:GLN:HB3	1.63	0.41
1:A:490:TYR:HB2	1:A:529:LEU:CD1	2.50	0.41
1:A:274:VAL:HG13	1:A:321:LYS:HG3	2.02	0.41
1:A:314:ARG:HE	1:A:315:ALA:N	2.17	0.41
1:B:583:ILE:HD13	1:B:774:ILE:HD11	2.03	0.41
1:B:1500:LEU:HG	1:B:1500:LEU:O	2.21	0.41
1:B:537:ASN:HB2	1:B:541:GLN:O	2.20	0.41
1:A:564:LYS:HG2	1:A:565:ASN:H	1.83	0.41
1:B:528:ARG:HD3	1:B:640:ALA:CB	2.51	0.41
1:A:1554:ASP:CA	1:A:1586:ILE:HD11	2.51	0.41
1:B:303:ARG:O	1:B:307:LEU:N	2.33	0.41
1:B:309:GLY:O	1:B:310:VAL:C	2.58	0.41
1:A:241:PHE:C	1:A:241:PHE:CD1	2.95	0.41
1:B:35:ARG:CG	1:B:38:SER:HB3	2.51	0.41
1:A:733:ARG:C	1:A:735:GLN:H	2.24	0.41
1:B:148:VAL:CG1	1:B:148:VAL:O	2.68	0.41
1:B:1600:TYR:CD2	1:B:1628:LEU:HG	2.55	0.41
1:B:482:GLN:HG2	1:B:482:GLN:O	2.21	0.41
1:B:285:HIS:HB2	1:B:305:VAL:HG13	2.03	0.41
1:B:1393:GLY:C	1:B:1395:GLN:H	2.23	0.41
1:B:730:THR:HG22	1:B:734:GLN:HE22	1.86	0.41
1:A:1457:LEU:HD12	1:A:1457:LEU:HA	1.77	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1215:GLU:O	1:B:1216:LYS:HB2	2.21	0.41
1:B:808:LEU:HA	1:B:814:ILE:HA	2.03	0.41
1:B:714:GLN:N	1:B:714:GLN:CD	2.74	0.41
1:A:421:THR:HG22	1:A:438:THR:CG2	2.51	0.41
1:A:541:GLN:C	1:A:543:GLU:H	2.25	0.41
1:A:1256:ASN:ND2	1:A:1259:ARG:NH1	2.68	0.41
1:A:30:THR:CG2	1:A:42:VAL:HG13	2.51	0.41
1:A:205:ILE:O	1:A:206:LYS:HB2	2.20	0.41
1:A:1225:LYS:HG3	1:A:1484:ASP:OD2	2.21	0.41
1:B:922:ASP:OD1	1:B:923:GLY:N	2.54	0.41
1:A:874:LEU:HA	1:A:874:LEU:HD23	1.84	0.41
1:B:381:SER:O	1:B:382:PRO:C	2.59	0.40
1:B:398:LEU:HD12	1:B:405:ALA:HB2	2.04	0.40
1:B:637:PHE:HB3	1:B:642:LEU:HB2	2.03	0.40
1:B:597:ASP:HB2	1:B:766:PRO:HG2	2.02	0.40
1:B:36:LEU:HB2	1:B:124:LEU:HD13	2.03	0.40
1:A:1567:ILE:HG23	1:A:1654:MET:CB	2.51	0.40
1:B:1551:LYS:HZ3	1:B:1581:LYS:HE2	1.86	0.40
1:B:1637:ASP:O	1:B:1641:GLN:HB2	2.21	0.40
1:B:708:ARG:HG2	1:B:708:ARG:H	1.70	0.40
1:B:1034:GLU:HG3	1:B:1035:LYS:N	2.35	0.40
1:B:276:ASP:OD2	1:B:321:LYS:NZ	2.50	0.40
1:A:1543:TYR:HB3	1:A:1563:ILE:HG23	2.02	0.40
1:A:312:PRO:O	1:A:317:ALA:HB3	2.20	0.40
1:A:806:VAL:HG22	1:A:816:VAL:HG13	2.01	0.40
1:A:750:ASP:O	1:A:751:ASP:C	2.59	0.40
1:A:507:GLU:CG	1:A:508:PRO:HD2	2.51	0.40
1:A:1362:LEU:HD23	1:A:1389:THR:HB	2.03	0.40
1:A:933:GLU:HG2	1:A:970:VAL:CG1	2.50	0.40
1:B:785:ILE:HG22	1:B:785:ILE:O	2.21	0.40
1:A:549:VAL:HG12	1:A:550:TRP:N	2.35	0.40
1:B:1308:HIS:ND1	1:B:1319:ARG:HD2	2.36	0.40
1:B:1505:HIS:CE1	1:B:1506:LYS:HG3	2.56	0.40
1:B:136:THR:CG2	1:B:607:ASN:HB2	2.51	0.40
1:B:847:ARG:HH11	1:B:847:ARG:HG2	1.86	0.40
1:A:319:VAL:HG12	1:A:320:GLY:N	2.36	0.40
1:A:1311:LEU:O	1:A:1312:TRP:C	2.60	0.40
1:B:633:TYR:O	1:B:637:PHE:CD2	2.53	0.40
1:B:832:LEU:HD21	1:B:909:VAL:HG12	2.03	0.40
1:B:1437:SER:O	1:B:1439:LYS:N	2.54	0.40
1:A:131:ILE:HB	1:A:219:ALA:HB2	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1265:TYR:CZ	1:B:1274:VAL:HG21	2.57	0.40
1:B:434:GLN:HG3	1:B:434:GLN:O	2.22	0.40
1:B:358:LYS:HB3	1:B:550:TRP:CZ3	2.56	0.40
1:A:1091:LEU:O	1:A:1092:ILE:HD13	2.22	0.40
1:A:478:ASP:O	1:A:479:PRO:C	2.59	0.40
1:B:148:VAL:O	1:B:148:VAL:HG13	2.20	0.40
1:B:1024:VAL:HG13	1:B:1033:TRP:CH2	2.56	0.40
1:B:534:THR:HG21	1:B:542:ARG:HE	1.86	0.40
1:B:1407:MET:HB2	1:B:1410:PHE:CD2	2.56	0.40
1:B:704:PRO:O	1:B:705:CYS:C	2.60	0.40
1:B:1278:LEU:HA	1:B:1278:LEU:HD23	1.88	0.40
1:B:629:SER:O	1:B:636:VAL:HA	2.21	0.40
1:B:712:ILE:CG2	1:B:719:VAL:HG22	2.52	0.40
1:B:128:TYR:CE1	1:B:618:VAL:HG13	2.57	0.40
1:A:1567:ILE:HG23	1:A:1654:MET:HB2	2.03	0.40
1:B:985:PRO:HB2	1:B:1256:ASN:ND2	2.37	0.40
1:B:756:GLU:O	1:B:757:GLU:C	2.59	0.40
1:A:804:LEU:HD22	1:A:804:LEU:N	2.36	0.40
1:A:574:ARG:O	1:A:575:PRO:O	2.39	0.40
1:B:852:ASN:C	1:B:854:ARG:N	2.75	0.40
1:A:269:PHE:N	1:A:269:PHE:CD2	2.90	0.40
1:A:270:VAL:O	1:A:287:LEU:HB3	2.21	0.40
1:B:481:GLU:O	1:B:483:ALA:N	2.55	0.40
1:A:481:GLU:OE2	1:A:538:ALA:HB2	2.21	0.40
1:B:1448:LYS:HD2	1:B:1449:VAL:N	2.36	0.40
1:A:1184:ARG:NH1	1:A:1184:ARG:HG2	2.36	0.40
1:A:1232:THR:O	1:A:1235:ALA:HB3	2.21	0.40
1:B:982:GLN:O	1:B:1339:GLY:HA3	2.21	0.40
1:B:1140:VAL:HG21	1:B:1182:LEU:HD21	2.04	0.40
1:A:609:LEU:HA	1:A:609:LEU:HD23	1.88	0.40
1:A:1352:LYS:HG3	1:A:1352:LYS:O	2.21	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 X-ray entries followed by that with respect to entries of similar resolution.

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	1602/1661 (96%)	1285 (80%)	213 (13%)	104 (6%)	1 8
1	B	1602/1661 (96%)	1268 (79%)	239 (15%)	95 (6%)	2 11
All	All	3204/3322 (96%)	2553 (80%)	452 (14%)	199 (6%)	2 10

All (199) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	63	PRO
1	A	91	PRO
1	A	187	ILE
1	A	212	SER
1	A	244	ILE
1	A	313	SER
1	A	384	ARG
1	A	482	GLN
1	A	526	SER
1	A	537	ASN
1	A	554	LYS
1	A	555	ASP
1	A	646	THR
1	A	757	GLU
1	A	778	LYS
1	A	780	ALA
1	A	794	LEU
1	A	817	ALA
1	A	888	PRO
1	A	971	PRO
1	A	1225	LYS
1	A	1245	TYR
1	A	1314	SER
1	A	1497	ASP
1	A	1506	LYS
1	A	1579	GLU
1	A	1613	LYS
1	A	1632	ALA
1	B	63	PRO
1	B	78	SER
1	B	140	PRO
1	B	219	ALA
1	B	302	LYS

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Mol	Chain	Res	Type
1	B	310	VAL
1	B	312	PRO
1	B	317	ALA
1	B	427	ASP
1	B	449	ASN
1	B	479	PRO
1	B	481	GLU
1	B	482	GLN
1	B	537	ASN
1	B	622	ASP
1	B	623	ILE
1	B	626	THR
1	B	653	GLN
1	B	716	ASP
1	B	757	GLU
1	B	785	ILE
1	B	798	ILE
1	B	817	ALA
1	B	1132	PHE
1	B	1225	LYS
1	B	1571	SER
1	B	1572	ASP
1	B	1632	ALA
1	A	78	SER
1	A	120	VAL
1	A	125	GLN
1	A	282	SER
1	A	309	GLY
1	A	483	ALA
1	A	543	GLU
1	A	576	GLY
1	A	616	ASP
1	A	629	SER
1	A	671	VAL
1	A	751	ASP
1	A	756	GLU
1	A	762	ARG
1	A	1010	GLY
1	A	1127	GLU
1	A	1350	LYS
1	A	1483	LEU
1	A	1493	PRO

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Mol	Chain	Res	Type
1	A	1502	LYS
1	A	1570	GLY
1	A	1580	ARG
1	B	215	GLN
1	B	244	ILE
1	B	248	ASP
1	B	282	SER
1	B	320	GLY
1	B	462	GLU
1	B	603	LEU
1	B	655	ARG
1	B	780	ALA
1	B	1010	GLY
1	B	1095	ASP
1	B	1266	GLY
1	B	1314	SER
1	B	1495	LYS
1	B	1570	GLY
1	B	1628	LEU
1	A	93	SER
1	A	219	ALA
1	A	250	LEU
1	A	283	LEU
1	A	335	SER
1	A	365	PRO
1	A	382	PRO
1	A	385	HIS
1	A	449	ASN
1	A	451	ASN
1	A	512	LEU
1	A	560	THR
1	A	603	LEU
1	A	752	ASP
1	A	889	ALA
1	A	918	HIS
1	A	1353	GLY
1	A	1372	THR
1	A	1438	ASN
1	A	1482	ASN
1	A	1653	ASN
1	B	82	TYR
1	B	126	SER

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Mol	Chain	Res	Type
1	B	134	ASP
1	B	157	PRO
1	B	174	VAL
1	B	283	LEU
1	B	525	PRO
1	B	571	LYS
1	B	687	ASP
1	B	755	PRO
1	B	812	LYS
1	B	987	ALA
1	B	1482	ASN
1	B	1613	LYS
1	B	1614	PRO
1	A	50	GLN
1	A	140	PRO
1	A	378	PRO
1	A	570	GLU
1	A	675	GLU
1	A	972	ASP
1	A	1435	ARG
1	A	1436	ASP
1	A	1657	PHE
1	B	47	HIS
1	B	185	PHE
1	B	251	LYS
1	B	378	PRO
1	B	384	ARG
1	B	464	LYS
1	B	540	GLY
1	B	671	VAL
1	B	702	LYS
1	B	971	PRO
1	B	1040	LYS
1	B	1372	THR
1	B	1438	ASN
1	B	1483	LEU
1	A	172	ILE
1	A	479	PRO
1	A	516	PRO
1	A	535	LEU
1	A	904	ILE
1	A	1555	ASP

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Mol	Chain	Res	Type
1	A	1565	ASN
1	B	237	PRO
1	B	448	GLY
1	B	657	ASP
1	B	724	ASP
1	B	840	ARG
1	B	1223	ASN
1	B	1565	ASN
1	B	1637	ASP
1	A	174	VAL
1	A	759	ILE
1	A	806	VAL
1	A	1540	ASP
1	B	172	ILE
1	B	334	GLY
1	B	577	GLN
1	B	661	PRO
1	B	822	VAL
1	B	1137	GLU
1	B	1597	GLY
1	A	360	PRO
1	A	466	GLY
1	A	575	PRO
1	A	623	ILE
1	A	657	ASP
1	A	1266	GLY
1	B	360	PRO
1	B	508	PRO
1	A	169	PRO
1	B	246	ASP
1	A	252	VAL
1	A	311	GLN
1	A	1538	GLY
1	B	373	VAL
1	B	461	VAL
1	B	806	VAL
1	A	766	PRO
1	A	658	PRO
1	A	1658	GLY
1	B	766	PRO

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 X-ray entries followed by that with respect to entries of similar resolution.

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	1420/1465 (97%)	1238 (87%)	182 (13%)	5 23
1	B	1420/1465 (97%)	1234 (87%)	186 (13%)	5 22
All	All	2840/2930 (97%)	2472 (87%)	368 (13%)	5 22

All (368) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	38	SER
1	A	41	THR
1	A	58	THR
1	A	61	ASP
1	A	75	GLN
1	A	80	ASN
1	A	83	LEU
1	A	95	GLU
1	A	98	SER
1	A	100	LYS
1	A	107	VAL
1	A	110	THR
1	A	113	ASN
1	A	114	VAL
1	A	118	LYS
1	A	120	VAL
1	A	121	LEU
1	A	125	GLN
1	A	128	TYR
1	A	135	LYS
1	A	139	THR
1	A	140	PRO
1	A	143	THR
1	A	146	TYR
1	A	151	VAL
1	A	164	ILE
1	A	174	VAL

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Mol	Chain	Res	Type
1	A	200	MET
1	A	218	SER
1	A	228	LEU
1	A	235	LEU
1	A	254	ILE
1	A	265	ASP
1	A	267	THR
1	A	270	VAL
1	A	278	ASP
1	A	287	LEU
1	A	288	THR
1	A	294	ASP
1	A	314	ARG
1	A	316	ASP
1	A	318	LEU
1	A	321	LYS
1	A	322	SER
1	A	328	THR
1	A	330	ILE
1	A	336	ASP
1	A	346	PRO
1	A	356	PHE
1	A	358	LYS
1	A	359	THR
1	A	361	LYS
1	A	399	THR
1	A	400	GLN
1	A	404	VAL
1	A	407	LEU
1	A	410	ASN
1	A	412	GLN
1	A	422	VAL
1	A	427	ASP
1	A	434	GLN
1	A	442	LEU
1	A	463	LEU
1	A	467	GLU
1	A	468	THR
1	A	471	VAL
1	A	476	ARG
1	A	479	PRO
1	A	484	LYS

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Mol	Chain	Res	Type
1	A	491	MET
1	A	501	VAL
1	A	504	GLN
1	A	513	VAL
1	A	535	LEU
1	A	537	ASN
1	A	541	GLN
1	A	555	ASP
1	A	565	ASN
1	A	600	VAL
1	A	601	PHE
1	A	605	LYS
1	A	618	VAL
1	A	631	ARG
1	A	633	TYR
1	A	650	LEU
1	A	654	GLN
1	A	658	PRO
1	A	673	LEU
1	A	677	ARG
1	A	687	ASP
1	A	692	CYS
1	A	701	MET
1	A	702	LYS
1	A	707	ARG
1	A	714	GLN
1	A	723	LEU
1	A	729	ILE
1	A	750	ASP
1	A	751	ASP
1	A	752	ASP
1	A	756	GLU
1	A	776	ASP
1	A	796	ASP
1	A	798	ILE
1	A	804	LEU
1	A	808	LEU
1	A	814	ILE
1	A	846	ILE
1	A	852	ASN
1	A	854	ARG
1	A	855	GLU

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Mol	Chain	Res	Type
1	A	859	LEU
1	A	867	TYR
1	A	871	PHE
1	A	881	HIS
1	A	906	LEU
1	A	927	THR
1	A	928	LEU
1	A	940	THR
1	A	945	THR
1	A	958	ARG
1	A	962	PRO
1	A	971	PRO
1	A	977	THR
1	A	978	LYS
1	A	988	GLN
1	A	999	LEU
1	A	1009	CYS
1	A	1012	GLN
1	A	1033	TRP
1	A	1039	GLU
1	A	1056	LEU
1	A	1077	LEU
1	A	1133	ARG
1	A	1134	ASP
1	A	1135	THR
1	A	1164	LEU
1	A	1190	ILE
1	A	1205	ARG
1	A	1207	THR
1	A	1217	ASN
1	A	1223	ASN
1	A	1244	ASP
1	A	1249	PRO
1	A	1257	GLU
1	A	1260	TYR
1	A	1275	PHE
1	A	1282	GLN
1	A	1289	LYS
1	A	1299	LEU
1	A	1306	VAL
1	A	1323	THR
1	A	1328	ARG

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Mol	Chain	Res	Type
1	A	1341	LEU
1	A	1345	THR
1	A	1351	LEU
1	A	1357	CYS
1	A	1358	LYS
1	A	1371	GLU
1	A	1375	LYS
1	A	1377	GLN
1	A	1380	LYS
1	A	1389	THR
1	A	1396	ASP
1	A	1422	THR
1	A	1435	ARG
1	A	1447	ASP
1	A	1448	LYS
1	A	1452	THR
1	A	1457	LEU
1	A	1489	ARG
1	A	1492	HIS
1	A	1496	GLU
1	A	1497	ASP
1	A	1527	LEU
1	A	1547	LEU
1	A	1549	GLN
1	A	1561	MET
1	A	1562	VAL
1	A	1563	ILE
1	A	1569	SER
1	A	1601	LEU
1	B	30	THR
1	B	32	ASN
1	B	44	LEU
1	B	50	GLN
1	B	54	GLN
1	B	55	VAL
1	B	58	THR
1	B	65	LYS
1	B	69	LEU
1	B	75	GLN
1	B	79	ASN
1	B	82	TYR
1	B	100	LYS

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Mol	Chain	Res	Type
1	B	105	VAL
1	B	110	THR
1	B	113	ASN
1	B	117	GLU
1	B	120	VAL
1	B	121	LEU
1	B	123	SER
1	B	140	PRO
1	B	143	THR
1	B	146	TYR
1	B	151	VAL
1	B	152	ASP
1	B	168	THR
1	B	182	GLN
1	B	183	ASN
1	B	184	GLN
1	B	200	MET
1	B	218	SER
1	B	243	TYR
1	B	246	ASP
1	B	278	ASP
1	B	288	THR
1	B	294	ASP
1	B	296	ASN
1	B	316	ASP
1	B	328	THR
1	B	350	SER
1	B	352	TYR
1	B	354	ILE
1	B	355	HIS
1	B	360	PRO
1	B	361	LYS
1	B	364	LYS
1	B	374	TYR
1	B	376	THR
1	B	382	PRO
1	B	400	GLN
1	B	407	LEU
1	B	408	SER
1	B	409	ILE
1	B	410	ASN
1	B	416	ASP

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Mol	Chain	Res	Type
1	B	422	VAL
1	B	423	ARG
1	B	429	ILE
1	B	433	ARG
1	B	438	THR
1	B	446	THR
1	B	455	HIS
1	B	478	ASP
1	B	479	PRO
1	B	486	ARG
1	B	487	TYR
1	B	491	MET
1	B	503	ARG
1	B	508	PRO
1	B	515	LEU
1	B	524	ILE
1	B	535	LEU
1	B	537	ASN
1	B	551	VAL
1	B	553	VAL
1	B	557	CYS
1	B	558	MET
1	B	565	ASN
1	B	570	GLU
1	B	618	VAL
1	B	626	THR
1	B	627	PRO
1	B	645	LYS
1	B	653	GLN
1	B	654	GLN
1	B	672	GLN
1	B	673	LEU
1	B	675	GLU
1	B	677	ARG
1	B	687	ASP
1	B	697	ARG
1	B	701	MET
1	B	708	ARG
1	B	718	CYS
1	B	750	ASP
1	B	798	ILE
1	B	799	THR

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Mol	Chain	Res	Type
1	B	804	LEU
1	B	808	LEU
1	B	812	LYS
1	B	818	ASP
1	B	830	ILE
1	B	839	VAL
1	B	846	ILE
1	B	859	LEU
1	B	867	TYR
1	B	881	HIS
1	B	918	HIS
1	B	927	THR
1	B	928	LEU
1	B	940	THR
1	B	945	THR
1	B	962	PRO
1	B	971	PRO
1	B	977	THR
1	B	986	VAL
1	B	988	GLN
1	B	997	GLU
1	B	999	LEU
1	B	1009	CYS
1	B	1012	GLN
1	B	1018	THR
1	B	1028	ASP
1	B	1033	TRP
1	B	1039	GLU
1	B	1040	LYS
1	B	1042	GLN
1	B	1056	LEU
1	B	1061	LYS
1	B	1129	ILE
1	B	1133	ARG
1	B	1134	ASP
1	B	1135	THR
1	B	1139	ASP
1	B	1160	GLN
1	B	1164	LEU
1	B	1190	ILE
1	B	1205	ARG
1	B	1206	LEU

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Mol	Chain	Res	Type
1	B	1207	THR
1	B	1217	ASN
1	B	1218	ARG
1	B	1223	ASN
1	B	1244	ASP
1	B	1258	GLN
1	B	1259	ARG
1	B	1260	TYR
1	B	1275	PHE
1	B	1280	GLN
1	B	1289	LYS
1	B	1298	GLN
1	B	1303	ASN
1	B	1306	VAL
1	B	1311	LEU
1	B	1328	ARG
1	B	1341	LEU
1	B	1345	THR
1	B	1346	VAL
1	B	1351	LEU
1	B	1357	CYS
1	B	1358	LYS
1	B	1375	LYS
1	B	1377	GLN
1	B	1396	ASP
1	B	1415	GLU
1	B	1422	THR
1	B	1445	TYR
1	B	1447	ASP
1	B	1448	LYS
1	B	1452	THR
1	B	1456	CYS
1	B	1484	ASP
1	B	1489	ARG
1	B	1535	CYS
1	B	1549	GLN
1	B	1561	MET
1	B	1563	ILE
1	B	1575	GLN
1	B	1577	LYS
1	B	1593	LYS
1	B	1603	TRP

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Mol	Chain	Res	Type
1	B	1610	TRP
1	B	1612	GLU
1	B	1634	GLU
1	B	1635	CYS
1	B	1653	ASN

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (85) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	47	HIS
1	A	54	GLN
1	A	71	ASN
1	A	80	ASN
1	A	183	ASN
1	A	193	ASN
1	A	199	ASN
1	A	296	ASN
1	A	308	ASN
1	A	353	GLN
1	A	377	ASN
1	A	440	GLN
1	A	494	ASN
1	A	510	GLN
1	A	537	ASN
1	A	541	GLN
1	A	653	GLN
1	A	654	GLN
1	A	841	ASN
1	A	883	GLN
1	A	1032	GLN
1	A	1054	GLN
1	A	1090	ASN
1	A	1160	GLN
1	A	1217	ASN
1	A	1223	ASN
1	A	1256	ASN
1	A	1282	GLN
1	A	1377	GLN
1	A	1434	ASN
1	A	1578	GLN
1	A	1585	HIS
1	A	1636	GLN

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Mol	Chain	Res	Type
1	A	1641	GLN
1	A	1643	GLN
1	A	1649	ASN
1	B	32	ASN
1	B	54	GLN
1	B	71	ASN
1	B	79	ASN
1	B	113	ASN
1	B	182	GLN
1	B	183	ASN
1	B	184	GLN
1	B	193	ASN
1	B	234	GLN
1	B	263	GLN
1	B	296	ASN
1	B	377	ASN
1	B	396	GLN
1	B	413	ASN
1	B	434	GLN
1	B	451	ASN
1	B	474	HIS
1	B	494	ASN
1	B	537	ASN
1	B	611	GLN
1	B	632	ASN
1	B	653	GLN
1	B	654	GLN
1	B	714	GLN
1	B	734	GLN
1	B	791	ASN
1	B	852	ASN
1	B	881	HIS
1	B	883	GLN
1	B	917	ASN
1	B	1013	ASN
1	B	1032	GLN
1	B	1042	GLN
1	B	1054	GLN
1	B	1069	GLN
1	B	1090	ASN
1	B	1160	GLN
1	B	1217	ASN

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Mol	Chain	Res	Type
1	B	1223	ASN
1	B	1258	GLN
1	B	1282	GLN
1	B	1298	GLN
1	B	1434	ASN
1	B	1585	HIS
1	B	1641	GLN
1	B	1643	GLN
1	B	1649	ASN
1	B	1653	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates

6 carbohydrates are modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
2	NAG	A	2001	1,2	14,14,15	0.56	0	15,19,21	0.78	0
2	NAG	A	2002	2	14,14,15	0.61	0	15,19,21	1.01	1 (6%)
2	BMA	A	2003	2	11,11,12	0.46	0	14,15,17	0.49	0
2	NAG	B	2001	1,2	14,14,15	0.57	0	15,19,21	0.84	0
2	NAG	B	2002	2	14,14,15	0.60	0	15,19,21	0.89	0
2	BMA	B	2003	2	11,11,12	0.47	0	14,15,17	0.67	0

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral

centers analysed, the number of these observed in the model and the number defined in the chemical component dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	NAG	A	2001	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	A	2002	2	-	0/6/23/26	0/1/1/1
2	BMA	A	2003	2	-	0/2/19/22	0/1/1/1
2	NAG	B	2001	1,2	1/1/5/7	0/6/23/26	0/1/1/1
2	NAG	B	2002	2	-	0/6/23/26	0/1/1/1
2	BMA	B	2003	2	-	0/2/19/22	0/1/1/1

There are no bond length outliers.

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
2	A	2002	NAG	C3-C4-C5	-2.37	106.06	110.20

All (2) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
2	A	2001	NAG	C1
2	B	2001	NAG	C1

There are no torsion outliers.

There are no ring outliers.

5 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	2001	NAG	3	0
2	A	2002	NAG	2	0
2	B	2001	NAG	1	0
2	B	2002	NAG	2	0
2	B	2003	BMA	1	0

5.6 Ligand geometry

There are no ligands in this entry.

5.7 Other polymers

There are no such residues in this entry.

5.8 Polymer linkage issues

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

In the following table, the column labelled '#RSRZ> 2' contains the number (and percentage) of RSRZ outliers, followed by percent RSRZ outliers for the chain as percentile scores relative to all X-ray entries and entries of similar resolution. The OWAB column contains the minimum, median, 95^{th} percentile and maximum values of the occupancy-weighted average B-factor per residue. The column labelled 'Q< 0.9' lists the number of (and percentage) of residues with an average occupancy less than 0.9.

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2			OWAB(Å^2)	Q<0.9
1	A	1610/1661 (96%)	-0.04	59 (3%)	45	19	15, 101, 169, 200	0
1	B	1610/1661 (96%)	-0.10	51 (3%)	51	23	17, 96, 169, 200	0
All	All	3220/3322 (96%)	-0.07	110 (3%)	49	21	15, 99, 169, 200	0

All (110) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	B	671	VAL	6.0
1	A	742	LEU	5.9
1	A	741	ALA	5.2
1	A	276	ASP	5.0
1	A	348	VAL	5.0
1	B	1654	MET	4.3
1	A	349	THR	4.2
1	A	431	GLU	3.9
1	A	278	ASP	3.9
1	A	125	GLN	3.8
1	A	52	THR	3.7
1	B	741	ALA	3.6
1	A	535	LEU	3.6
1	A	401	ASP	3.5
1	A	1661	ASN	3.5
1	A	1640	ASN	3.5
1	A	279	ARG	3.4
1	B	1659	CYS	3.4
1	B	1650	PHE	3.4
1	B	742	LEU	3.3
1	A	252	VAL	3.3
1	A	352	TYR	3.3
1	A	67	GLN	3.3
1	A	1133	ARG	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	375	VAL	3.3
1	A	99	ASP	3.2
1	B	57	VAL	3.2
1	A	829	PHE	3.2
1	B	273	GLY	3.2
1	A	70	SER	3.2
1	A	396	GLN	3.2
1	B	425	LYS	3.1
1	B	1661	ASN	3.1
1	A	277	GLY	3.1
1	B	92	ALA	3.0
1	A	736	HIS	3.0
1	B	1353	GLY	3.0
1	B	661	PRO	2.8
1	B	1647	LEU	2.8
1	A	121	LEU	2.8
1	B	1655	VAL	2.8
1	B	1651	THR	2.8
1	B	648	GLN	2.8
1	B	670	SER	2.8
1	B	1630	PRO	2.8
1	B	1641	GLN	2.8
1	A	1597	GLY	2.8
1	B	1638	GLU	2.8
1	B	1631	GLU	2.7
1	A	851	TYR	2.7
1	A	567	GLY	2.7
1	A	100	LYS	2.7
1	B	1657	PHE	2.7
1	B	304	GLN	2.7
1	A	320	GLY	2.7
1	B	1656	VAL	2.7
1	A	122	ILE	2.6
1	B	285	HIS	2.6
1	B	736	HIS	2.6
1	A	301	LEU	2.6
1	B	535	LEU	2.6
1	B	280	ARG	2.6
1	A	1532	ASP	2.6
1	A	740	GLY	2.5
1	A	254	ILE	2.5
1	A	288	THR	2.5

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Mol	Chain	Res	Type	RSRZ
1	B	1634	GLU	2.5
1	B	430	PRO	2.5
1	B	396	GLN	2.5
1	B	1643	GLN	2.4
1	A	120	VAL	2.4
1	A	76	LEU	2.4
1	B	472	ASN	2.4
1	A	1537	PRO	2.4
1	A	425	LYS	2.4
1	B	1606	SER	2.4
1	A	572	HIS	2.4
1	A	285	HIS	2.4
1	B	279	ARG	2.4
1	B	1652	GLU	2.4
1	B	91	PRO	2.3
1	B	415	ARG	2.3
1	B	1569	SER	2.3
1	A	853	TYR	2.3
1	A	274	VAL	2.3
1	A	321	LYS	2.3
1	B	1639	GLU	2.2
1	B	426	LYS	2.2
1	B	1498	GLY	2.2
1	A	97	LYS	2.2
1	B	750	ASP	2.2
1	A	779	GLN	2.1
1	A	91	PRO	2.1
1	B	388	VAL	2.1
1	A	53	ILE	2.1
1	A	785	ILE	2.1
1	A	1652	GLU	2.1
1	A	650	LEU	2.1
1	A	631	ARG	2.1
1	A	658	PRO	2.1
1	B	449	ASN	2.1
1	A	95	GLU	2.1
1	B	785	ILE	2.0
1	A	782	LYS	2.0
1	B	1626	VAL	2.0
1	A	322	SER	2.0
1	B	1501	SER	2.0
1	B	389	VAL	2.0

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Mol	Chain	Res	Type	RSRZ
1	A	634	ALA	2.0
1	B	74	THR	2.0

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

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

6.3 Carbohydrates (i)

In the following table, the Atoms column lists the number of modelled atoms in the group and the number defined in the chemical component dictionary. LLDF column lists the quality of electron density of the group with respect to its neighbouring residues in protein, DNA or RNA chains. The B-factors column lists the minimum, median, 95^{th} percentile and maximum values of B factors of atoms in the group. The column labelled 'Q< 0.9' lists the number of atoms with occupancy less than 0.9.

Mol	Type	Chain	Res	Atoms	RSCC	RSR	LLDF	B-factors(Å^2)	Q<0.9
2	NAG	A	2001	14/15	0.83	0.24	1.06	74,80,81,82	0
2	NAG	B	2002	14/15	0.88	0.26	0.81	80,80,81,82	0
2	BMA	A	2003	11/12	0.72	0.40	-	81,81,82,82	0
2	NAG	A	2002	14/15	0.80	0.32	-	80,81,82,82	0
2	NAG	B	2001	14/15	0.93	0.15	-	73,80,81,82	0
2	BMA	B	2003	11/12	0.79	0.23	-	80,81,81,82	0

6.4 Ligands (i)

There are no ligands in this entry.

6.5 Other polymers (i)

There are no such residues in this entry.