Full wwPDB X-ray Structure Validation Report (i)

Jan 31, 2016 – 11:39 PM GMT

PDB ID	:	1Y64
Title	:	Bni1p Formin Homology 2 Domain complexed with ATP-actin
Authors	:	Otomo, T.; Tomchick, D.R.; Otomo, C.; Panchal, S.C.; Machius, M.; Rosen, M.K.
Deposited on	:	2004-12-03
Resolution	:	3.05 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 (i) symbol.

The following versions of software and data (see references (1)) were used in the production of this report:

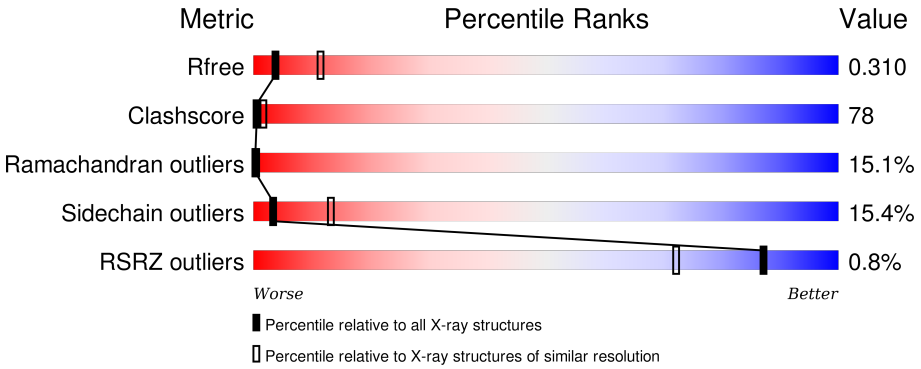
MolProbity	:	4.02b-467
Mogul	:	1.7 (RC4), CSD as536be (2015)
Xtriage (Phenix)	:	1.9-1692
EDS	:	rb-20026688
Percentile statistics	:	20151230.v01 (using entries in the PDB archive December 30th 2015)
Refmac	:	5.8.0135
CCP4	:	6.5.0
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	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 3.05 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	1191 (3.10-3.02)
Clashscore	102246	1303 (3.10-3.02)
Ramachandran outliers	100387	1254 (3.10-3.02)
Sidechain outliers	100360	1254 (3.10-3.02)
RSRZ outliers	91569	1197 (3.10-3.02)

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	375	% 17% 53% 21% • 5%
2	B	443	23% 51% 17% • 7%

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
3	CA	A	382	-	-	-	X
4	ATP	A	2000	-	-	X	-

2 Entry composition

There are 4 unique types of molecules in this entry. The entry contains 6162 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 Actin, alpha skeletal muscle.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	357	Total	C	N	O	S	0	0	0
			2795	1772	469	536	18			

There is a discrepancy between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	73	HIC	HIS	MODIFIED RESIDUE	UNP P68135

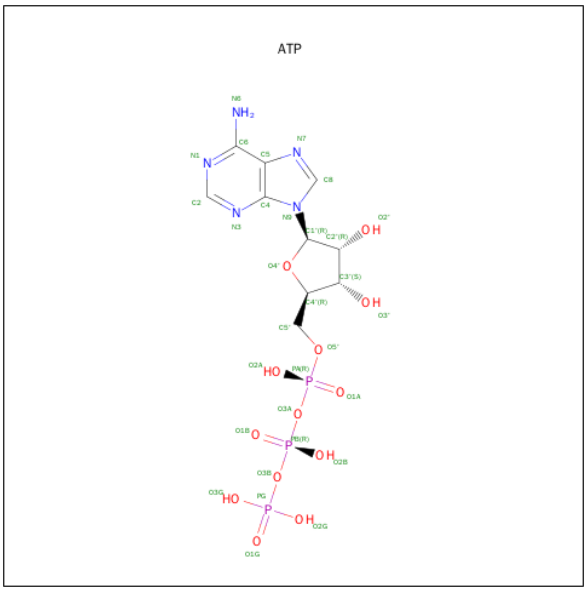
- Molecule 2 is a protein called BNI1 protein.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	411	Total	C	N	O	S	7	0	0
			3335	2124	560	641	10			

- Molecule 3 is CALCIUM ION (three-letter code: CA) (formula: Ca).

Mol	Chain	Residues	Atoms		ZeroOcc	AltConf
3	A	1	Total	Ca	0	0
			1	1		

- Molecule 4 is ADENOSINE-5'-TRIPHOSPHATE (three-letter code: ATP) (formula: $C_{10}H_{16}N_5O_{13}P_3$).



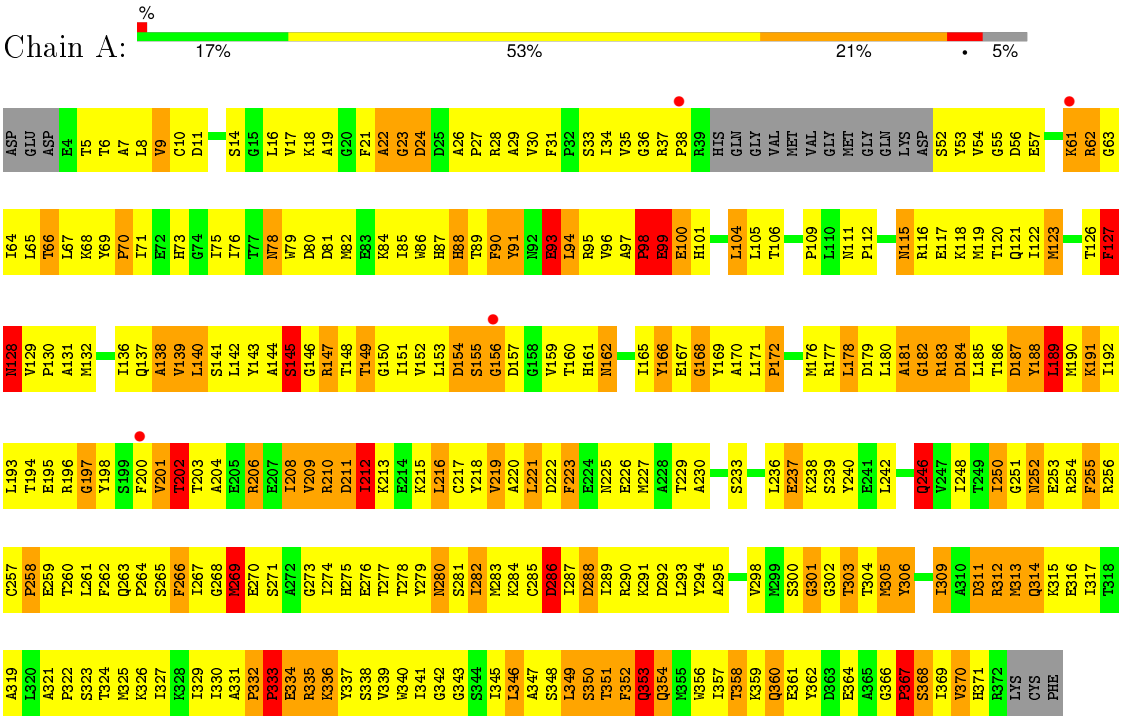
Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
4	A	1	Total	C	N	O	P	0	0
			31	10	5	13	3		

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.

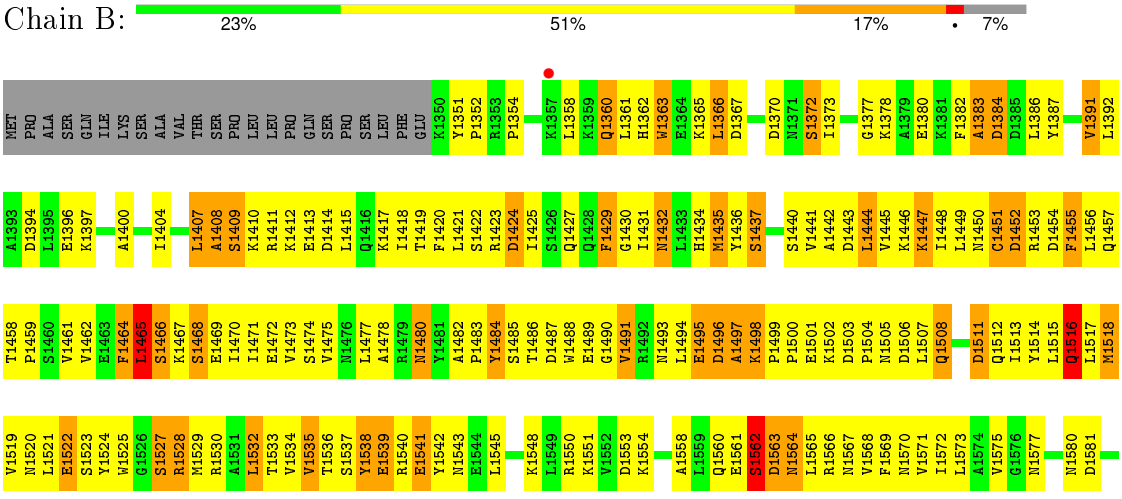
- Molecule 1: Actin, alpha skeletal muscle

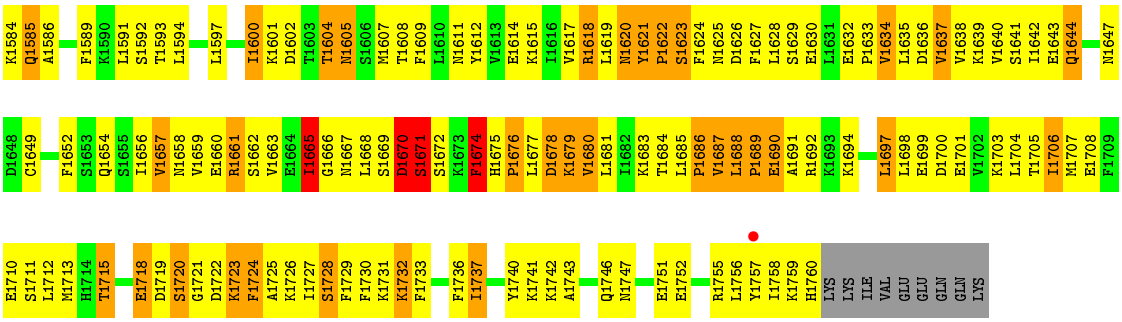
Chain A:



- Molecule 2: BNI1 protein

Chain B:




K1584 Q1585 A1586 F1589 K1590 L1591 S1592 T1593 L1594 L1597 I1600 K1601 D1602 T1603 T1604 N1605 S1606 M1607 T1608 F1609 L1610 N1611 Y1612 V1613 E1614 K1615 I1616 V1617 R1618 L1619 N1620 Y1621 P1622 S1623 F1624 N1625 D1626 F1627 L1628 S1629 E1630 L1631 E1632 P1633 V1634 L1635 D1636 V1637 V1638 K1639 V1640 S1641 I1642 E1643 Q1644 N1647
D1648 C1649 F1652 S1653 Q1654 S1655 I1656 V1657 N1658 V1659 E1660 R1661 S1662 V1663 E1664 I1665 G1666 N1667 L1668 S1669 D1670 S1671 S1672 K1673 F1674 H1675 P1676 L1677 D1678 K1679 V1680 L1681 I1682 K1683 T1684 L1685 P1686 V1687 L1688 P1689 E1690 A1691 R1692 K1693 K1694 L1697 L1698 E1699 D1700 E1701 V1702 K1703 L1704 T1705 I1706 M1707 E1708 F1709
E1710 S1711 L1712 M1713 H1714 T1715 E1718 D1719 S1720 G1721 D1722 K1723 F1724 A1725 K1726 I1727 S1728 F1729 F1730 K1731 K1732 F1733 F1736 I1737 Y1740 K1741 K1742 A1743 Q1746 N1747 E1751 E1752 R1755 L1756 Y1757 I1758 K1759 H1760 LYS LYS ILE VAL GLU GLU GLN GLN LYS

4 Data and refinement statistics (i)

Property	Value	Source
Space group	C 1 2 1	Depositor
Cell constants a, b, c, α, β, γ	232.00Å 56.23Å 100.94Å 90.00° 107.70° 90.00°	Depositor
Resolution (Å)	30.00 – 3.05 29.00 – 3.05	Depositor EDS
% Data completeness (in resolution range)	(Not available) (30.00-3.05) 99.2 (29.00-3.05)	Depositor EDS
R_{merge}	0.05	Depositor
R_{sym}	(Not available)	Depositor
$< I/\sigma(I) >$ [1]	2.64 (at 3.05Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.289 , 0.313 0.283 , 0.310	Depositor DCC
R_{free} test set	1145 reflections (4.79%)	DCC
Wilson B-factor (Å^2)	89.0	Xtriage
Anisotropy	0.721	Xtriage
Bulk solvent k_{sol}(e/Å^3), B_{sol}(Å^2)	0.26 , 70.0	EDS
Estimated twinning fraction	No twinning to report.	Xtriage
L-test for twinning[2]	$< \|L\| > = 0.49$, $< L^2 > = 0.33$	Xtriage
Outliers	4 of 23883 reflections (0.017%)	Xtriage
F_o,F_c correlation	0.93	EDS
Total number of atoms	6162	wwPDB-VP
Average B, all atoms (Å^2)	108.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 5.06% 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: CA, HIC, ATP

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	0.51	0/2842	0.97	10/3852 (0.3%)
2	B	0.45	0/3395	0.81	3/4577 (0.1%)
All	All	0.48	0/6237	0.89	13/8429 (0.2%)

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

There are no bond length outliers.

All (13) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	210	ARG	N-CA-C	-8.04	89.28	111.00
2	B	1429	PHE	N-CA-C	-7.39	91.03	111.00
1	A	127	PHE	O-C-N	-6.87	111.71	122.70
1	A	140	LEU	CA-CB-CG	6.57	130.40	115.30
1	A	306	TYR	N-CA-C	-6.14	94.43	111.00
1	A	154	ASP	N-CA-C	-5.87	95.14	111.00
1	A	189	LEU	CA-CB-CG	5.85	128.75	115.30
1	A	221	LEU	CA-CB-CG	-5.79	101.99	115.30
1	A	145	SER	N-CA-C	-5.72	95.56	111.00
1	A	105	LEU	CA-CB-CG	5.51	127.96	115.30
2	B	1465	LEU	CA-CB-CG	-5.42	102.84	115.30
1	A	212	ILE	N-CA-C	-5.17	97.04	111.00
2	B	1562	SER	N-CA-C	-5.08	97.28	111.00

There are no chirality outliers.

All (1) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	127	PHE	Mainchain

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	2795	0	2765	557	0
2	B	3335	0	3349	424	0
3	A	1	0	0	0	0
4	A	31	0	12	13	0
All	All	6162	0	6126	958	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 78.

All (958) close contacts within the same asymmetric unit are listed below, sorted by their clash magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:350:SER:OG	2:B:1411:ARG:HB3	1.39	1.21
1:A:350:SER:HB2	2:B:1411:ARG:HD3	1.27	1.15
1:A:259:GLU:HG3	1:A:263:GLN:HG3	1.29	1.11
2:B:1456:LEU:HD21	2:B:1532:LEU:HD23	1.25	1.10
1:A:196:ARG:HH22	1:A:251:GLY:HA3	1.15	1.09
2:B:1585:GLN:HA	2:B:1585:GLN:HE21	1.16	1.09
1:A:154:ASP:HA	1:A:300:SER:HB3	1.29	1.05
2:B:1474:SER:HB3	2:B:1477:LEU:HG	1.37	1.04
1:A:305:MET:HG3	1:A:305:MET:O	1.59	1.00
2:B:1473:VAL:HG22	2:B:1514:TYR:OH	1.61	1.00
2:B:1545:LEU:HD23	2:B:1649:CYS:SG	2.03	0.99
1:A:189:LEU:HD12	1:A:190:MET:N	1.80	0.97
2:B:1577:ASN:HA	2:B:1585:GLN:HE22	1.30	0.97
1:A:35:VAL:HG13	1:A:54:VAL:HG23	1.44	0.96
1:A:185:LEU:HD21	1:A:260:THR:OG1	1.64	0.96
1:A:217:CYS:H	1:A:254:ARG:HG2	1.31	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:313:MET:SD	1:A:317:ILE:HD11	2.05	0.95
1:A:37:ARG:HH22	1:A:84:LYS:HE2	1.30	0.94
1:A:8:LEU:HD13	1:A:94:LEU:CD1	1.96	0.94
2:B:1516:GLN:HE21	2:B:1516:GLN:N	1.65	0.94
1:A:150:GLY:HA2	1:A:293:LEU:HD23	1.47	0.93
1:A:189:LEU:HD11	1:A:209:VAL:HG12	1.50	0.91
1:A:160:THR:HB	1:A:178:LEU:HD23	1.50	0.91
1:A:350:SER:CB	2:B:1411:ARG:HB3	2.00	0.90
1:A:336:LYS:HE3	1:A:337:TYR:HE1	1.34	0.90
1:A:93:GLU:O	1:A:94:LEU:HD23	1.70	0.90
1:A:99:GLU:HG3	1:A:128:ASN:HB2	1.53	0.90
2:B:1550:ARG:HD3	2:B:1554:LYS:HE2	1.53	0.90
1:A:242:LEU:HD11	1:A:248:ILE:HG12	1.52	0.90
1:A:217:CYS:HA	1:A:254:ARG:CA	2.03	0.89
1:A:257:CYS:O	1:A:260:THR:HG23	1.72	0.89
1:A:26:ALA:HB1	1:A:27:PRO:HD2	1.52	0.89
1:A:213:LYS:HA	1:A:217:CYS:SG	2.13	0.88
2:B:1594:LEU:O	2:B:1597:LEU:HG	1.73	0.88
1:A:264:PRO:HG2	1:A:271:SER:O	1.73	0.88
1:A:295:ALA:HB2	1:A:326:LYS:HE2	1.56	0.87
1:A:180:LEU:HD23	1:A:181:ALA:N	1.90	0.86
1:A:257:CYS:SG	1:A:258:PRO:HD3	2.16	0.86
1:A:192:ILE:HD12	1:A:193:LEU:N	1.91	0.85
1:A:301:GLY:HA2	1:A:336:LYS:HA	1.58	0.85
1:A:350:SER:HB2	2:B:1411:ARG:CD	2.05	0.85
1:A:122:ILE:O	1:A:126:THR:HB	1.76	0.85
2:B:1626:ASP:O	2:B:1630:GLU:HG3	1.77	0.84
2:B:1628:LEU:HD11	2:B:1740:TYR:CD2	2.13	0.84
2:B:1513:ILE:HD12	2:B:1513:ILE:H	1.40	0.84
1:A:8:LEU:HD13	1:A:94:LEU:HD12	1.60	0.83
1:A:260:THR:HA	1:A:263:GLN:O	1.77	0.83
2:B:1742:LYS:O	2:B:1746:GLN:HG3	1.78	0.83
1:A:54:VAL:HG12	1:A:88:HIS:CD2	2.13	0.83
1:A:196:ARG:NH2	1:A:251:GLY:HA3	1.93	0.82
2:B:1519:VAL:O	2:B:1522:GLU:HB2	1.78	0.82
1:A:166:TYR:CD2	1:A:167:GLU:HG3	2.12	0.82
2:B:1642:ILE:HG22	2:B:1727:ILE:HG23	1.61	0.82
1:A:261:LEU:HD21	1:A:303:THR:CG2	2.09	0.82
2:B:1497:ALA:C	2:B:1499:PRO:HD3	2.00	0.82
1:A:73:HIC:HD2	1:A:179:ASP:OD1	1.78	0.82
1:A:217:CYS:HA	1:A:254:ARG:HA	1.60	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:157:ASP:HA	1:A:182:GLY:HA3	1.61	0.82
2:B:1700:ASP:O	2:B:1704:LEU:HG	1.77	0.82
2:B:1654:GLN:HE21	2:B:1658:ASN:ND2	1.78	0.82
1:A:215:LYS:O	1:A:216:LEU:HG	1.78	0.82
1:A:327:ILE:O	1:A:327:ILE:HG22	1.79	0.82
1:A:336:LYS:HG3	1:A:337:TYR:CD1	2.15	0.81
1:A:137:GLN:O	1:A:138:ALA:O	1.98	0.81
1:A:314:GLN:HA	1:A:329:ILE:HD12	1.61	0.80
1:A:277:THR:HA	1:A:280:ASN:HD21	1.46	0.80
1:A:330:ILE:HD12	1:A:330:ILE:H	1.47	0.80
2:B:1577:ASN:CA	2:B:1585:GLN:HE22	1.94	0.80
1:A:54:VAL:HG12	1:A:88:HIS:HD2	1.46	0.80
1:A:186:THR:HG23	1:A:210:ARG:HA	1.63	0.80
2:B:1562:SER:H	2:B:1566:ARG:NH2	1.79	0.80
2:B:1528:ARG:HH11	2:B:1528:ARG:HG2	1.45	0.80
1:A:165:ILE:HG22	1:A:166:TYR:H	1.47	0.79
1:A:287:ILE:HA	1:A:290:ARG:HE	1.45	0.79
1:A:262:PHE:HA	1:A:275:HIS:CE1	2.16	0.79
1:A:151:ILE:HD12	1:A:282:ILE:HG13	1.63	0.79
1:A:155:SER:HB2	1:A:160:THR:HG23	1.62	0.79
2:B:1688:LEU:N	2:B:1689:PRO:HD2	1.98	0.79
1:A:192:ILE:HA	1:A:195:GLU:HG3	1.64	0.78
1:A:223:PHE:CE2	1:A:259:GLU:HG2	2.18	0.78
1:A:306:TYR:O	1:A:309:ILE:HG22	1.83	0.78
2:B:1516:GLN:NE2	2:B:1516:GLN:N	2.32	0.78
1:A:162:ASN:HB2	1:A:176:MET:HB2	1.66	0.78
1:A:354:GLN:HE22	2:B:1415:LEU:HD21	1.48	0.78
2:B:1528:ARG:NH1	2:B:1532:LEU:HD13	1.98	0.78
2:B:1656:ILE:C	2:B:1658:ASN:H	1.87	0.78
2:B:1446:LYS:HE3	2:B:1677:LEU:HD21	1.64	0.77
2:B:1685:LEU:HD22	2:B:1685:LEU:H	1.50	0.77
2:B:1530:ARG:O	2:B:1534:VAL:HG23	1.85	0.77
2:B:1561:GLU:HA	2:B:1566:ARG:HH22	1.49	0.77
1:A:161:HIS:HD2	1:A:177:ARG:HA	1.51	0.76
2:B:1414:ASP:OD1	2:B:1508:GLN:HG2	1.85	0.76
2:B:1516:GLN:NE2	2:B:1516:GLN:H	1.82	0.76
1:A:359:LYS:HG2	2:B:1404:ILE:CD1	2.16	0.76
2:B:1585:GLN:HA	2:B:1585:GLN:NE2	1.99	0.76
1:A:282:ILE:HG12	1:A:293:LEU:HD13	1.66	0.76
1:A:176:MET:HG3	1:A:281:SER:HB2	1.68	0.76
1:A:335:ARG:C	1:A:337:TYR:H	1.87	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1445:VAL:HG12	2:B:1449:LEU:HD11	1.67	0.75
2:B:1674:PHE:HD2	2:B:1674:PHE:N	1.82	0.75
1:A:306:TYR:HD1	4:A:2000:ATP:H2	1.34	0.75
2:B:1571:VAL:O	2:B:1575:VAL:HG23	1.85	0.75
2:B:1668:LEU:HA	2:B:1674:PHE:HZ	1.51	0.74
1:A:336:LYS:HG3	1:A:337:TYR:HD1	1.51	0.74
2:B:1420:PHE:CD2	2:B:1480:ASN:HB3	2.22	0.74
1:A:227:MET:SD	1:A:252:ASN:ND2	2.61	0.74
1:A:316:GLU:O	1:A:319:ALA:HB3	1.87	0.74
1:A:190:MET:CE	1:A:206:ARG:HB2	2.18	0.74
2:B:1517:LEU:HD13	2:B:1525:TRP:CH2	2.23	0.74
2:B:1564:ASN:OD1	2:B:1624:PHE:HA	1.88	0.73
1:A:188:TYR:O	1:A:191:LYS:HB3	1.88	0.73
1:A:53:TYR:CD1	1:A:61:LYS:HD3	2.24	0.73
1:A:189:LEU:HD11	1:A:209:VAL:CG1	2.18	0.73
1:A:189:LEU:HD21	1:A:209:VAL:O	1.87	0.73
1:A:292:ASP:HA	1:A:295:ALA:HB3	1.70	0.73
1:A:116:ARG:O	1:A:120:THR:HG22	1.89	0.72
1:A:196:ARG:HH22	1:A:251:GLY:CA	1.98	0.72
1:A:261:LEU:HD21	1:A:303:THR:HG21	1.69	0.72
2:B:1514:TYR:HA	2:B:1518:MET:CE	2.19	0.72
1:A:301:GLY:CA	1:A:336:LYS:HA	2.18	0.72
1:A:305:MET:O	1:A:305:MET:CG	2.37	0.72
2:B:1687:VAL:C	2:B:1689:PRO:HD2	2.11	0.72
1:A:229:THR:HB	1:A:236:LEU:HD11	1.71	0.72
1:A:10:CYS:HA	1:A:19:ALA:HB2	1.71	0.72
2:B:1380:GLU:O	2:B:1383:ALA:HB3	1.90	0.72
1:A:35:VAL:HG22	1:A:54:VAL:CG2	2.19	0.71
1:A:37:ARG:HH12	1:A:52:SER:HB3	1.54	0.71
2:B:1694:LYS:HA	2:B:1697:LEU:HB2	1.72	0.71
2:B:1528:ARG:HH11	2:B:1528:ARG:CG	2.02	0.71
2:B:1608:THR:HG22	2:B:1611:ASN:ND2	2.05	0.71
1:A:160:THR:HB	1:A:178:LEU:CD2	2.21	0.71
1:A:218:TYR:O	1:A:255:PHE:HA	1.90	0.71
1:A:313:MET:HG3	1:A:317:ILE:HG13	1.71	0.71
1:A:109:PRO:HD2	1:A:161:HIS:ND1	2.06	0.71
2:B:1418:ILE:HB	2:B:1507:LEU:HD23	1.73	0.71
1:A:295:ALA:CB	1:A:326:LYS:HE2	2.21	0.71
1:A:34:ILE:HG12	1:A:69:TYR:CE1	2.24	0.71
2:B:1723:LYS:HA	2:B:1726:LYS:HD2	1.72	0.71
1:A:277:THR:HA	1:A:280:ASN:ND2	2.05	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1516:GLN:O	2:B:1517:LEU:HD23	1.92	0.70
1:A:112:PRO:HB2	1:A:115:ASN:HD21	1.56	0.70
1:A:196:ARG:HH12	1:A:251:GLY:N	1.88	0.70
2:B:1513:ILE:HD12	2:B:1513:ILE:N	2.06	0.70
2:B:1540:ARG:C	2:B:1542:TYR:H	1.95	0.70
1:A:306:TYR:CD1	4:A:2000:ATP:H2	2.09	0.70
2:B:1534:VAL:HG21	2:B:1659:VAL:HG21	1.74	0.70
2:B:1674:PHE:CD2	2:B:1674:PHE:N	2.56	0.70
2:B:1670:ASP:O	2:B:1672:SER:N	2.25	0.70
2:B:1621:TYR:C	2:B:1623:SER:H	1.95	0.70
2:B:1729:PHE:O	2:B:1732:LYS:HG3	1.92	0.70
2:B:1577:ASN:HA	2:B:1585:GLN:NE2	2.05	0.69
2:B:1457:GLN:O	2:B:1459:PRO:HD3	1.92	0.69
1:A:210:ARG:CG	1:A:211:ASP:N	2.56	0.69
1:A:350:SER:OG	2:B:1411:ARG:CB	2.31	0.69
1:A:353:GLN:HG2	1:A:356:TRP:CD1	2.28	0.69
1:A:176:MET:CG	1:A:281:SER:HB2	2.21	0.69
1:A:257:CYS:SG	1:A:258:PRO:CD	2.81	0.69
2:B:1540:ARG:HA	2:B:1543:ASN:HD22	1.58	0.69
1:A:201:VAL:HG23	1:A:202:THR:N	2.08	0.69
2:B:1654:GLN:HE21	2:B:1658:ASN:HD21	1.38	0.68
1:A:287:ILE:HA	1:A:290:ARG:NE	2.08	0.68
1:A:128:ASN:HD22	1:A:128:ASN:N	1.91	0.68
1:A:330:ILE:HD12	1:A:330:ILE:N	2.07	0.68
1:A:283:MET:HA	1:A:290:ARG:NH1	2.09	0.68
2:B:1480:ASN:HD22	2:B:1480:ASN:N	1.89	0.68
2:B:1486:THR:HG21	2:B:1488:TRP:CE2	2.28	0.68
1:A:8:LEU:CD1	1:A:94:LEU:CD1	2.68	0.68
2:B:1429:PHE:O	2:B:1431:ILE:N	2.26	0.68
1:A:210:ARG:HG3	1:A:211:ASP:N	2.07	0.68
2:B:1628:LEU:HD22	2:B:1741:LYS:HG2	1.75	0.68
1:A:367:PRO:O	1:A:369:ILE:N	2.27	0.68
2:B:1451:CYS:SG	2:B:1532:LEU:HD21	2.34	0.68
1:A:262:PHE:HA	1:A:275:HIS:HE1	1.57	0.68
1:A:54:VAL:HG13	1:A:55:GLY:N	2.09	0.68
1:A:242:LEU:HD11	1:A:248:ILE:CG1	2.24	0.68
2:B:1409:SER:HA	2:B:1412:LYS:HB3	1.76	0.68
1:A:146:GLY:O	2:B:1431:ILE:HG21	1.93	0.68
1:A:98:PRO:O	1:A:100:GLU:N	2.27	0.68
1:A:157:ASP:O	1:A:182:GLY:N	2.27	0.67
1:A:259:GLU:CG	1:A:263:GLN:HG3	2.16	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:165:ILE:HG22	1:A:166:TYR:N	2.08	0.67
2:B:1493:ASN:HD22	2:B:1495:GLU:HG2	1.59	0.67
1:A:139:VAL:H	1:A:165:ILE:HD11	1.57	0.67
1:A:287:ILE:HA	1:A:290:ARG:HG3	1.77	0.67
2:B:1498:LYS:HG2	2:B:1498:LYS:O	1.93	0.67
2:B:1681:LEU:O	2:B:1685:LEU:HD23	1.95	0.67
2:B:1366:LEU:HD12	2:B:1367:ASP:N	2.10	0.67
1:A:203:THR:O	1:A:206:ARG:HB3	1.96	0.66
1:A:37:ARG:HG2	1:A:37:ARG:HH11	1.60	0.66
2:B:1674:PHE:O	2:B:1675:HIS:C	2.32	0.66
2:B:1421:LEU:HD12	2:B:1511:ASP:OD1	1.96	0.66
1:A:11:ASP:HA	1:A:106:THR:OG1	1.95	0.66
1:A:218:TYR:H	1:A:254:ARG:HB3	1.59	0.66
1:A:281:SER:O	1:A:284:LYS:HB2	1.95	0.66
2:B:1608:THR:HG22	2:B:1611:ASN:CG	2.16	0.66
1:A:162:ASN:CB	1:A:176:MET:HB2	2.26	0.66
2:B:1431:ILE:O	2:B:1434:HIS:HB3	1.95	0.66
2:B:1464:PHE:HE1	2:B:1470:ILE:HG13	1.60	0.66
2:B:1618:ARG:HA	2:B:1622:PRO:HB3	1.78	0.66
2:B:1464:PHE:CE1	2:B:1470:ILE:HG13	2.31	0.66
1:A:330:ILE:HG22	1:A:331:ALA:N	2.09	0.66
1:A:38:PRO:CD	1:A:65:LEU:HD23	2.25	0.66
1:A:78:ASN:OD1	1:A:81:ASP:HB2	1.95	0.66
2:B:1708:GLU:O	2:B:1711:SER:HB3	1.96	0.66
2:B:1670:ASP:C	2:B:1672:SER:H	1.98	0.65
2:B:1632:GLU:N	2:B:1633:PRO:HD2	2.11	0.65
2:B:1643:GLU:O	2:B:1643:GLU:HG3	1.96	0.65
1:A:238:LYS:HE3	1:A:254:ARG:NH1	2.11	0.65
1:A:210:ARG:O	1:A:213:LYS:HB2	1.97	0.65
1:A:8:LEU:HD21	1:A:21:PHE:CD2	2.31	0.65
2:B:1497:ALA:O	2:B:1499:PRO:HD3	1.96	0.65
2:B:1480:ASN:ND2	2:B:1480:ASN:N	2.45	0.65
1:A:189:LEU:HD12	1:A:190:MET:CA	2.26	0.65
2:B:1422:SER:HB2	2:B:1424:ASP:OD1	1.96	0.65
1:A:62:ARG:HD3	1:A:63:GLY:N	2.11	0.65
4:A:2000:ATP:H8	4:A:2000:ATP:H3'	1.62	0.65
2:B:1513:ILE:CD1	2:B:1513:ILE:H	2.09	0.65
2:B:1681:LEU:HD23	2:B:1685:LEU:HD21	1.77	0.65
1:A:138:ALA:O	1:A:140:LEU:N	2.30	0.65
2:B:1737:ILE:O	2:B:1740:TYR:HB3	1.97	0.64
1:A:5:THR:HG21	2:B:1408:ALA:HA	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1446:LYS:HG3	2:B:1677:LEU:HD22	1.79	0.64
1:A:170:ALA:O	1:A:172:PRO:HD3	1.97	0.64
2:B:1540:ARG:HG3	2:B:1541:GLU:N	2.13	0.64
2:B:1713:MET:HG2	2:B:1718:GLU:HB2	1.80	0.64
2:B:1528:ARG:O	2:B:1532:LEU:HD12	1.97	0.64
1:A:336:LYS:HE3	1:A:337:TYR:CE1	2.26	0.64
2:B:1447:LYS:HA	2:B:1452:ASP:OD2	1.97	0.64
1:A:209:VAL:HG12	1:A:209:VAL:O	1.98	0.64
1:A:262:PHE:CA	1:A:275:HIS:HE1	2.10	0.64
1:A:290:ARG:O	1:A:294:TYR:HD2	1.80	0.64
1:A:240:TYR:HB3	1:A:248:ILE:HD11	1.80	0.64
2:B:1445:VAL:HG13	2:B:1517:LEU:HD21	1.80	0.64
2:B:1756:LEU:C	2:B:1758:ILE:H	2.00	0.64
2:B:1660:GLU:OE2	2:B:1692:ARG:HD2	1.98	0.63
1:A:312:ARG:HD2	1:A:312:ARG:O	1.97	0.63
1:A:31:PHE:HE1	1:A:93:GLU:HG3	1.64	0.63
1:A:262:PHE:HD1	1:A:275:HIS:ND1	1.97	0.63
1:A:185:LEU:HB3	1:A:213:LYS:HE3	1.78	0.63
1:A:81:ASP:O	1:A:84:LYS:HB2	1.98	0.63
2:B:1573:LEU:HD11	2:B:1586:ALA:O	1.98	0.63
2:B:1480:ASN:H	2:B:1480:ASN:ND2	1.95	0.63
1:A:194:THR:C	1:A:196:ARG:H	2.02	0.63
2:B:1528:ARG:NH1	2:B:1532:LEU:CD1	2.62	0.63
2:B:1656:ILE:C	2:B:1658:ASN:N	2.52	0.63
1:A:330:ILE:CD1	1:A:330:ILE:H	2.11	0.63
2:B:1573:LEU:O	2:B:1577:ASN:ND2	2.30	0.63
1:A:285:CYS:SG	1:A:289:ILE:HD11	2.39	0.63
2:B:1611:ASN:HD22	2:B:1743:ALA:HB1	1.63	0.63
2:B:1755:ARG:O	2:B:1758:ILE:HB	1.99	0.63
1:A:323:SER:HB3	2:B:1639:LYS:HD2	1.80	0.62
1:A:190:MET:SD	1:A:206:ARG:HG3	2.39	0.62
1:A:212:ILE:HG22	1:A:213:LYS:N	2.14	0.62
2:B:1539:GLU:O	2:B:1542:TYR:HB3	2.00	0.62
2:B:1677:LEU:O	2:B:1679:LYS:N	2.32	0.62
1:A:188:TYR:O	1:A:188:TYR:CD2	2.53	0.62
1:A:136:ILE:HD12	1:A:136:ILE:N	2.14	0.62
1:A:226:GLU:HG2	1:A:255:PHE:HE1	1.64	0.62
1:A:257:CYS:O	1:A:259:GLU:N	2.32	0.62
1:A:313:MET:O	1:A:315:LYS:N	2.33	0.62
2:B:1445:VAL:HG12	2:B:1449:LEU:CD1	2.29	0.62
2:B:1727:ILE:C	2:B:1729:PHE:H	2.03	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:304:THR:O	1:A:309:ILE:HD12	2.00	0.61
2:B:1675:HIS:O	2:B:1677:LEU:N	2.33	0.61
2:B:1498:LYS:O	2:B:1500:PRO:HD3	2.00	0.61
2:B:1542:TYR:HB2	2:B:1652:PHE:CZ	2.35	0.61
1:A:120:THR:HB	1:A:370:VAL:HG21	1.83	0.61
1:A:128:ASN:ND2	1:A:128:ASN:N	2.47	0.61
1:A:152:VAL:HG12	1:A:153:LEU:N	2.13	0.61
2:B:1516:GLN:HE21	2:B:1516:GLN:CA	2.12	0.61
1:A:342:GLY:HA2	1:A:345:ILE:HD12	1.83	0.61
2:B:1614:GLU:HG2	2:B:1740:TYR:CE2	2.36	0.61
2:B:1701:GLU:HA	2:B:1704:LEU:HD12	1.83	0.61
4:A:2000:ATP:C8	4:A:2000:ATP:H3'	2.35	0.61
1:A:10:CYS:HA	1:A:19:ALA:CB	2.30	0.61
1:A:350:SER:O	1:A:352:PHE:N	2.34	0.61
1:A:137:GLN:C	1:A:138:ALA:O	2.38	0.60
1:A:226:GLU:HG2	1:A:255:PHE:CE1	2.36	0.60
1:A:258:PRO:HB3	1:A:306:TYR:CE2	2.35	0.60
1:A:142:LEU:HD21	1:A:148:THR:HA	1.83	0.60
1:A:353:GLN:OE1	2:B:1412:LYS:HD3	2.01	0.60
1:A:359:LYS:HG2	2:B:1404:ILE:HD13	1.83	0.60
2:B:1611:ASN:HA	2:B:1747:ASN:HD21	1.65	0.60
2:B:1386:LEU:HD22	2:B:1391:VAL:HG21	1.84	0.60
2:B:1628:LEU:HD11	2:B:1740:TYR:HD2	1.66	0.60
2:B:1413:GLU:C	2:B:1415:LEU:H	2.05	0.60
1:A:157:ASP:HA	1:A:182:GLY:CA	2.32	0.60
1:A:171:LEU:HD12	1:A:171:LEU:N	2.16	0.60
2:B:1420:PHE:CE2	2:B:1480:ASN:HB3	2.37	0.60
1:A:182:GLY:HA2	4:A:2000:ATP:O2'	2.02	0.60
1:A:223:PHE:HZ	1:A:256:ARG:HA	1.66	0.60
2:B:1681:LEU:CD2	2:B:1685:LEU:HD21	2.31	0.60
2:B:1429:PHE:C	2:B:1431:ILE:H	2.05	0.60
1:A:121:GLN:HG2	1:A:367:PRO:HG3	1.83	0.60
1:A:306:TYR:CD1	4:A:2000:ATP:C2	2.90	0.60
2:B:1620:ASN:HB3	2:B:1621:TYR:CE1	2.36	0.60
1:A:185:LEU:CB	1:A:213:LYS:HE3	2.32	0.59
2:B:1444:LEU:HD12	2:B:1444:LEU:C	2.23	0.59
2:B:1493:ASN:ND2	2:B:1495:GLU:HG2	2.16	0.59
1:A:99:GLU:CG	1:A:128:ASN:HB2	2.27	0.59
2:B:1487:ASP:HB3	2:B:1489:GLU:HG3	1.85	0.59
2:B:1498:LYS:O	2:B:1500:PRO:CD	2.50	0.59
1:A:36:GLY:C	1:A:65:LEU:HD22	2.23	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:364:GLU:OE1	1:A:364:GLU:N	2.35	0.59
1:A:286:ASP:OD2	1:A:288:ASP:HB2	2.02	0.59
2:B:1540:ARG:O	2:B:1542:TYR:N	2.36	0.59
1:A:217:CYS:N	1:A:254:ARG:HG2	2.11	0.59
1:A:257:CYS:N	1:A:258:PRO:HD2	2.18	0.59
1:A:35:VAL:HG22	1:A:54:VAL:HG22	1.84	0.59
1:A:26:ALA:HA	1:A:340:TRP:CZ3	2.38	0.59
2:B:1632:GLU:O	2:B:1635:LEU:N	2.36	0.58
2:B:1615:LYS:HE2	2:B:1751:GLU:OE2	2.02	0.58
1:A:350:SER:CB	2:B:1411:ARG:CB	2.79	0.58
1:A:204:ALA:O	1:A:208:ILE:HG13	2.03	0.58
1:A:260:THR:O	1:A:263:GLN:C	2.42	0.58
1:A:31:PHE:CE1	1:A:93:GLU:HG3	2.37	0.58
2:B:1723:LYS:O	2:B:1726:LYS:HB2	2.03	0.58
2:B:1456:LEU:HD21	2:B:1532:LEU:CD2	2.17	0.58
2:B:1624:PHE:C	2:B:1626:ASP:H	2.06	0.58
2:B:1360:GLN:HE21	2:B:1360:GLN:HA	1.68	0.58
1:A:250:ILE:HG13	1:A:253:GLU:HB2	1.85	0.58
1:A:192:ILE:HD12	1:A:193:LEU:H	1.69	0.58
1:A:167:GLU:O	1:A:169:TYR:N	2.37	0.58
1:A:185:LEU:C	1:A:187:ASP:N	2.57	0.58
1:A:251:GLY:N	1:A:253:GLU:HG2	2.19	0.58
1:A:217:CYS:HA	1:A:254:ARG:CB	2.32	0.58
2:B:1674:PHE:HD2	2:B:1674:PHE:H	1.52	0.58
2:B:1514:TYR:HA	2:B:1518:MET:HE3	1.85	0.58
2:B:1409:SER:O	2:B:1412:LYS:N	2.37	0.58
2:B:1618:ARG:O	2:B:1619:LEU:HD23	2.04	0.58
1:A:157:ASP:OD1	1:A:183:ARG:N	2.30	0.58
2:B:1656:ILE:O	2:B:1658:ASN:N	2.37	0.58
1:A:22:ALA:O	1:A:23:GLY:C	2.42	0.58
1:A:368:SER:HA	1:A:371:HIS:HD2	1.69	0.58
1:A:248:ILE:O	1:A:248:ILE:HD12	2.04	0.57
1:A:9:VAL:O	1:A:9:VAL:HG12	2.04	0.57
1:A:334:GLU:HG2	1:A:334:GLU:O	2.04	0.57
1:A:223:PHE:C	1:A:225:ASN:H	2.07	0.57
2:B:1432:ASN:N	2:B:1432:ASN:OD1	2.37	0.57
1:A:150:GLY:HA2	1:A:293:LEU:CD2	2.27	0.57
1:A:192:ILE:HA	1:A:195:GLU:CG	2.34	0.57
1:A:265:SER:O	1:A:268:GLY:N	2.37	0.57
4:A:2000:ATP:C8	4:A:2000:ATP:C3'	2.88	0.57
2:B:1657:VAL:HG12	2:B:1657:VAL:O	2.04	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:201:VAL:HG23	1:A:202:THR:H	1.67	0.57
2:B:1528:ARG:HH12	2:B:1532:LEU:HD13	1.67	0.57
2:B:1627:PHE:CE1	2:B:1628:LEU:HG	2.39	0.57
2:B:1451:CYS:HB3	2:B:1456:LEU:HD11	1.87	0.57
2:B:1553:ASP:OD1	2:B:1705:THR:HG23	2.04	0.57
2:B:1542:TYR:HB2	2:B:1652:PHE:HZ	1.70	0.57
1:A:350:SER:HB2	2:B:1411:ARG:HB3	1.84	0.57
1:A:157:ASP:O	1:A:181:ALA:HB3	2.04	0.57
1:A:189:LEU:CD1	1:A:190:MET:N	2.61	0.57
2:B:1499:PRO:O	2:B:1501:GLU:HG3	2.05	0.57
1:A:362:TYR:O	1:A:366:GLY:N	2.37	0.57
1:A:186:THR:HG23	1:A:210:ARG:CA	2.34	0.57
1:A:8:LEU:CD2	1:A:21:PHE:CD2	2.88	0.57
2:B:1685:LEU:HB2	2:B:1686:PRO:HD3	1.87	0.57
1:A:335:ARG:C	1:A:337:TYR:N	2.56	0.57
1:A:161:HIS:CD2	1:A:177:ARG:HA	2.35	0.57
1:A:37:ARG:NH1	1:A:52:SER:HB3	2.19	0.56
2:B:1621:TYR:O	2:B:1623:SER:N	2.38	0.56
1:A:323:SER:HB3	2:B:1639:LYS:CD	2.34	0.56
1:A:279:TYR:HE1	1:A:321:ALA:HA	1.70	0.56
2:B:1413:GLU:C	2:B:1415:LEU:N	2.56	0.56
1:A:219:VAL:HA	1:A:255:PHE:HB2	1.86	0.56
1:A:154:ASP:CA	1:A:300:SER:HB3	2.20	0.56
1:A:188:TYR:C	1:A:188:TYR:CD2	2.78	0.56
2:B:1567:ASN:O	2:B:1570:ASN:HB2	2.05	0.56
2:B:1759:LYS:HD2	2:B:1760:HIS:CE1	2.40	0.56
1:A:152:VAL:CG1	1:A:153:LEU:N	2.68	0.56
2:B:1659:VAL:O	2:B:1663:VAL:HG23	2.05	0.56
2:B:1394:ASP:C	2:B:1396:GLU:N	2.59	0.56
1:A:311:ASP:N	1:A:311:ASP:OD2	2.30	0.56
1:A:87:HIS:O	1:A:88:HIS:C	2.44	0.56
1:A:8:LEU:HD21	1:A:21:PHE:CE2	2.40	0.56
1:A:300:SER:O	1:A:301:GLY:O	2.23	0.56
2:B:1712:LEU:O	2:B:1715:THR:HB	2.05	0.56
2:B:1618:ARG:HG2	2:B:1618:ARG:HH11	1.70	0.56
1:A:354:GLN:HE22	2:B:1415:LEU:CD2	2.17	0.56
2:B:1663:VAL:HG21	2:B:1688:LEU:HD11	1.88	0.56
1:A:301:GLY:HA2	1:A:336:LYS:CA	2.33	0.56
1:A:252:ASN:CG	1:A:252:ASN:O	2.43	0.56
2:B:1517:LEU:HD13	2:B:1525:TRP:HH2	1.70	0.56
2:B:1387:TYR:HA	2:B:1392:LEU:HG	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:128:ASN:H	1:A:128:ASN:ND2	2.03	0.55
2:B:1528:ARG:NH1	2:B:1528:ARG:CG	2.69	0.55
2:B:1723:LYS:N	2:B:1726:LYS:HE3	2.20	0.55
1:A:359:LYS:CG	2:B:1404:ILE:HD13	2.36	0.55
1:A:190:MET:HE1	1:A:206:ARG:HB2	1.87	0.55
1:A:198:TYR:HE2	1:A:248:ILE:HG22	1.72	0.55
1:A:312:ARG:HG2	1:A:312:ARG:HH11	1.70	0.55
1:A:264:PRO:CG	1:A:271:SER:O	2.50	0.55
2:B:1562:SER:H	2:B:1566:ARG:HH22	1.53	0.55
2:B:1628:LEU:HD22	2:B:1741:LYS:CG	2.36	0.55
1:A:252:ASN:N	1:A:253:GLU:OE2	2.39	0.55
1:A:139:VAL:HA	1:A:165:ILE:CD1	2.36	0.55
1:A:191:LYS:O	1:A:195:GLU:HG3	2.07	0.55
1:A:336:LYS:HG3	1:A:337:TYR:CE1	2.42	0.55
1:A:194:THR:O	1:A:197:GLY:N	2.40	0.55
1:A:70:PRO:HG3	1:A:81:ASP:HB3	1.88	0.55
1:A:327:ILE:O	1:A:327:ILE:CG2	2.52	0.55
1:A:196:ARG:HH12	1:A:251:GLY:H	1.54	0.55
1:A:9:VAL:HG12	1:A:340:TRP:NE1	2.21	0.55
1:A:149:THR:HG22	1:A:150:GLY:N	2.20	0.55
2:B:1491:VAL:HG13	2:B:1496:ASP:HB3	1.87	0.55
1:A:82:MET:HA	1:A:82:MET:HE3	1.87	0.55
1:A:99:GLU:HA	1:A:128:ASN:O	2.05	0.55
1:A:120:THR:HA	1:A:132:MET:CE	2.37	0.55
2:B:1366:LEU:HD12	2:B:1367:ASP:H	1.72	0.55
1:A:250:ILE:HG13	1:A:253:GLU:CG	2.37	0.55
1:A:262:PHE:O	1:A:264:PRO:HD3	2.06	0.55
1:A:277:THR:O	1:A:278:THR:C	2.45	0.55
1:A:78:ASN:OD1	1:A:81:ASP:N	2.39	0.54
2:B:1464:PHE:O	2:B:1467:LYS:HB2	2.07	0.54
2:B:1442:ALA:O	2:B:1443:ASP:C	2.46	0.54
1:A:78:ASN:CG	1:A:81:ASP:HB2	2.27	0.54
1:A:81:ASP:O	1:A:84:LYS:N	2.39	0.54
1:A:112:PRO:HD2	1:A:115:ASN:ND2	2.23	0.54
1:A:156:GLY:HA3	4:A:2000:ATP:PA	2.47	0.54
1:A:218:TYR:CE1	1:A:255:PHE:HB3	2.43	0.54
1:A:335:ARG:HA	1:A:338:SER:HB2	1.88	0.54
2:B:1496:ASP:O	2:B:1497:ALA:C	2.46	0.54
1:A:359:LYS:CG	2:B:1404:ILE:CD1	2.86	0.54
1:A:200:PHE:CD2	1:A:209:VAL:HG21	2.41	0.54
1:A:144:ALA:HB2	1:A:345:ILE:CD1	2.37	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:218:TYR:HD1	1:A:219:VAL:N	2.05	0.54
2:B:1675:HIS:CE1	2:B:1677:LEU:HD12	2.42	0.54
1:A:350:SER:CB	2:B:1411:ARG:HD3	2.19	0.54
1:A:252:ASN:ND2	1:A:252:ASN:O	2.40	0.54
1:A:345:ILE:C	1:A:347:ALA:H	2.11	0.54
2:B:1614:GLU:HG2	2:B:1740:TYR:CZ	2.43	0.54
2:B:1722:ASP:O	2:B:1723:LYS:C	2.46	0.54
1:A:38:PRO:HD3	1:A:65:LEU:HD23	1.90	0.54
2:B:1429:PHE:C	2:B:1431:ILE:N	2.62	0.54
1:A:112:PRO:O	1:A:115:ASN:ND2	2.40	0.54
1:A:196:ARG:NH1	1:A:251:GLY:H	2.05	0.53
1:A:21:PHE:CD1	1:A:21:PHE:N	2.75	0.53
1:A:69:TYR:O	1:A:71:ILE:N	2.42	0.53
1:A:262:PHE:CD1	1:A:275:HIS:ND1	2.74	0.53
2:B:1637:VAL:O	2:B:1640:VAL:HG12	2.08	0.53
2:B:1688:LEU:N	2:B:1689:PRO:CD	2.69	0.53
1:A:75:ILE:CD1	1:A:177:ARG:HH12	2.21	0.53
1:A:335:ARG:C	1:A:338:SER:H	2.11	0.53
2:B:1474:SER:CB	2:B:1477:LEU:HG	2.24	0.53
1:A:276:GLU:O	1:A:279:TYR:HB3	2.08	0.53
2:B:1483:PRO:O	2:B:1502:LYS:HB3	2.09	0.53
2:B:1670:ASP:C	2:B:1672:SER:N	2.62	0.53
2:B:1620:ASN:HB3	2:B:1621:TYR:CD1	2.43	0.53
1:A:238:LYS:O	1:A:250:ILE:N	2.40	0.53
1:A:258:PRO:HB3	1:A:306:TYR:CD2	2.43	0.53
2:B:1662:SER:O	2:B:1666:GLY:O	2.26	0.53
1:A:148:THR:O	1:A:149:THR:OG1	2.21	0.53
1:A:149:THR:CG2	1:A:150:GLY:N	2.72	0.53
1:A:54:VAL:CG1	1:A:55:GLY:N	2.72	0.53
1:A:359:LYS:HG2	2:B:1404:ILE:HD11	1.89	0.53
1:A:159:VAL:HG22	1:A:160:THR:N	2.23	0.53
1:A:180:LEU:O	1:A:181:ALA:HB2	2.09	0.53
1:A:66:THR:O	1:A:67:LEU:HD23	2.09	0.53
1:A:66:THR:C	1:A:67:LEU:HD23	2.29	0.53
1:A:27:PRO:HD2	1:A:337:TYR:CD2	2.44	0.53
1:A:127:PHE:HB2	1:A:129:VAL:HG13	1.91	0.53
1:A:29:ALA:O	1:A:30:VAL:HG23	2.09	0.53
1:A:240:TYR:CB	1:A:248:ILE:HD11	2.38	0.52
1:A:57:GLU:O	1:A:57:GLU:HG3	2.08	0.52
1:A:352:PHE:O	1:A:354:GLN:N	2.43	0.52
1:A:330:ILE:HG22	1:A:331:ALA:H	1.72	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:140:LEU:HD13	1:A:343:GLY:CA	2.38	0.52
1:A:24:ASP:OD2	1:A:28:ARG:NH2	2.43	0.52
2:B:1713:MET:CE	2:B:1720:SER:HA	2.39	0.52
2:B:1563:ASP:HA	2:B:1566:ARG:HE	1.73	0.52
2:B:1424:ASP:OD1	2:B:1424:ASP:N	2.42	0.52
2:B:1384:ASP:O	2:B:1387:TYR:HB3	2.10	0.52
1:A:336:LYS:O	1:A:337:TYR:CD1	2.62	0.52
2:B:1608:THR:O	2:B:1609:PHE:C	2.48	0.52
2:B:1643:GLU:O	2:B:1647:ASN:ND2	2.43	0.52
1:A:153:LEU:HD23	1:A:304:THR:CG2	2.39	0.52
1:A:221:LEU:HG	1:A:315:LYS:HD2	1.92	0.52
1:A:229:THR:O	1:A:229:THR:HG22	2.09	0.52
2:B:1486:THR:HB	2:B:1520:ASN:HD22	1.74	0.52
2:B:1719:ASP:C	2:B:1721:GLY:N	2.63	0.52
2:B:1453:ARG:O	2:B:1453:ARG:HG2	2.10	0.52
1:A:181:ALA:H	1:A:184:ASP:HB2	1.75	0.52
2:B:1455:PHE:HD2	2:B:1456:LEU:N	2.08	0.52
2:B:1573:LEU:HG	2:B:1577:ASN:ND2	2.25	0.52
2:B:1441:VAL:HG11	2:B:1512:GLN:OE1	2.09	0.52
2:B:1474:SER:O	2:B:1478:ALA:N	2.35	0.52
1:A:282:ILE:HG12	1:A:293:LEU:CD1	2.39	0.52
2:B:1540:ARG:HA	2:B:1543:ASN:ND2	2.23	0.52
1:A:70:PRO:HG3	1:A:81:ASP:CB	2.40	0.52
2:B:1525:TRP:NE1	2:B:1529:MET:HG3	2.23	0.52
2:B:1429:PHE:CD1	2:B:1464:PHE:HZ	2.27	0.52
1:A:147:ARG:HE	1:A:147:ARG:H	1.58	0.52
1:A:201:VAL:CG2	1:A:202:THR:H	2.23	0.52
1:A:17:VAL:C	1:A:18:LYS:HG3	2.30	0.52
2:B:1713:MET:HE1	2:B:1720:SER:HA	1.91	0.52
2:B:1756:LEU:C	2:B:1758:ILE:N	2.62	0.52
2:B:1605:ASN:ND2	2:B:1605:ASN:O	2.43	0.52
1:A:201:VAL:CG2	1:A:202:THR:N	2.72	0.51
1:A:203:THR:O	1:A:206:ARG:N	2.43	0.51
1:A:76:ILE:HD13	1:A:82:MET:HG2	1.92	0.51
1:A:8:LEU:CD1	1:A:94:LEU:HD12	2.33	0.51
2:B:1524:TYR:HE1	2:B:1678:ASP:OD1	1.93	0.51
1:A:112:PRO:HB2	1:A:115:ASN:ND2	2.25	0.51
2:B:1391:VAL:HG12	2:B:1392:LEU:N	2.25	0.51
1:A:186:THR:O	1:A:189:LEU:HG	2.09	0.51
2:B:1455:PHE:CD2	2:B:1456:LEU:N	2.78	0.51
2:B:1700:ASP:O	2:B:1703:LYS:HB2	2.10	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1563:ASP:N	2:B:1566:ARG:HH21	2.08	0.51
1:A:350:SER:HB2	2:B:1411:ARG:CG	2.39	0.51
1:A:180:LEU:HD23	1:A:180:LEU:C	2.31	0.51
1:A:208:ILE:HD12	1:A:208:ILE:O	2.11	0.51
1:A:210:ARG:O	1:A:213:LYS:N	2.43	0.51
1:A:335:ARG:CA	1:A:338:SER:HB2	2.41	0.51
2:B:1722:ASP:O	2:B:1724:PHE:N	2.44	0.51
2:B:1725:ALA:O	2:B:1729:PHE:HB2	2.10	0.51
2:B:1618:ARG:O	2:B:1622:PRO:HB3	2.09	0.51
1:A:260:THR:O	1:A:263:GLN:O	2.28	0.51
2:B:1503:ASP:CG	2:B:1504:PRO:HD2	2.30	0.51
1:A:305:MET:SD	1:A:336:LYS:HD3	2.50	0.51
1:A:335:ARG:NH1	1:A:335:ARG:HG2	2.25	0.51
2:B:1727:ILE:O	2:B:1729:PHE:N	2.44	0.51
1:A:229:THR:C	1:A:233:SER:HB3	2.31	0.51
2:B:1542:TYR:HA	2:B:1652:PHE:CE2	2.46	0.51
2:B:1486:THR:HG22	2:B:1487:ASP:N	2.26	0.51
1:A:180:LEU:HA	1:A:184:ASP:OD2	2.11	0.51
1:A:115:ASN:O	1:A:119:MET:HB2	2.10	0.51
2:B:1564:ASN:ND2	2:B:1626:ASP:HB2	2.26	0.51
2:B:1752:GLU:O	2:B:1755:ARG:HB2	2.10	0.51
1:A:306:TYR:HD1	4:A:2000:ATP:C2	2.22	0.51
2:B:1450:ASN:HA	2:B:1679:LYS:HG3	1.92	0.51
1:A:26:ALA:HB1	1:A:27:PRO:CD	2.35	0.51
1:A:330:ILE:CG2	1:A:331:ALA:N	2.74	0.51
1:A:353:GLN:O	1:A:353:GLN:NE2	2.40	0.51
1:A:36:GLY:O	1:A:65:LEU:HD22	2.11	0.50
2:B:1722:ASP:OD1	2:B:1724:PHE:HB2	2.10	0.50
1:A:64:ILE:HG13	1:A:65:LEU:H	1.76	0.50
1:A:8:LEU:HD23	1:A:21:PHE:HA	1.92	0.50
1:A:117:GLU:HB3	1:A:367:PRO:HB3	1.91	0.50
1:A:136:ILE:CD1	1:A:136:ILE:N	2.73	0.50
2:B:1712:LEU:HD12	2:B:1712:LEU:O	2.10	0.50
1:A:209:VAL:CG1	1:A:209:VAL:O	2.58	0.50
1:A:267:ILE:HD11	1:A:269:MET:HG3	1.93	0.50
1:A:250:ILE:HG13	1:A:253:GLU:HG2	1.92	0.50
1:A:257:CYS:C	1:A:259:GLU:N	2.64	0.50
1:A:118:LYS:O	1:A:122:ILE:HG12	2.12	0.50
2:B:1493:ASN:ND2	2:B:1496:ASP:H	2.09	0.50
2:B:1417:LYS:HB3	2:B:1506:ASP:O	2.11	0.50
2:B:1467:LYS:HB3	2:B:1470:ILE:HG12	1.94	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1567:ASN:O	2:B:1571:VAL:HG23	2.11	0.50
1:A:196:ARG:NH1	1:A:251:GLY:N	2.60	0.50
1:A:27:PRO:HD2	1:A:337:TYR:HD2	1.76	0.50
1:A:5:THR:CG2	2:B:1408:ALA:HA	2.42	0.50
1:A:218:TYR:CD1	1:A:219:VAL:N	2.79	0.50
1:A:313:MET:HG3	1:A:317:ILE:CG1	2.41	0.50
2:B:1458:THR:OG1	2:B:1461:VAL:HG23	2.12	0.50
1:A:269:MET:C	1:A:271:SER:H	2.13	0.50
2:B:1421:LEU:HD12	2:B:1511:ASP:HA	1.94	0.50
2:B:1727:ILE:C	2:B:1729:PHE:N	2.65	0.50
1:A:120:THR:HA	1:A:132:MET:HE1	1.93	0.50
2:B:1394:ASP:O	2:B:1397:LYS:N	2.45	0.50
1:A:185:LEU:HD21	1:A:260:THR:CB	2.42	0.50
2:B:1435:MET:HE2	2:B:1461:VAL:HG21	1.93	0.50
1:A:323:SER:HB3	2:B:1639:LYS:HB3	1.93	0.50
1:A:190:MET:SD	1:A:206:ARG:CG	3.00	0.49
1:A:257:CYS:C	1:A:259:GLU:H	2.14	0.49
2:B:1446:LYS:HE3	2:B:1677:LEU:CD2	2.39	0.49
1:A:265:SER:O	1:A:267:ILE:N	2.45	0.49
2:B:1611:ASN:CA	2:B:1747:ASN:HD21	2.25	0.49
2:B:1755:ARG:HG2	2:B:1755:ARG:HH11	1.77	0.49
2:B:1719:ASP:O	2:B:1721:GLY:N	2.45	0.49
2:B:1607:MET:SD	2:B:1612:TYR:HE1	2.34	0.49
1:A:157:ASP:CA	1:A:182:GLY:HA3	2.38	0.49
2:B:1484:TYR:HB2	2:B:1515:LEU:HD21	1.94	0.49
2:B:1581:ASP:O	2:B:1584:LYS:N	2.44	0.49
2:B:1354:PRO:HG3	2:B:1358:LEU:HD12	1.93	0.49
1:A:17:VAL:HG21	1:A:31:PHE:HE2	1.77	0.49
1:A:18:LYS:NZ	4:A:2000:ATP:O2A	2.45	0.49
1:A:261:LEU:C	1:A:274:ILE:HG22	2.32	0.49
1:A:99:GLU:O	1:A:130:PRO:HD3	2.12	0.49
2:B:1497:ALA:O	2:B:1499:PRO:CD	2.60	0.49
2:B:1537:SER:O	2:B:1539:GLU:N	2.46	0.49
2:B:1652:PHE:HD2	2:B:1698:LEU:HD22	1.77	0.49
1:A:27:PRO:CD	1:A:337:TYR:HD2	2.25	0.49
2:B:1591:LEU:C	2:B:1593:THR:H	2.15	0.49
1:A:237:GLU:HA	1:A:250:ILE:O	2.13	0.49
1:A:368:SER:HA	1:A:371:HIS:CD2	2.47	0.49
2:B:1565:LEU:HD11	2:B:1569:PHE:CE1	2.47	0.49
2:B:1607:MET:SD	2:B:1612:TYR:CE1	3.06	0.49
1:A:345:ILE:O	1:A:347:ALA:N	2.45	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1540:ARG:C	2:B:1542:TYR:N	2.63	0.49
2:B:1508:GLN:O	2:B:1511:ASP:N	2.46	0.49
1:A:215:LYS:O	1:A:216:LEU:CG	2.55	0.49
1:A:75:ILE:N	1:A:75:ILE:HD12	2.27	0.49
1:A:180:LEU:CD2	1:A:180:LEU:C	2.82	0.49
1:A:78:ASN:C	1:A:78:ASN:OD1	2.51	0.49
2:B:1624:PHE:O	2:B:1626:ASP:N	2.41	0.49
2:B:1414:ASP:CG	2:B:1508:GLN:HG2	2.34	0.49
1:A:129:VAL:O	1:A:129:VAL:HG23	2.12	0.49
1:A:194:THR:HA	1:A:198:TYR:H	1.78	0.48
1:A:37:ARG:HG2	1:A:37:ARG:NH1	2.27	0.48
2:B:1528:ARG:HH12	2:B:1532:LEU:CD1	2.24	0.48
2:B:1522:GLU:O	2:B:1524:TYR:N	2.46	0.48
2:B:1755:ARG:HG2	2:B:1755:ARG:NH1	2.28	0.48
1:A:360:GLN:O	1:A:364:GLU:OE1	2.31	0.48
1:A:185:LEU:C	1:A:187:ASP:H	2.16	0.48
1:A:123:MET:HG3	1:A:132:MET:HE2	1.95	0.48
2:B:1386:LEU:O	2:B:1391:VAL:HB	2.13	0.48
2:B:1515:LEU:HB3	2:B:1516:GLN:NE2	2.29	0.48
2:B:1527:SER:HA	2:B:1530:ARG:HG3	1.95	0.48
2:B:1663:VAL:HG11	2:B:1685:LEU:HD11	1.96	0.48
2:B:1414:ASP:O	2:B:1508:GLN:HG3	2.13	0.48
1:A:353:GLN:HG2	1:A:356:TRP:HD1	1.76	0.48
2:B:1429:PHE:CE1	2:B:1464:PHE:HZ	2.32	0.48
2:B:1455:PHE:C	2:B:1455:PHE:CD2	2.87	0.48
1:A:362:TYR:HE1	1:A:367:PRO:HD3	1.78	0.48
2:B:1486:THR:CG2	2:B:1487:ASP:N	2.77	0.48
1:A:34:ILE:CD1	1:A:69:TYR:HE1	2.26	0.48
2:B:1528:ARG:HH11	2:B:1532:LEU:HD13	1.77	0.48
2:B:1723:LYS:HA	2:B:1726:LYS:CD	2.42	0.48
2:B:1418:ILE:N	2:B:1506:ASP:O	2.46	0.48
1:A:130:PRO:O	1:A:358:THR:HA	2.14	0.48
1:A:165:ILE:CG2	1:A:166:TYR:H	2.24	0.48
2:B:1424:ASP:O	2:B:1427:GLN:HB3	2.14	0.48
1:A:143:TYR:CE2	1:A:346:LEU:HD22	2.48	0.48
1:A:208:ILE:HD12	1:A:209:VAL:HG23	1.95	0.48
2:B:1444:LEU:HD12	2:B:1444:LEU:O	2.14	0.48
1:A:350:SER:HB2	2:B:1411:ARG:CB	2.43	0.47
1:A:261:LEU:HB3	1:A:274:ILE:HG21	1.95	0.47
1:A:332:PRO:HB3	1:A:333:PRO:HD2	1.94	0.47
1:A:362:TYR:CD1	1:A:366:GLY:HA2	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:367:PRO:C	1:A:369:ILE:H	2.17	0.47
1:A:22:ALA:O	1:A:24:ASP:N	2.47	0.47
2:B:1665:ILE:HG13	2:B:1665:ILE:O	2.14	0.47
1:A:18:LYS:HZ3	4:A:2000:ATP:PA	2.37	0.47
1:A:262:PHE:CA	1:A:275:HIS:CE1	2.88	0.47
1:A:194:THR:C	1:A:196:ARG:N	2.66	0.47
2:B:1663:VAL:HG21	2:B:1688:LEU:CD1	2.44	0.47
1:A:341:ILE:HG22	1:A:342:GLY:N	2.28	0.47
1:A:119:MET:O	1:A:122:ILE:HB	2.14	0.47
2:B:1719:ASP:C	2:B:1721:GLY:H	2.17	0.47
1:A:185:LEU:HD21	1:A:260:THR:CG2	2.45	0.47
2:B:1685:LEU:CD2	2:B:1685:LEU:H	2.25	0.47
2:B:1591:LEU:C	2:B:1593:THR:N	2.68	0.47
2:B:1490:GLY:O	2:B:1491:VAL:C	2.53	0.47
1:A:273:GLY:O	1:A:276:GLU:HB2	2.13	0.47
1:A:62:ARG:HD3	1:A:62:ARG:C	2.35	0.47
1:A:155:SER:OG	1:A:155:SER:O	2.24	0.47
1:A:213:LYS:O	1:A:217:CYS:HB2	2.14	0.47
1:A:217:CYS:HA	1:A:254:ARG:C	2.34	0.47
1:A:309:ILE:HA	1:A:312:ARG:HB3	1.96	0.47
2:B:1662:SER:OG	2:B:1668:LEU:HD12	2.15	0.47
2:B:1372:SER:OG	2:B:1373:ILE:N	2.48	0.47
2:B:1533:THR:HG22	2:B:1534:VAL:N	2.30	0.47
2:B:1668:LEU:HA	2:B:1674:PHE:CZ	2.41	0.47
1:A:120:THR:HG21	1:A:370:VAL:HB	1.96	0.47
2:B:1710:GLU:HB3	2:B:1720:SER:HB3	1.95	0.47
2:B:1602:ASP:HB3	2:B:1607:MET:HB2	1.97	0.47
1:A:339:VAL:HG13	1:A:340:TRP:N	2.30	0.47
1:A:142:LEU:HD23	1:A:142:LEU:C	2.35	0.47
2:B:1550:ARG:CD	2:B:1554:LYS:HE2	2.34	0.47
2:B:1652:PHE:CD2	2:B:1698:LEU:HD22	2.50	0.47
1:A:6:THR:HG22	1:A:7:ALA:N	2.30	0.47
1:A:144:ALA:HB2	1:A:345:ILE:HD12	1.97	0.47
1:A:293:LEU:HD23	1:A:293:LEU:HA	1.81	0.47
2:B:1422:SER:O	2:B:1423:ARG:C	2.53	0.47
2:B:1436:TYR:O	2:B:1437:SER:C	2.53	0.47
2:B:1618:ARG:C	2:B:1619:LEU:HD23	2.36	0.46
1:A:147:ARG:HD2	1:A:298:VAL:HG22	1.97	0.46
1:A:265:SER:OG	1:A:266:PHE:N	2.48	0.46
2:B:1618:ARG:CG	2:B:1618:ARG:HH11	2.27	0.46
1:A:218:TYR:CD1	1:A:255:PHE:HB3	2.50	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:78:ASN:ND2	1:A:81:ASP:OD2	2.49	0.46
1:A:8:LEU:CD1	1:A:94:LEU:HD13	2.45	0.46
1:A:140:LEU:HD13	1:A:343:GLY:HA2	1.98	0.46
2:B:1628:LEU:CD2	2:B:1737:ILE:HG23	2.44	0.46
2:B:1600:ILE:HB	2:B:1609:PHE:HB2	1.97	0.46
1:A:350:SER:CB	2:B:1411:ARG:CG	2.94	0.46
1:A:206:ARG:HH11	1:A:206:ARG:HG3	1.80	0.46
1:A:306:TYR:O	1:A:309:ILE:CG2	2.61	0.46
1:A:34:ILE:CG1	1:A:69:TYR:CE1	2.95	0.46
2:B:1448:ILE:HG23	2:B:1455:PHE:CE1	2.50	0.46
2:B:1515:LEU:HD12	2:B:1519:VAL:HB	1.98	0.46
1:A:9:VAL:HG22	1:A:104:LEU:HB3	1.97	0.46
1:A:98:PRO:CB	1:A:127:PHE:HB3	2.46	0.46
1:A:348:SER:C	1:A:350:SER:H	2.19	0.46
1:A:160:THR:OG1	1:A:181:ALA:HB2	2.15	0.46
1:A:260:THR:CA	1:A:263:GLN:O	2.57	0.46
2:B:1432:ASN:C	2:B:1434:HIS:H	2.18	0.46
1:A:142:LEU:HD21	1:A:148:THR:CA	2.45	0.46
2:B:1503:ASP:OD1	2:B:1504:PRO:HD2	2.15	0.46
2:B:1675:HIS:HE1	2:B:1677:LEU:HD12	1.80	0.46
2:B:1573:LEU:HG	2:B:1577:ASN:HD21	1.80	0.46
2:B:1698:LEU:O	2:B:1699:GLU:C	2.54	0.46
1:A:86:TRP:O	1:A:90:PHE:CD2	2.68	0.46
1:A:204:ALA:C	1:A:206:ARG:H	2.19	0.46
1:A:210:ARG:CG	1:A:211:ASP:H	2.29	0.46
1:A:88:HIS:HE1	1:A:93:GLU:HG2	1.81	0.46
1:A:139:VAL:N	1:A:165:ILE:HD11	2.29	0.46
1:A:330:ILE:HG22	1:A:332:PRO:HD3	1.96	0.46
1:A:91:TYR:HE1	1:A:97:ALA:HB1	1.81	0.46
1:A:330:ILE:CG2	1:A:331:ALA:H	2.28	0.46
2:B:1550:ARG:NH2	2:B:1553:ASP:OD2	2.48	0.46
2:B:1409:SER:O	2:B:1412:LYS:HB3	2.15	0.46
1:A:186:THR:HA	1:A:213:LYS:HD3	1.98	0.46
1:A:253:GLU:O	1:A:254:ARG:C	2.53	0.46
1:A:155:SER:O	1:A:303:THR:HB	2.16	0.46
2:B:1449:LEU:C	2:B:1451:CYS:H	2.17	0.46
2:B:1656:ILE:HG21	2:B:1692:ARG:HA	1.98	0.46
1:A:140:LEU:O	1:A:342:GLY:HA3	2.16	0.46
1:A:190:MET:HE3	1:A:206:ARG:HB2	1.98	0.46
1:A:166:TYR:HD2	1:A:167:GLU:HG3	1.73	0.46
2:B:1638:VAL:HG12	2:B:1639:LYS:HG2	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:182:GLY:CA	4:A:2000:ATP:O2'	2.65	0.45
2:B:1449:LEU:HD21	2:B:1521:LEU:HD11	1.98	0.45
2:B:1680:VAL:O	2:B:1684:THR:N	2.49	0.45
2:B:1540:ARG:CG	2:B:1541:GLU:N	2.78	0.45
2:B:1417:LYS:HD3	2:B:1505:ASN:O	2.17	0.45
2:B:1713:MET:HE3	2:B:1718:GLU:HB3	1.99	0.45
1:A:85:ILE:O	1:A:86:TRP:C	2.53	0.45
1:A:143:TYR:OH	1:A:168:GLY:HA3	2.16	0.45
1:A:37:ARG:HA	1:A:38:PRO:HD3	1.76	0.45
2:B:1591:LEU:O	2:B:1593:THR:N	2.49	0.45
2:B:1601:LYS:HG3	2:B:1605:ASN:OD1	2.16	0.45
2:B:1473:VAL:HG22	2:B:1514:TYR:HH	1.75	0.45
1:A:166:TYR:HE1	1:A:289:ILE:HG22	1.81	0.45
1:A:325:MET:HG3	1:A:326:LYS:O	2.16	0.45
1:A:166:TYR:HD2	1:A:166:TYR:O	1.99	0.45
2:B:1418:ILE:HG22	2:B:1419:THR:N	2.31	0.45
2:B:1621:TYR:C	2:B:1623:SER:N	2.65	0.45
1:A:250:ILE:HG13	1:A:253:GLU:CB	2.46	0.45
2:B:1518:MET:HE2	2:B:1518:MET:HB2	1.59	0.45
1:A:7:ALA:O	1:A:22:ALA:N	2.50	0.45
1:A:14:SER:O	1:A:33:SER:HB2	2.17	0.45
1:A:157:ASP:C	1:A:157:ASP:OD1	2.55	0.45
2:B:1534:VAL:O	2:B:1535:VAL:C	2.56	0.45
2:B:1660:GLU:O	2:B:1662:SER:N	2.49	0.45
2:B:1675:HIS:HE1	2:B:1677:LEU:CD1	2.30	0.45
1:A:145:SER:OG	1:A:147:ARG:HG2	2.17	0.45
1:A:117:GLU:O	1:A:121:GLN:HG3	2.17	0.45
1:A:285:CYS:SG	1:A:293:LEU:HD11	2.56	0.45
1:A:147:ARG:NH1	1:A:330:ILE:HG12	2.31	0.45
2:B:1562:SER:C	2:B:1564:ASN:N	2.66	0.45
2:B:1382:PHE:O	2:B:1383:ALA:O	2.35	0.45
1:A:262:PHE:HB3	1:A:275:HIS:CE1	2.52	0.45
1:A:216:LEU:CD2	1:A:238:LYS:HD3	2.48	0.44
1:A:38:PRO:N	1:A:65:LEU:HD23	2.33	0.44
2:B:1494:LEU:HD21	2:B:1677:LEU:HD11	1.99	0.44
1:A:142:LEU:HG	1:A:147:ARG:HG3	1.98	0.44
1:A:325:MET:O	1:A:327:ILE:HG12	2.17	0.44
1:A:37:ARG:NH2	1:A:84:LYS:HE2	2.14	0.44
2:B:1422:SER:CB	2:B:1424:ASP:OD1	2.63	0.44
1:A:78:ASN:HD21	1:A:81:ASP:CG	2.19	0.44
1:A:87:HIS:CD2	1:A:91:TYR:CD2	3.05	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1482:ALA:C	2:B:1484:TYR:H	2.21	0.44
1:A:16:LEU:O	1:A:18:LYS:HG3	2.18	0.44
1:A:312:ARG:O	1:A:313:MET:O	2.35	0.44
1:A:167:GLU:C	1:A:169:TYR:H	2.21	0.44
1:A:185:LEU:HA	1:A:185:LEU:HD23	1.58	0.44
2:B:1482:ALA:HB3	2:B:1483:PRO:HD3	1.99	0.44
2:B:1449:LEU:HA	2:B:1528:ARG:HH21	1.82	0.44
1:A:188:TYR:HB2	1:A:267:ILE:CG2	2.48	0.44
1:A:120:THR:O	1:A:121:GLN:C	2.55	0.44
2:B:1757:TYR:N	2:B:1757:TYR:CD2	2.85	0.44
1:A:185:LEU:HD12	1:A:306:TYR:OH	2.18	0.44
1:A:203:THR:O	1:A:204:ALA:C	2.55	0.44
1:A:213:LYS:HA	1:A:217:CYS:CB	2.47	0.44
1:A:91:TYR:HE1	1:A:97:ALA:CB	2.30	0.44
2:B:1589:PHE:CD1	2:B:1589:PHE:C	2.91	0.44
1:A:239:SER:HA	1:A:248:ILE:O	2.18	0.44
2:B:1660:GLU:O	2:B:1661:ARG:C	2.56	0.44
1:A:139:VAL:HG22	1:A:165:ILE:HD13	2.00	0.44
2:B:1652:PHE:HD2	2:B:1698:LEU:CD2	2.30	0.44
2:B:1358:LEU:HD23	2:B:1400:ALA:HA	1.99	0.44
1:A:350:SER:O	1:A:351:THR:C	2.56	0.44
1:A:35:VAL:HG21	1:A:81:ASP:HB3	1.99	0.44
1:A:191:LYS:HG3	1:A:192:ILE:N	2.32	0.44
1:A:112:PRO:CB	1:A:115:ASN:HD21	2.28	0.44
1:A:156:GLY:HA2	1:A:302:GLY:HA3	1.99	0.44
2:B:1562:SER:O	2:B:1563:ASP:C	2.57	0.44
2:B:1706:ILE:O	2:B:1707:MET:C	2.56	0.43
1:A:290:ARG:O	1:A:291:LYS:C	2.57	0.43
1:A:34:ILE:CD1	1:A:69:TYR:CE1	3.01	0.43
2:B:1675:HIS:HA	2:B:1676:PRO:HD2	1.85	0.43
2:B:1470:ILE:O	2:B:1518:MET:HG2	2.18	0.43
1:A:166:TYR:HE2	1:A:167:GLU:OE2	2.01	0.43
2:B:1407:LEU:HB2	2:B:1408:ALA:H	1.38	0.43
2:B:1604:THR:O	2:B:1604:THR:OG1	2.35	0.43
2:B:1365:LYS:H	2:B:1365:LYS:HG2	1.56	0.43
1:A:131:ALA:HA	1:A:357:ILE:O	2.19	0.43
1:A:17:VAL:O	1:A:18:LYS:HG3	2.19	0.43
2:B:1431:ILE:HA	2:B:1431:ILE:HD13	1.70	0.43
2:B:1725:ALA:O	2:B:1726:LYS:C	2.56	0.43
1:A:75:ILE:H	1:A:75:ILE:HD12	1.83	0.43
2:B:1361:LEU:O	2:B:1363:TRP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:16:LEU:O	1:A:18:LYS:HE3	2.18	0.43
1:A:185:LEU:O	1:A:187:ASP:N	2.51	0.43
1:A:251:GLY:C	1:A:253:GLU:H	2.21	0.43
1:A:69:TYR:CE2	1:A:183:ARG:NH1	2.87	0.43
2:B:1515:LEU:O	2:B:1517:LEU:N	2.52	0.43
2:B:1450:ASN:HD21	2:B:1679:LYS:HE3	1.83	0.43
1:A:151:ILE:O	1:A:151:ILE:HG23	2.18	0.43
2:B:1722:ASP:O	2:B:1726:LYS:HG3	2.18	0.43
1:A:123:MET:HB3	1:A:129:VAL:HG21	1.99	0.43
1:A:261:LEU:O	1:A:274:ILE:HG22	2.19	0.43
2:B:1534:VAL:HG21	2:B:1659:VAL:CG2	2.46	0.43
2:B:1518:MET:HE2	2:B:1518:MET:H	1.83	0.43
1:A:147:ARG:HD2	1:A:298:VAL:CG2	2.48	0.43
1:A:171:LEU:CD2	1:A:285:CYS:HB2	2.48	0.43
2:B:1710:GLU:HB3	2:B:1720:SER:CB	2.49	0.43
2:B:1580:ASN:HB3	2:B:1584:LYS:HB3	1.99	0.43
2:B:1620:ASN:C	2:B:1621:TYR:CD1	2.92	0.43
1:A:136:ILE:CD1	1:A:136:ILE:H	2.32	0.43
1:A:213:LYS:HE2	1:A:306:TYR:OH	2.19	0.43
2:B:1572:ILE:O	2:B:1573:LEU:C	2.56	0.43
2:B:1632:GLU:O	2:B:1634:VAL:N	2.52	0.43
1:A:303:THR:HG22	1:A:303:THR:O	2.19	0.43
2:B:1422:SER:OG	2:B:1425:ILE:HG12	2.18	0.43
2:B:1730:PHE:O	2:B:1733:PHE:N	2.46	0.43
1:A:223:PHE:HE2	1:A:259:GLU:HG2	1.76	0.42
1:A:335:ARG:HH11	1:A:335:ARG:HG2	1.84	0.42
2:B:1496:ASP:HB3	2:B:1497:ALA:H	1.62	0.42
2:B:1699:GLU:O	2:B:1700:ASP:C	2.57	0.42
2:B:1608:THR:O	2:B:1608:THR:CG2	2.67	0.42
1:A:354:GLN:NE2	2:B:1415:LEU:CD2	2.81	0.42
2:B:1446:LYS:O	2:B:1448:ILE:N	2.52	0.42
2:B:1614:GLU:HA	2:B:1740:TYR:OH	2.18	0.42
1:A:279:TYR:O	1:A:283:MET:HG2	2.19	0.42
1:A:27:PRO:CD	1:A:337:TYR:CD2	3.03	0.42
2:B:1545:LEU:O	2:B:1548:LYS:N	2.52	0.42
2:B:1705:THR:O	2:B:1708:GLU:HB2	2.19	0.42
2:B:1644:GLN:HA	2:B:1644:GLN:HE21	1.84	0.42
1:A:192:ILE:HG22	1:A:195:GLU:OE2	2.20	0.42
1:A:73:HIC:HZ2	1:A:179:ASP:HB3	2.02	0.42
2:B:1525:TRP:CZ2	2:B:1529:MET:HE3	2.54	0.42
2:B:1674:PHE:O	2:B:1676:PRO:N	2.53	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1474:SER:O	2:B:1477:LEU:HB2	2.19	0.42
2:B:1642:ILE:CG2	2:B:1727:ILE:HG23	2.41	0.42
2:B:1456:LEU:HD22	2:B:1536:THR:HG23	2.00	0.42
2:B:1525:TRP:CZ2	2:B:1529:MET:CE	3.02	0.42
2:B:1507:LEU:HB3	2:B:1511:ASP:HB3	2.01	0.42
1:A:210:ARG:HG2	1:A:211:ASP:H	1.85	0.42
1:A:311:ASP:HA	1:A:314:GLN:HB3	2.01	0.42
1:A:312:ARG:HD2	1:A:312:ARG:C	2.38	0.42
1:A:37:ARG:O	1:A:66:THR:N	2.53	0.42
2:B:1656:ILE:HG22	2:B:1657:VAL:N	2.34	0.42
1:A:336:LYS:C	1:A:337:TYR:CD1	2.93	0.42
1:A:165:ILE:CG2	1:A:166:TYR:N	2.80	0.42
1:A:287:ILE:HG12	1:A:290:ARG:NH2	2.34	0.42
1:A:123:MET:HG3	1:A:132:MET:CE	2.49	0.42
2:B:1618:ARG:CA	2:B:1622:PRO:HB3	2.48	0.42
2:B:1447:LYS:CE	2:B:1454:ASP:OD2	2.67	0.42
2:B:1757:TYR:HD2	2:B:1757:TYR:N	2.18	0.42
2:B:1533:THR:O	2:B:1534:VAL:C	2.58	0.42
2:B:1681:LEU:C	2:B:1683:LYS:N	2.73	0.42
2:B:1464:PHE:CD1	2:B:1464:PHE:C	2.91	0.42
1:A:151:ILE:HD12	1:A:282:ILE:CG1	2.42	0.42
1:A:156:GLY:HA3	4:A:2000:ATP:O1A	2.20	0.42
2:B:1591:LEU:CD2	2:B:1594:LEU:HD11	2.50	0.42
2:B:1729:PHE:HA	2:B:1732:LYS:HE3	2.01	0.42
1:A:246:GLN:HE21	1:A:246:GLN:HB3	1.68	0.42
1:A:76:ILE:HD12	1:A:79:TRP:CH2	2.55	0.42
1:A:166:TYR:CE1	1:A:289:ILE:HG22	2.54	0.42
2:B:1513:ILE:CD1	2:B:1513:ILE:N	2.76	0.42
2:B:1459:PRO:HA	2:B:1462:VAL:HB	2.02	0.42
2:B:1464:PHE:O	2:B:1466:SER:N	2.53	0.41
2:B:1545:LEU:CD2	2:B:1649:CYS:HA	2.50	0.41
2:B:1624:PHE:C	2:B:1626:ASP:N	2.73	0.41
1:A:180:LEU:CD2	1:A:181:ALA:N	2.73	0.41
2:B:1591:LEU:HD22	2:B:1594:LEU:HD11	2.01	0.41
2:B:1564:ASN:O	2:B:1565:LEU:C	2.58	0.41
2:B:1421:LEU:HB2	2:B:1511:ASP:OD1	2.21	0.41
1:A:98:PRO:CG	1:A:127:PHE:HB3	2.50	0.41
1:A:34:ILE:HD11	1:A:69:TYR:CE1	2.55	0.41
1:A:357:ILE:HA	1:A:361:GLU:OE2	2.20	0.41
1:A:5:THR:CG2	1:A:6:THR:N	2.84	0.41
1:A:240:TYR:HB3	1:A:248:ILE:CD1	2.48	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:242:LEU:HD21	1:A:248:ILE:HG21	2.03	0.41
2:B:1585:GLN:HE21	2:B:1585:GLN:CA	2.00	0.41
1:A:138:ALA:O	1:A:139:VAL:C	2.57	0.41
1:A:142:LEU:HD11	1:A:149:THR:C	2.41	0.41
1:A:312:ARG:HG2	1:A:312:ARG:NH1	2.35	0.41
1:A:317:ILE:H	1:A:317:ILE:HG12	1.68	0.41
2:B:1484:TYR:CE2	2:B:1503:ASP:O	2.73	0.41
2:B:1568:VAL:O	2:B:1572:ILE:HG13	2.20	0.41
1:A:151:ILE:H	1:A:293:LEU:HD22	1.86	0.41
2:B:1421:LEU:HD22	2:B:1425:ILE:HG21	2.01	0.41
1:A:95:ARG:NH1	1:A:95:ARG:HG2	2.34	0.41
1:A:96:VAL:HG11	1:A:101:HIS:CE1	2.56	0.41
1:A:14:SER:HA	1:A:71:ILE:HB	2.02	0.41
2:B:1449:LEU:HA	2:B:1528:ARG:NH2	2.35	0.41
1:A:335:ARG:O	1:A:337:TYR:N	2.54	0.41
1:A:142:LEU:HD11	1:A:149:THR:O	2.20	0.41
1:A:277:THR:C	1:A:279:TYR:N	2.72	0.41
1:A:287:ILE:O	1:A:290:ARG:HG3	2.21	0.41
1:A:321:ALA:HA	1:A:322:PRO:HD3	1.86	0.41
2:B:1690:GLU:O	2:B:1691:ALA:C	2.56	0.41
1:A:34:ILE:HA	1:A:68:LYS:O	2.20	0.41
1:A:38:PRO:HD3	1:A:65:LEU:CD2	2.50	0.41
2:B:1687:VAL:C	2:B:1689:PRO:CD	2.85	0.41
1:A:111:ASN:HA	1:A:112:PRO:HD3	1.80	0.41
1:A:313:MET:O	1:A:314:GLN:C	2.59	0.41
1:A:81:ASP:O	1:A:82:MET:C	2.58	0.41
1:A:99:GLU:C	1:A:101:HIS:H	2.24	0.41
2:B:1684:THR:HB	2:B:1685:LEU:HD22	2.03	0.41
1:A:171:LEU:CD1	1:A:171:LEU:N	2.82	0.41
2:B:1419:THR:OG1	2:B:1508:GLN:HB2	2.21	0.41
1:A:346:LEU:HD11	1:A:352:PHE:CD2	2.54	0.41
1:A:216:LEU:HD22	1:A:238:LYS:HD3	2.02	0.41
1:A:242:LEU:N	1:A:242:LEU:HD12	2.36	0.41
1:A:223:PHE:CZ	1:A:256:ARG:HA	2.52	0.41
2:B:1517:LEU:HD13	2:B:1525:TRP:CZ3	2.55	0.41
2:B:1674:PHE:CE1	2:B:1681:LEU:HD11	2.55	0.41
1:A:27:PRO:C	1:A:29:ALA:H	2.23	0.41
2:B:1467:LYS:O	2:B:1468:SER:C	2.59	0.41
2:B:1722:ASP:C	2:B:1726:LYS:HG3	2.41	0.41
1:A:287:ILE:CA	1:A:290:ARG:HG3	2.47	0.41
2:B:1618:ARG:HA	2:B:1622:PRO:CB	2.49	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1377:GLY:O	2:B:1378:LYS:C	2.60	0.41
1:A:208:ILE:CD1	1:A:208:ILE:O	2.69	0.41
1:A:38:PRO:HA	1:A:65:LEU:HA	2.02	0.41
1:A:298:VAL:HA	1:A:330:ILE:HB	2.02	0.41
2:B:1736:PHE:O	2:B:1737:ILE:C	2.59	0.41
2:B:1722:ASP:OD1	2:B:1722:ASP:O	2.38	0.41
1:A:284:LYS:HA	1:A:284:LYS:HD2	1.88	0.41
1:A:120:THR:HA	1:A:132:MET:HE3	2.02	0.41
1:A:38:PRO:HG3	1:A:65:LEU:HD23	2.03	0.40
1:A:87:HIS:NE2	1:A:91:TYR:CD2	2.90	0.40
2:B:1432:ASN:O	2:B:1435:MET:SD	2.79	0.40
2:B:1604:THR:O	2:B:1605:ASN:C	2.60	0.40
1:A:223:PHE:O	1:A:227:MET:HB2	2.21	0.40
1:A:35:VAL:CG1	1:A:54:VAL:HG23	2.32	0.40
1:A:94:LEU:HB3	1:A:96:VAL:HG23	2.03	0.40
2:B:1465:LEU:HD22	2:B:1525:TRP:CZ2	2.56	0.40
2:B:1740:TYR:C	2:B:1742:LYS:N	2.75	0.40
2:B:1728:SER:O	2:B:1732:LYS:HE2	2.21	0.40
2:B:1542:TYR:HD1	2:B:1652:PHE:HE2	1.69	0.40
2:B:1441:VAL:HG11	2:B:1512:GLN:HB2	2.03	0.40
2:B:1351:TYR:HA	2:B:1352:PRO:HD3	1.81	0.40
1:A:223:PHE:C	1:A:225:ASN:N	2.74	0.40
1:A:259:GLU:HA	1:A:259:GLU:OE1	2.21	0.40
2:B:1516:GLN:C	2:B:1517:LEU:HD23	2.40	0.40
2:B:1525:TRP:HE1	2:B:1529:MET:HG3	1.86	0.40
2:B:1474:SER:O	2:B:1477:LEU:N	2.54	0.40
1:A:345:ILE:O	1:A:349:LEU:CB	2.69	0.40
1:A:130:PRO:HG2	1:A:131:ALA:H	1.87	0.40
1:A:189:LEU:CD1	1:A:190:MET:HG3	2.52	0.40
1:A:223:PHE:CD2	1:A:259:GLU:HG2	2.54	0.40
2:B:1517:LEU:HB3	2:B:1525:TRP:CZ3	2.56	0.40
1:A:115:ASN:O	1:A:119:MET:N	2.48	0.40
1:A:120:THR:O	1:A:123:MET:N	2.55	0.40
2:B:1394:ASP:O	2:B:1396:GLU:N	2.53	0.40
1:A:223:PHE:HE1	1:A:255:PHE:CE1	2.40	0.40
1:A:26:ALA:CA	1:A:340:TRP:CZ3	3.03	0.40
2:B:1419:THR:HG1	2:B:1508:GLN:HB2	1.86	0.40
1:A:120:THR:HG23	1:A:121:GLN:H	1.87	0.40
1:A:7:ALA:O	1:A:22:ALA:HB2	2.21	0.40
2:B:1669:SER:O	2:B:1671:SER:N	2.54	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

In the following table, the Percentiles column shows the percent Ramachandran outliers of the chain as a percentile score with respect to all 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	352/375 (94%)	205 (58%)	91 (26%)	56 (16%)	0 0
2	B	409/443 (92%)	232 (57%)	118 (29%)	59 (14%)	0 1
All	All	761/818 (93%)	437 (57%)	209 (28%)	115 (15%)	0 0

All (115) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	23	GLY
1	A	61	LYS
1	A	90	PHE
1	A	98	PRO
1	A	99	GLU
1	A	128	ASN
1	A	138	ALA
1	A	139	VAL
1	A	216	LEU
1	A	220	ALA
1	A	230	ALA
1	A	266	PHE
1	A	301	GLY
1	A	314	GLN
1	A	324	THR
1	A	332	PRO
1	A	351	THR
1	A	353	GLN
1	A	368	SER
2	B	1370	ASP
2	B	1383	ALA
2	B	1391	VAL
2	B	1451	CYS
2	B	1491	VAL
2	B	1496	ASP

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Mol	Chain	Res	Type
2	B	1497	ALA
2	B	1498	LYS
2	B	1523	SER
2	B	1538	TYR
2	B	1539	GLU
2	B	1541	GLU
2	B	1620	ASN
2	B	1670	ASP
2	B	1671	SER
2	B	1676	PRO
2	B	1678	ASP
1	A	91	TYR
1	A	123	MET
1	A	145	SER
1	A	156	GLY
1	A	168	GLY
1	A	181	ALA
1	A	182	GLY
1	A	197	GLY
1	A	202	THR
1	A	269	MET
1	A	303	THR
1	A	313	MET
1	A	346	LEU
1	A	350	SER
1	A	360	GLN
2	B	1362	HIS
2	B	1430	GLY
2	B	1437	SER
2	B	1447	LYS
2	B	1465	LEU
2	B	1485	SER
2	B	1564	ASN
2	B	1600	ILE
2	B	1605	ASN
2	B	1618	ARG
2	B	1657	VAL
2	B	1723	LYS
2	B	1724	PHE
2	B	1728	SER
1	A	166	TYR
1	A	288	ASP

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Mol	Chain	Res	Type
2	B	1452	ASP
2	B	1472	GLU
2	B	1522	GLU
2	B	1625	ASN
2	B	1661	ARG
2	B	1715	THR
2	B	1720	SER
1	A	22	ALA
1	A	70	PRO
1	A	89	THR
1	A	100	GLU
1	A	149	THR
1	A	208	ILE
1	A	349	LEU
2	B	1409	SER
2	B	1410	LYS
2	B	1471	ILE
2	B	1535	VAL
2	B	1562	SER
2	B	1592	SER
2	B	1665	ILE
2	B	1667	ASN
2	B	1689	PRO
1	A	93	GLU
1	A	155	SER
1	A	183	ARG
1	A	211	ASP
1	A	258	PRO
1	A	286	ASP
1	A	367	PRO
2	B	1464	PHE
2	B	1516	GLN
2	B	1558	ALA
2	B	1674	PHE
2	B	1706	ILE
1	A	88	HIS
1	A	209	VAL
1	A	246	GLN
1	A	336	LYS
2	B	1372	SER
2	B	1408	ALA
2	B	1679	LYS

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Mol	Chain	Res	Type
2	B	1617	VAL
2	B	1737	ILE
1	A	201	VAL
1	A	333	PRO
2	B	1637	VAL
2	B	1622	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	302/317 (95%)	249 (82%)	53 (18%)	2 9
2	B	374/404 (93%)	323 (86%)	51 (14%)	5 18
All	All	676/721 (94%)	572 (85%)	104 (15%)	3 13

All (104) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	9	VAL
1	A	24	ASP
1	A	56	ASP
1	A	62	ARG
1	A	66	THR
1	A	78	ASN
1	A	80	ASP
1	A	93	GLU
1	A	94	LEU
1	A	98	PRO
1	A	99	GLU
1	A	104	LEU
1	A	115	ASN
1	A	128	ASN
1	A	141	SER
1	A	147	ARG
1	A	162	ASN

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Mol	Chain	Res	Type
1	A	172	PRO
1	A	178	LEU
1	A	184	ASP
1	A	187	ASP
1	A	188	TYR
1	A	189	LEU
1	A	191	LYS
1	A	202	THR
1	A	206	ARG
1	A	212	ILE
1	A	219	VAL
1	A	222	ASP
1	A	223	PHE
1	A	237	GLU
1	A	246	GLN
1	A	250	ILE
1	A	252	ASN
1	A	255	PHE
1	A	269	MET
1	A	270	GLU
1	A	280	ASN
1	A	282	ILE
1	A	286	ASP
1	A	305	MET
1	A	309	ILE
1	A	311	ASP
1	A	312	ARG
1	A	333	PRO
1	A	334	GLU
1	A	335	ARG
1	A	352	PHE
1	A	353	GLN
1	A	354	GLN
1	A	358	THR
1	A	367	PRO
1	A	370	VAL
2	B	1360	GLN
2	B	1363	TRP
2	B	1366	LEU
2	B	1384	ASP
2	B	1407	LEU
2	B	1424	ASP

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Mol	Chain	Res	Type
2	B	1432	ASN
2	B	1435	MET
2	B	1440	SER
2	B	1444	LEU
2	B	1455	PHE
2	B	1466	SER
2	B	1468	SER
2	B	1469	GLU
2	B	1475	VAL
2	B	1480	ASN
2	B	1484	TYR
2	B	1495	GLU
2	B	1508	GLN
2	B	1511	ASP
2	B	1516	GLN
2	B	1518	MET
2	B	1527	SER
2	B	1528	ARG
2	B	1532	LEU
2	B	1538	TYR
2	B	1551	LYS
2	B	1560	GLN
2	B	1563	ASP
2	B	1585	GLN
2	B	1604	THR
2	B	1621	TYR
2	B	1623	SER
2	B	1629	SER
2	B	1634	VAL
2	B	1636	ASP
2	B	1641	SER
2	B	1644	GLN
2	B	1665	ILE
2	B	1670	ASP
2	B	1671	SER
2	B	1674	PHE
2	B	1680	VAL
2	B	1686	PRO
2	B	1687	VAL
2	B	1688	LEU
2	B	1690	GLU
2	B	1697	LEU

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Mol	Chain	Res	Type
2	B	1718	GLU
2	B	1731	LYS
2	B	1732	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (28) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	88	HIS
1	A	92	ASN
1	A	115	ASN
1	A	121	GLN
1	A	128	ASN
1	A	246	GLN
1	A	252	ASN
1	A	263	GLN
1	A	280	ASN
1	A	354	GLN
2	B	1360	GLN
2	B	1450	ASN
2	B	1457	GLN
2	B	1476	ASN
2	B	1480	ASN
2	B	1493	ASN
2	B	1508	GLN
2	B	1516	GLN
2	B	1543	ASN
2	B	1585	GLN
2	B	1611	ASN
2	B	1620	ASN
2	B	1625	ASN
2	B	1644	GLN
2	B	1658	ASN
2	B	1675	HIS
2	B	1744	GLN
2	B	1747	ASN

5.3.3 RNA

There are no RNA molecules in this entry.

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

1 non-standard protein/DNA/RNA residue is modelled in this entry.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\| > 2$	Counts	RMSZ	$\#\|Z\| > 2$
1	HIC	A	73	1	8,11,12	0.76	0	5,14,16	1.68	2 (40%)

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
1	HIC	A	73	1	-	0/4/6/8	0/1/1/1

There are no bond length outliers.

All (2) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
1	A	73	HIC	O-C-CA	-2.27	119.57	125.49
1	A	73	HIC	CZ-NE2-CD2	2.31	134.86	126.33

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 2 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
1	A	73	HIC	2	0

5.5 Carbohydrates (i)

There are no carbohydrates in this entry.

5.6 Ligand geometry (i)

Of 2 ligands modelled in this entry, 1 is monoatomic - leaving 1 for Mogul analysis.

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	$\#\|Z\| > 2$
4	ATP	A	2000	3	24,33,33	1.79	3 (12%)	31,52,52	2.17	4 (12%)

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
4	ATP	A	2000	3	-	0/18/38/38	0/3/3/3

All (3) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	A	2000	ATP	C5-N7	-2.07	1.32	1.39
4	A	2000	ATP	O4'-C1'	2.49	1.44	1.41
4	A	2000	ATP	C2-N1	7.02	1.47	1.33

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
4	A	2000	ATP	N3-C2-N1	-9.97	121.26	128.89
4	A	2000	ATP	PB-O3B-PG	-3.79	119.95	132.67
4	A	2000	ATP	C4-C5-N7	-2.55	107.13	109.48
4	A	2000	ATP	N6-C6-N1	2.20	123.92	119.20

There are no chirality outliers.

There are no torsion outliers.

There are no ring outliers.

1 monomer is involved in 13 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
4	A	2000	ATP	13	0

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	356/375 (94%)	-0.22	4 (1%)	82	63	41, 99, 154, 190	0
2	B	411/443 (92%)	-0.46	2 (0%)	91	81	57, 109, 159, 207	2 (0%)
All	All	767/818 (93%)	-0.35	6 (0%)	87	72	41, 103, 157, 207	2 (0%)

All (6) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	38	PRO	3.4
2	B	1757	TYR	2.6
1	A	156	GLY	2.6
1	A	200	PHE	2.3
1	A	61	LYS	2.1
2	B	1357	LYS	2.1

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

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
1	HIC	A	73	11/12	0.95	0.15	-	57,67,67,67	0

6.3 Carbohydrates

There are no carbohydrates in this entry.

6.4 Ligands

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
3	CA	A	382	1/1	0.94	0.78	5.95	97,97,97,97	0
4	ATP	A	2000	31/31	0.86	0.34	1.25	97,97,97,97	0

6.5 Other polymers

There are no such residues in this entry.