



# Full wwPDB X-ray Structure Validation Report ⓘ

Aug 7, 2020 – 12:12 PM BST

PDB ID : 3PVM  
Title : Structure of Complement C5 in Complex with CVF  
Authors : Laursen, N.S.; Andersen, K.R.; Braren, I.; Sottrup-Jensen, L.; Spillner, E.; Andersen, G.R.  
Deposited on : 2010-12-07  
Resolution : 4.30 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](mailto:validation@mail.wwpdb.org)

A user guide is available at

<https://www.wwpdb.org/validation/2017/XrayValidationReportHelp>

with specific help available everywhere you see the ⓘ symbol.

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

MolProbity : 4.02b-467  
Mogul : 1.8.5 (274361), CSD as541be (2020)  
Xtriage (Phenix) : 1.13  
EDS : 2.13.1  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Refmac : 5.8.0158  
CCP4 : 7.0.044 (Gargrove)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.13.1

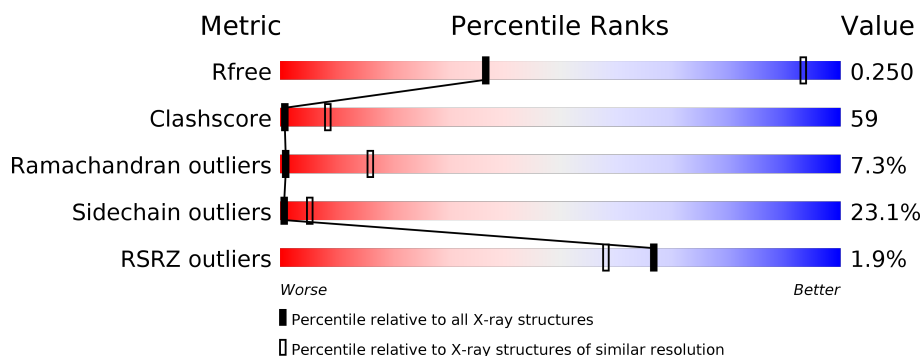
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*X-RAY DIFFRACTION*

The reported resolution of this entry is 4.30 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))
$R_{free}$	130704	1014 (4.80-3.80)
Clashscore	141614	1077 (4.80-3.80)
Ramachandran outliers	138981	1029 (4.80-3.80)
Sidechain outliers	138945	1012 (4.80-3.80)
RSRZ outliers	127900	1075 (4.90-3.70)

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  $\geq 3$ , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions  $\leq 5\%$ . 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	1676	<div> <div>2%</div> <div>24% 52% 20%</div> <div>• •</div> </div>
1	C	1676	<div> <div>2%</div> <div>24% 52% 20%</div> <div>• •</div> </div>
2	B	1642	<div> <div>2%</div> <div>23% 38% 13% 25%</div> <div>•</div> </div>
2	D	1642	<div> <div>%</div> <div>23% 38% 13% 25%</div> <div>•</div> </div>

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 crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
3	NAG	B	2002	-	-	-	X
3	NAG	D	2002	-	-	-	X

## 2 Entry composition [i](#)

There are 3 unique types of molecules in this entry. The entry contains 45268 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.

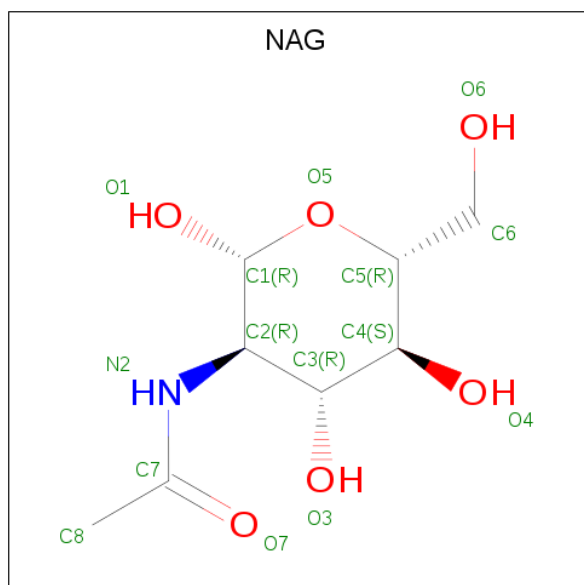
- Molecule 1 is a protein called Complement C5.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1627	Total	C	N	O	S	0	0	0
			12881	8246	2114	2469	52			
1	C	1627	Total	C	N	O	S	0	0	0
			12881	8246	2114	2469	52			

- Molecule 2 is a protein called Cobra venom factor.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
2	B	1225	Total	C	N	O	S	0	0	0
			9711	6187	1633	1851	40			
2	D	1225	Total	C	N	O	S	0	0	0
			9711	6187	1633	1851	40			

- Molecule 3 is 2-acetamido-2-deoxy-beta-D-glucopyranose (three-letter code: NAG) (formula:  $C_8H_{15}NO_6$ ).

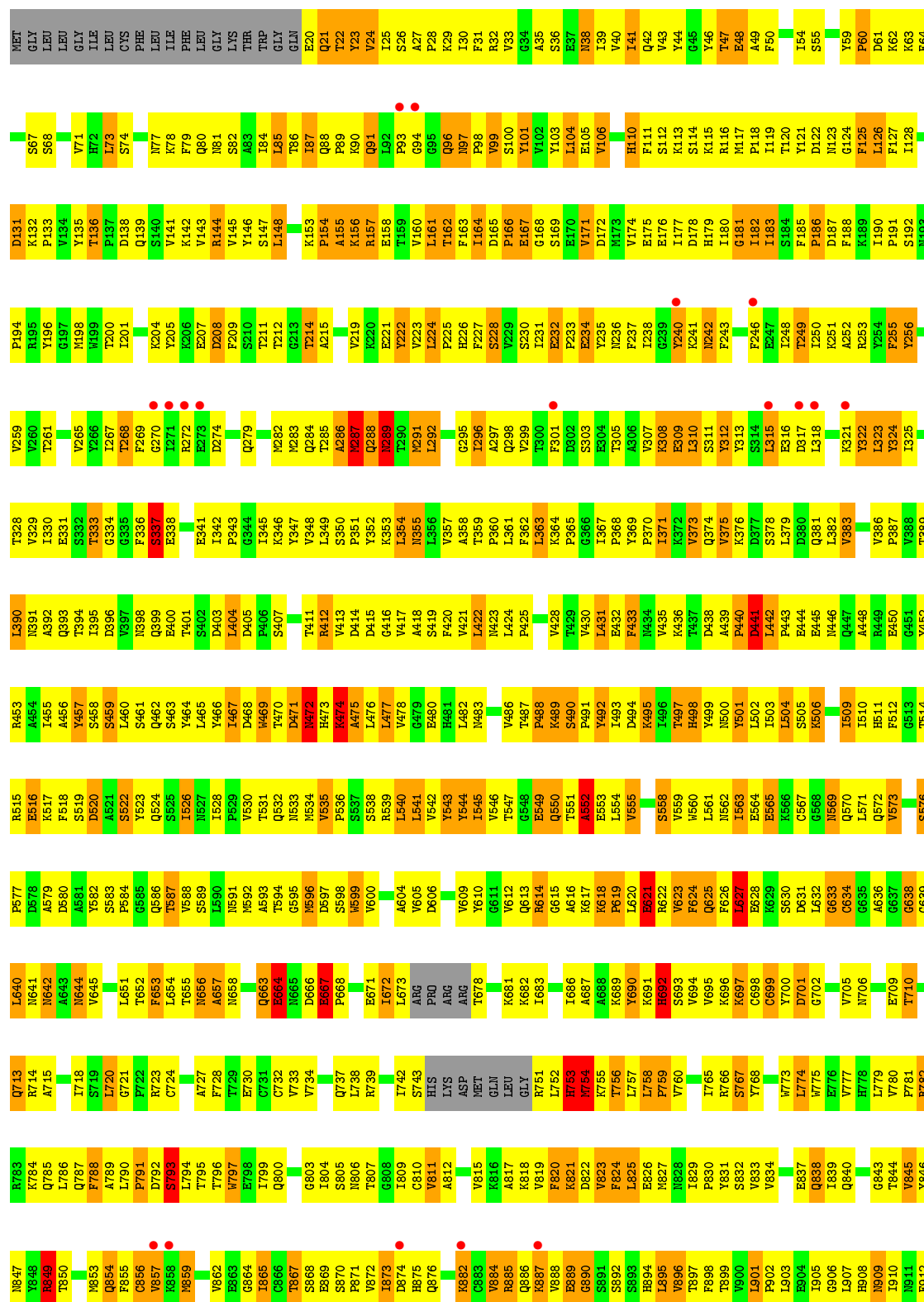
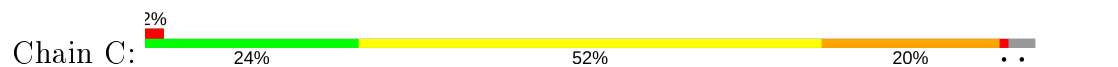


Mol	Chain	Residues	Atoms				ZeroOcc	AltConf
3	A	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	B	1	Total	C	N	O	0	0
			14	8	1	5		
3	C	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		
3	D	1	Total	C	N	O	0	0
			14	8	1	5		



K1628	T1566	Q1504	L1432	T1362	S1301	K1285	F1174	W1106	I1040	R975	H909	G843	L779	C704
Y1629	S1567	C1505	S1433	T1363	L1302	D1286	L1175	L1107	E1041	R976	I910	T844	V780	V705
N1630	I1568	C1506	V1364	V1365	V1303	S1237	S1176	E1108	E1042	L977	N911	V845	R782	M706
F1631	T1569	M1507	K1366	H1366	K1306	V1239	E1177	N1110	Q1043	V979	S913	N847	R783	E710
S1632	V1570	F1508	L1439	K1367	Q1305	P1240	N1178	Y1111	L1045	K980	L914	K784	K785	T709
F1633	E1571	F1509	K1440	T1368	D1307	P1240	T1179	Q1112	K1046	G981	E915	R843	R786	E709
R1634	N1572	S1510	V1446	S1369	R1308	G1243	L1180	Q1112	K1047	G982	T916	R843	R787	Q713
Y1635	V1573	T1511	V1446	T1370	R1309	T1244	P1181	D1114	K1048	L982	N917	T850	R788	R714
S1512	F1574	S1512	F1450	S1370	L1309	A1245	A1182	S1117	L1049	G985	F918	M853	F788	R174
N1513	K1576	N1513	T1451	S1371	M1311	A1246	Q1183	Q1117	Q984	G985	V923	K854	L730	L720
L1514	K1577	L1514	T1452	S1372	D1312	M1247	S1184	K1118	M1053	E986	L923	F855	L730	A789
I1515	V1578	I1515	V1453	E1373	I1313	V1248	F1185	K1119	L1054	R987	V924	C856	L790	G721
Q1516	A1579	Q1516	Q1454	C1375	D1314	E1249	F1186	E1120	S1055	L988	K925	V857	P722	P722
L1517	L1580	L1517	L1455	S1376	V1316	T1250	T1187	M1121	M1056	S989	R928	K858	D792	R723
T1518	T1581	T1518	L1456	F1377	S1316	T1251	L1188	S1122	I1057	A990	V929	M859	S793	C724
C1519	C1582	C1519	D1457	V1378	Y1317	Y1263	L1190	Q1123	R1060	S993	V930	V862	L794	R727
G1520	G1583	G1520	G1458	L1379	Y1317	Y1263	L1190	Q1123	R1060	S993	V930	V862	L794	A727
L1521	L1584	L1521	L1461	K1380	K1320	A1254	S1191	Y1124	M1061	Q994	V930	V862	L794	T727
A1522	A1585	A1522	L1462	L1381	G1321	L1285	A1192	Y1124	M1061	Q994	V930	V862	L794	T727
C1523	C1586	C1523	Q1463	D1382	A1322	L1286	A1192	Y1124	M1061	Q994	V930	V862	L794	T727
S1524	S1587	S1524	L1464	T1383	H1323	L1287	A1194	L1129	S1065	G995	V930	V862	L794	T727
L1525	L1588	L1525	N1465	T1383	H1323	S1258	L1195	L1129	S1065	G995	V930	V862	L794	T727
A1526	A1589	A1526	S1466	I1386	N1325	L1259	S1196	L1133	S1067	G995	V930	V862	L794	T727
T1527	T1590	T1527	L1467	E1387	Y1326	N1280	L1197	L1133	S1067	G995	V930	V862	L794	T727
R1528	R1591	R1528	P1468	ALA	K1327	L1281	G1198	P1134	M1069	T1001	S988	S870	S805	Q737
G1529	G1592	G1529	S1469	SER	M1328	L1281	G1198	P1134	M1069	T1001	S988	S870	S805	Q737
H1530	H1593	H1530	S1470	HIS	T1329	L1281	G1198	P1134	M1069	T1001	S988	S870	S805	Q737
L1531	L1594	L1531	F1471	TRP	D1330	N1265	H1202	E1139	A1074	S1007	A1008	K882	S805	Q737
K1532	K1595	K1532	F1472	ARG	K1331	N1266	H1202	E1139	A1074	S1007	A1008	K882	S805	Q737
G1533	G1596	G1533	L1473	GLY	N1332	N1267	P1203	Q1204	A1074	S1007	A1008	K882	S805	Q737
S1534	S1597	S1534	G1474	GLY	N1332	N1267	P1203	Q1204	A1074	S1007	A1008	K882	S805	Q737
A1535	A1598	A1535	G1475	GLY	N1332	N1267	P1203	Q1204	A1074	S1007	A1008	K882	S805	Q737
T1536	T1599	T1536	L1476	ASN	L1335	N1270	T1209	Y1143	A1080	P946	L945	K882	S805	Q737
E1537	E1600	E1537	R1476	ASN	L1335	N1270	T1209	Y1143	A1080	P946	L945	K882	S805	Q737
G1538	G1603	G1538	L1479	S1397	L1336	I1271	V1209	Y1143	A1080	P946	L945	K882	S805	Q737
L1539	L1604	L1539	F1480	T1402	P1337	K1273	S1210	T1145	F1081	G948	V942	K882	S805	Q737
T1540	T1607	T1540	L1482	V1403	V1338	K1273	S1210	T1145	F1081	G948	V942	K882	S805	Q737
L1541	L1608	L1541	E1483	A1404	E1339	L1274	A1211	L1146	L1082	Y950	V950	K882	S805	Q737
T1542	T1609	T1542	E1484	A1404	E1339	L1274	A1211	L1146	L1082	Y950	V950	K882	S805	Q737
S1543	S1612	S1543	V1485	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
A1544	A1613	A1544	L1486	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
S1545	S1614	S1545	L1487	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
A1546	A1615	A1546	L1488	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
T1547	T1616	T1547	L1489	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
R1548	R1617	R1548	L1490	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
G1549	G1618	G1549	L1491	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
Q1550	Q1619	Q1550	L1492	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
T1551	T1620	T1551	L1493	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
L1552	L1621	L1552	L1494	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
C1553	C1622	C1553	L1495	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
K1554	K1623	K1554	L1496	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
P1555	P1624	P1555	L1497	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
E1556	E1625	E1556	L1498	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
L1557	L1626	L1557	L1499	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
Q1558	Q1627	Q1558	L1500	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
A1559	A1628	A1559	L1501	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
S1560	S1629	S1560	L1502	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
T1561	T1630	T1561	L1503	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
K1562	K1631	K1562	L1504	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
L1563	L1632	L1563	L1505	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
S1564	S1633	S1564	L1506	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
V1565	V1634	V1565	L1507	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737
I1566	I1635	I1566	L1508	V1408	V1340	E1277	K1213	T1146	R1084	G951	V950	K882	S805	Q737

● Molecule 1: Complement C5





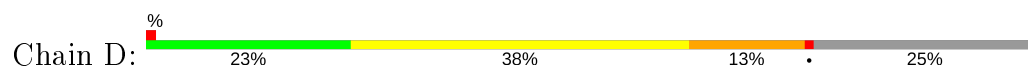




VAL	ARG	ASP	R1289	V1349	N1415	I1484	R1557	D1626	R1557	I1484	N1415	V1349	R1289	ARG	ASP	
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SER	THR	THR	R1291	N1351	M1417			F1628			M1417	N1351	R1291	THR	THR	
GLY	THR	GLY	I1292	I1352	A1418	C1490	H1561	A1629	H1561	C1490	A1418	I1352	I1292	THR	GLY	
THR	THR	PRO	M1293	R1353	Q1419	R1491	Q1562	Q1630	Q1562	R1491	Q1419	R1353	M1293	THR	PRO	
MET	ALA	ILE	Y1294	L1354	K1420	C1492	Y1563	F1631	Y1563	C1492	K1420	L1354	Y1294	ALA	ILE	
GLN	LEU	VAL	E1295	M1355	V1421	G1494	Q1566	S1632	Q1566	G1494	V1421	M1355	E1295	LEU	VAL	
GLY	THR	TRP	A1296	ALA	A1422	E1495				E1495	A1422	ALA	A1296	THR	TRP	
ILE	ALA	THR	L1298	GLY	I1423	T1496	C1569	T1636	C1569	T1496	I1423	GLY	L1298	ALA	THR	
GLN	ALA	THR	L1299	ALA	I1425	C1497	Q1570	E1637	Q1570	C1497	I1425	ALA	L1299	GLN	ALA	
GLY	LEU	ASP	A1300	K1360	Y1426	S1498	E1571	F1638	E1571	S1498	Y1426	K1360	A1300	LEU	ASP	
ALA	ALA	ASN	R1301	L1363	N1427	L1500	A1572	G1639	A1572	L1500	N1427	L1363	R1301	ALA	ASN	
GLU	ALA	PHE	T1302	M1364	N1428	M1501	N1574	T1642	N1574	M1501	N1428	M1364	T1302	GLU	PHE	
GLU	GLU	TVR	V1303	L1365	K1429	H1502	L1575		L1575	H1502	K1429	L1365	V1303	GLU	GLU	
VAL	GLN	GLY	T1304	K1366	S1431	Q1503	K1576		K1576	Q1503	S1431	K1366	T1304	VAL	GLN	
TYR	LEU	GLY	K1306	I1367	H1432	E1504	Y1577		Y1577	E1504	H1432	I1367	K1306	TYR	GLY	
LEU	ASN	THR	L1307	C1368	S1433	R1505	N1578		N1578	R1505	S1433	C1368	L1307	LEU	ASN	
THR	ASP	TYR	M1308	T1369	C1437	D1507	Y1581		Y1581	D1507	C1437	T1369	M1308	THR	ASP	
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PHE	ARG	GLN	D1310	Y1371	H1439	P1509	L1583		L1583	P1509	H1439	Y1371	D1310	PHE	ARG	
ILE	VAL	THR	I1311	L1372		L1510	W1584		W1584	L1510		L1372	I1311	ILE	VAL	
LEU	LEU	GLN	T1312	G1373		Q1511				Q1511		G1373	T1312	LEU	LEU	
VAL	MET	ALA	V1313	E1374		I1512				I1512		E1374	V1313	VAL	MET	
ALA	ALA	THR	T1314	V1375		L1513				L1513		T1314	T1314	ALA	ALA	
LEU	ALA	VAL	A1315	D1376		E1513				E1513		A1315	VAL	LEU	ALA	
SER	SER	MET	S1316	S1377		K1514				K1514		S1377	MET	SER	SER	
GLU	THR	GLY	G1317	T1378		A1515				A1515		T1378	GLY	GLU	THR	
SER	GLY	PHE	D1318	M1379		C1516				C1516		M1379	PHE	SER	GLY	
LVS	ARG	GLN	G1319	T1380		E1517				E1517		T1380	GLN	LVS	ARG	
THR	ASP	ALA	K1320	I1381		T1518				T1518		I1381	K1320	THR	ASP	
ILE	HIS	LEU	A1321	I1382		M1519				M1519		A1321	A1321	ILE	HIS	
CYS	TRP	ALA	T1322	D1383		V1520				V1520		T1322	ALA	CYS	TRP	
ASN	GLU	GLU	M1323	I1384		D1521				D1521		I1384	GLU	ASN	GLU	
ASP	GLY	TVR	T1324	S1385		Y1522				Y1522		T1324	TVR	ASP	GLY	
TYR	TYR	GLY	I1325	M1386		I1601				I1601		I1325	TYR	TYR	GLY	
VAL	ASN	ILE	L1326	L1387		T1602				T1602		L1326	ASN	VAL	ASN	
ASN	ALA	GLN	T1327	T1388		M1604				M1604		T1327	GLN	ASN	ALA	
SER	HIS	MET	F1328	G1389		T1605				T1605		F1328	MET	SER	HIS	
LEU	THR	PRO	Y1329	F1390		K1606				K1606		Y1329	PRO	LEU	THR	
ASP	HIS	THR	M1330	L1391		L1607				L1607		M1330	THR	ASP	HIS	
SER	ASN	THR	A1331	P1392		E1608				E1608		A1331	THR	SER	ASN	
SER	ILE	GLY	Q1332	D1393		R1609				R1609		Q1332	THR	SER	ILE	
ILE	GLY	GLY	L1333	D1396		W1610				W1610		L1333	GLY	ILE	GLY	
LVS	THR	LVS	N1274	L1397		P1611				P1611		N1274	GLY	LVS	THR	
ALA	SER	ALA	D1276	L1398		H1612				H1612		D1276	LYS	ALA	SER	
THR	TYR	ALA	I1277	R1399		Q1613				Q1613		I1277	ALA	THR	TYR	
ASN	ALA	ASN	T1278	L1400		D1614				D1614		T1278	ASN	ASN	ALA	
TVR	LEU	LEU	I1279	S1401		E1615				E1615		I1279	LEU	TVR	LEU	
LEU	LEU	ALA	E1280	K1402		C1616				C1616		E1280	ALA	LEU	LEU	
ALA	ALA	ALA	L1281			Q1617				Q1617		L1281	ALA	ALA	ALA	
LVS	LYS	LYS	P1282	R1406		E1618				E1618		P1282	LYS	LVS	LYS	
LVS	LVS	LVS	D1283	I1407		E1619				E1619		D1283	LVS	LVS	LVS	
TVR	LVS	LVS	E1285	I1408		E1620				E1620		E1285	TVR	TVR	TVR	
GLU	MET	LEU	P1286	I1408		F1621				F1621		P1286	GLU	GLU	MET	
LVS	LVS	LVS	P1287	E1412		Q1622				Q1622		P1287	LVS	LVS	LVS	
LEU	PHE	PHE	I1288	V1413		K1623				K1623		I1288	LEU	LEU	PHE	
				D1414		L1480				L1480						
						L1481				L1481						
						N1482				N1482						
						P1556				P1556						

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● Molecule 2: Cobra venom factor



MET	R63	S125	L188	R250	GLU	R64	S126	P189	R251	ARG	Q65	F127	P190	Y252	THR	R65	F128	L191	L253	Y253	
	R66	S127	P191	Y254	ARG	R66	T67	F129	S193	ALA	T67	F130	P192	Y255	LEU	R67	F131	L192	L254	Y254	
	R68	S128	P193	Y256	LEU	R68	F69	Q131	E194	TVR	F69	Q132	L194	Y257	LEU	R69	F132	L195	L255	Y256	
	R70	S129	P194	Y258	LEU	R70	T71	D133	G195	VAL	T71	D134	L196	Y259	VAL	R71	F133	L197	L256	Y258	
	R72	S130	P195	Y260	ALA	R72	R73	G135	L198	ALA	R73	G136	L199	Y261	ALA	R74	F134	L198	L257	Y260	
	R74	S131	P196	Y262	ALA	R74	D75	L136	E199	ALA	D75	L137	L200	Y263	ALA	R75	F135	L199	L258	Y262	
	R76	S132	P197	Y264	LEU	R76	M75	L137	F200	LEU	M75	L138	L201	Y265	LEU	R77	F136	L200	L259	Y264	
	R78	S133	P198	Y266	LEU	R78	P77	T139	F201	ILE	P77	T140	L202	Y267	ILE	R79	F137	L201	L260	Y266	
	R80	S134	P199	Y268	GLY	R80	A78	G202	G266	GLY	A78	G203	L203	Y269	GLY	R81	F138	L202	L261	Y268	
	R82	S135	P200	Y270	LEU	R82	G80	V143	K267	SER	G80	V144	L204	Y271	SER	R83	F139	L203	L262	Y270	
GLY	R84	S136	P201	Y272	SER	R84	H81	L144	E204	SER	H81	L145	L205	Y273	SER	R85	F140	L204	L263	Y272	
	R86	S137	P202	Y274	HIS	R86	L82	Y145	E205	HIS	L82	Y146	L206	Y275	HIS	R87	F141	L205	L264	Y274	
	R88	S138	P203	Y276	THR	R88	T84	R146	E206	THR	T84	R147	L207	Y277	THR	R89	F142	L206	L265	Y276	
	R90	S139	P204	Y278	ALA	R90	P85	Y147	E207	ALA	P85	Y148	L208	Y279	ALA	R91	F143	L207	L266	Y278	
	R92	S140	P205	Y280	LEU	R92	T86	S149	E208	LEU	T86	S150	L209	Y281	LEU	R93	F144	L208	L267	Y280	
	R94	S141	P206	Y282	LEU	R94	L87	N150	E209	LEU	L87	N151	L210	Y283	LEU	R95	F145	L209	L268	Y282	
	R96	S142	P207	Y284	LEU	R96	E88	D151	E210	LEU	E88	D152	L211	Y285	LEU	R97	F146	L210	L269	Y284	
	R98	S143	P208	Y286	ILE	R98	A91	T154	E211	ILE	A91	T155	L212	Y287	ILE	R99	F147	L211	L270	Y286	
	R100	S144	P209	Y288	GLY	R100	V94	S155	E212	GLY	V94	S156	L213	Y289	GLY	R101	F148	L212	L271	Y288	
	R102	S145	P210	Y290	THR	R102	S95	N157	E213	THR	S95	N158	L214	Y291	THR	R103	F149	L213	L272	Y290	
P30	R104	S146	P211	Y292	ALA	R104	T96	H158	E214	ALA	T96	H159	L215	Y293	ALA	R105	F150	L214	L273	Y292	
	R106	S147	P212	Y294	ALA	R106	R99	T160	E215	ALA	R99	T161	L216	Y295	ALA	R107	F151	L215	L274	Y294	
	R108	S148	P213	Y296	LEU	R108	Q100	I162	E216	LEU	Q100	I163	L217	Y297	LEU	R109	F152	L216	L275	Y296	
	R110	S149	P214	Y298	LEU	R110	N101	V163	E217	LEU	N101	V164	L218	Y299	LEU	R111	F153	L217	L276	Y298	
	R112	S150	P215	Y300	LEU	R112	Q102	E164	E218	LEU	Q102	E165	L219	Y301	LEU	R113	F154	L218	L277	Y300	
	R114	S151	P216	Y302	LEU	R114	Y103	F166	E219	LEU	Y103	F167	L220	Y303	LEU	R115	F155	L219	L278	Y302	
	R116	S152	P217	Y304	LEU	R116	Y104	Q166	E220	LEU	Y104	Q167	L221	Y305	LEU	R117	F156	L220	L279	Y304	
	R118	S153	P218	Y306	LEU	R118	Y105	Q167	E221	LEU	Y105	Q168	L222	Y307	LEU	R119	F157	L221	L280	Y306	
	R120	S154	P219	Y308	LEU	R120	Y106	Q168	E222	LEU	Y106	Q169	L223	Y309	LEU	R121	F158	L222	L281	Y308	
	R122	S155	P220	Y310	LEU	R122	Q107	V108	E223	LEU	Q107	V109	F169	L224	LEU	R123	F159	L223	L282	Y310	
A45	R124	S156	P221	Y312	LEU	R124	Q108	E224	LEU	Q108	E225	L225	Y313	LEU	R125	F160	L224	L283	Y312	Y313	
	R126	S157	P222	Y314	LEU	R126	Q109	E225	LEU	Q109	E226	L226	Y315	LEU	R127	F161	L225	L284	Y314	Y315	
	R128	S158	P223	Y316	LEU	R128	Y107	F170	E226	LEU	Y107	F171	L227	LEU	R129	F162	L226	L285	Y316	Y317	
	R130	S159	P224	Y318	LEU	R130	Y108	F171	E227	LEU	Y108	F172	L228	Y319	LEU	R131	F163	L227	L286	Y318	Y319
	R132	S160	P225	Y320	LEU	R132	Y109	F172	E228	LEU	Y109	F173	L229	Y321	LEU	R133	F164	L228	L287	Y320	Y321
	R134	S161	P226	Y322	LEU	R134	Y110	F173	E229	LEU	Y110	F174	L230	Y323	LEU	R135	F165	L229	L288	Y322	Y323
	R136	S162	P227	Y324	LEU	R136	Y111	F174	E230	LEU	Y111	F175	L231	Y325	LEU	R137	F166	L230	L289	Y324	Y325
	R138	S163	P228	Y326	LEU	R138	Y112	F175	E231	LEU	Y112	F176	L232	Y327	LEU	R139	F167	L231	L290	Y326	Y327
	R140	S164	P229	Y328	LEU	R140	Y113	F176	E232	LEU	Y113	F177	L233	Y329	LEU	R141	F168	L232	L291	Y328	Y329
	R142	S165	P230	Y330	LEU	R142	Y114	F177	E233	LEU	Y114	F178	L234	Y331	LEU	R143	F169	L233	L292	Y330	Y331
R52	R144	S166	P231	Y332	LEU	R144	Y115	F178	E234	LEU	Y115	F179	L235	Y333	LEU	R145	F170	L234	L293	Y332	Y333
	R146	S167	P232	Y334	LEU	R146	Y116	F179	E235	LEU	Y116	F180	L236	Y335	LEU	R147	F171	L235	L294	Y334	Y335
	R148	S168	P233	Y336	LEU	R148	Y117	F180	E236	LEU	Y117	F181	L237	Y337	LEU	R149	F172	L236	L295	Y336	Y337
	R150	S169	P234	Y338	LEU	R150	Y118	F181	E237	LEU	Y118	F182	L238	Y339	LEU	R151	F173	L237	L296	Y338	Y339
	R152	S170	P235	Y340	LEU	R152	Y119	F182	E238	LEU	Y119	F183	L239	Y341	LEU	R153	F174	L238	L297	Y340	Y341
	R154	S171	P236	Y342	LEU	R154	Y120	F183	E239	LEU	Y120	F184	L240	Y343	LEU	R155	F175	L239	L298	Y342	Y343
	R156	S172	P237	Y344	LEU	R156	Y121	F184	E240	LEU	Y121	F185	L241	Y345	LEU	R157	F176	L240	L299	Y344	Y345
	R158	S173	P238	Y346	LEU	R158	Y122	F185	E241	LEU	Y122	F186	L242	Y347	LEU	R159	F177	L241	L300	Y346	Y347
	R160	S174	P239	Y348	LEU	R160	Y123	F186	E242	LEU	Y123	F187	L243	Y349	LEU	R161	F178	L242	L301	Y348	Y349
	R162	S175	P240	Y350	LEU	R162	Y124	F187	E243	LEU	Y124	F188	L244	Y351	LEU	R163	F179	L243	L302	Y350	Y351
Q53	R164	S176	P241	Y352	LEU	R164	Y125	F188	E244	LEU	Y125	F189	L245	Y353	LEU	R165	F180	L244	L303	Y352	Y353
	R166	S177	P242	Y354	LEU	R166	Y126	F189	E245	LEU	Y126	F190	L246	Y355	LEU	R167	F181	L245	L304	Y354	Y355
	R168	S178	P243	Y356	LEU	R168	Y127	F190	E246	LEU	Y127	F191	L247	Y357	LEU	R169	F182	L246	L305	Y356	Y357
	R170	S179	P244	Y358	LEU	R170	Y128	F191	E247	LEU	Y128	F192	L248	Y359	LEU	R171	F183	L247	L306	Y358	Y359
	R172	S180	P245	Y360	LEU	R172	Y129	F192	E248	LEU	Y129	F193	L249	Y361	LEU	R173	F184	L248	L307	Y360	Y361
	R174	S181	P246	Y362	LEU	R174	Y130	F193	E249	LEU	Y130	F194	L250	Y363	LEU	R175	F185	L249	L308	Y362	Y363
	R176	S182	P247	Y364	LEU	R176	Y131	F194	E250	LEU	Y131	F195	L251	Y365	LEU	R177	F186	L250	L309	Y364	Y365
	R178	S183	P248	Y366	LEU	R178	Y132	F195	E251	LEU	Y132	F196	L252	Y367	LEU	R179	F187	L251	L310	Y366	Y367
	R180	S184	P249	Y368	LEU	R180	Y133	F196	E252	LEU	Y133	F197	L253	Y369	LEU	R181	F188	L252	L311	Y368	Y369
	R182	S185	P250	Y370	LEU	R182	Y134	F197	E253	LEU	Y134	F198	L254	Y371	LEU	R183	F189	L253	L312	Y370	Y371
R58	R184	S186	P251	Y372	LEU	R184	Y135	F198	E254	LEU	Y135	F199	L255	Y373	LEU	R185	F190	L254	L313	Y372	Y373
	R186	S187	P252	Y374	LEU	R186	Y136	F199	E255	LEU	Y136	F200	L256	Y375	LEU	R187	F191	L255	L314	Y374	Y375
	R188	S188	P253	Y376	LEU	R188	Y137	F200	E256	LEU	Y137	F201	L257	Y377	LEU	R189	F192	L256	L315	Y376	Y377
	R190	S189	P254	Y378	LEU	R190	Y138	F201	E257	LEU	Y138	F202	L258	Y379	LEU	R191	F193	L257	L316	Y378	Y379
	R192	S190	P255	Y380	LEU	R192	Y139	F202	E258	LEU	Y139	F203	L259	Y381	LEU	R193	F194	L258	L317	Y380	Y381
	R194	S191	P256	Y382	LEU	R194	Y140	F203	E259	LEU	Y140	F204	L260	Y383	LEU	R195	F195	L259	L318	Y382	Y383
	R196	S192	P257	Y384	LEU	R196	Y141	F204	E260	LEU	Y141	F205	L261	Y385	LEU	R197	F196	L260	L319	Y384	Y385
	R198	S193	P258	Y386	LEU	R198	Y142	F205	E261	LEU	Y142	F206	L262	Y387	LEU	R199	F197	L261	L320	Y386	Y387
	R200	S194	P259	Y388	LEU	R200	Y143	F206	E262	LEU	Y143	F207	L263	Y389	LEU	R201	F198	L262	L321	Y388	Y389
	R202	S195	P260	Y390	LEU	R202	Y144	F207	E263	LEU	Y144	F208	L264	Y391	LEU	R203	F199	L263	L322	Y390	Y391
R55	R204	S196	P261	Y392	LEU	R204	Y145	F208	E264	LEU	Y145	F209	L265	Y393	LEU	R205	F200	L264	L323	Y392	Y393
	R206	S197	P262	Y394	LEU	R206	Y146	F209	E265	LEU	Y146	F210	L266	Y395	LEU	R207	F201	L265	L324	Y394	Y395
	R208	S198	P263	Y396	LEU	R208	Y147	F210	E266	LEU	Y147	F211	L267	Y397	LEU	R209	F202	L266	L325		



K1623	L1624	C1625	D1626	D1627	F1628	A1629	Q1630	F1631	S1632	L1635	T1636	E1637	T1642																																							
D1553	P1556	P1557	A1558	K1559	T1560	H1561	Q1562	Y1563	Q1566	Q1570	E1571	A1572	L1573	N1574	L1575	K1576	V1577	N1578	Y1581	L1582	T1583	W1584	L1590	L1591	P1592	T1593	K1594	I1597	S1598	Y1599	I1600	I1601	T1602	N1604	T1605	W1606	I1607	E1608	R1609	W1610	P1611	H1612	E1613	D1614	E1615	C1616	Q1617	E1618	E1619	E1620	F1621	Q1622
L1481	M1482	K1483	I1484	C1485	G1490	R1491	C1492	A1493	G1494	E1495	T1496	C1497	L1500	M1501	H1502	Q1503	E1504	R1505	I1506	D1507	V1508	P1509	L1510	Q1511	I1512	E1513	K1514	A1515	C1516	E1517	T1518	M1519	V1520	D1521	Y1522	V1523	Y1524	K1525	T1526	K1527	L1528	L1529	R1530	I1531	Q1534	D1535	I1539	Y1540	V1541	M1542	L1545	I1548
R1406	Y1407	I1408	E1412	M1417	A1418	Q1419	K1420	V1421	A1422	V1423	I1424	I1425	Y1426	L1427	N1428	K1429	V1430	S1431	H1432	S1433	C1437	L1438	H1439	I1442	L1443	K1444	H1445	F1446	E1447	V1448	G1449	F1450	I1451	S1455	V1456	K1457	V1458	Y1459	S1460	L1464	D1465	E1466	K1467	C1468	T1469	K1470	F1471	Y1472	H1473	P1474	D1475	L1480

## 4 Data and refinement statistics

Property	Value	Source
Space group	P 2 2 21	Depositor
Cell constants a, b, c, $\alpha$ , $\beta$ , $\gamma$	176.52Å 179.20Å 389.69Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	49.47 – 4.30 49.47 – 4.30	Depositor EDS
% Data completeness (in resolution range)	94.2 (49.47-4.30) 94.3 (49.47-4.30)	Depositor EDS
$R_{merge}$	(Not available)	Depositor
$R_{sym}$	0.14	Depositor
$\langle I/\sigma(I) \rangle$ <sup>1</sup>	3.12 (at 4.29Å)	Xtriage
Refinement program	PHENIX (phenix.refine: 1.6.4_486)	Depositor
R, $R_{free}$	0.233 , 0.262 0.225 , 0.250	Depositor DCC
$R_{free}$ test set	1734 reflections (2.17%)	wwPDB-VP
Wilson B-factor (Å <sup>2</sup> )	135.2	Xtriage
Anisotropy	0.503	Xtriage
Bulk solvent $k_{sol}$ (e/Å <sup>3</sup> ), $B_{sol}$ (Å <sup>2</sup> )	0.30 , 172.4	EDS
L-test for twinning <sup>2</sup>	$\langle  L  \rangle = 0.48$ , $\langle L^2 \rangle = 0.31$	Xtriage
Estimated twinning fraction	0.026 for k,h,-l	Xtriage
$F_o, F_c$ correlation	0.90	EDS
Total number of atoms	45268	wwPDB-VP
Average B, all atoms (Å <sup>2</sup> )	192.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.37% of the height of the origin peak. No significant pseudotranslation is detected.*

<sup>1</sup>Intensities estimated from amplitudes.

<sup>2</sup>Theoretical values of  $\langle |L| \rangle$ ,  $\langle L^2 \rangle$  for acentric reflections are 0.5, 0.333 respectively for untwinned datasets, and 0.375, 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: 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	0.57	1/13158 (0.0%)	0.77	6/17851 (0.0%)
1	C	0.58	0/13158	0.76	5/17851 (0.0%)
2	B	0.55	0/9912	0.74	1/13454 (0.0%)
2	D	0.55	0/9912	0.74	2/13454 (0.0%)
All	All	0.57	1/46140 (0.0%)	0.75	14/62610 (0.0%)

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	3
1	C	0	3
2	B	0	1
2	D	0	1
All	All	0	8

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	810	CYS	CB-SG	-5.27	1.73	1.81

All (14) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	C	1539	LEU	CA-CB-CG	6.88	131.12	115.30
1	A	1539	LEU	CA-CB-CG	6.87	131.10	115.30
1	A	1195	LEU	CA-CB-CG	-6.42	100.53	115.30
1	C	1195	LEU	CA-CB-CG	-6.27	100.87	115.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	1346	ASN	CA-CB-CG	5.54	125.58	113.40
2	D	1346	ASN	CA-CB-CG	5.53	125.56	113.40
1	A	1000	LEU	CA-CB-CG	-5.35	102.99	115.30
1	A	181	GLY	N-CA-C	5.32	126.40	113.10
1	A	1105	LEU	CA-CB-CG	-5.28	103.16	115.30
2	D	1492	CYS	CA-CB-SG	-5.22	104.59	114.00
1	C	982	LEU	CA-CB-CG	-5.19	103.36	115.30
1	C	1000	LEU	CA-CB-CG	-5.19	103.37	115.30
1	A	982	LEU	CA-CB-CG	-5.17	103.40	115.30
1	C	181	GLY	N-CA-C	5.09	125.83	113.10

There are no chirality outliers.

All (8) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	472	ASN	Peptide
1	A	552	ALA	Peptide
1	A	667	GLU	Peptide
2	B	1351	ASN	Peptide
1	C	472	ASN	Peptide
1	C	552	ALA	Peptide
1	C	667	GLU	Peptide
2	D	1351	ASN	Peptide

## 5.2 Too-close contacts

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

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	12881	0	12821	1676	0
1	C	12881	0	12821	1666	0
2	B	9711	0	9702	1046	0
2	D	9711	0	9702	1061	0
3	A	14	0	13	2	0
3	B	28	0	26	1	0
3	C	14	0	13	2	0
3	D	28	0	26	1	0
All	All	45268	0	45124	5374	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 59.

All (5374) 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)
2:D:380:VAL:HG12	2:D:387:MET:HB3	1.26	1.15
2:B:380:VAL:HG12	2:B:387:MET:HB3	1.24	1.15
2:D:1609:ARG:HH11	2:D:1609:ARG:HG2	1.12	1.13
1:A:386:VAL:H	1:A:411:THR:HG22	1.02	1.12
1:C:386:VAL:H	1:C:411:THR:HG22	1.00	1.11
2:D:261:ALA:HB2	2:D:320:VAL:HG23	1.30	1.11
2:B:1609:ARG:HG2	2:B:1609:ARG:HH11	1.13	1.10
1:A:1228:TRP:H	1:A:1251:THR:HG22	1.13	1.10
1:C:979:VAL:HG21	1:C:1326:TYR:CE1	1.85	1.10
1:A:59:TYR:CE2	1:A:99:VAL:HG21	1.85	1.09
1:A:1278:GLN:OE1	1:A:1283:GLY:HA2	1.49	1.09
1:A:1494:THR:HB	1:A:1506:THR:HG23	1.32	1.07
1:C:1278:GLN:OE1	1:C:1283:GLY:HA2	1.53	1.07
2:D:850:LEU:HB2	2:D:882:PHE:HE1	1.20	1.07
1:C:1228:TRP:H	1:C:1251:THR:HG22	1.12	1.06
2:B:261:ALA:HB2	2:B:320:VAL:HG23	1.36	1.05
2:B:851:LEU:HD23	2:B:852:TYR:H	1.18	1.05
1:A:979:VAL:HG21	1:A:1326:TYR:CE1	1.90	1.05
2:B:344:GLN:HA	2:B:344:GLN:HE21	1.19	1.04
1:C:1228:TRP:H	1:C:1251:THR:CG2	1.70	1.03
2:D:526:VAL:HG23	2:D:530:GLU:HB3	1.37	1.03
2:B:1473:HIS:CD2	2:B:1474:PRO:HD2	1.93	1.03
1:C:492:TYR:CD2	1:C:493:ILE:N	2.27	1.03
1:C:535:VAL:HG23	1:C:536:PRO:HD3	1.40	1.03
1:A:492:TYR:CD2	1:A:493:ILE:N	2.27	1.03
1:C:1494:THR:HB	1:C:1506:THR:HG23	1.39	1.03
1:C:1584:ILE:HG22	1:C:1585:TYR:H	1.24	1.03
1:C:59:TYR:CE2	1:C:99:VAL:HG21	1.92	1.03
2:B:526:VAL:HG23	2:B:530:GLU:HB3	1.39	1.02
1:C:42:GLN:HB2	1:C:80:GLN:HE21	1.24	1.02
2:B:1607:ILE:H	2:B:1607:ILE:HD12	1.22	1.02
1:A:535:VAL:HG23	1:A:536:PRO:HD3	1.40	1.02
2:B:1590:LEU:HD23	2:B:1591:LEU:H	1.21	1.02
1:A:42:GLN:HB2	1:A:80:GLN:HE21	1.25	1.01
1:A:224:LEU:HD22	1:A:225:PRO:HD2	1.39	1.01
1:C:24:VAL:CA	1:C:655:THR:HG21	1.88	1.01
1:A:1228:TRP:H	1:A:1251:THR:CG2	1.73	1.01

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1473:HIS:CD2	2:D:1474:PRO:HD2	1.96	1.01
2:D:344:GLN:HA	2:D:344:GLN:HE21	1.18	1.01
2:D:1523:VAL:HG22	2:D:1584:TRP:HB2	1.39	1.01
1:C:87:ILE:H	1:C:87:ILE:HD13	1.23	1.00
1:C:1008:ALA:HB3	1:C:1078:LEU:HD11	1.40	1.00
1:C:222:TYR:HE1	1:C:768:TYR:HB2	1.25	1.00
1:A:1584:ILE:HG22	1:A:1585:TYR:H	1.27	1.00
1:A:87:ILE:HD13	1:A:87:ILE:H	1.21	1.00
1:C:24:VAL:HA	1:C:655:THR:CG2	1.89	1.00
2:D:851:LEU:HD23	2:D:852:TYR:H	1.21	1.00
1:A:44:TYR:HE1	1:A:497:THR:HG21	1.24	1.00
2:B:850:LEU:HB2	2:B:882:PHE:HE1	1.25	0.99
1:A:24:VAL:HA	1:A:655:THR:HG21	1.02	0.99
1:A:24:VAL:HA	1:A:655:THR:CG2	1.91	0.99
1:C:831:TYR:O	1:C:928:ARG:HD2	1.63	0.99
1:A:1056:ILE:HD11	1:A:1066:TYR:HE2	1.25	0.99
1:A:24:VAL:CA	1:A:655:THR:HG21	1.91	0.99
2:B:548:LEU:HD22	2:B:793:SER:HB3	1.43	0.99
1:A:222:TYR:HE1	1:A:768:TYR:HB2	1.28	0.99
1:A:831:TYR:O	1:A:928:ARG:HD2	1.62	0.99
2:D:548:LEU:HD22	2:D:793:SER:HB3	1.42	0.99
1:A:576:SER:HB3	1:A:577:PRO:HD3	1.44	0.98
2:D:1607:ILE:H	2:D:1607:ILE:HD12	1.28	0.98
1:C:386:VAL:N	1:C:411:THR:HG22	1.76	0.98
1:A:1008:ALA:HB3	1:A:1078:LEU:HD11	1.44	0.97
1:C:111:PHE:HE2	1:C:113:LYS:HB2	1.26	0.97
2:D:556:ILE:H	2:D:556:ILE:HD12	1.26	0.97
1:C:224:LEU:HD22	1:C:225:PRO:HD2	1.42	0.97
1:C:682:LYS:HZ2	1:C:686:ILE:HD11	1.28	0.97
1:A:1068:VAL:HA	1:A:1078:LEU:HD12	1.47	0.97
1:C:24:VAL:HA	1:C:655:THR:HG21	1.00	0.97
1:C:1056:ILE:HD11	1:C:1066:TYR:HE2	1.27	0.97
1:A:44:TYR:HB2	1:A:545:ILE:HD12	1.47	0.97
2:B:531:ILE:HD11	2:B:634:LEU:HD23	1.42	0.97
1:C:44:TYR:HB2	1:C:545:ILE:HD12	1.47	0.97
1:A:386:VAL:N	1:A:411:THR:HG22	1.79	0.96
2:D:1590:LEU:HD23	2:D:1591:LEU:H	1.27	0.96
2:B:556:ILE:H	2:B:556:ILE:HD12	1.29	0.96
1:C:576:SER:HB3	1:C:577:PRO:HD3	1.44	0.96
1:A:111:PHE:HE2	1:A:113:LYS:HB2	1.27	0.96
2:B:1523:VAL:HG22	2:B:1584:TRP:HB2	1.47	0.96

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:421:VAL:HG11	2:B:505:THR:HG22	1.47	0.96
1:C:386:VAL:H	1:C:411:THR:CG2	1.78	0.96
2:D:531:ILE:HD11	2:D:634:LEU:HD23	1.46	0.96
1:C:44:TYR:HE1	1:C:497:THR:HG21	1.28	0.95
1:C:236:ASN:HB2	1:C:379:LEU:HD21	1.48	0.95
2:D:954:VAL:HB	2:D:957:THR:HG21	1.47	0.95
1:A:853:MET:O	1:A:888:VAL:HG12	1.66	0.95
1:C:395:ILE:HG22	1:C:401:THR:HG22	1.49	0.95
2:D:1284:ARG:CD	2:D:1285:GLU:H	1.80	0.95
1:A:395:ILE:HG22	1:A:401:THR:HG22	1.49	0.95
1:A:386:VAL:H	1:A:411:THR:CG2	1.79	0.95
1:A:702:GLY:HA2	1:A:728:PHE:CE1	2.02	0.94
1:C:330:ILE:HG22	1:C:337:SER:HB2	1.46	0.94
1:C:1068:VAL:HA	1:C:1078:LEU:HD12	1.48	0.94
1:C:1228:TRP:N	1:C:1251:THR:HG22	1.82	0.94
2:B:1284:ARG:CD	2:B:1285:GLU:H	1.81	0.94
1:C:111:PHE:CE2	1:C:113:LYS:HB2	2.02	0.94
1:A:1012:LEU:HD22	1:A:1085:VAL:HG21	1.49	0.94
1:A:236:ASN:HB2	1:A:379:LEU:HD21	1.47	0.94
1:C:145:VAL:HB	1:C:183:ILE:HD12	1.49	0.94
2:D:1450:PHE:HD1	2:D:1451:ILE:H	1.12	0.94
2:B:120:LEU:HD12	2:B:121:LEU:H	1.30	0.94
2:B:1610:TRP:HA	2:B:1628:PHE:HE2	1.33	0.94
2:B:481:TYR:HB2	2:B:520:PHE:HE1	1.30	0.94
2:D:1610:TRP:HA	2:D:1628:PHE:HE2	1.33	0.94
2:D:787:TRP:HB2	2:D:808:ILE:HG22	1.49	0.94
1:A:1585:TYR:HD1	1:A:1671:ILE:HG12	1.33	0.94
1:A:653:PHE:O	1:A:653:PHE:HD1	1.51	0.94
1:C:1585:TYR:HD1	1:C:1671:ILE:HG12	1.33	0.94
1:A:1615:ARG:HH21	1:A:1650:ARG:HH22	1.09	0.93
1:A:374:GLN:HA	1:A:416:GLY:O	1.68	0.93
1:C:853:MET:O	1:C:888:VAL:HG12	1.67	0.93
2:B:1273:LEU:HB2	2:B:1319:GLY:HA3	1.51	0.93
2:B:1491:ARG:HG3	2:B:1492:CYS:H	1.33	0.93
2:D:265:PHE:CD2	2:D:294:LEU:HB2	2.03	0.93
1:A:682:LYS:NZ	1:A:686:ILE:HD11	1.84	0.93
2:B:787:TRP:HB2	2:B:808:ILE:HG22	1.50	0.93
2:B:285:ILE:HD12	2:B:285:ILE:H	1.32	0.92
1:A:1056:ILE:HD11	1:A:1066:TYR:CE2	2.04	0.92
1:A:135:TYR:CZ	1:A:141:VAL:HG13	2.05	0.92
2:D:120:LEU:HD12	2:D:121:LEU:H	1.30	0.92

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1607:ILE:N	2:B:1607:ILE:HD12	1.85	0.92
2:B:510:ILE:HG23	2:B:514:LEU:HD12	1.52	0.92
2:B:954:VAL:HB	2:B:957:THR:HG21	1.51	0.92
2:D:1273:LEU:HB2	2:D:1319:GLY:HA3	1.51	0.92
2:D:510:ILE:HG23	2:D:514:LEU:HD12	1.50	0.92
1:C:1585:TYR:CD1	1:C:1671:ILE:HG12	2.05	0.92
2:D:1491:ARG:HG3	2:D:1492:CYS:H	1.35	0.92
1:A:371:ILE:HD11	1:A:433:PHE:CE2	2.04	0.91
1:C:1615:ARG:HH21	1:C:1650:ARG:HH22	1.06	0.91
2:D:285:ILE:HD12	2:D:285:ILE:H	1.33	0.91
1:A:145:VAL:HB	1:A:183:ILE:HD12	1.51	0.91
1:A:884:VAL:O	1:A:885:ARG:HB2	1.67	0.91
1:C:135:TYR:CZ	1:C:141:VAL:HG13	2.06	0.91
1:C:222:TYR:CE1	1:C:768:TYR:HB2	2.04	0.91
1:A:351:PRO:HG2	1:A:352:TYR:CD2	2.06	0.91
1:C:489:LYS:C	1:C:491:PRO:HD3	1.91	0.91
2:B:1424:ILE:H	2:B:1424:ILE:HD13	1.34	0.91
1:C:493:ILE:HG22	1:C:495:LYS:H	1.36	0.91
2:D:197:TRP:HB2	2:D:214:PHE:CE1	2.05	0.91
1:A:330:ILE:HG22	1:A:337:SER:HB2	1.51	0.91
2:B:1450:PHE:HD1	2:B:1451:ILE:H	1.13	0.91
1:A:111:PHE:CE2	1:A:113:LYS:HB2	2.06	0.91
1:A:1404:ALA:HB1	1:A:1493:PHE:CE2	2.06	0.91
2:B:435:TYR:HD1	2:B:436:GLN:H	0.94	0.91
1:C:371:ILE:HD11	1:C:433:PHE:CE2	2.06	0.91
1:C:702:GLY:HA2	1:C:728:PHE:CE1	2.06	0.91
2:D:42:LEU:HD11	2:D:82:LEU:HD12	1.52	0.91
1:A:1228:TRP:N	1:A:1251:THR:HG22	1.85	0.90
1:A:489:LYS:C	1:A:491:PRO:HD3	1.91	0.90
2:B:239:GLY:H	2:B:296:ARG:NH2	1.69	0.90
1:C:682:LYS:NZ	1:C:686:ILE:HD11	1.85	0.90
2:B:646:GLN:HB3	2:B:647:PRO:HD2	1.51	0.90
2:D:239:GLY:H	2:D:296:ARG:NH2	1.69	0.90
1:A:1585:TYR:CD1	1:A:1671:ILE:HG12	2.07	0.90
2:B:481:TYR:O	2:B:481:TYR:HD2	1.54	0.90
1:C:374:GLN:HA	1:C:416:GLY:O	1.72	0.90
1:A:60:PRO:HD2	1:A:61:ASP:H	1.36	0.90
1:A:222:TYR:CE1	1:A:768:TYR:HB2	2.06	0.90
1:A:423:ASN:HB3	2:B:501:GLN:NE2	1.86	0.90
1:A:702:GLY:HA2	1:A:728:PHE:HE1	1.37	0.90
2:B:1331:ALA:O	2:B:1332:GLN:HB3	1.70	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:482:LEU:HB3	2:B:492:VAL:HG23	1.54	0.90
1:A:500:ASN:OD1	1:A:514:THR:HG23	1.71	0.89
1:C:888:VAL:HG23	1:C:894:HIS:HB2	1.52	0.89
2:D:481:TYR:HB2	2:D:520:PHE:HE1	1.36	0.89
1:C:884:VAL:O	1:C:885:ARG:HB2	1.70	0.89
2:D:435:TYR:HD1	2:D:436:GLN:H	0.94	0.89
1:A:884:VAL:HG12	1:A:886:GLN:HG2	1.52	0.89
1:A:849:ARG:HH11	1:A:849:ARG:HG3	1.37	0.89
2:B:927:ILE:HG23	2:B:1324:THR:HG23	1.54	0.89
1:A:493:ILE:HG22	1:A:495:LYS:H	1.36	0.89
1:A:584:PRO:HB3	1:A:792:ASP:HA	1.54	0.89
1:C:539:ARG:NH2	1:C:634:CYS:H	1.69	0.89
2:D:1424:ILE:HD13	2:D:1424:ILE:H	1.36	0.89
2:D:964:ILE:HG13	2:D:1302:THR:HG23	1.55	0.89
1:C:1056:ILE:HD11	1:C:1066:TYR:CE2	2.07	0.89
1:C:584:PRO:HB3	1:C:792:ASP:HA	1.54	0.89
2:D:435:TYR:HD1	2:D:436:GLN:N	1.69	0.89
2:D:850:LEU:HB2	2:D:882:PHE:CE1	2.08	0.89
2:D:646:GLN:HB3	2:D:647:PRO:HD2	1.52	0.89
2:B:42:LEU:HD11	2:B:82:LEU:HD12	1.51	0.89
2:D:1607:ILE:N	2:D:1607:ILE:HD12	1.88	0.89
2:B:265:PHE:CD2	2:B:294:LEU:HB2	2.08	0.88
1:C:653:PHE:HD1	1:C:653:PHE:O	1.56	0.88
2:D:482:LEU:HB3	2:D:492:VAL:HG23	1.55	0.88
1:A:490:SER:N	1:A:491:PRO:CD	2.36	0.88
1:C:1086:LEU:HD12	1:C:1095:GLN:HG3	1.55	0.88
1:C:470:THR:HG22	2:D:450:THR:HG22	1.55	0.88
1:C:60:PRO:HD2	1:C:61:ASP:H	1.38	0.88
1:C:849:ARG:HH11	1:C:849:ARG:HG3	1.37	0.88
1:C:1315:VAL:HG12	1:C:1324:HIS:O	1.72	0.88
2:D:161:VAL:HG21	2:D:180:LEU:HD21	1.55	0.88
2:D:221:LEU:HD11	2:D:753:LYS:HG2	1.55	0.88
2:D:218:LYS:HB3	2:D:822:TYR:CD2	2.08	0.88
2:D:850:LEU:HG	2:D:851:LEU:N	1.89	0.88
1:A:1102:ASN:HD21	1:C:1162:VAL:H	1.20	0.88
2:B:435:TYR:HD1	2:B:436:GLN:N	1.70	0.87
2:D:415:THR:HG1	2:D:425:GLN:HB3	1.39	0.87
1:C:174:VAL:HG22	1:C:175:GLU:H	1.40	0.87
1:C:351:PRO:HG2	1:C:352:TYR:CD2	2.10	0.87
1:A:250:ILE:HD11	1:A:265:VAL:HG11	1.56	0.87
1:C:1012:LEU:HD22	1:C:1085:VAL:HG21	1.57	0.87

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:VAL:HG22	1:C:1102:ASN:ND2	1.89	0.87
2:D:481:TYR:O	2:D:481:TYR:HD2	1.57	0.87
1:A:979:VAL:HG12	1:A:1359:VAL:HG22	1.55	0.87
1:A:1162:VAL:H	1:C:1102:ASN:HD21	1.16	0.87
1:A:1627:ILE:HD12	1:A:1629:TYR:HB3	1.57	0.87
1:A:869:GLU:C	1:A:871:PRO:HD3	1.95	0.87
2:B:221:LEU:HD11	2:B:753:LYS:HG2	1.56	0.87
1:C:127:PHE:HE2	1:C:623:VAL:HG13	1.39	0.87
1:C:614:ARG:HD2	1:C:615:GLY:H	1.39	0.87
2:D:1331:ALA:O	2:D:1332:GLN:HB3	1.70	0.87
1:A:362:PHE:HE1	1:A:640:LEU:HD22	1.39	0.86
1:A:614:ARG:HD2	1:A:615:GLY:H	1.41	0.86
2:B:948:ARG:HH21	2:B:948:ARG:HB2	1.40	0.86
1:C:869:GLU:C	1:C:871:PRO:HD3	1.95	0.86
2:B:192:VAL:HG22	2:B:193:SER:H	1.39	0.86
1:C:884:VAL:HG12	1:C:886:GLN:HG2	1.55	0.86
1:A:999:ILE:HG13	1:A:1000:LEU:H	1.41	0.86
1:C:182:ILE:HG12	1:C:804:ILE:HD11	1.58	0.86
1:C:490:SER:N	1:C:491:PRO:CD	2.38	0.86
1:A:796:THR:HG23	1:A:818:LYS:HB3	1.55	0.86
1:C:504:LEU:HD21	1:C:651:LEU:HG	1.57	0.86
1:C:430:VAL:HG11	1:C:453:ARG:HH21	1.41	0.86
2:B:161:VAL:HG21	2:B:180:LEU:HD21	1.57	0.86
1:A:162:THR:HG21	1:A:204:LYS:HE2	1.56	0.86
1:A:1086:LEU:HD12	1:A:1095:GLN:HG3	1.57	0.85
2:B:850:LEU:HG	2:B:851:LEU:N	1.91	0.85
2:D:508:LEU:HD12	2:D:509:HIS:H	1.40	0.85
1:A:504:LEU:HD21	1:A:651:LEU:HG	1.57	0.85
2:B:415:THR:HG1	2:B:425:GLN:HB3	1.38	0.85
1:C:1144:LEU:O	1:C:1148:THR:HG23	1.75	0.85
1:A:1549:LYS:NZ	1:A:1667:PHE:HB3	1.90	0.85
1:A:967:LEU:HD12	1:A:968:VAL:N	1.91	0.85
2:D:44:GLU:HG2	2:D:82:LEU:HB2	1.58	0.85
2:B:218:LYS:HB3	2:B:822:TYR:CD2	2.10	0.85
1:C:250:ILE:HD11	1:C:265:VAL:HG11	1.58	0.85
1:A:174:VAL:HG22	1:A:175:GLU:H	1.41	0.85
1:A:979:VAL:HG21	1:A:1326:TYR:HE1	1.36	0.85
1:A:539:ARG:NH2	1:A:634:CYS:H	1.72	0.85
1:A:1278:GLN:OE1	1:A:1283:GLY:CA	2.25	0.85
1:C:44:TYR:CE1	1:C:497:THR:HG21	2.12	0.85
1:A:471:ASP:OD2	1:A:474:LYS:HB3	1.76	0.85

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:44:GLU:HG2	2:B:82:LEU:HB2	1.57	0.85
2:D:114:ARG:O	2:D:115:LEU:HD23	1.76	0.85
1:A:470:THR:HG22	2:B:450:THR:HG22	1.57	0.84
1:C:1490:PRO:HB3	1:C:1510:SER:HB2	1.58	0.84
1:A:1315:VAL:HG12	1:A:1324:HIS:O	1.77	0.84
1:A:623:VAL:HG12	1:A:624:PHE:N	1.92	0.84
1:C:623:VAL:HG12	1:C:624:PHE:N	1.92	0.84
1:C:982:LEU:H	1:C:982:LEU:HD12	1.41	0.84
2:D:1450:PHE:CD1	2:D:1451:ILE:N	2.45	0.84
2:D:948:ARG:HB2	2:D:948:ARG:HH21	1.43	0.84
1:A:1109:GLU:HG2	1:C:1163:LYS:HZ1	1.41	0.84
1:A:44:TYR:CE1	1:A:497:THR:HG21	2.10	0.84
2:D:1561:HIS:CE1	2:D:1597:ILE:HD13	2.12	0.84
1:A:1576:LYS:HG2	1:A:1601:ILE:HG22	1.58	0.84
1:A:888:VAL:HG23	1:A:894:HIS:HB2	1.57	0.84
1:C:471:ASP:OD2	1:C:474:LYS:HB3	1.77	0.84
1:C:999:ILE:HG13	1:C:1000:LEU:H	1.42	0.84
1:A:830:PRO:HG3	1:A:1483:PHE:CZ	2.13	0.84
1:A:1490:PRO:HB3	1:A:1510:SER:HB2	1.58	0.84
1:C:1068:VAL:HG21	1:C:1124:TYR:CD1	2.13	0.84
1:A:113:LYS:HG2	1:A:114:SER:H	1.41	0.84
1:C:979:VAL:HG21	1:C:1326:TYR:HE1	1.33	0.84
2:D:482:LEU:HD12	2:D:482:LEU:H	1.43	0.84
1:A:87:ILE:HD13	1:A:87:ILE:N	1.91	0.84
1:C:476:LEU:HD21	1:C:482:LEU:HD12	1.57	0.84
1:A:489:LYS:HZ3	2:B:502:ASN:H	1.24	0.84
1:C:796:THR:HG23	1:C:818:LYS:HB3	1.58	0.84
2:D:1274:ASN:ND2	2:D:1293:ASN:HB3	1.93	0.84
2:B:482:LEU:H	2:B:482:LEU:HD12	1.43	0.83
1:C:549:GLU:H	1:C:549:GLU:CD	1.80	0.83
1:A:546:VAL:O	1:A:553:GLU:HB3	1.78	0.83
1:C:1383:THR:HG21	1:C:1511:THR:HG22	1.60	0.83
1:C:889:GLU:HB2	1:C:892:SER:HB2	1.59	0.83
1:A:127:PHE:HE2	1:A:623:VAL:HG13	1.42	0.83
1:C:1127:ILE:HD12	1:C:1127:ILE:H	1.44	0.83
1:C:467:ILE:HG22	1:C:486:VAL:HG22	1.60	0.83
1:C:113:LYS:HG2	1:C:114:SER:H	1.44	0.83
1:C:830:PRO:HG3	1:C:1483:PHE:CZ	2.12	0.83
1:A:265:VAL:HG22	1:A:329:VAL:HG22	1.61	0.83
2:B:964:ILE:HG13	2:B:1302:THR:HG23	1.60	0.83
1:C:87:ILE:N	1:C:87:ILE:HD13	1.93	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1576:LYS:HG2	1:C:1601:ILE:HG22	1.60	0.83
1:A:884:VAL:CG1	1:A:886:GLN:HG2	2.08	0.83
1:C:131:ASP:HB3	1:C:142:LYS:HB2	1.60	0.83
1:C:1370:THR:HG23	1:C:1373:GLU:OE1	1.79	0.83
1:A:42:GLN:HB2	1:A:80:GLN:NE2	1.93	0.83
2:B:1274:ASN:ND2	2:B:1293:ASN:HB3	1.94	0.83
2:B:285:ILE:HD12	2:B:285:ILE:N	1.94	0.83
1:C:42:GLN:HB2	1:C:80:GLN:NE2	1.93	0.83
2:B:508:LEU:HD12	2:B:509:HIS:H	1.44	0.83
1:C:1320:LYS:HD2	1:C:1321:GLY:H	1.42	0.83
1:C:1549:LYS:NZ	1:C:1667:PHE:HB3	1.93	0.83
1:C:162:THR:HG21	1:C:204:LYS:HE2	1.58	0.83
1:C:546:VAL:O	1:C:553:GLU:HB3	1.78	0.83
1:A:491:PRO:HG2	1:A:494:ASP:HB3	1.60	0.82
2:D:344:GLN:HA	2:D:344:GLN:NE2	1.93	0.82
1:A:1127:ILE:HD12	1:A:1127:ILE:H	1.44	0.82
1:A:955:ARG:HG2	1:A:1350:THR:HG23	1.60	0.82
1:A:549:GLU:CD	1:A:549:GLU:H	1.81	0.82
1:A:838:GLN:HA	1:A:901:LEU:HB2	1.59	0.82
2:B:25:TYR:HB2	2:B:631:SER:HB3	1.60	0.82
1:C:443:PRO:HD2	1:C:446:ASN:HB2	1.61	0.82
1:A:905:ILE:HD12	1:A:931:PRO:HD3	1.61	0.82
2:B:476:ILE:O	2:B:497:ARG:HG2	1.78	0.82
1:A:153:LYS:HB2	1:A:154:PRO:HD2	1.58	0.82
1:C:153:LYS:HB2	1:C:154:PRO:HD2	1.60	0.82
1:C:905:ILE:HD12	1:C:931:PRO:HD3	1.60	0.82
1:A:1144:LEU:O	1:A:1148:THR:HG23	1.80	0.82
2:B:1561:HIS:CE1	2:B:1597:ILE:HD13	2.14	0.82
1:C:362:PHE:HE1	1:C:640:LEU:HD22	1.44	0.82
1:C:967:LEU:HD12	1:C:968:VAL:N	1.94	0.82
1:C:743:SER:HB2	1:C:751:ARG:N	1.95	0.82
1:A:238:ILE:HG23	1:A:242:ASN:HD22	1.41	0.82
2:B:1450:PHE:CD1	2:B:1451:ILE:N	2.47	0.82
1:A:1068:VAL:HG21	1:A:1124:TYR:CD1	2.13	0.82
1:A:1320:LYS:HD2	1:A:1321:GLY:H	1.43	0.82
1:C:1561:TYR:CD1	1:C:1581:LEU:HD21	2.14	0.82
1:A:1561:TYR:CD1	1:A:1581:LEU:HD21	2.14	0.82
1:C:979:VAL:HG12	1:C:1359:VAL:HG22	1.60	0.82
1:A:1626:GLN:HB2	1:A:1635:TYR:HD1	1.44	0.82
1:A:857:VAL:HG23	1:A:884:VAL:HG21	1.59	0.82
1:C:1402:ILE:HG13	1:C:1479:ILE:HD12	1.59	0.82

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1533:GLY:O	1:A:1534:GLN:HB3	1.80	0.81
1:C:1278:GLN:OE1	1:C:1283:GLY:CA	2.28	0.81
1:C:35:ALA:O	1:C:86:THR:HG22	1.80	0.81
1:C:491:PRO:HG2	1:C:494:ASP:HB3	1.60	0.81
2:D:818:LEU:HD21	2:D:820:MET:HE3	1.61	0.81
2:B:339:VAL:HG23	2:B:341:SER:H	1.46	0.81
1:C:160:VAL:HG22	1:C:175:GLU:HB3	1.61	0.81
1:C:857:VAL:HG23	1:C:884:VAL:HG21	1.62	0.81
1:A:1383:THR:HG21	1:A:1511:THR:HG22	1.63	0.81
1:C:702:GLY:HA2	1:C:728:PHE:HE1	1.45	0.81
2:D:1284:ARG:CG	2:D:1285:GLU:H	1.94	0.81
2:D:745:ILE:CG2	2:D:897:LYS:HD3	2.11	0.81
1:A:375:VAL:O	1:A:383:VAL:HG13	1.80	0.81
1:A:773:TRP:HZ3	1:A:788:PHE:CE1	1.98	0.81
1:A:936:ARG:HG3	1:A:936:ARG:HH11	1.44	0.81
1:A:944:LEU:HD12	1:A:1313:ILE:HD11	1.63	0.81
1:A:982:LEU:HD12	1:A:982:LEU:H	1.44	0.81
2:B:344:GLN:HA	2:B:344:GLN:NE2	1.94	0.81
1:C:42:GLN:HG2	1:C:43:VAL:H	1.45	0.81
2:D:339:VAL:HG23	2:D:341:SER:H	1.46	0.81
1:A:182:ILE:HG12	1:A:804:ILE:HD11	1.62	0.81
1:A:520:ASP:OD2	2:B:404:LEU:HB2	1.81	0.81
1:A:113:LYS:HG2	1:A:114:SER:N	1.96	0.81
1:A:753:HIS:O	1:A:754:MET:HB3	1.81	0.81
2:B:294:LEU:HD12	2:B:295:LYS:N	1.95	0.81
1:C:1570:VAL:HA	1:C:1574:PHE:O	1.79	0.81
2:D:422:ARG:HD3	2:D:422:ARG:H	1.45	0.81
1:A:1590:ALA:HB1	1:A:1635:TYR:CE1	2.16	0.81
2:B:850:LEU:HB2	2:B:882:PHE:CE1	2.14	0.81
1:C:838:GLN:HA	1:C:901:LEU:HB2	1.62	0.81
1:A:1370:THR:HG23	1:A:1373:GLU:OE1	1.81	0.81
1:C:1623:GLU:HB2	1:C:1638:PRO:HG2	1.63	0.81
1:C:917:TRP:HB3	2:D:558:MET:SD	2.21	0.81
1:A:160:VAL:HG22	1:A:175:GLU:HB3	1.61	0.81
1:A:1549:LYS:HZ1	1:A:1667:PHE:HB3	1.44	0.81
1:A:309:GLU:HG2	1:A:310:LEU:H	1.44	0.81
1:A:889:GLU:HB2	1:A:892:SER:HB2	1.62	0.81
2:B:415:THR:OG1	2:B:425:GLN:HB3	1.81	0.81
1:C:1176:LEU:HD21	1:C:1195:LEU:CD2	2.10	0.81
1:C:309:GLU:HG2	1:C:310:LEU:H	1.43	0.81
2:B:481:TYR:HE1	2:B:506:MET:SD	2.04	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1404:ALA:HB1	1:C:1493:PHE:CE2	2.16	0.80
2:D:1347:VAL:HG22	2:D:1367:ILE:HG23	1.62	0.80
1:A:131:ASP:HB3	1:A:142:LYS:HB2	1.62	0.80
1:A:1620:MET:HB2	1:A:1644:TRP:HB3	1.64	0.80
1:C:1615:ARG:HH21	1:C:1650:ARG:NH2	1.79	0.80
1:C:753:HIS:O	1:C:754:MET:HB3	1.78	0.80
2:D:415:THR:OG1	2:D:425:GLN:HB3	1.81	0.80
1:A:1570:VAL:HA	1:A:1574:PHE:O	1.80	0.80
1:A:596:MET:HA	1:A:782:ARG:HG2	1.62	0.80
2:B:1284:ARG:HG3	2:B:1286:VAL:H	1.47	0.80
1:A:924:VAL:HG21	3:A:2003:NAG:H82	1.64	0.80
1:A:476:LEU:HD21	1:A:482:LEU:HD12	1.61	0.80
1:C:837:GLU:O	1:C:901:LEU:HD12	1.81	0.80
2:D:927:ILE:HG23	2:D:1324:THR:HG23	1.63	0.80
2:B:1506:ILE:HD12	2:B:1627:ASP:HB2	1.64	0.80
1:C:463:SER:HB3	1:C:491:PRO:HA	1.64	0.80
1:C:470:THR:HG22	2:D:450:THR:CG2	2.11	0.80
1:A:743:SER:HB2	1:A:751:ARG:N	1.96	0.80
1:C:969:PRO:HG3	1:C:1601:ILE:HD12	1.64	0.80
1:C:265:VAL:HG22	1:C:329:VAL:HG22	1.64	0.80
1:C:500:ASN:CB	1:C:543:TYR:CE1	2.65	0.80
1:A:1102:ASN:ND2	1:C:1162:VAL:H	1.79	0.80
1:A:35:ALA:O	1:A:86:THR:HG22	1.82	0.80
2:B:484:LEU:HB2	2:B:519:ARG:HB2	1.63	0.80
2:B:262:PHE:CE1	2:B:282:ARG:HG3	2.17	0.80
1:A:1152:ILE:HG21	1:A:1168:LEU:HD21	1.64	0.79
1:A:443:PRO:HD2	1:A:446:ASN:HB2	1.63	0.79
1:C:238:ILE:HG23	1:C:242:ASN:HD22	1.44	0.79
1:C:733:VAL:O	1:C:737:GLN:HG2	1.82	0.79
2:D:25:TYR:HB2	2:D:631:SER:HB3	1.63	0.79
1:A:1176:LEU:HD21	1:A:1195:LEU:CD2	2.12	0.79
1:C:884:VAL:CG1	1:C:886:GLN:HG2	2.11	0.79
2:D:563:MET:HG3	2:D:780:LEU:HD23	1.64	0.79
1:A:1244:THR:HG22	1:A:1247:MET:H	1.47	0.79
1:A:500:ASN:HB3	1:A:543:TYR:HE1	1.47	0.79
2:B:563:MET:SD	2:B:808:ILE:HD11	2.21	0.79
1:C:126:LEU:HD11	1:C:205:TYR:CE2	2.17	0.79
1:C:773:TRP:HZ3	1:C:788:PHE:CE1	2.00	0.79
2:D:164:GLU:HG2	2:D:175:SER:HB2	1.63	0.79
1:A:1309:LEU:HD11	1:A:1328:MET:HG3	1.64	0.79
1:A:315:LEU:HD13	1:A:317:ASP:HB2	1.62	0.79

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:961:THR:HG22	2:B:1327:THR:HG23	1.64	0.79
2:B:1393:ASP:HB2	2:B:1443:LEU:HD11	1.63	0.79
1:A:500:ASN:CB	1:A:543:TYR:CE1	2.65	0.79
2:B:422:ARG:HD3	2:B:422:ARG:H	1.46	0.79
1:C:1590:ALA:HB1	1:C:1635:TYR:CE1	2.18	0.79
2:D:285:ILE:N	2:D:285:ILE:HD12	1.96	0.79
2:D:294:LEU:HD12	2:D:295:LYS:N	1.98	0.79
1:C:1549:LYS:HZ1	1:C:1667:PHE:HB3	1.45	0.79
2:D:262:PHE:CE1	2:D:282:ARG:HG3	2.17	0.79
2:D:518:PHE:CE2	2:D:538:VAL:HB	2.18	0.79
1:A:492:TYR:CG	1:A:493:ILE:N	2.50	0.79
1:A:91:GLN:HA	1:A:91:GLN:OE1	1.77	0.79
1:C:1100:ILE:HG21	1:C:1158:ILE:HD12	1.65	0.79
1:C:924:VAL:HG21	3:C:2003:NAG:H82	1.65	0.79
1:C:596:MET:HA	1:C:782:ARG:HG2	1.64	0.79
1:A:430:VAL:HG11	1:A:453:ARG:HH21	1.46	0.78
2:D:476:ILE:O	2:D:497:ARG:HG2	1.82	0.78
1:A:837:GLU:O	1:A:901:LEU:HD12	1.83	0.78
1:A:1623:GLU:HB2	1:A:1638:PRO:HG2	1.66	0.78
2:B:83:VAL:C	2:B:85:PRO:HD3	2.03	0.78
1:C:1620:MET:HB2	1:C:1644:TRP:HB3	1.65	0.78
1:C:20:GLU:HG2	1:C:20:GLU:O	1.83	0.78
2:B:197:TRP:HB2	2:B:214:PHE:CE1	2.18	0.78
1:C:576:SER:HB2	1:C:589:SER:H	1.48	0.78
2:D:1482:ASN:HB2	2:D:1495:GLU:HG2	1.65	0.78
2:B:1347:VAL:HG22	2:B:1367:ILE:HG23	1.63	0.78
1:C:1186:PHE:HD1	1:C:1250:THR:HG22	1.49	0.78
2:D:476:ILE:HG23	2:D:476:ILE:O	1.82	0.78
1:A:489:LYS:NZ	2:B:502:ASN:H	1.82	0.78
2:D:1444:LYS:HE2	2:D:1447:GLU:HA	1.64	0.78
2:D:563:MET:SD	2:D:808:ILE:HD11	2.24	0.78
1:A:1411:SER:N	1:A:1414:GLU:HG3	1.99	0.78
2:B:165:PHE:CZ	2:B:199:ILE:HD11	2.19	0.78
1:C:500:ASN:HB2	1:C:543:TYR:CD1	2.19	0.78
1:C:506:LYS:HD2	1:C:536:PRO:HD2	1.66	0.78
1:C:91:GLN:HA	1:C:91:GLN:OE1	1.72	0.78
2:D:127:PHE:HE2	2:D:602:ILE:HG23	1.49	0.78
1:A:733:VAL:O	1:A:737:GLN:HG2	1.83	0.78
2:B:244:HIS:HB3	2:B:291:LYS:HD2	1.64	0.78
1:C:1244:THR:HG22	1:C:1247:MET:H	1.49	0.78
1:C:1627:ILE:HD12	1:C:1629:TYR:HB3	1.65	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1614:ASP:O	2:D:1617:GLN:HG2	1.83	0.78
1:A:1109:GLU:HG2	1:C:1163:LYS:NZ	1.98	0.77
1:A:1153:ARG:HD2	1:A:1197:LEU:HB3	1.66	0.77
1:C:500:ASN:OD1	1:C:514:THR:HG23	1.83	0.77
2:D:563:MET:HB3	2:D:778:PHE:CE2	2.19	0.77
2:D:83:VAL:C	2:D:85:PRO:HD3	2.04	0.77
1:A:126:LEU:HD11	1:A:205:TYR:CE2	2.19	0.77
1:A:267:ILE:HD12	1:A:299:VAL:HG11	1.67	0.77
1:A:682:LYS:HZ3	1:A:686:ILE:HD11	1.47	0.77
2:B:1482:ASN:HB2	2:B:1495:GLU:HG2	1.66	0.77
1:C:1386:ILE:HG13	1:C:1387:GLU:H	1.50	0.77
1:C:1533:GLY:O	1:C:1534:GLN:HB3	1.83	0.77
1:C:315:LEU:HD13	1:C:317:ASP:HB2	1.64	0.77
2:D:484:LEU:HB2	2:D:519:ARG:HB2	1.66	0.77
1:A:1615:ARG:HH21	1:A:1650:ARG:NH2	1.83	0.77
2:B:1382:ILE:CD1	2:B:1458:VAL:HG22	2.14	0.77
1:A:1053:MET:HE2	1:A:1089:VAL:HG21	1.65	0.77
2:B:1444:LYS:HE2	2:B:1447:GLU:HA	1.65	0.77
2:D:961:THR:HG22	2:D:1327:THR:HG23	1.67	0.77
1:A:179:HIS:O	1:A:180:ILE:HG12	1.85	0.77
1:A:514:THR:O	1:A:515:ARG:HD3	1.84	0.77
2:B:518:PHE:CE2	2:B:538:VAL:HB	2.18	0.77
2:B:818:LEU:HD21	2:B:820:MET:HE3	1.67	0.77
1:A:1186:PHE:HD1	1:A:1250:THR:HG22	1.50	0.77
1:A:465:LEU:HG	1:A:466:TYR:N	2.00	0.77
2:B:1614:ASP:O	2:B:1617:GLN:HG2	1.84	0.77
1:C:1176:LEU:HD21	1:C:1195:LEU:HD22	1.67	0.77
1:C:365:PRO:HD2	1:C:464:TYR:CD2	2.19	0.77
1:C:365:PRO:HG2	1:C:464:TYR:CE2	2.20	0.77
1:C:465:LEU:HG	1:C:466:TYR:N	2.00	0.77
1:C:500:ASN:HB3	1:C:543:TYR:HE1	1.49	0.77
1:A:126:LEU:HD11	1:A:205:TYR:CZ	2.20	0.77
1:C:1645:ILE:O	1:C:1646:GLU:HG3	1.83	0.77
1:C:773:TRP:CE3	1:C:774:LEU:HB2	2.20	0.77
1:A:23:TYR:CD1	1:A:23:TYR:N	2.46	0.77
1:A:362:PHE:CE1	1:A:640:LEU:HD22	2.19	0.77
2:B:462:VAL:HG21	2:B:520:PHE:HE2	1.48	0.77
2:D:194:LEU:CD1	2:D:217:ARG:HA	2.15	0.77
1:A:488:PRO:HG3	1:A:499:TYR:OH	1.84	0.77
1:C:135:TYR:CE1	1:C:141:VAL:HA	2.19	0.77
1:C:1411:SER:N	1:C:1414:GLU:HG3	2.00	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:576:SER:HB2	1:A:589:SER:H	1.49	0.76
1:C:144:ARG:HD2	1:C:146:TYR:CE1	2.20	0.76
1:C:1623:GLU:CB	1:C:1638:PRO:HG2	2.15	0.76
2:D:462:VAL:HG21	2:D:520:PHE:HE2	1.48	0.76
2:D:221:LEU:CD1	2:D:753:LYS:HG2	2.15	0.76
1:A:1213:LYS:HG2	1:A:1266:TYR:HE2	1.49	0.76
1:C:1176:LEU:HB3	1:C:1204:GLN:HG2	1.68	0.76
1:C:375:VAL:O	1:C:383:VAL:HG13	1.84	0.76
1:C:25:ILE:H	1:C:655:THR:CG2	1.97	0.76
1:A:1176:LEU:HD21	1:A:1195:LEU:HD22	1.67	0.76
1:A:42:GLN:HG2	1:A:43:VAL:H	1.49	0.76
2:B:1284:ARG:CG	2:B:1285:GLU:H	1.98	0.76
1:C:492:TYR:CG	1:C:493:ILE:N	2.50	0.76
1:C:493:ILE:CG2	1:C:495:LYS:HB2	2.14	0.76
2:D:518:PHE:HE2	2:D:538:VAL:HB	1.50	0.76
1:A:773:TRP:CE3	1:A:774:LEU:HB2	2.20	0.76
1:C:132:LYS:NZ	1:C:139:GLN:HE22	1.84	0.76
1:C:563:ILE:HG13	1:C:564:GLU:N	1.98	0.76
2:D:922:LYS:HE3	2:D:1329:TYR:CZ	2.20	0.76
1:A:104:LEU:HD12	1:A:105:GLU:H	1.50	0.76
1:A:493:ILE:HG22	1:A:495:LYS:N	2.01	0.76
1:A:618:LYS:N	1:A:619:PRO:HD2	2.01	0.76
1:C:1152:ILE:HG21	1:C:1168:LEU:HD21	1.68	0.76
1:C:470:THR:HG22	2:D:450:THR:CB	2.15	0.76
1:C:133:PRO:HD2	1:C:609:VAL:HG11	1.67	0.76
1:A:1100:ILE:HG21	1:A:1158:ILE:HD12	1.68	0.76
1:A:1320:LYS:CD	1:A:1321:GLY:H	1.98	0.76
1:A:563:ILE:HG13	1:A:564:GLU:N	1.98	0.76
2:B:114:ARG:O	2:B:115:LEU:HD23	1.85	0.76
1:C:666:ASP:O	1:C:668:PRO:HD2	1.84	0.76
2:D:1393:ASP:HB2	2:D:1443:LEU:HD11	1.66	0.76
1:A:493:ILE:CG2	1:A:495:LYS:HB2	2.14	0.76
2:B:1387:LEU:HD21	2:B:1472:TYR:CE1	2.20	0.76
1:C:1626:GLN:HB2	1:C:1635:TYR:HD1	1.49	0.76
1:C:412:ARG:HH22	1:C:472:ASN:ND2	1.83	0.76
2:D:137:TYR:HB2	2:D:216:VAL:HG23	1.68	0.76
1:A:284:GLN:HG2	1:A:310:LEU:HD22	1.68	0.76
1:A:322:TYR:N	1:A:322:TYR:HD2	1.84	0.76
1:A:467:ILE:HG22	1:A:486:VAL:HG22	1.68	0.76
1:C:1365:VAL:HG22	1:C:1366:HIS:H	1.51	0.76
1:C:59:TYR:CD1	1:C:60:PRO:HD3	2.21	0.76

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:132:LYS:NZ	1:A:139:GLN:HE22	1.84	0.76
1:A:1626:GLN:HB2	1:A:1635:TYR:CD1	2.20	0.76
1:C:1560:ALA:CB	1:C:1620:MET:HG2	2.16	0.76
1:C:618:LYS:N	1:C:619:PRO:HD2	2.01	0.76
1:C:944:LEU:HD12	1:C:1313:ILE:HD11	1.66	0.76
1:A:222:TYR:OH	1:A:224:LEU:HD23	1.86	0.76
1:A:666:ASP:O	1:A:668:PRO:HD2	1.85	0.76
2:B:476:ILE:O	2:B:476:ILE:HG23	1.83	0.76
1:C:873:ILE:O	1:C:873:ILE:HD12	1.85	0.76
1:A:690:TYR:HE1	1:A:696:LYS:HD2	1.51	0.75
2:B:1450:PHE:HD1	2:B:1451:ILE:N	1.82	0.75
2:B:851:LEU:CD2	2:B:852:TYR:H	1.98	0.75
1:C:1176:LEU:HD23	1:C:1176:LEU:N	2.00	0.75
1:C:126:LEU:HD11	1:C:205:TYR:CZ	2.21	0.75
1:C:936:ARG:HG3	1:C:936:ARG:HH11	1.50	0.75
2:D:218:LYS:HD3	2:D:822:TYR:HE2	1.50	0.75
1:A:480:GLU:O	1:A:530:VAL:HG12	1.85	0.75
1:A:77:ASN:ND2	1:A:81:ASN:HB2	2.01	0.75
1:C:1320:LYS:CD	1:C:1321:GLY:H	1.97	0.75
1:C:267:ILE:HD12	1:C:299:VAL:HG11	1.68	0.75
2:D:1450:PHE:HD1	2:D:1451:ILE:N	1.81	0.75
2:D:1609:ARG:CG	2:D:1609:ARG:HH11	1.94	0.75
1:A:873:ILE:HD12	1:A:873:ILE:O	1.87	0.75
1:A:1386:ILE:HG13	1:A:1387:GLU:H	1.52	0.75
2:B:235:PHE:HB3	2:B:338:ILE:HG22	1.68	0.75
2:B:127:PHE:HE2	2:B:602:ILE:HG23	1.52	0.75
2:B:891:LEU:HB3	2:B:912:LYS:HD3	1.66	0.75
1:C:77:ASN:ND2	1:C:81:ASN:HB2	2.01	0.75
2:D:462:VAL:HG21	2:D:520:PHE:CE2	2.21	0.75
1:C:1244:THR:HG23	1:C:1502:ASP:OD2	1.87	0.75
1:C:284:GLN:HG2	1:C:310:LEU:HD22	1.67	0.75
2:D:481:TYR:HE1	2:D:506:MET:SD	2.09	0.75
1:A:1159:CYS:SG	1:A:1161:LEU:HD23	2.27	0.75
2:B:410:PRO:HA	2:B:431:THR:HG22	1.68	0.75
2:B:469:ASN:OD1	2:B:472:SER:HB2	1.85	0.75
2:B:563:MET:HB3	2:B:778:PHE:CE2	2.21	0.75
2:D:1506:ILE:HD12	2:D:1627:ASP:HB2	1.68	0.75
2:B:1583:ILE:HG23	2:B:1607:ILE:HG23	1.67	0.75
2:B:221:LEU:CD1	2:B:753:LYS:HG2	2.17	0.75
1:C:243:PHE:CE1	1:C:316:GLU:HB3	2.22	0.75
2:B:494:ARG:HG3	2:B:494:ARG:HH11	1.51	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1085:VAL:O	1:C:1089:VAL:HG23	1.86	0.75
2:D:960:GLU:OE1	2:D:1306:LYS:HE2	1.87	0.75
1:A:765:ILE:O	1:A:765:ILE:HD12	1.87	0.75
2:B:299:PHE:HE1	2:B:303:PHE:HD2	1.35	0.75
1:C:493:ILE:HG22	1:C:495:LYS:N	2.01	0.75
2:D:1284:ARG:HG3	2:D:1286:VAL:H	1.51	0.75
1:A:975:ARG:NH2	1:A:1346:LEU:HD22	2.02	0.74
1:C:111:PHE:HE2	1:C:113:LYS:CB	2.00	0.74
1:C:955:ARG:HG2	1:C:1350:THR:HG23	1.69	0.74
2:D:244:HIS:HB3	2:D:291:LYS:HD2	1.68	0.74
2:B:462:VAL:HG21	2:B:520:PHE:CE2	2.22	0.74
2:B:745:ILE:CG2	2:B:897:LYS:HD3	2.17	0.74
2:B:948:ARG:NH2	2:B:948:ARG:HB2	2.02	0.74
2:D:296:ARG:HG3	2:D:296:ARG:HH11	1.53	0.74
1:A:20:GLU:O	1:A:20:GLU:HG2	1.85	0.74
1:A:500:ASN:HB2	1:A:543:TYR:CD1	2.22	0.74
1:A:506:LYS:HD2	1:A:536:PRO:HD2	1.69	0.74
2:B:518:PHE:HE2	2:B:538:VAL:HB	1.52	0.74
1:C:690:TYR:HE1	1:C:696:LYS:HD2	1.52	0.74
2:D:1457:LYS:HG2	2:D:1469:THR:OG1	1.87	0.74
1:A:322:TYR:CD2	1:A:322:TYR:N	2.55	0.74
1:A:829:ILE:HG12	1:A:925:LYS:HG2	1.69	0.74
1:C:620:LEU:O	1:C:622:ARG:N	2.21	0.74
2:D:825:VAL:HB	2:D:828:GLU:CD	2.08	0.74
1:A:120:THR:HG22	1:A:122:ASP:H	1.52	0.74
1:A:423:ASN:OD1	2:B:504:VAL:HG22	1.87	0.74
1:A:809:ILE:HG12	1:A:810:CYS:N	2.03	0.74
1:A:849:ARG:NH1	2:B:555:LEU:HD13	2.02	0.74
1:C:1033:ILE:HG22	1:C:1034:PHE:CD1	2.22	0.74
1:C:113:LYS:HG2	1:C:114:SER:N	1.99	0.74
1:C:1309:LEU:HD11	1:C:1328:MET:HG3	1.69	0.74
1:A:412:ARG:HH22	1:A:472:ASN:ND2	1.86	0.74
2:B:481:TYR:HB2	2:B:520:PHE:CE1	2.20	0.74
1:C:1584:ILE:HG22	1:C:1585:TYR:N	2.02	0.74
1:C:222:TYR:OH	1:C:224:LEU:HD23	1.87	0.74
2:D:192:VAL:HG22	2:D:193:SER:H	1.51	0.74
1:A:969:PRO:HG3	1:A:1601:ILE:HD12	1.70	0.74
1:A:59:TYR:CD1	1:A:60:PRO:HD3	2.23	0.74
1:A:88:GLN:O	1:A:90:LYS:HD3	1.88	0.74
2:B:825:VAL:HB	2:B:828:GLU:CD	2.07	0.74
1:C:132:LYS:O	1:C:135:TYR:HE2	1.70	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:809:ILE:HG12	1:C:810:CYS:N	2.03	0.74
2:B:952:ASP:N	2:B:952:ASP:OD1	2.21	0.73
2:D:1520:VAL:HG11	2:D:1584:TRP:CD1	2.23	0.73
2:D:435:TYR:CD1	2:D:436:GLN:N	2.49	0.73
1:C:937:GLU:O	1:C:1363:THR:HG23	1.88	0.73
1:C:473:HIS:CE1	2:D:455:LYS:HZ1	2.05	0.73
2:D:1387:LEU:HD21	2:D:1472:TYR:CE1	2.23	0.73
2:D:353:TYR:HB2	2:D:613:SER:OG	1.88	0.73
1:A:25:ILE:H	1:A:655:THR:CG2	2.00	0.73
1:A:830:PRO:HG3	1:A:1483:PHE:CE2	2.23	0.73
2:B:380:VAL:CG1	2:B:387:MET:HB3	2.13	0.73
1:C:182:ILE:HG12	1:C:804:ILE:CD1	2.18	0.73
2:D:848:VAL:HG22	2:D:898:ALA:HB2	1.70	0.73
1:C:1627:ILE:O	1:C:1627:ILE:HG13	1.88	0.73
1:C:871:PRO:HB3	1:C:882:LYS:HG3	1.70	0.73
2:D:1514:LYS:O	2:D:1517:GLU:HB2	1.89	0.73
1:A:1402:ILE:HG13	1:A:1479:ILE:HD12	1.70	0.73
1:C:135:TYR:HE1	1:C:141:VAL:HA	1.54	0.73
1:A:538:SER:O	1:A:561:LEU:HB2	1.88	0.73
1:A:60:PRO:CD	1:A:61:ASP:H	2.00	0.73
2:B:1457:LYS:HG2	2:B:1469:THR:OG1	1.88	0.73
2:B:1609:ARG:CG	2:B:1609:ARG:HH11	1.95	0.73
1:C:538:SER:O	1:C:561:LEU:HB2	1.88	0.73
1:C:907:LEU:HD12	1:C:908:HIS:H	1.52	0.73
2:D:548:LEU:CD2	2:D:793:SER:HB3	2.16	0.73
1:A:1560:ALA:CB	1:A:1620:MET:HG2	2.19	0.73
1:A:1623:GLU:CB	1:A:1638:PRO:HG2	2.19	0.73
1:A:977:LEU:HD22	1:A:978:SER:N	2.04	0.73
2:D:1520:VAL:HG11	2:D:1584:TRP:HD1	1.52	0.73
2:D:961:THR:CG2	2:D:1327:THR:HG23	2.19	0.73
1:A:1244:THR:HG23	1:A:1502:ASP:OD2	1.89	0.73
1:A:1323:LEU:HD12	1:A:1324:HIS:H	1.54	0.73
1:C:154:PRO:O	1:C:155:ALA:CB	2.37	0.73
2:D:320:VAL:HG12	2:D:329:VAL:HG22	1.71	0.73
1:A:871:PRO:HB3	1:A:882:LYS:HG3	1.70	0.73
2:B:1408:ILE:HD11	2:B:1425:ILE:HG12	1.71	0.73
2:B:750:ASP:O	2:B:782:ASP:HB2	1.88	0.73
1:C:393:GLN:HG2	1:C:403:ASP:OD1	1.89	0.73
1:C:977:LEU:HD22	1:C:978:SER:N	2.03	0.73
2:D:563:MET:HE2	2:D:564:LYS:H	1.54	0.73
1:A:1176:LEU:HD23	1:A:1176:LEU:N	2.02	0.73

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1627:ILE:CD1	1:A:1629:TYR:HB3	2.17	0.73
1:A:182:ILE:HG12	1:A:804:ILE:CD1	2.19	0.73
2:B:435:TYR:CD1	2:B:436:GLN:N	2.50	0.73
2:B:960:GLU:OE1	2:B:1306:LYS:HE2	1.89	0.73
1:C:1333:PHE:O	1:C:1334:LEU:HB2	1.88	0.73
1:C:830:PRO:HG3	1:C:1483:PHE:CE2	2.22	0.73
1:A:104:LEU:HD12	1:A:105:GLU:N	2.03	0.72
1:A:144:ARG:HD2	1:A:146:TYR:CE1	2.24	0.72
1:C:1159:CYS:SG	1:C:1161:LEU:HD23	2.29	0.72
1:C:20:GLU:HB2	1:C:551:THR:HA	1.70	0.72
1:C:480:GLU:O	1:C:530:VAL:HG12	1.89	0.72
2:D:137:TYR:CZ	2:D:143:VAL:HG22	2.24	0.72
1:A:1090:ASN:O	1:A:1092:TYR:N	2.22	0.72
1:A:1549:LYS:HZ2	1:A:1667:PHE:HD1	1.35	0.72
1:A:500:ASN:HB3	1:A:543:TYR:CE1	2.24	0.72
2:B:104:VAL:HG22	2:B:105:VAL:H	1.54	0.72
2:B:961:THR:CG2	2:B:1327:THR:HG23	2.19	0.72
1:C:1323:LEU:HD12	1:C:1324:HIS:H	1.54	0.72
1:C:88:GLN:O	1:C:90:LYS:HD3	1.89	0.72
1:C:975:ARG:NH1	1:C:1340:VAL:HG11	2.05	0.72
2:D:165:PHE:CZ	2:D:199:ILE:HD11	2.24	0.72
1:A:1083:LEU:HD22	1:A:1104:LEU:HD21	1.70	0.72
2:B:1473:HIS:HD2	2:B:1474:PRO:HD2	1.54	0.72
2:B:618:LEU:HD22	2:B:636:THR:HA	1.70	0.72
1:C:362:PHE:CE1	1:C:640:LEU:HD22	2.23	0.72
1:A:720:LEU:HD13	1:A:724:CYS:HB3	1.72	0.72
2:B:1613:GLU:O	2:B:1616:CYS:HB2	1.89	0.72
1:C:371:ILE:HG22	1:C:420:PHE:HB2	1.70	0.72
1:C:60:PRO:CD	1:C:61:ASP:H	2.01	0.72
1:C:934:VAL:HG22	1:C:1366:HIS:CD2	2.23	0.72
1:A:62:LYS:HD3	1:A:103:TYR:CD2	2.24	0.72
2:B:120:LEU:HD12	2:B:121:LEU:N	2.03	0.72
2:B:164:GLU:HG2	2:B:175:SER:HB2	1.70	0.72
2:B:262:PHE:HE1	2:B:282:ARG:HG3	1.54	0.72
1:A:934:VAL:HG22	1:A:1366:HIS:CD2	2.23	0.72
1:A:1573:VAL:O	1:A:1603:LYS:HD2	1.88	0.72
1:A:786:LEU:H	1:A:786:LEU:HD23	1.54	0.72
1:A:796:THR:HG23	1:A:818:LYS:CB	2.18	0.72
1:C:1568:ILE:HG23	1:C:1577:TYR:HE1	1.54	0.72
1:C:1549:LYS:HZ2	1:C:1667:PHE:HD1	1.35	0.72
1:C:489:LYS:HG2	1:C:490:SER:N	2.04	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:104:VAL:HG22	2:D:105:VAL:H	1.54	0.72
2:D:127:PHE:CE2	2:D:602:ILE:HG23	2.23	0.72
1:A:1645:ILE:O	1:A:1646:GLU:HG3	1.89	0.72
1:C:1365:VAL:HG22	1:C:1366:HIS:N	2.05	0.72
1:C:720:LEU:HD13	1:C:724:CYS:HB3	1.72	0.72
2:D:120:LEU:HD12	2:D:121:LEU:N	2.04	0.72
2:D:1382:ILE:CD1	2:D:1458:VAL:HG22	2.19	0.72
2:D:829:GLN:HE22	2:D:883:VAL:HG13	1.53	0.72
2:D:948:ARG:HB2	2:D:948:ARG:NH2	2.04	0.72
2:B:922:LYS:HE3	2:B:1329:TYR:CZ	2.24	0.72
1:C:1083:LEU:HD22	1:C:1104:LEU:HD21	1.69	0.72
1:C:614:ARG:HD2	1:C:615:GLY:N	2.04	0.72
1:C:697:LYS:O	1:C:700:TYR:HB3	1.90	0.72
1:A:620:LEU:O	1:A:622:ARG:N	2.23	0.72
2:B:851:LEU:HD23	2:B:852:TYR:N	2.01	0.72
1:C:1153:ARG:HD2	1:C:1197:LEU:HB3	1.71	0.72
1:A:30:ILE:HG23	1:A:118:PRO:HB2	1.71	0.72
1:C:1660:PHE:HE2	1:C:1664:LEU:HD12	1.54	0.72
2:B:1514:LYS:O	2:B:1517:GLU:HB2	1.90	0.71
1:C:1271:ILE:HD13	1:C:1300:TYR:CE1	2.24	0.71
1:C:786:LEU:H	1:C:786:LEU:HD23	1.53	0.71
2:D:925:VAL:HG13	2:D:1326:LEU:HD23	1.71	0.71
2:D:422:ARG:CD	2:D:422:ARG:H	2.02	0.71
2:D:449:ILE:HD13	2:D:462:VAL:HG23	1.71	0.71
2:B:296:ARG:HH11	2:B:296:ARG:HG3	1.54	0.71
2:B:824:VAL:HG21	2:B:830:VAL:HG11	1.70	0.71
1:C:115:LYS:HB2	1:C:654:LEU:HD11	1.71	0.71
1:C:461:SER:HB2	1:C:553:GLU:OE2	1.90	0.71
1:C:554:LEU:HB3	1:C:642:ASN:OD1	1.90	0.71
2:D:745:ILE:HG21	2:D:897:LYS:HD3	1.72	0.71
1:A:1132:THR:HG22	1:A:1133:LEU:H	1.55	0.71
1:A:1333:PHE:O	1:A:1334:LEU:HB2	1.88	0.71
2:B:194:LEU:CD1	2:B:217:ARG:HA	2.20	0.71
2:B:548:LEU:CD2	2:B:793:SER:HB3	2.18	0.71
1:C:148:LEU:HD12	1:C:154:PRO:O	1.91	0.71
1:C:154:PRO:O	1:C:155:ALA:HB3	1.89	0.71
1:C:628:GLU:C	1:C:630:SER:H	1.91	0.71
1:A:115:LYS:HB2	1:A:654:LEU:HD11	1.71	0.71
1:A:365:PRO:HD2	1:A:464:TYR:CD2	2.25	0.71
1:A:393:GLN:HG2	1:A:403:ASP:OD1	1.90	0.71
2:B:137:TYR:CZ	2:B:143:VAL:HG22	2.26	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:765:ILE:O	1:C:765:ILE:HD12	1.91	0.71
1:A:135:TYR:CE1	1:A:141:VAL:HA	2.25	0.71
1:A:20:GLU:HB2	1:A:551:THR:HA	1.71	0.71
2:B:1305:THR:HG23	2:B:1307:LEU:H	1.54	0.71
2:B:1610:TRP:HA	2:B:1628:PHE:CE2	2.23	0.71
2:B:208:GLU:OE1	2:B:210:TYR:HB2	1.91	0.71
1:A:1098:ASN:OD1	1:C:1160:PRO:HG2	1.90	0.71
1:C:322:TYR:N	1:C:322:TYR:HD2	1.89	0.71
2:D:106:VAL:HG23	2:D:117:LYS:O	1.89	0.71
1:A:133:PRO:HD2	1:A:609:VAL:HG11	1.71	0.71
1:A:638:GLY:HA2	1:A:645:VAL:HG22	1.73	0.71
2:B:106:VAL:HG23	2:B:117:LYS:O	1.89	0.71
1:C:1136:GLU:O	1:C:1139:GLU:HB2	1.91	0.71
1:C:638:GLY:HA2	1:C:645:VAL:HG22	1.72	0.71
2:D:1613:GLU:O	2:D:1616:CYS:HB2	1.91	0.71
1:A:1227:PHE:HD1	1:A:1227:PHE:C	1.93	0.71
1:A:1365:VAL:HG22	1:A:1366:HIS:H	1.55	0.71
1:A:614:ARG:HD2	1:A:615:GLY:N	2.05	0.71
2:B:320:VAL:HG12	2:B:329:VAL:HG22	1.73	0.71
1:C:1056:ILE:C	1:C:1056:ILE:HD13	2.09	0.71
1:C:156:LYS:O	1:C:157:ARG:HG2	1.91	0.71
1:C:1626:GLN:HB2	1:C:1635:TYR:CD1	2.25	0.71
2:D:494:ARG:HG3	2:D:494:ARG:HH11	1.55	0.71
2:D:824:VAL:HG21	2:D:830:VAL:HG11	1.71	0.71
2:B:848:VAL:HG22	2:B:898:ALA:HB2	1.72	0.71
1:C:1650:ARG:H	1:C:1650:ARG:HD2	1.56	0.71
1:C:796:THR:HG23	1:C:818:LYS:CB	2.20	0.71
1:A:1012:LEU:HD13	1:A:1081:PHE:HD2	1.54	0.71
1:A:489:LYS:HG2	1:A:490:SER:N	2.04	0.71
1:A:682:LYS:HZ2	1:A:686:ILE:HD11	1.55	0.71
1:A:1176:LEU:HB3	1:A:1204:GLN:HG2	1.73	0.71
1:A:506:LYS:HE2	1:A:533:ASN:O	1.90	0.71
1:A:595:GLY:HA2	1:A:782:ARG:HH11	1.56	0.71
1:A:907:LEU:HD12	1:A:908:HIS:H	1.55	0.71
1:C:1581:LEU:CD1	1:C:1598:ILE:HD11	2.21	0.71
1:C:322:TYR:CD2	1:C:322:TYR:N	2.59	0.71
2:D:1288:ILE:HD12	2:D:1303:VAL:HG21	1.71	0.71
2:D:1610:TRP:HA	2:D:1628:PHE:CE2	2.24	0.71
1:A:1479:ILE:N	1:A:1479:ILE:HD13	2.06	0.70
1:A:576:SER:CB	1:A:577:PRO:HD3	2.19	0.70
2:B:294:LEU:HD12	2:B:295:LYS:H	1.56	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:989:SER:O	1:C:993:SER:HB2	1.91	0.70
2:D:1341:ASN:ND2	2:D:1342:LYS:HG2	2.06	0.70
2:D:262:PHE:HE1	2:D:282:ARG:HG3	1.54	0.70
1:A:371:ILE:HG22	1:A:420:PHE:HB2	1.72	0.70
1:A:365:PRO:HG2	1:A:464:TYR:CE2	2.26	0.70
1:C:983:LEU:HD21	1:C:1271:ILE:HD12	1.74	0.70
2:D:218:LYS:HD3	2:D:822:TYR:CE2	2.25	0.70
2:D:299:PHE:HE1	2:D:303:PHE:HD2	1.39	0.70
2:D:380:VAL:CG1	2:D:387:MET:HB3	2.16	0.70
2:B:1288:ILE:HD12	2:B:1303:VAL:HG21	1.71	0.70
2:B:1590:LEU:HD23	2:B:1591:LEU:N	2.02	0.70
2:D:1442:ILE:C	2:D:1443:LEU:HD12	2.11	0.70
1:A:1085:VAL:O	1:A:1089:VAL:HG23	1.91	0.70
1:A:1627:ILE:HG13	1:A:1627:ILE:O	1.88	0.70
1:A:625:GLN:HG2	1:A:626:PHE:N	2.06	0.70
2:B:1382:ILE:HD12	2:B:1458:VAL:HG22	1.72	0.70
2:B:353:TYR:HB2	2:B:613:SER:OG	1.92	0.70
2:B:449:ILE:HD13	2:B:462:VAL:HG23	1.72	0.70
1:C:595:GLY:HA2	1:C:782:ARG:HH11	1.56	0.70
1:C:849:ARG:NH1	1:C:849:ARG:HG3	2.06	0.70
2:D:1305:THR:HG23	2:D:1307:LEU:H	1.55	0.70
2:D:216:VAL:HG12	2:D:216:VAL:O	1.90	0.70
2:D:829:GLN:HA	2:D:885:VAL:HG12	1.72	0.70
1:A:983:LEU:HD21	1:A:1271:ILE:HD12	1.73	0.70
2:B:422:ARG:H	2:B:422:ARG:CD	2.04	0.70
2:B:54:LEU:HD21	2:B:75:MET:HE2	1.72	0.70
1:A:1584:ILE:HG22	1:A:1585:TYR:N	2.04	0.70
1:A:628:GLU:C	1:A:630:SER:H	1.92	0.70
1:C:1145:THR:O	1:C:1149:VAL:HG23	1.92	0.70
2:D:1408:ILE:HD11	2:D:1425:ILE:HG12	1.73	0.70
1:A:1033:ILE:HG22	1:A:1034:PHE:CD1	2.26	0.70
1:C:1450:PHE:HZ	1:C:1475:VAL:HB	1.57	0.70
1:C:1534:GLN:HG3	1:C:1534:GLN:O	1.91	0.70
1:C:640:LEU:H	1:C:644:ASN:HB3	1.57	0.70
1:A:1427:SER:HB3	1:A:1492:THR:HG23	1.74	0.70
2:D:481:TYR:HB2	2:D:520:PHE:CE1	2.25	0.70
1:A:1145:THR:O	1:A:1149:VAL:HG23	1.92	0.70
1:A:1271:ILE:HD13	1:A:1300:TYR:CE1	2.26	0.70
1:A:148:LEU:HD12	1:A:154:PRO:O	1.92	0.70
1:A:554:LEU:HB3	1:A:642:ASN:OD1	1.91	0.70
1:C:506:LYS:HE2	1:C:533:ASN:O	1.92	0.70

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1013:MET:O	1:A:1016:VAL:HG23	1.91	0.70
1:A:495:LYS:HA	1:A:495:LYS:HE2	1.72	0.70
2:B:127:PHE:CE2	2:B:602:ILE:HG23	2.26	0.70
2:B:1341:ASN:ND2	2:B:1342:LYS:HG2	2.07	0.70
2:B:525:GLN:HA	2:B:530:GLU:O	1.91	0.70
1:C:1226:ARG:CZ	1:C:1266:TYR:HE1	2.05	0.70
2:D:1275:LEU:HD21	2:D:1319:GLY:O	1.91	0.70
2:D:834:ALA:O	2:D:835:ILE:HD13	1.91	0.70
1:A:931:PRO:HB2	1:A:1366:HIS:CD2	2.27	0.69
1:A:955:ARG:HG2	1:A:1350:THR:CG2	2.22	0.69
2:B:1275:LEU:HD21	2:B:1319:GLY:O	1.92	0.69
2:B:239:GLY:H	2:B:296:ARG:HH22	1.37	0.69
1:C:104:LEU:HD12	1:C:105:GLU:H	1.56	0.69
1:C:1090:ASN:O	1:C:1092:TYR:N	2.25	0.69
1:C:33:VAL:HG21	1:C:121:TYR:CD1	2.26	0.69
1:C:1227:PHE:C	1:C:1227:PHE:HD1	1.95	0.69
1:C:180:ILE:O	1:C:182:ILE:N	2.24	0.69
1:C:23:TYR:N	1:C:23:TYR:CD1	2.54	0.69
1:C:576:SER:CB	1:C:577:PRO:HD3	2.18	0.69
2:D:1383:ASP:O	2:D:1456:VAL:HA	1.92	0.69
1:A:1581:LEU:CD1	1:A:1598:ILE:HD11	2.23	0.69
1:A:687:ALA:O	1:A:690:TYR:HB3	1.92	0.69
2:B:481:TYR:O	2:B:481:TYR:CD2	2.42	0.69
1:C:495:LYS:HE2	1:C:495:LYS:HA	1.73	0.69
1:C:625:GLN:HG2	1:C:626:PHE:N	2.06	0.69
1:A:154:PRO:O	1:A:155:ALA:CB	2.40	0.69
1:A:361:LEU:N	1:A:361:LEU:HD12	2.08	0.69
2:B:818:LEU:HD23	2:B:911:LYS:HD2	1.73	0.69
1:C:1213:LYS:HG2	1:C:1266:TYR:HE2	1.56	0.69
1:C:975:ARG:NH2	1:C:1346:LEU:HD22	2.07	0.69
1:C:463:SER:CB	1:C:491:PRO:HA	2.23	0.69
2:B:524:TYR:CE1	2:B:532:VAL:HG12	2.27	0.69
2:D:618:LEU:HD22	2:D:636:THR:HA	1.73	0.69
2:D:218:LYS:HB3	2:D:822:TYR:HD2	1.56	0.69
1:A:1108:VAL:HG11	1:A:1164:ILE:HG22	1.74	0.69
1:C:1244:THR:O	1:C:1247:MET:HB3	1.93	0.69
1:C:62:LYS:HD3	1:C:103:TYR:CD2	2.27	0.69
2:D:750:ASP:O	2:D:782:ASP:HB2	1.91	0.69
1:A:955:ARG:NH1	1:A:1352:PHE:HA	2.06	0.69
2:B:1590:LEU:CD2	2:B:1591:LEU:H	2.03	0.69
2:B:953:ARG:CG	2:B:954:VAL:H	2.05	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1162:VAL:H	1:C:1102:ASN:ND2	1.88	0.69
1:C:495:LYS:CE	1:C:495:LYS:HA	2.21	0.69
2:D:168:PRO:HG3	2:D:196:THR:C	2.12	0.69
2:D:891:LEU:HB3	2:D:912:LYS:HD3	1.73	0.69
1:A:1136:GLU:O	1:A:1139:GLU:HB2	1.92	0.69
1:A:493:ILE:HG22	1:A:495:LYS:HB2	1.73	0.69
2:B:137:TYR:HB2	2:B:216:VAL:HG23	1.75	0.69
2:B:603:GLU:O	2:B:605:SER:N	2.25	0.69
1:C:120:THR:HG22	1:C:122:ASP:H	1.57	0.69
1:C:1450:PHE:CZ	1:C:1475:VAL:HB	2.28	0.69
2:D:598:ILE:CD1	2:D:800:ILE:HG21	2.22	0.69
1:A:1244:THR:O	1:A:1247:MET:HB3	1.91	0.69
1:A:697:LYS:O	1:A:700:TYR:HB3	1.93	0.69
1:A:824:PHE:HD2	1:A:824:PHE:H	1.39	0.69
2:B:312:HIS:O	2:B:338:ILE:HG12	1.92	0.69
1:C:363:LEU:HD12	1:C:363:LEU:O	1.93	0.69
1:C:752:LEU:HD12	1:C:753:HIS:N	2.06	0.69
1:C:834:VAL:HB	1:C:837:GLU:CD	2.13	0.69
2:B:1273:LEU:CB	2:B:1319:GLY:HA3	2.22	0.69
1:C:1013:MET:O	1:C:1016:VAL:HG23	1.92	0.69
1:C:1068:VAL:HG13	1:C:1069:TRP:H	1.58	0.69
1:C:1431:GLY:C	1:C:1432:ILE:HD13	2.13	0.69
1:C:1575:VAL:HB	1:C:1602:LYS:O	1.93	0.69
1:C:196:TYR:CE1	1:C:221:GLU:HB2	2.28	0.69
1:C:234:GLU:HG3	1:C:235:TYR:CD2	2.27	0.69
1:C:654:LEU:O	1:C:655:THR:HG23	1.92	0.69
1:C:906:GLY:O	1:C:908:HIS:CE1	2.46	0.69
2:D:1391:LEU:HB2	2:D:1417:MET:HE2	1.75	0.69
2:D:235:PHE:HB3	2:D:338:ILE:HG22	1.74	0.69
1:A:1084:ARG:HD2	1:A:1154:LYS:HG3	1.75	0.69
2:B:1383:ASP:O	2:B:1456:VAL:HA	1.92	0.69
1:C:1211:ALA:HA	1:C:1214:ARG:HH11	1.57	0.69
2:D:469:ASN:OD1	2:D:472:SER:HB2	1.93	0.69
1:A:421:VAL:HG11	2:B:505:THR:CG2	2.20	0.69
1:C:145:VAL:HB	1:C:183:ILE:CD1	2.22	0.69
1:C:931:PRO:HB2	1:C:1366:HIS:CD2	2.27	0.69
1:C:982:LEU:HD12	1:C:982:LEU:N	2.08	0.69
2:D:194:LEU:HD12	2:D:217:ARG:HA	1.73	0.69
2:D:269:ILE:HA	2:D:312:HIS:CD2	2.27	0.69
2:D:603:GLU:O	2:D:605:SER:N	2.26	0.69
2:B:925:VAL:HG13	2:B:1326:LEU:HD23	1.72	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:500:ASN:HB2	1:C:543:TYR:CE1	2.27	0.68
2:D:1284:ARG:CG	2:D:1285:GLU:N	2.55	0.68
1:A:1211:ALA:HA	1:A:1214:ARG:HH11	1.57	0.68
1:A:1421:HIS:HD2	1:A:1422:ALA:N	1.91	0.68
1:A:1534:GLN:HG3	1:A:1534:GLN:O	1.93	0.68
1:C:1573:VAL:O	1:C:1603:LYS:HD2	1.93	0.68
1:C:514:THR:O	1:C:515:ARG:HD3	1.93	0.68
2:D:1583:ILE:HG23	2:D:1607:ILE:HG23	1.75	0.68
2:D:513:ASP:N	2:D:513:ASP:OD2	2.25	0.68
2:D:76:ASN:HB2	2:D:77:PRO:HD2	1.75	0.68
1:A:1660:PHE:HE2	1:A:1664:LEU:HD12	1.57	0.68
1:C:1279:ARG:HD3	1:C:1280:TYR:N	2.08	0.68
1:C:493:ILE:HG22	1:C:495:LYS:HB2	1.73	0.68
2:B:1442:ILE:C	2:B:1443:LEU:HD12	2.14	0.68
2:B:24:LEU:HB3	2:B:46:HIS:HB2	1.76	0.68
2:B:844:ILE:HG13	2:B:872:ILE:HG12	1.76	0.68
1:C:360:PRO:HB3	1:C:636:ALA:HB3	1.75	0.68
2:D:481:TYR:CD2	2:D:481:TYR:O	2.45	0.68
1:A:154:PRO:O	1:A:155:ALA:HB3	1.92	0.68
1:A:243:PHE:CE1	1:A:316:GLU:HB3	2.28	0.68
1:A:654:LEU:O	1:A:655:THR:HG23	1.93	0.68
2:B:513:ASP:OD2	2:B:513:ASP:N	2.26	0.68
1:C:1024:TYR:HA	1:C:1302:LEU:HD21	1.75	0.68
1:C:1487:PHE:CD2	1:C:1487:PHE:N	2.61	0.68
1:C:222:TYR:CD2	1:C:223:VAL:N	2.62	0.68
1:A:1019:PHE:CD2	1:A:1019:PHE:C	2.67	0.68
1:A:1450:PHE:HZ	1:A:1475:VAL:HB	1.59	0.68
1:A:156:LYS:O	1:A:157:ARG:HG2	1.94	0.68
1:C:1053:MET:HE2	1:C:1089:VAL:HG21	1.75	0.68
1:C:500:ASN:HB3	1:C:543:TYR:CE1	2.29	0.68
2:D:208:GLU:OE1	2:D:210:TYR:HB2	1.94	0.68
2:D:622:GLU:OE2	2:D:637:LYS:HD3	1.93	0.68
1:A:1219:LYS:HE2	1:A:1239:VAL:HG21	1.76	0.68
1:A:224:LEU:HD22	1:A:225:PRO:CD	2.21	0.68
1:A:439:ALA:HB3	1:A:442:LEU:HD12	1.76	0.68
2:B:194:LEU:HD12	2:B:217:ARG:HA	1.75	0.68
1:C:1024:TYR:HD2	1:C:1025:LEU:N	1.92	0.68
1:C:1008:ALA:CB	1:C:1078:LEU:HD11	2.22	0.68
2:D:548:LEU:HD22	2:D:793:SER:CB	2.20	0.68
2:D:818:LEU:HD23	2:D:911:LYS:HD2	1.75	0.68
1:A:936:ARG:HG3	1:A:936:ARG:NH1	2.09	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:938:SER:C	1:A:940:SER:H	1.97	0.68
2:B:128:LEU:O	2:B:129:PHE:CD1	2.47	0.68
1:A:145:VAL:HB	1:A:183:ILE:CD1	2.24	0.68
1:A:977:LEU:HD23	1:A:1361:VAL:HG13	1.76	0.68
2:B:218:LYS:HB3	2:B:822:TYR:HD2	1.57	0.68
1:A:1561:TYR:HD1	1:A:1581:LEU:HD21	1.57	0.68
1:C:42:GLN:HG2	1:C:43:VAL:N	2.09	0.68
2:D:916:VAL:HG23	2:D:917:PRO:HD2	1.76	0.68
1:A:1227:PHE:CD1	1:A:1227:PHE:C	2.67	0.67
1:A:1365:VAL:HG22	1:A:1366:HIS:N	2.08	0.67
1:A:594:THR:O	1:A:782:ARG:HD3	1.94	0.67
1:A:906:GLY:O	1:A:908:HIS:CE1	2.47	0.67
2:B:168:PRO:HD3	2:B:197:TRP:CD1	2.29	0.67
2:B:563:MET:HE2	2:B:564:LYS:H	1.59	0.67
1:C:1644:TRP:NE1	1:C:1646:GLU:OE1	2.26	0.67
1:C:269:PHE:HE1	1:C:287:MET:HB3	1.58	0.67
2:D:1501:ASN:H	2:D:1501:ASN:HD22	1.40	0.67
2:D:312:HIS:O	2:D:338:ILE:HG12	1.93	0.67
1:C:1108:VAL:HG11	1:C:1164:ILE:HG22	1.76	0.67
1:C:1174:PHE:O	1:C:1178:ASN:HB2	1.95	0.67
1:C:179:HIS:O	1:C:180:ILE:HG12	1.95	0.67
2:D:1474:PRO:HG2	2:D:1475:ASP:OD1	1.93	0.67
2:D:214:PHE:CD1	2:D:214:PHE:O	2.47	0.67
2:D:482:LEU:HD12	2:D:482:LEU:N	2.09	0.67
1:A:1450:PHE:CZ	1:A:1475:VAL:HB	2.29	0.67
1:A:222:TYR:CD2	1:A:223:VAL:N	2.63	0.67
1:A:539:ARG:HE	1:A:633:GLY:HA3	1.59	0.67
2:D:511:THR:O	2:D:514:LEU:HG	1.93	0.67
1:A:1244:THR:HB	1:A:1247:MET:HE3	1.75	0.67
1:A:937:GLU:O	1:A:1363:THR:HG23	1.94	0.67
1:A:269:PHE:HE1	1:A:287:MET:HB3	1.57	0.67
2:B:829:GLN:HE22	2:B:883:VAL:HG13	1.59	0.67
2:D:1382:ILE:HD12	2:D:1458:VAL:HG22	1.75	0.67
2:D:168:PRO:HD3	2:D:197:TRP:CD1	2.30	0.67
2:D:129:PHE:CE2	2:D:598:ILE:HG23	2.30	0.67
1:A:33:VAL:HG21	1:A:121:TYR:CD1	2.29	0.67
1:A:132:LYS:O	1:A:135:TYR:HE2	1.77	0.67
1:A:432:GLU:HG2	1:A:453:ARG:HB3	1.76	0.67
2:B:521:VAL:HG13	2:B:535:SER:HB3	1.76	0.67
1:C:576:SER:HB3	1:C:577:PRO:CD	2.22	0.67
2:D:239:GLY:H	2:D:296:ARG:HH22	1.39	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:24:LEU:HB3	2:D:46:HIS:HB2	1.77	0.67
1:A:1102:ASN:ND2	1:C:1162:VAL:HG22	2.10	0.67
1:A:975:ARG:NH1	1:A:1340:VAL:HG11	2.10	0.67
1:A:1650:ARG:H	1:A:1650:ARG:HD2	1.60	0.67
1:A:228:SER:O	1:A:252:ALA:HA	1.95	0.67
1:A:425:PRO:O	1:A:428:VAL:HG12	1.94	0.67
1:A:576:SER:HB3	1:A:577:PRO:CD	2.23	0.67
1:A:591:ASN:HB3	1:A:785:GLN:HE21	1.59	0.67
1:A:791:PRO:CG	1:A:797:TRP:HE1	2.06	0.67
2:B:192:VAL:HG22	2:B:193:SER:N	2.09	0.67
2:B:76:ASN:HB2	2:B:77:PRO:HD2	1.75	0.67
1:C:1003:LEU:HD11	1:C:1286:SER:HA	1.75	0.67
1:C:1560:ALA:HB1	1:C:1620:MET:HG2	1.77	0.67
1:C:174:VAL:HG22	1:C:175:GLU:N	2.09	0.67
1:C:489:LYS:CG	1:C:490:SER:N	2.58	0.67
1:C:500:ASN:CB	1:C:543:TYR:HE1	2.06	0.67
1:C:941:GLY:O	1:C:942:VAL:HG13	1.94	0.67
1:A:234:GLU:HG3	1:A:235:TYR:CD2	2.29	0.67
2:B:1284:ARG:CG	2:B:1285:GLU:N	2.58	0.67
2:B:1520:VAL:HG11	2:B:1584:TRP:CD1	2.30	0.67
2:B:563:MET:HG3	2:B:780:LEU:HD23	1.76	0.67
2:B:829:GLN:HA	2:B:885:VAL:HG12	1.76	0.67
1:C:1127:ILE:HG13	1:C:1143:TYR:HE2	1.60	0.67
1:C:516:GLU:H	1:C:516:GLU:CD	1.97	0.67
2:D:1273:LEU:CB	2:D:1319:GLY:HA3	2.24	0.67
1:A:475:ALA:HB1	1:A:477:LEU:HD21	1.76	0.67
1:A:765:ILE:HD13	1:A:767:SER:O	1.94	0.67
2:B:482:LEU:HD12	2:B:482:LEU:N	2.10	0.67
2:B:548:LEU:HD22	2:B:793:SER:CB	2.21	0.67
1:A:1056:ILE:HD13	1:A:1056:ILE:C	2.15	0.67
1:A:174:VAL:HG22	1:A:175:GLU:N	2.09	0.67
1:A:415:ASP:HB2	1:A:417:VAL:HB	1.77	0.67
2:B:29:THR:HB	2:B:41:ILE:HG22	1.77	0.67
1:C:551:THR:O	1:C:552:ALA:HB2	1.93	0.67
1:C:591:ASN:HB3	1:C:785:GLN:HE21	1.60	0.67
2:D:265:PHE:CE2	2:D:294:LEU:HB2	2.30	0.67
2:D:563:MET:HB3	2:D:778:PHE:HE2	1.57	0.67
2:B:218:LYS:HD3	2:B:822:TYR:HE2	1.59	0.67
1:C:39:ILE:HD11	1:C:104:LEU:HD21	1.78	0.67
1:C:489:LYS:C	1:C:491:PRO:CD	2.63	0.67
1:C:710:THR:HG23	1:C:713:GLN:NE2	2.10	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:90:LYS:O	1:C:91:GLN:NE2	2.28	0.67
2:D:183:PHE:CD2	2:D:183:PHE:N	2.62	0.67
2:D:508:LEU:HD12	2:D:509:HIS:N	2.10	0.67
1:A:504:LEU:HD21	1:A:651:LEU:CG	2.26	0.66
1:A:500:ASN:HB2	1:A:543:TYR:CE1	2.30	0.66
1:C:1561:TYR:HD1	1:C:1581:LEU:HD21	1.57	0.66
1:C:180:ILE:HG21	1:C:599:TRP:CE3	2.30	0.66
1:C:473:HIS:CE1	2:D:455:LYS:NZ	2.63	0.66
1:A:490:SER:N	1:A:491:PRO:HD2	2.09	0.66
1:A:640:LEU:H	1:A:644:ASN:HB3	1.60	0.66
2:B:511:THR:O	2:B:514:LEU:HG	1.95	0.66
1:C:1239:VAL:O	1:C:1239:VAL:HG12	1.96	0.66
1:C:791:PRO:CG	1:C:797:TRP:HE1	2.08	0.66
2:D:214:PHE:HD1	2:D:214:PHE:O	1.78	0.66
1:A:101:TYR:HE1	1:A:116:ARG:CZ	2.07	0.66
1:A:153:LYS:HB2	1:A:154:PRO:CD	2.25	0.66
1:A:1539:LEU:O	1:A:1540:ASP:HB3	1.94	0.66
1:A:1560:ALA:HB3	1:A:1585:TYR:CE2	2.31	0.66
1:A:982:LEU:N	1:A:982:LEU:HD12	2.10	0.66
2:B:531:ILE:HD11	2:B:634:LEU:CD2	2.24	0.66
1:C:1127:ILE:CG1	1:C:1143:TYR:CE2	2.79	0.66
1:C:1227:PHE:CD1	1:C:1227:PHE:C	2.68	0.66
1:C:1244:THR:HB	1:C:1247:MET:HE3	1.76	0.66
1:C:1563:VAL:HG21	1:C:1619:ILE:HD12	1.77	0.66
2:D:147:VAL:H	2:D:183:PHE:HZ	1.42	0.66
2:D:410:PRO:HA	2:D:431:THR:HG22	1.77	0.66
2:D:844:ILE:HG13	2:D:872:ILE:HG12	1.77	0.66
2:D:889:GLN:HE21	2:D:890:GLY:N	1.93	0.66
1:A:160:VAL:O	1:A:160:VAL:HG12	1.94	0.66
2:B:524:TYR:HE1	2:B:532:VAL:HG12	1.61	0.66
1:C:1012:LEU:HD13	1:C:1081:PHE:HD2	1.59	0.66
1:C:1132:THR:HG22	1:C:1133:LEU:H	1.61	0.66
1:C:1493:PHE:HD1	1:C:1494:THR:N	1.92	0.66
2:D:851:LEU:HD23	2:D:852:TYR:N	2.05	0.66
1:A:1381:ILE:HD12	1:A:1493:PHE:CD2	2.30	0.66
1:A:1573:VAL:HG12	1:A:1603:LYS:HB3	1.76	0.66
1:A:1568:ILE:HG23	1:A:1577:TYR:HE1	1.60	0.66
1:A:495:LYS:HA	1:A:495:LYS:CE	2.21	0.66
1:C:1186:PHE:CD1	1:C:1250:THR:HG22	2.30	0.66
1:C:30:ILE:HG23	1:C:118:PRO:HB2	1.77	0.66
1:C:1016:VAL:HG11	1:C:1291:ILE:HG13	1.76	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:439:ALA:HB3	1:C:442:LEU:HD12	1.78	0.66
2:D:29:THR:HB	2:D:41:ILE:HG22	1.76	0.66
1:A:1226:ARG:CZ	1:A:1266:TYR:HE1	2.09	0.66
1:A:1239:VAL:HG12	1:A:1239:VAL:O	1.96	0.66
1:A:551:THR:O	1:A:552:ALA:HB2	1.94	0.66
1:C:1381:ILE:O	1:C:1382:ASP:HB3	1.96	0.66
1:C:1479:ILE:N	1:C:1479:ILE:HD13	2.11	0.66
1:C:373:VAL:HG23	1:C:418:ALA:HB3	1.78	0.66
1:C:365:PRO:HG2	1:C:464:TYR:HE2	1.57	0.66
1:C:475:ALA:HB1	1:C:477:LEU:HD21	1.76	0.66
1:C:792:ASP:O	1:C:793:SER:HB3	1.94	0.66
2:D:1443:LEU:N	2:D:1443:LEU:HD12	2.10	0.66
2:D:54:LEU:HD21	2:D:75:MET:HE2	1.77	0.66
1:A:111:PHE:HE2	1:A:113:LYS:CB	2.05	0.66
2:B:183:PHE:CD2	2:B:183:PHE:N	2.63	0.66
2:D:347:PHE:O	2:D:349:LYS:N	2.29	0.66
2:D:769:GLN:HB3	2:D:771:ILE:HG12	1.77	0.66
1:A:22:THR:HG21	1:A:656:ASN:O	1.96	0.66
1:A:47:THR:O	1:A:48:GLU:HB2	1.94	0.66
1:A:90:LYS:O	1:A:91:GLN:NE2	2.29	0.66
2:B:266:GLY:HA2	2:B:276:ILE:HG13	1.76	0.66
2:B:613:SER:HA	2:B:620:VAL:HG22	1.78	0.66
1:C:104:LEU:HD12	1:C:105:GLU:N	2.10	0.66
1:C:1053:MET:CE	1:C:1086:LEU:HD22	2.25	0.66
1:C:1627:ILE:CD1	1:C:1629:TYR:HB3	2.25	0.66
1:C:361:LEU:N	1:C:361:LEU:HD12	2.11	0.66
1:C:576:SER:HB2	1:C:589:SER:HB2	1.78	0.66
1:C:470:THR:CG2	2:D:450:THR:HG22	2.25	0.66
2:D:525:GLN:HA	2:D:530:GLU:O	1.95	0.66
2:D:953:ARG:CG	2:D:954:VAL:H	2.07	0.66
1:A:135:TYR:HE1	1:A:141:VAL:HA	1.61	0.66
1:A:128:ILE:HG22	1:A:145:VAL:HG22	1.77	0.66
1:C:228:SER:O	1:C:252:ALA:HA	1.96	0.66
1:C:474:LYS:HD3	1:C:474:LYS:H	1.61	0.66
2:D:1590:LEU:HD23	2:D:1591:LEU:N	2.07	0.66
1:A:1068:VAL:HG13	1:A:1069:TRP:H	1.61	0.65
1:A:1127:ILE:HG13	1:A:1143:TYR:HE2	1.62	0.65
1:A:535:VAL:O	1:A:563:ILE:HG12	1.96	0.65
1:A:887:LYS:H	1:A:887:LYS:HD2	1.61	0.65
1:A:989:SER:O	1:A:993:SER:HB2	1.96	0.65
1:A:412:ARG:HD2	2:B:458:ASP:OD1	1.96	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:615:GLN:HB2	2:B:616:ASN:HD22	1.60	0.65
1:C:123:ASN:OD1	1:C:123:ASN:C	2.33	0.65
1:C:492:TYR:HD2	1:C:493:ILE:H	1.33	0.65
1:C:829:ILE:HG12	1:C:925:LYS:HG2	1.77	0.65
2:D:417:HIS:O	2:D:419:ASP:N	2.28	0.65
1:A:653:PHE:O	1:A:653:PHE:CD1	2.43	0.65
2:B:144:LEU:H	2:B:144:LEU:HD23	1.62	0.65
2:B:769:GLN:HB3	2:B:771:ILE:HG12	1.78	0.65
1:C:594:THR:O	1:C:782:ARG:HD3	1.96	0.65
1:C:681:LYS:HD2	1:C:738:LEU:HD21	1.77	0.65
1:C:781:PRO:O	1:C:782:ARG:HB2	1.96	0.65
2:D:1563:TYR:HB3	2:D:1601:ILE:HD11	1.76	0.65
2:D:476:ILE:HG12	2:D:524:TYR:CD2	2.31	0.65
1:A:576:SER:HB2	1:A:589:SER:HB2	1.78	0.65
2:B:963:ILE:HD11	2:B:1311:ILE:HG12	1.77	0.65
2:B:1474:PRO:HG2	2:B:1475:ASP:OD1	1.96	0.65
2:B:1601:ILE:HD12	2:B:1601:ILE:N	2.12	0.65
1:C:1180:LEU:O	1:C:1182:ALA:N	2.30	0.65
1:C:171:VAL:HG12	1:C:172:ASP:N	2.11	0.65
1:A:1024:TYR:HD2	1:A:1025:LEU:N	1.94	0.65
2:B:1458:VAL:O	2:B:1466:GLU:HG2	1.97	0.65
2:B:269:ILE:HA	2:B:312:HIS:CD2	2.31	0.65
2:B:800:ILE:HG23	2:B:801:CYS:N	2.10	0.65
1:C:1539:LEU:O	1:C:1540:ASP:HB3	1.95	0.65
1:C:955:ARG:NH1	1:C:1352:PHE:HA	2.12	0.65
1:C:955:ARG:O	1:C:1349:SER:HA	1.96	0.65
2:D:1429:LYS:HE3	2:D:1429:LYS:N	2.12	0.65
1:A:1219:LYS:CE	1:A:1239:VAL:HG21	2.27	0.65
1:A:474:LYS:H	1:A:474:LYS:HD3	1.61	0.65
1:A:752:LEU:HD12	1:A:753:HIS:N	2.12	0.65
2:B:958:GLU:HA	2:B:958:GLU:OE1	1.95	0.65
1:C:1031:TRP:CZ3	1:C:1042:LYS:HA	2.30	0.65
1:C:160:VAL:HG12	1:C:160:VAL:O	1.97	0.65
1:C:539:ARG:HE	1:C:633:GLY:HA3	1.61	0.65
1:C:687:ALA:O	1:C:690:TYR:HB3	1.97	0.65
2:D:1473:HIS:HD2	2:D:1474:PRO:HD2	1.59	0.65
2:D:919:GLY:HA2	2:D:1332:GLN:HB3	1.79	0.65
1:A:1024:TYR:HA	1:A:1302:LEU:HD21	1.77	0.65
1:A:849:ARG:HH12	2:B:555:LEU:HD13	1.59	0.65
2:B:237:ILE:O	2:B:306:LEU:HD11	1.95	0.65
1:C:1016:VAL:N	1:C:1017:PRO:CD	2.60	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:506:LYS:HD2	1:C:536:PRO:CD	2.26	0.65
2:D:476:ILE:CG2	2:D:476:ILE:O	2.44	0.65
2:D:218:LYS:HB3	2:D:822:TYR:CE2	2.32	0.65
2:D:40:GLN:HG3	2:D:86:THR:HG23	1.78	0.65
2:B:1408:ILE:CD1	2:B:1425:ILE:HG12	2.27	0.65
2:B:172:LEU:HD12	2:B:173:VAL:H	1.62	0.65
2:B:168:PRO:HG3	2:B:196:THR:C	2.16	0.65
1:C:1024:TYR:CD2	1:C:1025:LEU:N	2.64	0.65
1:C:1219:LYS:HE2	1:C:1239:VAL:HG21	1.79	0.65
1:C:1226:ARG:CZ	1:C:1266:TYR:CE1	2.80	0.65
1:C:1584:ILE:CG2	1:C:1585:TYR:H	2.02	0.65
1:C:490:SER:N	1:C:491:PRO:HD2	2.11	0.65
1:A:99:VAL:HG22	1:A:100:SER:O	1.97	0.65
2:B:115:LEU:HD13	2:B:629:THR:HG22	1.79	0.65
2:B:1500:LEU:C	2:B:1500:LEU:HD12	2.17	0.65
2:B:172:LEU:HD12	2:B:173:VAL:N	2.11	0.65
2:B:417:HIS:O	2:B:419:ASP:N	2.30	0.65
1:C:797:TRP:HA	1:C:797:TRP:CE3	2.32	0.65
2:D:136:ILE:HA	2:D:215:ASP:O	1.95	0.65
1:A:976:ILE:HB	1:A:1362:THR:HG22	1.78	0.65
1:A:1562:LYS:HD2	1:A:1648:TRP:HZ2	1.61	0.65
1:A:196:TYR:CE1	1:A:221:GLU:HB2	2.32	0.65
2:B:1446:PHE:HD2	2:B:1448:VAL:HG22	1.62	0.65
2:B:241:GLU:O	2:B:296:ARG:HD3	1.97	0.65
1:C:1113:LEU:HD23	1:C:1114:ASP:H	1.61	0.65
1:C:1581:LEU:HD12	1:C:1598:ILE:HD11	1.79	0.65
1:C:425:PRO:O	1:C:428:VAL:HG12	1.96	0.65
1:C:127:PHE:CE2	1:C:623:VAL:HG13	2.29	0.65
2:D:613:SER:HA	2:D:620:VAL:HG22	1.79	0.65
1:A:1113:LEU:HD23	1:A:1114:ASP:H	1.61	0.65
1:A:123:ASN:C	1:A:123:ASN:OD1	2.35	0.65
1:A:1575:VAL:HB	1:A:1602:LYS:O	1.97	0.65
2:B:622:GLU:OE2	2:B:637:LYS:HD3	1.97	0.65
2:B:889:GLN:HE21	2:B:890:GLY:N	1.95	0.65
1:C:1431:GLY:O	1:C:1432:ILE:HD13	1.97	0.65
1:C:1124:TYR:HA	1:C:1465:ASN:OD1	1.96	0.65
1:C:47:THR:O	1:C:48:GLU:HB2	1.96	0.65
2:D:1277:ILE:CG2	2:D:1290:TYR:HB2	2.27	0.65
1:A:180:ILE:O	1:A:182:ILE:N	2.30	0.64
1:A:864:GLY:HA3	1:A:907:LEU:CD2	2.27	0.64
1:C:442:LEU:HD23	1:C:443:PRO:HD2	1.79	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1408:ILE:CD1	2:D:1425:ILE:HG12	2.27	0.64
1:A:1186:PHE:CD1	1:A:1250:THR:HG22	2.31	0.64
1:A:1487:PHE:N	1:A:1487:PHE:CD2	2.64	0.64
2:B:919:GLY:HA2	2:B:1332:GLN:HB3	1.79	0.64
1:C:238:ILE:HG12	1:C:246:PHE:CE1	2.32	0.64
1:C:432:GLU:HG2	1:C:453:ARG:HB3	1.78	0.64
1:C:824:PHE:HD2	1:C:824:PHE:H	1.43	0.64
1:C:871:PRO:CB	1:C:882:LYS:HG3	2.27	0.64
1:C:938:SER:C	1:C:940:SER:H	2.00	0.64
2:D:1274:ASN:HD21	2:D:1293:ASN:HB3	1.62	0.64
1:A:1381:ILE:O	1:A:1382:ASP:HB3	1.98	0.64
1:A:830:PRO:HG3	1:A:1483:PHE:HZ	1.60	0.64
1:A:1493:PHE:HD1	1:A:1494:THR:N	1.94	0.64
1:A:489:LYS:CG	1:A:490:SER:N	2.61	0.64
1:A:849:ARG:NH1	1:A:849:ARG:HG3	2.08	0.64
2:B:1501:ASN:HD22	2:B:1501:ASN:H	1.45	0.64
1:C:415:ASP:HB2	1:C:417:VAL:HB	1.80	0.64
1:C:773:TRP:HZ2	1:C:797:TRP:CD1	2.16	0.64
1:C:969:PRO:O	1:C:971:THR:HG23	1.98	0.64
1:A:681:LYS:HD2	1:A:738:LEU:HD21	1.79	0.64
2:B:1424:ILE:HD13	2:B:1424:ILE:N	2.10	0.64
2:B:547:THR:HG22	2:B:548:LEU:H	1.63	0.64
2:D:294:LEU:HD12	2:D:295:LYS:H	1.62	0.64
1:A:1127:ILE:CG1	1:A:1143:TYR:CE2	2.81	0.64
1:A:1174:PHE:O	1:A:1178:ASN:HB2	1.97	0.64
1:A:1279:ARG:HD3	1:A:1280:TYR:N	2.11	0.64
1:A:1124:TYR:HA	1:A:1465:ASN:OD1	1.97	0.64
1:A:1587:THR:HB	1:A:1591:VAL:HG22	1.80	0.64
1:A:811:VAL:HG12	1:A:811:VAL:O	1.97	0.64
2:B:1285:GLU:O	2:B:1287:PRO:HD3	1.98	0.64
1:C:1019:PHE:C	1:C:1019:PHE:CD2	2.70	0.64
1:C:1084:ARG:HD2	1:C:1154:LYS:HG3	1.80	0.64
1:C:1427:SER:HB3	1:C:1492:THR:HG23	1.79	0.64
2:D:531:ILE:HD11	2:D:634:LEU:CD2	2.26	0.64
1:A:516:GLU:H	1:A:516:GLU:CD	1.99	0.64
1:A:977:LEU:HA	1:A:1361:VAL:CG1	2.27	0.64
2:B:285:ILE:CD1	2:B:285:ILE:H	2.08	0.64
2:B:316:ALA:HB3	2:B:333:GLN:HB3	1.79	0.64
2:B:481:TYR:HE2	2:B:493:GLY:CA	2.11	0.64
2:B:481:TYR:CB	2:B:520:PHE:HE1	2.10	0.64
2:B:598:ILE:CD1	2:B:800:ILE:HG21	2.27	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:762:LEU:N	2:B:762:LEU:HD12	2.12	0.64
2:D:967:GLY:HA2	2:D:1321:ALA:HA	1.80	0.64
2:D:316:ALA:HB3	2:D:333:GLN:HB3	1.78	0.64
2:D:735:ASN:HB3	2:D:869:GLN:HE22	1.63	0.64
1:A:146:TYR:CD1	1:A:182:ILE:HG23	2.32	0.64
1:A:1581:LEU:HD12	1:A:1598:ILE:HD11	1.80	0.64
1:A:363:LEU:O	1:A:363:LEU:HD12	1.97	0.64
1:A:375:VAL:HG11	1:A:386:VAL:HG11	1.79	0.64
1:A:492:TYR:HD2	1:A:493:ILE:H	1.33	0.64
1:A:44:TYR:CB	1:A:545:ILE:HD12	2.26	0.64
1:C:1573:VAL:HG12	1:C:1603:LYS:HB3	1.79	0.64
1:C:307:VAL:HG13	1:C:313:TYR:HB2	1.79	0.64
1:C:905:ILE:HD12	1:C:931:PRO:CD	2.27	0.64
2:D:1429:LYS:HE3	2:D:1429:LYS:H	1.63	0.64
2:D:482:LEU:HD11	2:D:521:VAL:HB	1.79	0.64
1:A:1204:GLN:O	1:A:1208:ILE:HG13	1.98	0.64
2:B:1365:LEU:HD12	2:B:1366:LYS:H	1.62	0.64
1:C:1584:ILE:O	1:C:1585:TYR:HB3	1.97	0.64
1:C:85:LEU:HD22	1:C:85:LEU:N	2.12	0.64
1:A:353:LYS:HE3	1:A:378:SER:HA	1.80	0.64
1:A:871:PRO:CB	1:A:882:LYS:HG3	2.28	0.64
2:B:476:ILE:HG12	2:B:524:TYR:CD2	2.33	0.64
1:C:1053:MET:HE3	1:C:1086:LEU:HD22	1.80	0.64
1:C:146:TYR:CD1	1:C:182:ILE:HG23	2.33	0.64
1:C:1562:LYS:HD2	1:C:1648:TRP:HZ2	1.63	0.64
1:C:243:PHE:CZ	1:C:316:GLU:HB3	2.33	0.64
2:D:1417:MET:HG2	2:D:1443:LEU:HD22	1.80	0.64
1:A:476:LEU:HB3	1:A:563:ILE:HA	1.80	0.64
2:B:1274:ASN:HD21	2:B:1293:ASN:HB3	1.63	0.64
2:B:1417:MET:HG2	2:B:1443:LEU:HD22	1.80	0.64
2:B:476:ILE:O	2:B:476:ILE:CG2	2.46	0.64
1:C:1554:LYS:HG3	1:C:1555:PRO:HD2	1.80	0.64
1:C:24:VAL:HG11	1:C:543:TYR:CE2	2.33	0.64
2:D:521:VAL:HG13	2:D:535:SER:HB3	1.78	0.64
1:A:1644:TRP:NE1	1:A:1646:GLU:OE1	2.31	0.63
1:A:315:LEU:HD12	1:A:318:LEU:HG	1.79	0.63
1:A:33:VAL:HG21	1:A:121:TYR:CE1	2.32	0.63
1:A:710:THR:HG23	1:A:713:GLN:NE2	2.12	0.63
1:C:1421:HIS:HD2	1:C:1422:ALA:N	1.95	0.63
1:C:830:PRO:HG3	1:C:1483:PHE:HZ	1.60	0.63
1:C:984:VAL:HG22	1:C:987:ILE:HD12	1.79	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:115:LEU:HD13	2:D:629:THR:HG22	1.81	0.63
1:A:1082:ALA:O	1:A:1086:LEU:HD23	1.99	0.63
1:A:1560:ALA:HB1	1:A:1620:MET:HG2	1.81	0.63
1:A:1627:ILE:O	1:A:1627:ILE:CG1	2.45	0.63
1:A:788:PHE:HD2	1:A:788:PHE:N	1.96	0.63
1:A:797:TRP:HA	1:A:797:TRP:CE3	2.32	0.63
2:B:563:MET:HB3	2:B:778:PHE:HE2	1.63	0.63
1:C:705:VAL:HA	1:C:739:ARG:NH1	2.13	0.63
1:C:38:ASN:HA	1:C:84:ILE:HG22	1.79	0.63
2:D:1365:LEU:HD12	2:D:1366:LYS:H	1.61	0.63
2:D:738:GLY:O	2:D:901:GLN:HA	1.99	0.63
1:A:44:TYR:HB2	1:A:545:ILE:CD1	2.27	0.63
1:A:781:PRO:O	1:A:782:ARG:HB2	1.97	0.63
2:B:1427:LEU:N	2:B:1427:LEU:HD13	2.14	0.63
2:B:416:ASN:HA	2:B:425:GLN:HE22	1.63	0.63
2:B:464:PHE:HB2	2:B:504:VAL:O	1.97	0.63
1:C:1315:VAL:HG23	1:C:1348:VAL:HG22	1.81	0.63
1:C:219:VAL:O	1:C:219:VAL:HG12	1.98	0.63
1:C:535:VAL:O	1:C:563:ILE:HG12	1.99	0.63
1:A:1234:HIS:HD2	1:A:1236:ASP:H	1.46	0.63
2:B:137:TYR:CE2	2:B:143:VAL:HG22	2.34	0.63
2:B:1609:ARG:HG2	2:B:1609:ARG:NH1	1.94	0.63
2:B:745:ILE:HG21	2:B:897:LYS:HD3	1.80	0.63
1:C:1033:ILE:HG22	1:C:1034:PHE:N	2.12	0.63
1:C:753:HIS:O	1:C:754:MET:CB	2.46	0.63
1:C:765:ILE:HD13	1:C:767:SER:O	1.98	0.63
2:D:175:SER:H	2:D:1300:ALA:HB2	1.63	0.63
2:D:416:ASN:HA	2:D:425:GLN:HE22	1.64	0.63
1:A:1031:TRP:CZ3	1:A:1042:LYS:HA	2.33	0.63
1:A:1431:GLY:HA3	1:A:1483:PHE:CE1	2.34	0.63
1:A:392:ALA:HB2	1:A:433:PHE:HB3	1.79	0.63
1:C:307:VAL:CG1	1:C:313:TYR:HB2	2.28	0.63
1:C:491:PRO:CG	1:C:494:ASP:HB3	2.29	0.63
1:C:572:GLN:HB2	1:C:593:ALA:HB3	1.80	0.63
2:D:851:LEU:CD2	2:D:852:TYR:H	2.02	0.63
1:A:1431:GLY:CA	1:A:1483:PHE:CE1	2.81	0.63
1:A:599:TRP:NE1	1:A:779:LEU:HA	2.14	0.63
2:B:1284:ARG:HD2	2:B:1285:GLU:H	1.62	0.63
2:B:967:GLY:HA2	2:B:1321:ALA:HA	1.81	0.63
1:C:1133:LEU:HB2	1:C:1134:PRO:HD3	1.81	0.63
1:C:1255:LEU:O	1:C:1255:LEU:HD12	1.98	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:820:PHE:O	1:C:821:LYS:HG2	1.98	0.63
1:C:887:LYS:HD2	1:C:887:LYS:H	1.62	0.63
2:D:1458:VAL:O	2:D:1466:GLU:HG2	1.98	0.63
2:D:26:THR:HG22	2:D:630:THR:HG22	1.79	0.63
2:D:524:TYR:CE1	2:D:532:VAL:HG12	2.33	0.63
1:A:1008:ALA:CB	1:A:1078:LEU:HD11	2.26	0.63
1:A:955:ARG:O	1:A:1349:SER:HA	1.98	0.63
1:A:422:LEU:HD12	1:A:422:LEU:H	1.63	0.63
1:A:523:TYR:CZ	2:B:359:PRO:HD2	2.34	0.63
2:B:1491:ARG:HG3	2:B:1492:CYS:N	2.11	0.63
2:B:189:PRO:C	2:B:191:LEU:H	2.02	0.63
1:C:33:VAL:HG21	1:C:121:TYR:CE1	2.33	0.63
1:C:932:GLU:N	1:C:932:GLU:OE1	2.32	0.63
2:D:1289:ARG:O	2:D:1290:TYR:HD1	1.81	0.63
2:D:144:LEU:HD23	2:D:144:LEU:H	1.64	0.63
1:A:171:VAL:HG12	1:A:172:ASP:N	2.13	0.63
1:A:373:VAL:HG23	1:A:418:ALA:HB3	1.81	0.63
1:A:987:ILE:HD11	1:A:1294:ILE:HG23	1.80	0.63
2:B:129:PHE:CE2	2:B:598:ILE:HG23	2.34	0.63
1:C:1128:LYS:C	1:C:1129:LEU:HD23	2.19	0.63
2:D:762:LEU:HD12	2:D:762:LEU:N	2.13	0.63
2:D:82:LEU:HG	2:D:83:VAL:N	2.12	0.63
1:A:1305:LYS:O	1:A:1307:LEU:HD13	1.99	0.63
1:A:1671:ILE:O	1:A:1671:ILE:HG13	1.98	0.63
1:A:627:LEU:HD13	1:A:627:LEU:O	1.99	0.63
1:A:360:PRO:HB3	1:A:636:ALA:HB3	1.80	0.63
1:C:101:TYR:HE1	1:C:116:ARG:CZ	2.12	0.63
1:C:44:TYR:HB2	1:C:545:ILE:CD1	2.28	0.63
1:C:907:LEU:HD12	1:C:908:HIS:N	2.14	0.63
2:D:216:VAL:CG1	2:D:216:VAL:O	2.46	0.63
2:D:856:PHE:CD1	2:D:884:ILE:HD11	2.33	0.63
1:A:1226:ARG:CZ	1:A:1266:TYR:CE1	2.82	0.62
1:A:1304:VAL:HG12	1:A:1305:LYS:N	2.13	0.62
1:A:503:ILE:HB	1:A:511:HIS:HB2	1.81	0.62
2:B:1528:LEU:HD21	2:B:1531:ILE:HD11	1.81	0.62
2:B:595:GLN:O	2:B:598:ILE:HB	1.99	0.62
1:C:1219:LYS:CE	1:C:1239:VAL:HG21	2.28	0.62
1:C:128:ILE:HD11	1:C:214:THR:C	2.19	0.62
1:C:392:ALA:HB2	1:C:433:PHE:HB3	1.80	0.62
2:D:1387:LEU:HB2	2:D:1390:PHE:CD2	2.34	0.62
2:D:1446:PHE:HD2	2:D:1448:VAL:HG22	1.64	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:481:TYR:HE2	2:D:493:GLY:CA	2.12	0.62
2:D:595:GLN:O	2:D:598:ILE:HB	1.99	0.62
2:D:872:ILE:HG22	2:D:878:ARG:HG3	1.81	0.62
1:A:491:PRO:CG	1:A:494:ASP:HB3	2.29	0.62
1:A:941:GLY:O	1:A:942:VAL:HG13	1.99	0.62
1:A:969:PRO:O	1:A:971:THR:HG23	1.99	0.62
2:B:326:SER:HB2	2:B:819:GLN:HG3	1.81	0.62
2:D:128:LEU:O	2:D:129:PHE:CD1	2.52	0.62
2:D:1623:LYS:HB3	2:D:1623:LYS:HZ2	1.64	0.62
2:D:326:SER:HB2	2:D:819:GLN:HG3	1.81	0.62
1:A:1097:GLN:O	1:A:1098:ASN:C	2.37	0.62
1:A:1180:LEU:O	1:A:1182:ALA:N	2.32	0.62
1:A:1213:LYS:HG2	1:A:1266:TYR:CE2	2.32	0.62
1:A:981:GLY:CA	1:A:1333:PHE:HB2	2.29	0.62
2:B:175:SER:H	2:B:1300:ALA:HB2	1.64	0.62
2:B:1443:LEU:HD12	2:B:1443:LEU:N	2.13	0.62
1:C:1304:VAL:HG12	1:C:1305:LYS:N	2.14	0.62
1:C:1560:ALA:HB3	1:C:1585:TYR:CE2	2.34	0.62
1:C:627:LEU:O	1:C:627:LEU:HD13	1.99	0.62
1:C:986:GLU:HG2	1:C:987:ILE:N	2.13	0.62
2:D:1609:ARG:NH1	2:D:1609:ARG:HG2	1.93	0.62
2:D:237:ILE:O	2:D:306:LEU:HD11	1.97	0.62
2:D:247:ILE:HD11	2:D:318:VAL:HG21	1.81	0.62
2:D:407:GLN:NE2	2:D:407:GLN:HA	2.15	0.62
1:A:1593:GLU:HB2	1:A:1596:SER:OG	1.99	0.62
1:A:292:LEU:HA	1:A:297:ALA:HB2	1.80	0.62
1:A:38:ASN:HA	1:A:84:ILE:HG22	1.81	0.62
1:A:42:GLN:HG2	1:A:43:VAL:N	2.15	0.62
1:A:642:ASN:C	1:A:642:ASN:HD22	2.03	0.62
1:C:1127:ILE:CG1	1:C:1143:TYR:HE2	2.12	0.62
1:C:838:GLN:OE1	1:C:1528:VAL:HG12	2.00	0.62
1:C:623:VAL:O	1:C:624:PHE:C	2.38	0.62
2:D:464:PHE:HB2	2:D:504:VAL:O	1.99	0.62
1:A:1008:ALA:O	1:A:1009:GLU:C	2.38	0.62
1:A:1133:LEU:HB2	1:A:1134:PRO:HD3	1.81	0.62
1:A:1431:GLY:C	1:A:1432:ILE:HD13	2.19	0.62
1:A:376:LYS:HA	1:A:381:GLN:O	2.00	0.62
1:A:461:SER:HB2	1:A:553:GLU:OE2	1.99	0.62
1:A:834:VAL:HB	1:A:837:GLU:CD	2.20	0.62
1:A:968:VAL:HG13	1:A:1366:HIS:O	2.00	0.62
2:B:1386:MET:HE2	2:B:1386:MET:HA	1.81	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:216:VAL:HG12	2:B:216:VAL:O	1.97	0.62
1:C:788:PHE:HD2	1:C:788:PHE:N	1.97	0.62
1:C:804:ILE:HG22	1:C:809:ILE:HG13	1.79	0.62
1:C:909:ASN:O	1:C:910:ILE:HG12	1.99	0.62
1:C:936:ARG:NH1	1:C:936:ARG:HG3	2.14	0.62
2:D:137:TYR:CE2	2:D:143:VAL:HG22	2.34	0.62
2:D:958:GLU:OE1	2:D:958:GLU:HA	1.97	0.62
1:A:1024:TYR:CD2	1:A:1025:LEU:N	2.67	0.62
1:A:1068:VAL:HA	1:A:1078:LEU:CD1	2.27	0.62
1:A:1255:LEU:O	1:A:1255:LEU:HD12	1.99	0.62
1:A:504:LEU:HD12	1:A:509:ILE:HA	1.81	0.62
1:A:506:LYS:HD2	1:A:536:PRO:CD	2.29	0.62
1:A:596:MET:CA	1:A:782:ARG:HG2	2.29	0.62
2:B:950:LEU:HD22	2:B:1329:TYR:CE1	2.34	0.62
2:B:200:VAL:O	2:B:200:VAL:HG23	1.99	0.62
2:B:218:LYS:HD3	2:B:822:TYR:CE2	2.34	0.62
1:A:849:ARG:NH2	2:B:555:LEU:HB2	2.15	0.62
1:C:981:GLY:CA	1:C:1333:PHE:HB2	2.29	0.62
1:C:371:ILE:CD1	1:C:433:PHE:CE2	2.82	0.62
1:C:476:LEU:HB3	1:C:563:ILE:HA	1.82	0.62
2:D:1284:ARG:HG3	2:D:1285:GLU:N	2.15	0.62
2:D:1427:LEU:N	2:D:1427:LEU:HD13	2.15	0.62
2:D:131:GLN:OE1	2:D:146:ARG:NH1	2.32	0.62
2:B:40:GLN:HG3	2:B:86:THR:HG23	1.81	0.62
1:C:1143:TYR:CE1	1:C:1147:PHE:HB2	2.34	0.62
1:C:1560:ALA:HB2	1:C:1620:MET:HG2	1.81	0.62
1:C:308:LYS:HG3	1:C:309:GLU:N	2.15	0.62
2:D:944:VAL:HG22	2:D:1312:THR:OG1	1.99	0.62
2:D:285:ILE:CD1	2:D:285:ILE:H	2.10	0.62
1:A:39:ILE:HD11	1:A:104:LEU:HD21	1.82	0.62
1:A:1570:VAL:HG22	1:A:1575:VAL:HG22	1.81	0.62
1:A:970:LYS:HD3	1:A:1640:ASP:OD2	1.99	0.62
2:B:955:PRO:O	2:B:957:THR:HG23	2.00	0.62
1:C:132:LYS:O	1:C:135:TYR:CE2	2.53	0.62
1:C:1431:GLY:CA	1:C:1483:PHE:CE1	2.82	0.62
1:C:353:LYS:HE3	1:C:378:SER:HA	1.82	0.62
1:A:1199:ASP:O	1:A:1199:ASP:CG	2.37	0.62
1:A:1431:GLY:HA3	1:A:1483:PHE:HE1	1.64	0.62
1:A:788:PHE:N	1:A:788:PHE:CD2	2.67	0.62
1:A:792:ASP:O	1:A:793:SER:HB3	1.99	0.62
1:A:999:ILE:HG13	1:A:1000:LEU:N	2.13	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:494:ARG:NH1	2:B:494:ARG:HG3	2.13	0.62
2:B:951:ASP:C	2:B:953:ARG:H	2.02	0.62
1:C:128:ILE:HG22	1:C:145:VAL:HG22	1.81	0.62
1:C:1271:ILE:HD13	1:C:1300:TYR:CZ	2.35	0.62
1:C:1429:PRO:HB2	1:C:1432:ILE:HG13	1.81	0.62
1:C:571:LEU:HA	1:C:593:ALA:O	2.00	0.62
2:D:241:GLU:O	2:D:296:ARG:HD3	2.00	0.62
1:A:1227:PHE:HD2	1:A:1273:TRP:CE2	2.17	0.62
1:A:1315:VAL:HG23	1:A:1348:VAL:HG22	1.82	0.62
1:A:85:LEU:HD22	1:A:85:LEU:N	2.14	0.62
1:A:961:TYR:OH	1:A:1343:ASN:CG	2.37	0.62
2:B:179:ASP:OD1	2:B:181:ASN:HB2	2.00	0.62
2:B:218:LYS:HB3	2:B:822:TYR:CE2	2.35	0.62
2:B:482:LEU:HD11	2:B:521:VAL:HB	1.80	0.62
2:B:82:LEU:HG	2:B:83:VAL:N	2.14	0.62
2:B:953:ARG:CZ	2:B:959:ILE:HD11	2.30	0.62
1:C:1199:ASP:O	1:C:1199:ASP:CG	2.37	0.62
1:C:1234:HIS:HD2	1:C:1236:ASP:H	1.46	0.62
1:C:1587:THR:HB	1:C:1591:VAL:HG22	1.82	0.62
1:C:977:LEU:HD23	1:C:1361:VAL:HG13	1.81	0.62
2:D:1284:ARG:CD	2:D:1285:GLU:N	2.58	0.62
1:A:773:TRP:HZ2	1:A:797:TRP:CD1	2.18	0.61
1:A:905:ILE:HD12	1:A:931:PRO:CD	2.29	0.61
1:C:1012:LEU:O	1:C:1015:VAL:HG12	2.00	0.61
1:C:1127:ILE:HD11	1:C:1143:TYR:CD2	2.35	0.61
1:C:1188:LEU:HD23	1:C:1212:LEU:HD22	1.81	0.61
1:C:696:LYS:NZ	1:C:759:PRO:HG2	2.15	0.61
1:C:797:TRP:HE3	1:C:797:TRP:HA	1.63	0.61
1:C:895:LEU:HD12	1:C:896:VAL:N	2.15	0.61
1:A:754:MET:SD	1:A:755:LYS:N	2.73	0.61
2:B:147:VAL:H	2:B:183:PHE:HZ	1.45	0.61
2:B:247:ILE:HD11	2:B:318:VAL:HG21	1.82	0.61
1:A:423:ASN:CG	2:B:504:VAL:HG22	2.20	0.61
2:B:615:GLN:HB2	2:B:616:ASN:ND2	2.14	0.61
1:C:1083:LEU:CD2	1:C:1104:LEU:HD21	2.30	0.61
1:C:811:VAL:O	1:C:811:VAL:HG12	1.99	0.61
2:D:137:TYR:HB2	2:D:216:VAL:CG2	2.30	0.61
2:D:1601:ILE:HD12	2:D:1601:ILE:N	2.15	0.61
2:D:172:LEU:HD12	2:D:173:VAL:N	2.15	0.61
2:D:31:ALA:O	2:D:119:VAL:HG12	2.00	0.61
2:D:951:ASP:C	2:D:953:ARG:H	2.02	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1271:ILE:HD13	1:A:1300:TYR:CZ	2.36	0.61
1:A:1554:LYS:HG3	1:A:1555:PRO:HD2	1.83	0.61
1:A:551:THR:O	1:A:552:ALA:CB	2.47	0.61
1:A:977:LEU:HA	1:A:1361:VAL:HG13	1.80	0.61
2:B:945:ILE:HD13	2:B:1311:ILE:HB	1.82	0.61
2:B:214:PHE:O	2:B:214:PHE:CD1	2.53	0.61
1:C:25:ILE:H	1:C:655:THR:HG23	1.63	0.61
2:D:1606:TRP:CD1	2:D:1606:TRP:C	2.73	0.61
2:D:1610:TRP:CA	2:D:1628:PHE:HE2	2.11	0.61
2:D:423:GLU:N	2:D:423:GLU:OE2	2.33	0.61
2:D:838:ASN:OD1	2:D:840:VAL:HG23	1.99	0.61
1:A:1127:ILE:HD11	1:A:1143:TYR:CD2	2.35	0.61
1:A:160:VAL:CG2	1:A:175:GLU:HB3	2.30	0.61
1:A:284:GLN:CG	1:A:310:LEU:HD22	2.30	0.61
2:B:1520:VAL:HG11	2:B:1584:TRP:HD1	1.63	0.61
2:B:322:THR:HG21	2:B:326:SER:OG	2.01	0.61
1:C:1451:THR:O	1:C:1452:ASP:CB	2.49	0.61
1:A:1166:THR:O	1:A:1170:LYS:HG2	2.01	0.61
1:A:311:SER:O	1:A:313:TYR:N	2.33	0.61
1:A:655:THR:O	1:A:657:ALA:N	2.33	0.61
1:A:696:LYS:NZ	1:A:759:PRO:HG2	2.16	0.61
1:A:932:GLU:N	1:A:932:GLU:OE1	2.34	0.61
1:A:986:GLU:HG2	1:A:987:ILE:N	2.14	0.61
1:C:1082:ALA:O	1:C:1086:LEU:HD23	2.01	0.61
1:C:520:ASP:OD2	2:D:404:LEU:HB2	2.00	0.61
1:C:754:MET:SD	1:C:755:LYS:N	2.74	0.61
1:C:949:ILE:O	1:C:950:TYR:CD1	2.54	0.61
2:D:1517:GLU:HA	2:D:1517:GLU:OE1	1.98	0.61
2:D:266:GLY:HA2	2:D:276:ILE:HG13	1.81	0.61
1:A:1033:ILE:HG22	1:A:1034:PHE:N	2.14	0.61
1:A:371:ILE:CD1	1:A:433:PHE:CE2	2.83	0.61
1:A:572:GLN:HB2	1:A:593:ALA:HB3	1.81	0.61
1:A:702:GLY:CA	1:A:728:PHE:CE1	2.80	0.61
2:B:407:GLN:NE2	2:B:407:GLN:HA	2.14	0.61
2:B:501:GLN:HG2	2:B:504:VAL:HG23	1.81	0.61
1:C:1229:LYS:NZ	1:C:1240:PRO:HD2	2.15	0.61
1:C:1570:VAL:O	1:C:1571:GLU:HG3	2.01	0.61
1:C:970:LYS:HD3	1:C:1640:ASP:OD2	2.00	0.61
1:C:551:THR:O	1:C:552:ALA:CB	2.48	0.61
1:C:642:ASN:HD22	1:C:642:ASN:C	2.04	0.61
1:A:1117:SER:HB3	1:A:1174:PHE:CE2	2.36	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1188:LEU:HD23	1:A:1212:LEU:HD22	1.82	0.61
1:A:532:GLN:HE21	1:A:807:THR:HB	1.66	0.61
2:B:28:ILE:HD12	2:B:42:LEU:HD23	1.82	0.61
1:C:292:LEU:HA	1:C:297:ALA:HB2	1.81	0.61
1:C:690:TYR:CE1	1:C:696:LYS:HD2	2.35	0.61
1:C:990:ALA:HB1	1:C:1000:LEU:HD11	1.82	0.61
2:D:358:MET:HE1	2:D:467:LYS:HD2	1.83	0.61
2:D:745:ILE:O	2:D:745:ILE:HG22	2.00	0.61
1:A:1034:PHE:CE2	1:A:1041:GLU:HG2	2.36	0.61
1:A:231:ILE:HG12	1:A:231:ILE:O	1.99	0.61
1:A:251:LYS:HG2	1:A:296:ILE:HD11	1.82	0.61
1:A:373:VAL:O	1:A:417:VAL:HA	2.01	0.61
1:A:820:PHE:O	1:A:821:LYS:HG2	2.00	0.61
1:A:847:ASN:HD22	1:A:888:VAL:HG13	1.66	0.61
1:A:895:LEU:HD12	1:A:896:VAL:N	2.16	0.61
1:C:1068:VAL:HA	1:C:1078:LEU:CD1	2.28	0.61
1:C:1283:GLY:HA3	1:C:1290:THR:HG23	1.82	0.61
1:C:1381:ILE:HG12	1:C:1382:ASP:N	2.14	0.61
1:C:23:TYR:HA	1:C:43:VAL:HA	1.81	0.61
1:C:742:ILE:HG13	1:C:742:ILE:O	2.01	0.61
1:C:976:ILE:HB	1:C:1362:THR:HG22	1.82	0.61
2:D:1284:ARG:HG3	2:D:1285:GLU:H	1.64	0.61
1:A:1431:GLY:O	1:A:1432:ILE:HD13	2.01	0.61
1:A:265:VAL:O	1:A:289:ASN:HA	2.01	0.61
1:A:838:GLN:OE1	1:A:1528:VAL:HG12	2.01	0.61
2:B:1429:LYS:HE3	2:B:1429:LYS:N	2.14	0.61
2:B:1517:GLU:HA	2:B:1517:GLU:OE1	2.00	0.61
2:B:508:LEU:HD12	2:B:509:HIS:N	2.14	0.61
2:B:735:ASN:HB3	2:B:869:GLN:HE22	1.65	0.61
1:C:455:ILE:HG22	1:C:456:ALA:H	1.66	0.61
2:D:1399:ARG:HG2	2:D:1399:ARG:HH11	1.66	0.61
2:D:261:ALA:N	2:D:285:ILE:HD11	2.15	0.61
2:D:800:ILE:HG23	2:D:801:CYS:N	2.14	0.61
1:A:1003:LEU:HD11	1:A:1286:SER:HA	1.82	0.61
2:B:1534:GLN:HB2	2:B:1539:ILE:HD11	1.83	0.61
2:B:365:TYR:HD1	2:B:395:THR:HG22	1.66	0.61
2:B:816:ILE:HD13	2:B:896:ILE:HG22	1.83	0.61
1:C:161:LEU:HD11	1:C:185:PHE:CD1	2.36	0.61
2:D:1285:GLU:O	2:D:1287:PRO:HD3	2.01	0.61
2:D:524:TYR:HE1	2:D:532:VAL:HG12	1.66	0.61
1:A:238:ILE:HG12	1:A:246:PHE:CE1	2.35	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:270:GLY:HA3	1:A:282:MET:HG3	1.82	0.60
1:A:690:TYR:CE1	1:A:696:LYS:HD2	2.35	0.60
1:A:797:TRP:HA	1:A:797:TRP:HE3	1.64	0.60
1:A:804:ILE:HG22	1:A:809:ILE:HG13	1.83	0.60
2:B:265:PHE:CE2	2:B:294:LEU:HB2	2.36	0.60
1:A:1226:ARG:NH1	1:A:1266:TYR:HE1	1.99	0.60
1:A:180:ILE:HG21	1:A:599:TRP:CE3	2.36	0.60
2:B:916:VAL:HG23	2:B:917:PRO:HD2	1.82	0.60
1:C:1176:LEU:HD21	1:C:1195:LEU:HD21	1.82	0.60
1:C:532:GLN:HE21	1:C:807:THR:HB	1.67	0.60
1:C:591:ASN:HB3	1:C:785:GLN:HG3	1.82	0.60
2:D:963:ILE:HD11	2:D:1311:ILE:HG12	1.81	0.60
2:B:1391:LEU:HB2	2:B:1417:MET:HE2	1.83	0.60
2:B:423:GLU:N	2:B:423:GLU:OE2	2.33	0.60
1:C:160:VAL:CG2	1:C:175:GLU:HB3	2.31	0.60
1:C:1625:LEU:HB3	1:C:1636:ILE:HG22	1.83	0.60
1:C:640:LEU:H	1:C:644:ASN:CB	2.14	0.60
1:C:950:TYR:OH	1:C:1307:LEU:HD21	2.02	0.60
2:D:251:TYR:CE2	2:D:257:VAL:HG22	2.36	0.60
1:A:1000:LEU:O	1:A:1001:THR:HG23	2.01	0.60
1:A:1016:VAL:N	1:A:1017:PRO:CD	2.64	0.60
1:A:1127:ILE:CG1	1:A:1143:TYR:HE2	2.14	0.60
1:A:1016:VAL:HG11	1:A:1291:ILE:HG13	1.82	0.60
1:A:1479:ILE:H	1:A:1479:ILE:HD13	1.65	0.60
1:A:1423:VAL:HG11	1:A:1496:TYR:CZ	2.36	0.60
1:A:307:VAL:CG1	1:A:313:TYR:HB2	2.31	0.60
1:A:84:ILE:HD12	1:A:84:ILE:O	2.01	0.60
2:B:1429:LYS:H	2:B:1429:LYS:HE3	1.66	0.60
2:B:165:PHE:CE2	2:B:199:ILE:HD11	2.35	0.60
1:C:1593:GLU:HB2	1:C:1596:SER:OG	2.01	0.60
2:D:263:VAL:HG23	2:D:283:ILE:HD13	1.83	0.60
2:D:870:PHE:HB2	2:D:871:PRO:HD2	1.82	0.60
1:A:1112:GLN:HB2	1:A:1118:PHE:HE1	1.66	0.60
1:A:930:VAL:HG22	1:A:931:PRO:HD2	1.84	0.60
1:C:39:ILE:CD1	1:C:104:LEU:HD21	2.31	0.60
1:C:596:MET:CA	1:C:782:ARG:HG2	2.32	0.60
2:D:322:THR:HG21	2:D:326:SER:OG	2.01	0.60
1:A:502:LEU:HD22	1:A:509:ILE:HG21	1.83	0.60
1:A:990:ALA:HB1	1:A:1000:LEU:HD11	1.82	0.60
2:B:1387:LEU:HB2	2:B:1390:PHE:CD2	2.37	0.60
2:B:358:MET:HE1	2:B:467:LYS:HD2	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1191:SER:O	1:C:1194:ALA:HB3	2.02	0.60
1:C:1568:ILE:HG23	1:C:1577:TYR:CE1	2.36	0.60
2:D:236:TYR:C	2:D:238:ASP:H	2.05	0.60
2:D:28:ILE:HD12	2:D:42:LEU:HD23	1.83	0.60
2:D:547:THR:HG22	2:D:548:LEU:H	1.67	0.60
2:D:955:PRO:O	2:D:957:THR:HG23	2.00	0.60
1:A:355:ASN:HD22	1:A:355:ASN:N	2.00	0.60
2:B:785:THR:OG1	2:B:786:THR:N	2.29	0.60
1:C:311:SER:O	1:C:313:TYR:N	2.34	0.60
1:C:961:TYR:OH	1:C:1343:ASN:CG	2.40	0.60
1:A:128:ILE:HD11	1:A:214:THR:C	2.22	0.60
1:A:1560:ALA:HB2	1:A:1620:MET:HG2	1.82	0.60
2:B:1611:PRO:HD2	2:B:1628:PHE:CE2	2.37	0.60
1:C:830:PRO:CG	1:C:1483:PHE:HZ	2.14	0.60
2:D:148:PHE:CE2	2:D:792:VAL:HG11	2.36	0.60
1:A:455:ILE:HG22	1:A:456:ALA:H	1.67	0.60
1:A:907:LEU:HD12	1:A:908:HIS:N	2.16	0.60
1:C:1431:GLY:HA3	1:C:1483:PHE:CE1	2.37	0.60
1:C:308:LYS:HG3	1:C:309:GLU:H	1.66	0.60
1:C:599:TRP:NE1	1:C:779:LEU:HA	2.16	0.60
1:C:788:PHE:CD2	1:C:788:PHE:N	2.68	0.60
1:C:844:THR:HG22	1:C:895:LEU:HB2	1.83	0.60
2:D:615:GLN:HB2	2:D:616:ASN:HD22	1.66	0.60
1:A:1132:THR:H	1:A:1135:VAL:HB	1.66	0.60
1:A:1563:VAL:HG21	1:A:1619:ILE:HD12	1.84	0.60
2:B:31:ALA:O	2:B:119:VAL:HG12	2.02	0.60
2:B:148:PHE:CE2	2:B:792:VAL:HG11	2.36	0.60
1:C:1317:TYR:HD2	1:C:1344:ASP:HB3	1.67	0.60
1:C:955:ARG:HG2	1:C:1350:THR:CG2	2.31	0.60
1:C:1431:GLY:CA	1:C:1483:PHE:HE1	2.15	0.60
1:C:1483:PHE:HD1	1:C:1483:PHE:O	1.85	0.60
1:C:177:ILE:HG22	1:C:178:ASP:H	1.67	0.60
1:C:44:TYR:CB	1:C:545:ILE:HD12	2.27	0.60
1:C:655:THR:O	1:C:657:ALA:N	2.35	0.60
1:C:875:HIS:HB2	2:D:901:GLN:NE2	2.17	0.60
1:A:1625:LEU:HB3	1:A:1636:ILE:HG22	1.84	0.59
1:A:492:TYR:CE2	1:A:493:ILE:HB	2.37	0.59
2:B:261:ALA:N	2:B:285:ILE:HD11	2.17	0.59
2:B:745:ILE:O	2:B:745:ILE:HG22	2.01	0.59
1:C:999:ILE:HG13	1:C:1000:LEU:N	2.14	0.59
1:C:1671:ILE:HG13	1:C:1671:ILE:O	2.02	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LEU:HD12	1:C:318:LEU:HG	1.83	0.59
1:C:22:THR:HG21	1:C:656:ASN:O	2.02	0.59
1:C:830:PRO:CG	1:C:1483:PHE:CZ	2.84	0.59
1:C:934:VAL:CG2	1:C:1366:HIS:CD2	2.85	0.59
2:D:1442:ILE:CA	2:D:1443:LEU:HD12	2.32	0.59
2:D:494:ARG:HG3	2:D:494:ARG:NH1	2.14	0.59
2:D:785:THR:OG1	2:D:786:THR:N	2.34	0.59
1:A:864:GLY:HA3	1:A:907:LEU:HD23	1.84	0.59
2:B:1591:LEU:C	2:B:1591:LEU:HD23	2.22	0.59
2:B:478:TYR:CD1	2:B:478:TYR:O	2.55	0.59
2:B:838:ASN:OD1	2:B:840:VAL:HG23	2.03	0.59
1:C:470:THR:HG22	2:D:450:THR:HB	1.84	0.59
2:D:958:GLU:O	2:D:959:ILE:HG13	2.02	0.59
1:A:128:ILE:HD11	1:A:215:ALA:N	2.17	0.59
1:A:1377:PHE:CE1	1:A:1408:TYR:HD1	2.21	0.59
1:A:1434:ALA:HA	1:A:1479:ILE:HG22	1.83	0.59
1:A:219:VAL:HG12	1:A:219:VAL:O	2.00	0.59
1:A:243:PHE:O	1:A:303:SER:HB2	2.02	0.59
2:B:315:TYR:CD1	2:B:315:TYR:O	2.55	0.59
1:C:628:GLU:HA	1:C:630:SER:OG	2.01	0.59
1:C:790:LEU:HD12	1:C:790:LEU:H	1.66	0.59
1:C:968:VAL:HG23	1:C:971:THR:HG21	1.83	0.59
2:D:189:PRO:C	2:D:191:LEU:H	2.05	0.59
1:A:1013:MET:SD	1:A:1016:VAL:HG21	2.42	0.59
1:A:367:ILE:HD13	1:A:466:TYR:CD2	2.38	0.59
1:A:430:VAL:HG22	1:A:455:ILE:HG23	1.83	0.59
1:C:1133:LEU:H	1:C:1133:LEU:HD12	1.67	0.59
1:C:987:ILE:HD11	1:C:1294:ILE:HG23	1.83	0.59
1:C:1431:GLY:HA3	1:C:1483:PHE:HE1	1.67	0.59
1:C:373:VAL:O	1:C:417:VAL:HA	2.03	0.59
1:C:492:TYR:CE2	1:C:493:ILE:HB	2.37	0.59
1:C:133:PRO:HD2	1:C:609:VAL:CG1	2.33	0.59
2:D:133:ASP:HA	2:D:757:TRP:HZ3	1.67	0.59
2:D:1456:VAL:HG12	2:D:1456:VAL:O	2.01	0.59
1:A:101:TYR:CZ	1:C:1305:LYS:HG3	2.38	0.59
1:A:442:LEU:HD23	1:A:443:PRO:HD2	1.83	0.59
1:A:968:VAL:HG23	1:A:971:THR:HG21	1.83	0.59
1:A:974:LYS:O	1:A:1364:VAL:HG12	2.03	0.59
2:B:857:CYS:H	2:B:887:LEU:HD21	1.67	0.59
1:C:1084:ARG:HD2	1:C:1154:LYS:HE3	1.83	0.59
1:C:1186:PHE:HA	1:C:1250:THR:HG22	1.84	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:25:ILE:HB	1:C:654:LEU:O	2.03	0.59
1:C:689:LYS:HG2	1:C:699:CYS:SG	2.41	0.59
2:D:1591:LEU:C	2:D:1591:LEU:HD23	2.22	0.59
2:D:355:LYS:N	2:D:355:LYS:HD2	2.17	0.59
2:D:803:ALA:O	2:D:805:PRO:HD3	2.02	0.59
2:D:857:CYS:H	2:D:887:LEU:HD21	1.67	0.59
1:A:128:ILE:HG13	1:A:215:ALA:HB2	1.84	0.59
1:A:640:LEU:HB2	1:A:644:ASN:OD1	2.03	0.59
1:A:595:GLY:HA2	1:A:782:ARG:NH1	2.18	0.59
2:B:1277:ILE:CG2	2:B:1290:TYR:HB2	2.32	0.59
2:B:236:TYR:C	2:B:238:ASP:H	2.06	0.59
2:B:28:ILE:HG12	2:B:628:LEU:HD13	1.83	0.59
2:B:529:ASN:OD1	2:B:529:ASN:O	2.21	0.59
1:C:1008:ALA:O	1:C:1009:GLU:C	2.41	0.59
1:C:1623:GLU:HB2	1:C:1638:PRO:CG	2.33	0.59
1:C:284:GLN:CG	1:C:310:LEU:HD22	2.32	0.59
1:C:382:LEU:HD22	1:C:416:GLY:HA3	1.85	0.59
1:C:504:LEU:HD21	1:C:651:LEU:CG	2.32	0.59
2:D:1534:GLN:HB2	2:D:1539:ILE:HD11	1.85	0.59
2:D:159:LYS:HD3	2:D:180:LEU:HD12	1.85	0.59
2:D:202:LYS:HG3	2:D:203:TYR:N	2.18	0.59
2:D:257:VAL:CG1	2:D:258:GLU:N	2.65	0.59
2:D:786:THR:OG1	2:D:809:ARG:HG3	2.03	0.59
1:A:1429:PRO:HB2	1:A:1432:ILE:HG13	1.85	0.59
1:A:23:TYR:HD1	1:A:23:TYR:O	1.84	0.59
1:A:591:ASN:HB3	1:A:785:GLN:HG3	1.83	0.59
2:B:234:PHE:CD1	2:B:234:PHE:C	2.76	0.59
1:C:1423:VAL:HG11	1:C:1496:TYR:CZ	2.36	0.59
2:D:1500:LEU:HD12	2:D:1500:LEU:C	2.23	0.59
2:D:376:HIS:O	2:D:378:PRO:HD3	2.02	0.59
1:A:1381:ILE:HG12	1:A:1382:ASP:N	2.16	0.59
1:A:1431:GLY:CA	1:A:1483:PHE:HE1	2.16	0.59
2:B:1610:TRP:CA	2:B:1628:PHE:HE2	2.12	0.59
2:B:856:PHE:CD1	2:B:884:ILE:HD11	2.37	0.59
2:B:965:ILE:HG13	2:B:1301:ARG:HB2	1.85	0.59
1:C:1627:ILE:O	1:C:1627:ILE:CG1	2.50	0.59
1:C:265:VAL:O	1:C:289:ASN:HA	2.03	0.59
1:C:488:PRO:HG3	1:C:499:TYR:OH	2.02	0.59
1:A:1012:LEU:HD13	1:A:1081:PHE:CD2	2.37	0.59
1:A:1083:LEU:CD2	1:A:1104:LEU:HD21	2.33	0.59
1:A:1229:LYS:NZ	1:A:1240:PRO:HD2	2.16	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:347:PHE:O	2:B:349:LYS:N	2.36	0.59
2:B:485:ASN:OD1	2:B:486:LYS:HD2	2.03	0.59
1:C:430:VAL:HG11	1:C:453:ARG:NH2	2.16	0.59
1:C:465:LEU:HD12	1:C:488:PRO:HA	1.85	0.59
1:C:632:LEU:HD23	1:C:632:LEU:N	2.17	0.59
2:D:1284:ARG:HD2	2:D:1285:GLU:H	1.65	0.59
2:D:243:PHE:CD1	2:D:314:LEU:HD23	2.38	0.59
2:D:54:LEU:N	2:D:54:LEU:HD23	2.17	0.59
1:A:39:ILE:CD1	1:A:104:LEU:HD21	2.32	0.59
1:A:1307:LEU:H	1:A:1307:LEU:HD22	1.68	0.59
1:A:1421:HIS:CD2	1:A:1421:HIS:C	2.75	0.59
1:A:1451:THR:O	1:A:1452:ASP:CB	2.51	0.59
1:A:1576:LYS:HG2	1:A:1601:ILE:CG2	2.32	0.59
1:A:25:ILE:H	1:A:655:THR:HG23	1.67	0.59
1:A:505:SER:OG	1:A:506:LYS:HD3	2.03	0.59
1:A:753:HIS:O	1:A:754:MET:CB	2.49	0.59
1:A:799:ILE:HG22	1:A:815:VAL:O	2.01	0.59
2:B:26:THR:HG22	2:B:630:THR:HG22	1.85	0.59
1:C:99:VAL:HG22	1:C:100:SER:O	2.02	0.59
1:C:270:GLY:HA3	1:C:282:MET:HG3	1.84	0.59
1:C:505:SER:OG	1:C:506:LYS:HD3	2.02	0.59
1:C:653:PHE:O	1:C:653:PHE:CD1	2.48	0.59
1:C:949:ILE:O	1:C:949:ILE:HG22	2.03	0.59
2:D:104:VAL:HG22	2:D:105:VAL:N	2.17	0.59
1:A:1128:LYS:C	1:A:1129:LEU:HD23	2.23	0.58
1:A:571:LEU:HA	1:A:593:ALA:O	2.04	0.58
1:A:790:LEU:H	1:A:790:LEU:HD12	1.67	0.58
1:A:833:VAL:O	1:A:929:VAL:HA	2.02	0.58
2:B:299:PHE:HE1	2:B:303:PHE:CD2	2.20	0.58
2:B:247:ILE:CD1	2:B:318:VAL:HG21	2.33	0.58
1:C:1226:ARG:NH1	1:C:1266:TYR:HE1	2.00	0.58
1:C:1446:VAL:O	1:C:1446:VAL:HG12	2.01	0.58
1:C:23:TYR:HD1	1:C:23:TYR:O	1.86	0.58
1:C:502:LEU:HD22	1:C:509:ILE:HG21	1.85	0.58
2:D:47:GLY:O	2:D:48:ASP:HB2	2.02	0.58
2:D:745:ILE:O	2:D:745:ILE:CG2	2.51	0.58
2:D:39:GLU:O	2:D:87:ILE:HD12	2.03	0.58
2:D:35:THR:HB	2:D:91:ALA:HB2	1.84	0.58
1:A:1180:LEU:CD2	1:A:1208:ILE:HG12	2.33	0.58
1:A:1232:LEU:O	1:A:1233:GLN:HB3	2.02	0.58
1:A:1560:ALA:O	1:A:1585:TYR:HD2	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:623:VAL:O	1:A:624:PHE:C	2.39	0.58
1:A:125:PHE:CD1	1:A:627:LEU:HD21	2.38	0.58
1:A:87:ILE:CD1	1:A:87:ILE:N	2.63	0.58
2:B:137:TYR:HB2	2:B:216:VAL:CG2	2.33	0.58
2:B:844:ILE:O	2:B:871:PRO:HA	2.04	0.58
1:C:1204:GLN:O	1:C:1208:ILE:HG13	2.03	0.58
1:C:128:ILE:HD11	1:C:215:ALA:N	2.18	0.58
1:C:1305:LYS:O	1:C:1307:LEU:HD13	2.02	0.58
1:C:503:ILE:HB	1:C:511:HIS:HB2	1.85	0.58
2:D:1620:GLU:HG2	2:D:1621:PHE:CE2	2.38	0.58
2:D:266:GLY:O	2:D:314:LEU:HD12	2.03	0.58
2:D:478:TYR:CD1	2:D:478:TYR:O	2.56	0.58
2:D:950:LEU:HD22	2:D:1329:TYR:CE1	2.37	0.58
1:A:1053:MET:HE2	1:A:1089:VAL:CG2	2.33	0.58
1:A:625:GLN:HG2	1:A:626:PHE:H	1.68	0.58
2:B:266:GLY:O	2:B:314:LEU:HD12	2.02	0.58
2:B:748:ARG:HH12	2:B:784:ILE:HG12	1.68	0.58
2:B:891:LEU:CB	2:B:912:LYS:HD3	2.31	0.58
1:C:171:VAL:HG13	1:C:1054:LEU:HD21	1.84	0.58
1:C:355:ASN:N	1:C:355:ASN:HD22	2.02	0.58
1:C:833:VAL:O	1:C:929:VAL:HA	2.02	0.58
2:D:1527:LYS:HE2	2:D:1578:ASN:OD1	2.03	0.58
2:D:384:PHE:CD1	2:D:400:LEU:HG	2.38	0.58
1:A:830:PRO:CG	1:A:1483:PHE:CZ	2.86	0.58
1:A:573:VAL:HG12	1:A:592:MET:HG2	1.84	0.58
1:A:689:LYS:HG2	1:A:699:CYS:SG	2.43	0.58
1:A:734:VAL:O	1:A:737:GLN:HB2	2.04	0.58
2:B:1442:ILE:CA	2:B:1443:LEU:HD12	2.34	0.58
2:B:1475:ASP:N	2:B:1475:ASP:OD1	2.27	0.58
2:B:476:ILE:HD11	2:B:524:TYR:HB2	1.86	0.58
2:B:133:ASP:HA	2:B:757:TRP:HZ3	1.68	0.58
2:B:870:PHE:HB2	2:B:871:PRO:HD2	1.85	0.58
2:B:39:GLU:O	2:B:87:ILE:HD12	2.03	0.58
2:B:69:PHE:CG	2:B:87:ILE:HG22	2.38	0.58
2:B:953:ARG:CG	2:B:954:VAL:N	2.67	0.58
1:C:375:VAL:HG11	1:C:386:VAL:HG11	1.85	0.58
1:C:862:VAL:HB	1:C:865:ILE:HD11	1.86	0.58
1:C:980:LYS:HD3	1:C:986:GLU:HA	1.86	0.58
2:D:1371:TYR:CG	2:D:1377:SER:HB3	2.38	0.58
2:D:172:LEU:HD12	2:D:173:VAL:H	1.67	0.58
1:A:117:MET:HB2	1:A:118:PRO:CD	2.33	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:292:LEU:HD13	1:A:296:ILE:O	2.03	0.58
1:A:308:LYS:HG3	1:A:309:GLU:N	2.19	0.58
1:A:469:TRP:N	1:A:469:TRP:HE3	2.01	0.58
2:B:606:ASP:OD1	2:B:606:ASP:O	2.21	0.58
2:B:885:VAL:HG23	2:B:885:VAL:O	2.01	0.58
1:C:1000:LEU:O	1:C:1001:THR:HG23	2.03	0.58
1:C:550:GLN:O	1:C:550:GLN:HG2	2.03	0.58
1:C:640:LEU:HB2	1:C:644:ASN:OD1	2.04	0.58
1:C:23:TYR:CD1	1:C:655:THR:HB	2.38	0.58
1:C:84:ILE:O	1:C:84:ILE:HD12	2.03	0.58
1:C:977:LEU:HA	1:C:1361:VAL:CG1	2.34	0.58
2:D:261:ALA:CB	2:D:285:ILE:HD11	2.33	0.58
2:D:476:ILE:HD11	2:D:524:TYR:CG	2.38	0.58
2:D:558:MET:HE3	2:D:559:PRO:HD2	1.86	0.58
2:D:628:LEU:HD12	2:D:629:THR:H	1.69	0.58
1:A:640:LEU:H	1:A:644:ASN:CB	2.16	0.58
2:B:100:GLN:HG3	2:B:101:ASN:N	2.19	0.58
2:B:953:ARG:HA	2:B:1330:ASN:O	2.03	0.58
2:B:1606:TRP:CD1	2:B:1606:TRP:C	2.76	0.58
2:B:1620:GLU:HG2	2:B:1621:PHE:CE2	2.39	0.58
2:B:315:TYR:CD1	2:B:315:TYR:C	2.77	0.58
2:B:263:VAL:HG13	2:B:318:VAL:HG23	1.85	0.58
1:C:1381:ILE:HD12	1:C:1493:PHE:CD2	2.38	0.58
1:C:1576:LYS:HG2	1:C:1601:ILE:CG2	2.33	0.58
1:C:502:LEU:HB2	1:C:541:LEU:HD23	1.85	0.58
1:C:576:SER:HB2	1:C:589:SER:CB	2.33	0.58
1:C:799:ILE:HG22	1:C:815:VAL:O	2.04	0.58
2:D:1611:PRO:HD2	2:D:1628:PHE:CE2	2.39	0.58
2:D:243:PHE:HD1	2:D:314:LEU:HD23	1.67	0.58
2:D:69:PHE:CG	2:D:87:ILE:HG22	2.38	0.58
1:A:1012:LEU:O	1:A:1015:VAL:HG12	2.04	0.58
1:A:1147:PHE:O	1:A:1150:ILE:HB	2.04	0.58
2:B:243:PHE:CD1	2:B:314:LEU:HD23	2.38	0.58
1:C:1628:LYS:HB3	1:C:1633:PHE:CD1	2.38	0.58
1:C:243:PHE:O	1:C:303:SER:HB2	2.04	0.58
1:C:469:TRP:HE3	1:C:469:TRP:N	2.01	0.58
1:C:493:ILE:HG21	1:C:495:LYS:HB2	1.85	0.58
1:C:628:GLU:C	1:C:630:SER:N	2.56	0.58
2:D:628:LEU:HD12	2:D:629:THR:N	2.19	0.58
1:A:113:LYS:CG	1:A:114:SER:H	2.14	0.58
1:A:1176:LEU:HD21	1:A:1195:LEU:HD21	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1641:SER:C	1:A:1643:THR:H	2.06	0.58
1:A:357:VAL:O	1:A:359:THR:HG22	2.04	0.58
1:A:705:VAL:HA	1:A:739:ARG:NH1	2.18	0.58
1:A:77:ASN:HD22	1:A:81:ASN:HB2	1.68	0.58
1:A:857:VAL:CG2	1:A:884:VAL:HG21	2.31	0.58
2:B:263:VAL:HG23	2:B:283:ILE:HD13	1.84	0.58
1:C:1474:CYS:HB3	1:C:1476:ARG:HH12	1.67	0.58
1:C:177:ILE:HG22	1:C:178:ASP:N	2.19	0.58
1:C:367:ILE:HD13	1:C:466:TYR:CD2	2.39	0.58
1:C:625:GLN:HG2	1:C:626:PHE:H	1.68	0.58
2:D:963:ILE:HG12	2:D:1325:ILE:HG12	1.86	0.58
2:D:476:ILE:HG12	2:D:524:TYR:HD2	1.66	0.58
2:D:221:LEU:HD11	2:D:753:LYS:CG	2.29	0.58
1:A:1143:TYR:CE1	1:A:1147:PHE:HB2	2.38	0.58
1:A:243:PHE:CZ	1:A:316:GLU:HB3	2.39	0.58
1:A:382:LEU:HD22	1:A:416:GLY:HA3	1.86	0.58
1:A:23:TYR:HA	1:A:43:VAL:HA	1.84	0.58
2:B:107:GLN:HG3	2:B:116:GLU:HG3	1.86	0.58
2:B:1284:ARG:CD	2:B:1285:GLU:N	2.60	0.58
2:B:1365:LEU:HD12	2:B:1366:LYS:N	2.18	0.58
2:B:1386:MET:HA	2:B:1386:MET:CE	2.34	0.58
2:B:1602:THR:C	2:B:1604:ASN:H	2.05	0.58
2:B:628:LEU:HD12	2:B:629:THR:H	1.69	0.58
2:B:738:GLY:O	2:B:901:GLN:HA	2.03	0.58
1:C:31:PHE:HB2	1:C:119:ILE:HG22	1.86	0.58
1:C:854:GLN:CD	1:C:854:GLN:H	2.07	0.58
2:D:179:ASP:OD1	2:D:181:ASN:HB2	2.03	0.58
1:A:1084:ARG:HD2	1:A:1154:LYS:HE3	1.85	0.58
1:A:1221:ASN:HA	1:A:1222:PRO:C	2.24	0.58
1:A:1568:ILE:HG12	1:A:1577:TYR:CE1	2.39	0.58
1:A:307:VAL:HG13	1:A:313:TYR:HB2	1.84	0.58
1:A:489:LYS:C	1:A:491:PRO:CD	2.63	0.58
1:A:985:GLY:O	1:A:986:GLU:C	2.42	0.58
2:B:130:ILE:HB	2:B:212:ALA:HB2	1.86	0.58
2:B:339:VAL:HG23	2:B:341:SER:N	2.18	0.58
2:B:628:LEU:HD12	2:B:629:THR:N	2.19	0.58
1:C:1033:ILE:CG2	1:C:1034:PHE:CD1	2.87	0.58
1:C:1570:VAL:HG22	1:C:1575:VAL:HG22	1.85	0.58
2:D:1371:TYR:CD1	2:D:1377:SER:HB3	2.39	0.58
2:D:247:ILE:CD1	2:D:318:VAL:HG21	2.34	0.58
2:D:342:PRO:HG2	2:D:420:LEU:HD13	1.84	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:224:LEU:CD2	1:A:225:PRO:HD2	2.24	0.57
1:A:395:ILE:HD12	1:A:395:ILE:O	2.04	0.57
2:B:476:ILE:HD11	2:B:524:TYR:CG	2.39	0.57
1:C:1097:GLN:O	1:C:1098:ASN:C	2.41	0.57
1:C:251:LYS:HG2	1:C:296:ILE:HD11	1.86	0.57
2:D:1365:LEU:HD12	2:D:1366:LYS:N	2.18	0.57
2:D:825:VAL:HB	2:D:828:GLU:OE2	2.04	0.57
2:D:861:THR:O	2:D:863:GLY:N	2.37	0.57
1:A:1033:ILE:HD13	1:A:1333:PHE:HZ	1.69	0.57
1:A:1574:PHE:HA	1:A:1603:LYS:CD	2.35	0.57
1:A:1584:ILE:O	1:A:1585:TYR:HB3	2.02	0.57
1:A:457:TYR:C	1:A:457:TYR:CD2	2.78	0.57
1:A:576:SER:HB2	1:A:589:SER:CB	2.34	0.57
2:B:243:PHE:HD1	2:B:314:LEU:HD23	1.68	0.57
1:C:117:MET:HB2	1:C:118:PRO:CD	2.34	0.57
1:C:128:ILE:HG13	1:C:215:ALA:HB2	1.84	0.57
1:C:316:GLU:O	1:C:349:LEU:HD21	2.04	0.57
1:C:862:VAL:HB	1:C:865:ILE:CD1	2.34	0.57
1:C:903:LEU:HD22	1:C:903:LEU:N	2.19	0.57
1:C:969:PRO:HG3	1:C:1601:ILE:CD1	2.32	0.57
2:D:100:GLN:HG3	2:D:101:ASN:N	2.18	0.57
2:D:234:PHE:C	2:D:234:PHE:CD1	2.77	0.57
1:A:101:TYR:CE1	1:A:116:ARG:NH2	2.73	0.57
1:A:1227:PHE:HD2	1:A:1273:TRP:NE1	2.02	0.57
1:A:161:LEU:HD11	1:A:185:PHE:CD1	2.40	0.57
1:A:502:LEU:HB2	1:A:541:LEU:HD23	1.86	0.57
1:A:24:VAL:HG11	1:A:543:TYR:CE2	2.39	0.57
2:B:953:ARG:HG2	2:B:954:VAL:H	1.69	0.57
1:C:1147:PHE:O	1:C:1150:ILE:HB	2.05	0.57
1:C:469:TRP:CE3	1:C:469:TRP:N	2.72	0.57
2:D:1573:LEU:HB3	2:D:1575:LEU:HD23	1.86	0.57
2:D:23:ALA:HB3	2:D:528:ASN:HD22	1.67	0.57
1:A:1019:PHE:HD2	1:A:1020:TYR:N	2.03	0.57
1:A:614:ARG:NE	1:A:614:ARG:H	2.01	0.57
2:B:885:VAL:HG23	2:B:887:LEU:HD21	1.86	0.57
2:B:961:THR:HG22	2:B:1327:THR:CG2	2.34	0.57
1:C:1132:THR:H	1:C:1135:VAL:HB	1.69	0.57
1:C:1227:PHE:HD2	1:C:1273:TRP:NE1	2.02	0.57
1:C:249:THR:HG23	1:C:298:GLN:HE21	1.69	0.57
1:A:1562:LYS:HD3	1:A:1664:LEU:HD21	1.87	0.57
1:A:238:ILE:HG23	1:A:242:ASN:ND2	2.15	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:250:ILE:HD11	1:A:265:VAL:CG1	2.32	0.57
1:A:365:PRO:HG2	1:A:464:TYR:HE2	1.66	0.57
1:A:692:HIS:HA	1:A:696:LYS:HD3	1.85	0.57
1:A:844:THR:HG22	1:A:895:LEU:HB2	1.85	0.57
1:A:59:TYR:CZ	1:A:99:VAL:HG21	2.39	0.57
2:B:1426:TYR:CD2	2:B:1426:TYR:N	2.72	0.57
1:C:1221:ASN:HA	1:C:1222:PRO:C	2.25	0.57
1:C:1227:PHE:HB2	1:C:1251:THR:HG21	1.86	0.57
1:C:1568:ILE:HG12	1:C:1577:TYR:CE1	2.39	0.57
1:C:1622:LYS:HZ2	1:C:1642:LEU:HD13	1.68	0.57
1:C:231:ILE:O	1:C:231:ILE:HG12	2.02	0.57
1:C:292:LEU:HD13	1:C:296:ILE:O	2.05	0.57
1:C:734:VAL:O	1:C:737:GLN:HB2	2.05	0.57
2:D:315:TYR:CD1	2:D:315:TYR:O	2.58	0.57
2:D:390:THR:HG22	2:D:394:GLY:C	2.24	0.57
1:A:1507:MET:HG3	1:A:1508:PHE:O	2.04	0.57
2:B:944:VAL:HG22	2:B:1312:THR:OG1	2.04	0.57
2:B:1563:TYR:HB3	2:B:1601:ILE:HD11	1.85	0.57
2:B:257:VAL:CG1	2:B:258:GLU:N	2.67	0.57
1:C:395:ILE:O	1:C:395:ILE:HD12	2.04	0.57
1:C:461:SER:O	1:C:462:GLN:HB2	2.02	0.57
1:C:595:GLY:HA2	1:C:782:ARG:NH1	2.20	0.57
2:D:200:VAL:O	2:D:200:VAL:HG23	2.04	0.57
2:D:384:PHE:CE1	2:D:400:LEU:HG	2.39	0.57
2:D:953:ARG:CG	2:D:954:VAL:N	2.68	0.57
1:A:308:LYS:HG3	1:A:309:GLU:H	1.69	0.57
1:A:315:LEU:CD1	1:A:318:LEU:HG	2.34	0.57
1:A:493:ILE:HG21	1:A:495:LYS:HB2	1.85	0.57
1:A:742:ILE:O	1:A:742:ILE:HG13	2.04	0.57
1:A:980:LYS:HD3	1:A:986:GLU:HA	1.87	0.57
2:B:640:SER:O	2:B:641:ALA:HB2	2.04	0.57
1:C:1333:PHE:O	1:C:1334:LEU:CB	2.52	0.57
1:C:161:LEU:HD11	1:C:185:PHE:CG	2.39	0.57
1:C:977:LEU:HD13	1:C:977:LEU:C	2.24	0.57
2:D:1424:ILE:HD13	2:D:1424:ILE:N	2.12	0.57
2:D:1602:THR:C	2:D:1604:ASN:H	2.07	0.57
2:D:226:VAL:HG21	2:D:320:VAL:HG11	1.87	0.57
2:D:953:ARG:CZ	2:D:959:ILE:HD11	2.35	0.57
1:A:1127:ILE:HD11	1:A:1143:TYR:HD2	1.70	0.57
1:A:1323:LEU:HD12	1:A:1324:HIS:N	2.18	0.57
1:A:1570:VAL:O	1:A:1571:GLU:HG3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:470:THR:HG22	2:B:450:THR:CG2	2.30	0.57
1:A:540:LEU:C	1:A:540:LEU:HD12	2.25	0.57
1:A:979:VAL:C	1:A:980:LYS:HG2	2.24	0.57
2:B:963:ILE:HG12	2:B:1325:ILE:HG12	1.86	0.57
2:B:793:SER:OG	2:B:801:CYS:HB3	2.04	0.57
2:B:958:GLU:O	2:B:959:ILE:HG13	2.04	0.57
1:C:1034:PHE:CE2	1:C:1041:GLU:HG2	2.40	0.57
1:C:1450:PHE:HB3	1:C:1463:GLN:O	2.04	0.57
1:C:267:ILE:HG22	1:C:268:THR:N	2.20	0.57
1:C:422:LEU:HD12	1:C:422:LEU:H	1.67	0.57
1:C:709:GLU:HB3	1:C:713:GLN:OE1	2.05	0.57
2:D:197:TRP:CB	2:D:214:PHE:CE1	2.85	0.57
1:A:830:PRO:CG	1:A:1483:PHE:HZ	2.16	0.57
1:A:469:TRP:N	1:A:469:TRP:CE3	2.73	0.57
1:A:599:TRP:HE1	1:A:779:LEU:HD13	1.69	0.57
1:A:182:ILE:CG1	1:A:804:ILE:HD11	2.34	0.57
1:A:81:ASN:CG	1:A:82:SER:H	2.09	0.57
1:A:944:LEU:HD12	1:A:1313:ILE:CD1	2.33	0.57
2:B:221:LEU:HD11	2:B:753:LYS:CG	2.31	0.57
2:B:251:TYR:CE2	2:B:257:VAL:HG22	2.39	0.57
1:C:1084:ARG:CD	1:C:1154:LYS:HE3	2.35	0.57
1:C:1352:PHE:CD2	1:C:1353:GLY:N	2.73	0.57
1:C:1617:TYR:HA	1:C:1646:GLU:O	2.04	0.57
1:C:516:GLU:OE1	1:C:516:GLU:N	2.38	0.57
1:C:39:ILE:HG21	1:C:54:ILE:HD13	1.87	0.57
2:D:263:VAL:HG13	2:D:318:VAL:HG23	1.85	0.57
2:D:953:ARG:HA	2:D:1330:ASN:O	2.04	0.57
2:D:965:ILE:HG13	2:D:1301:ARG:HB2	1.87	0.57
1:A:1421:HIS:CD2	1:A:1422:ALA:N	2.72	0.57
1:A:1560:ALA:HB3	1:A:1585:TYR:HE2	1.68	0.57
1:A:457:TYR:C	1:A:457:TYR:HD2	2.08	0.57
1:A:957:LYS:HD2	1:A:958:GLU:H	1.70	0.57
2:B:202:LYS:HG3	2:B:203:TYR:N	2.20	0.57
2:B:766:PRO:HA	2:B:771:ILE:O	2.05	0.57
2:B:825:VAL:HB	2:B:828:GLU:OE2	2.05	0.57
2:B:872:ILE:HG22	2:B:878:ARG:HG3	1.87	0.57
1:C:1166:THR:O	1:C:1170:LYS:HG2	2.05	0.57
1:C:1488:LEU:HD12	1:C:1488:LEU:O	2.05	0.57
1:C:957:LYS:HD2	1:C:958:GLU:H	1.69	0.57
1:C:985:GLY:O	1:C:986:GLU:C	2.42	0.57
2:D:756:LEU:HD22	2:D:778:PHE:CE1	2.40	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:632:LEU:N	1:A:632:LEU:HD23	2.19	0.56
1:A:934:VAL:CG2	1:A:1366:HIS:CD2	2.88	0.56
1:A:967:LEU:HD12	1:A:968:VAL:H	1.70	0.56
2:B:1399:ARG:HG2	2:B:1399:ARG:HH11	1.70	0.56
1:C:1551:THR:O	1:C:1557:ILE:HG13	2.05	0.56
1:C:442:LEU:HD23	1:C:443:PRO:CD	2.35	0.56
1:C:779:LEU:O	1:C:781:PRO:HD3	2.05	0.56
1:C:869:GLU:O	1:C:871:PRO:HD3	2.05	0.56
1:A:1081:PHE:O	1:A:1084:ARG:N	2.38	0.56
1:A:269:PHE:CG	1:A:301:PHE:CE1	2.92	0.56
1:A:501:TYR:O	1:A:501:TYR:HD1	1.88	0.56
1:A:949:ILE:O	1:A:950:TYR:CD1	2.58	0.56
2:B:1512:ILE:O	2:B:1516:CYS:HB2	2.06	0.56
2:B:745:ILE:CG2	2:B:745:ILE:O	2.53	0.56
1:C:1053:MET:HE3	1:C:1086:LEU:CD2	2.34	0.56
1:C:1232:LEU:O	1:C:1233:GLN:HB3	2.05	0.56
1:C:1377:PHE:CE1	1:C:1408:TYR:HD1	2.23	0.56
1:C:224:LEU:HD22	1:C:225:PRO:CD	2.25	0.56
1:C:539:ARG:NE	1:C:633:GLY:HA3	2.19	0.56
2:D:1426:TYR:CD2	2:D:1426:TYR:N	2.73	0.56
2:D:495:GLN:NE2	2:D:496:PRO:HD2	2.20	0.56
2:D:820:MET:CE	2:D:832:ILE:HD13	2.35	0.56
1:A:1227:PHE:CD2	1:A:1273:TRP:CE2	2.93	0.56
1:A:696:LYS:HZ3	1:A:759:PRO:HG2	1.71	0.56
1:C:1420:SER:O	1:C:1421:HIS:C	2.44	0.56
1:C:654:LEU:O	1:C:655:THR:CG2	2.53	0.56
2:D:1346:ASN:O	2:D:1368:CYS:HB2	2.05	0.56
2:D:237:ILE:HD11	2:D:309:LEU:CB	2.34	0.56
1:A:165:ASP:OD2	1:A:165:ASP:C	2.44	0.56
1:A:361:LEU:H	1:A:361:LEU:HD12	1.71	0.56
1:A:39:ILE:HG21	1:A:54:ILE:HD13	1.87	0.56
1:A:869:GLU:O	1:A:871:PRO:HD3	2.05	0.56
2:B:239:GLY:N	2:B:296:ARG:NH2	2.48	0.56
2:B:23:ALA:HB3	2:B:528:ASN:HD22	1.70	0.56
2:B:556:ILE:H	2:B:556:ILE:CD1	1.99	0.56
1:C:1150:ILE:HG22	1:C:1151:GLY:N	2.20	0.56
1:C:1431:GLY:HA2	1:C:1483:PHE:CE1	2.39	0.56
1:C:153:LYS:HB2	1:C:154:PRO:CD	2.31	0.56
1:C:1561:TYR:CE1	1:C:1581:LEU:HD21	2.40	0.56
1:C:443:PRO:HD2	1:C:446:ASN:CB	2.33	0.56
1:C:614:ARG:H	1:C:614:ARG:NE	2.03	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:77:ASN:HD22	1:C:81:ASN:HB2	1.68	0.56
1:C:87:ILE:CD1	1:C:87:ILE:N	2.64	0.56
2:D:165:PHE:CE2	2:D:199:ILE:HD11	2.39	0.56
2:D:191:LEU:HD13	2:D:960:GLU:HB3	1.87	0.56
2:D:523:TYR:CD1	2:D:523:TYR:C	2.79	0.56
2:D:804:GLU:OE1	2:D:805:PRO:HD2	2.05	0.56
2:D:961:THR:HG22	2:D:1327:THR:CG2	2.35	0.56
2:B:1573:LEU:HB3	2:B:1575:LEU:HD23	1.87	0.56
2:B:376:HIS:O	2:B:378:PRO:HD3	2.06	0.56
2:B:476:ILE:HG12	2:B:524:TYR:HD2	1.69	0.56
2:B:803:ALA:O	2:B:805:PRO:HD3	2.05	0.56
1:C:1164:ILE:O	1:C:1165:ASP:C	2.41	0.56
1:C:1479:ILE:H	1:C:1479:ILE:HD13	1.70	0.56
1:C:565:GLU:HG3	1:C:624:PHE:CB	2.35	0.56
1:C:73:LEU:H	1:C:73:LEU:HD23	1.71	0.56
1:C:803:GLY:O	1:C:810:CYS:CB	2.53	0.56
2:D:1491:ARG:HG3	2:D:1492:CYS:N	2.13	0.56
2:D:1607:ILE:H	2:D:1607:ILE:CD1	2.11	0.56
2:D:130:ILE:HB	2:D:212:ALA:HB2	1.88	0.56
2:D:477:LYS:HD3	2:D:477:LYS:N	2.20	0.56
2:D:615:GLN:HB2	2:D:616:ASN:ND2	2.20	0.56
2:D:563:MET:HG3	2:D:780:LEU:CD2	2.35	0.56
2:D:885:VAL:HG23	2:D:885:VAL:O	2.05	0.56
1:A:171:VAL:HG13	1:A:1054:LEU:HD21	1.86	0.56
1:A:1049:LEU:HD11	1:A:1089:VAL:HG13	1.88	0.56
1:A:101:TYR:HE1	1:A:116:ARG:NH2	2.03	0.56
1:A:1474:CYS:HB3	1:A:1476:ARG:HH12	1.69	0.56
1:A:249:THR:HG23	1:A:298:GLN:HE21	1.71	0.56
2:B:1387:LEU:HD12	2:B:1442:ILE:HD11	1.88	0.56
2:B:54:LEU:HD23	2:B:54:LEU:N	2.19	0.56
1:A:116:ARG:HH21	1:C:1305:LYS:CB	2.17	0.56
1:C:1641:SER:C	1:C:1643:THR:H	2.07	0.56
1:C:539:ARG:NH2	1:C:634:CYS:N	2.49	0.56
2:D:173:VAL:O	2:D:173:VAL:HG12	2.06	0.56
2:D:228:LEU:HD22	2:D:247:ILE:HG12	1.87	0.56
2:D:299:PHE:HE1	2:D:303:PHE:CD2	2.23	0.56
1:A:1053:MET:CE	1:A:1086:LEU:HD22	2.34	0.56
1:A:1403:VAL:HG22	1:A:1476:ARG:HB3	1.88	0.56
1:A:1483:PHE:O	1:A:1483:PHE:HD1	1.88	0.56
1:A:23:TYR:CD1	1:A:655:THR:HB	2.40	0.56
2:B:127:PHE:O	2:B:149:SER:HA	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1560:ALA:O	1:C:1585:TYR:HD2	1.89	0.56
1:C:535:VAL:HG23	1:C:536:PRO:CD	2.27	0.56
2:D:192:VAL:HG22	2:D:193:SER:N	2.19	0.56
2:D:236:TYR:O	2:D:238:ASP:N	2.38	0.56
2:D:582:LYS:O	2:D:583:ALA:O	2.23	0.56
1:A:455:ILE:HG22	1:A:456:ALA:N	2.21	0.56
1:A:628:GLU:HA	1:A:630:SER:OG	2.05	0.56
1:A:653:PHE:CD1	1:A:653:PHE:C	2.79	0.56
1:A:634:CYS:HA	1:A:671:GLU:OE2	2.06	0.56
1:A:690:TYR:HE1	1:A:696:LYS:CD	2.19	0.56
2:B:235:PHE:CE2	2:B:299:PHE:CE2	2.93	0.56
2:B:518:PHE:HE2	2:B:538:VAL:CB	2.19	0.56
1:C:1033:ILE:HD13	1:C:1333:PHE:HZ	1.70	0.56
1:C:1112:GLN:NE2	1:C:1171:ALA:HB2	2.20	0.56
1:C:1224:ILE:HG22	1:C:1225:TYR:CD2	2.41	0.56
1:C:1451:THR:O	1:C:1452:ASP:HB2	2.06	0.56
1:C:576:SER:CB	1:C:589:SER:H	2.18	0.56
2:D:1367:ILE:HD13	2:D:1456:VAL:HG21	1.88	0.56
2:D:541:LYS:O	2:D:543:THR:HG23	2.05	0.56
1:A:1016:VAL:HG21	1:A:1291:ILE:HD12	1.88	0.56
1:A:132:LYS:O	1:A:135:TYR:CE2	2.59	0.56
1:A:1446:VAL:O	1:A:1446:VAL:HG12	2.05	0.56
1:A:1450:PHE:HB3	1:A:1463:GLN:O	2.05	0.56
1:A:1617:TYR:HA	1:A:1646:GLU:O	2.05	0.56
2:B:1305:THR:CG2	2:B:1307:LEU:H	2.17	0.56
2:B:214:PHE:O	2:B:214:PHE:HD1	1.88	0.56
2:B:136:ILE:HA	2:B:215:ASP:O	2.04	0.56
2:B:541:LYS:O	2:B:543:THR:HG23	2.05	0.56
2:B:603:GLU:C	2:B:605:SER:H	2.09	0.56
2:B:861:THR:O	2:B:863:GLY:N	2.38	0.56
1:C:1139:GLU:OE1	1:C:1184:SER:HB3	2.05	0.56
1:C:540:LEU:HD12	1:C:540:LEU:C	2.26	0.56
1:C:827:MET:SD	1:C:843:GLY:HA3	2.46	0.56
2:D:1387:LEU:HD12	2:D:1442:ILE:HD11	1.88	0.56
2:D:501:GLN:HG2	2:D:504:VAL:HG23	1.88	0.56
1:A:1139:GLU:O	1:A:1142:LEU:N	2.38	0.56
1:A:1333:PHE:O	1:A:1334:LEU:CB	2.52	0.56
1:A:1618:LEU:HD13	1:A:1618:LEU:O	2.06	0.56
1:A:1623:GLU:HB2	1:A:1638:PRO:CG	2.35	0.56
1:A:231:ILE:HA	1:A:250:ILE:HG22	1.88	0.56
1:A:628:GLU:C	1:A:630:SER:N	2.57	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:889:GLU:O	1:A:890:GLY:O	2.24	0.56
1:A:96:GLN:HG3	1:A:97:ASN:ND2	2.20	0.56
2:B:104:VAL:HG22	2:B:105:VAL:N	2.18	0.56
2:B:1284:ARG:HG3	2:B:1285:GLU:N	2.20	0.56
2:B:1548:ILE:N	2:B:1548:ILE:HD13	2.21	0.56
2:B:173:VAL:O	2:B:173:VAL:HG12	2.06	0.56
2:B:547:THR:HG22	2:B:548:LEU:N	2.21	0.56
2:B:959:ILE:HG22	2:B:959:ILE:O	2.05	0.56
1:C:1117:SER:HB3	1:C:1174:PHE:CE2	2.41	0.56
1:C:455:ILE:HG22	1:C:456:ALA:N	2.21	0.56
1:A:1554:LYS:HE3	1:A:1556:GLU:OE1	2.06	0.56
1:A:1564:SER:HB2	1:A:1616:GLN:HG3	1.88	0.56
1:A:373:VAL:HG11	1:A:435:VAL:HG11	1.87	0.56
1:A:950:TYR:OH	1:A:1307:LEU:HD21	2.06	0.56
2:B:236:TYR:O	2:B:238:ASP:N	2.39	0.56
2:B:342:PRO:HG2	2:B:420:LEU:HD13	1.86	0.56
2:B:786:THR:OG1	2:B:809:ARG:HG3	2.06	0.56
2:B:829:GLN:HB3	2:B:1471:PHE:HE2	1.71	0.56
1:C:968:VAL:HG13	1:C:1366:HIS:O	2.06	0.56
1:C:182:ILE:CG1	1:C:804:ILE:HD11	2.33	0.56
2:D:963:ILE:CG1	2:D:1325:ILE:HG12	2.36	0.56
1:A:1264:ILE:O	1:A:1267:VAL:HB	2.06	0.55
1:A:1628:LYS:HB3	1:A:1633:PHE:CD1	2.41	0.55
1:A:161:LEU:HD11	1:A:185:PHE:CG	2.42	0.55
1:A:267:ILE:CD1	1:A:299:VAL:HG11	2.34	0.55
1:A:709:GLU:HB3	1:A:713:GLN:OE1	2.06	0.55
2:B:482:LEU:CD1	2:B:521:VAL:HB	2.34	0.55
2:B:757:TRP:O	2:B:758:LEU:HD23	2.06	0.55
2:B:756:LEU:HD22	2:B:778:PHE:CE1	2.41	0.55
1:C:1127:ILE:HD11	1:C:1143:TYR:HD2	1.70	0.55
1:C:125:PHE:CD1	1:C:627:LEU:HD21	2.41	0.55
1:C:1562:LYS:HD3	1:C:1664:LEU:HD21	1.89	0.55
1:C:1574:PHE:HA	1:C:1603:LYS:CD	2.36	0.55
1:C:906:GLY:O	1:C:908:HIS:NE2	2.39	0.55
1:C:930:VAL:HG22	1:C:931:PRO:HD2	1.88	0.55
2:D:518:PHE:HE2	2:D:538:VAL:CB	2.19	0.55
2:D:756:LEU:HD12	2:D:758:LEU:HG	1.88	0.55
2:D:885:VAL:HG23	2:D:887:LEU:HD21	1.87	0.55
1:A:862:VAL:HB	1:A:865:ILE:CD1	2.36	0.55
2:B:191:LEU:HD13	2:B:960:GLU:HB3	1.88	0.55
2:B:355:LYS:HD2	2:B:355:LYS:N	2.21	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:944:LEU:HD12	1:C:1313:ILE:CD1	2.35	0.55
1:C:1377:PHE:CD2	1:C:1495:VAL:HG22	2.41	0.55
1:C:1577:TYR:HB2	1:C:1600:PHE:O	2.06	0.55
1:C:599:TRP:HE1	1:C:779:LEU:HD13	1.71	0.55
1:C:977:LEU:HA	1:C:1361:VAL:HG13	1.86	0.55
2:D:1273:LEU:HD12	2:D:1273:LEU:C	2.27	0.55
2:D:1443:LEU:CD1	2:D:1443:LEU:N	2.69	0.55
2:D:1623:LYS:HZ3	2:D:1623:LYS:HA	1.71	0.55
2:D:322:THR:HG22	2:D:327:ASP:O	2.06	0.55
2:D:485:ASN:OD1	2:D:486:LYS:HD2	2.06	0.55
2:D:870:PHE:HB2	2:D:871:PRO:CD	2.36	0.55
1:A:1118:PHE:HD2	1:A:1148:THR:HG1	1.52	0.55
1:A:1159:CYS:O	1:A:1161:LEU:N	2.32	0.55
1:A:1549:LYS:NZ	1:A:1667:PHE:CB	2.67	0.55
1:A:267:ILE:HG22	1:A:268:THR:N	2.21	0.55
1:A:269:PHE:HB2	1:A:283:MET:HE3	1.87	0.55
1:A:422:LEU:HD12	1:A:422:LEU:N	2.20	0.55
1:A:654:LEU:O	1:A:655:THR:CG2	2.53	0.55
1:A:949:ILE:O	1:A:949:ILE:HG22	2.06	0.55
1:A:981:GLY:HA3	1:A:1333:PHE:HB2	1.87	0.55
2:B:199:ILE:O	2:B:199:ILE:HG22	2.05	0.55
2:B:322:THR:HG22	2:B:327:ASP:O	2.06	0.55
2:B:523:TYR:HB3	2:B:533:ALA:HB2	1.88	0.55
2:B:750:ASP:OD1	2:B:752:PRO:HD3	2.06	0.55
1:C:1139:GLU:O	1:C:1142:LEU:N	2.40	0.55
1:C:1487:PHE:HD2	1:C:1487:PHE:N	2.04	0.55
1:C:1562:LYS:C	1:C:1563:VAL:HG13	2.26	0.55
1:C:1562:LYS:HD2	1:C:1582:LEU:HD11	1.88	0.55
1:C:1622:LYS:NZ	1:C:1642:LEU:HB3	2.21	0.55
1:C:221:GLU:HG2	1:C:222:TYR:O	2.07	0.55
1:C:250:ILE:HD11	1:C:265:VAL:CG1	2.31	0.55
1:C:371:ILE:O	1:C:371:ILE:HG22	2.07	0.55
1:C:457:TYR:C	1:C:457:TYR:CD2	2.79	0.55
1:C:59:TYR:CG	1:C:60:PRO:HD3	2.41	0.55
1:C:653:PHE:HD1	1:C:653:PHE:C	2.09	0.55
2:D:315:TYR:CD1	2:D:315:TYR:C	2.78	0.55
1:A:1186:PHE:HA	1:A:1250:THR:HG22	1.87	0.55
1:A:1622:LYS:HZ2	1:A:1642:LEU:HD13	1.72	0.55
1:A:25:ILE:HB	1:A:654:LEU:O	2.06	0.55
1:A:936:ARG:HH11	1:A:936:ARG:CG	2.17	0.55
1:A:942:VAL:HG11	1:A:957:LYS:CB	2.36	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1447:GLU:HG3	2:B:1447:GLU:O	2.06	0.55
2:B:469:ASN:ND2	2:B:469:ASN:C	2.57	0.55
2:B:850:LEU:HD13	2:B:882:PHE:CD1	2.42	0.55
1:C:1129:LEU:N	1:C:1129:LEU:HD23	2.18	0.55
1:C:1323:LEU:HD12	1:C:1324:HIS:N	2.19	0.55
1:C:560:TRP:CH2	1:C:562:ASN:HB2	2.42	0.55
1:C:919:GLY:HA2	2:D:813:VAL:HG11	1.88	0.55
2:D:529:ASN:O	2:D:529:ASN:OD1	2.24	0.55
1:A:1133:LEU:HD12	1:A:1133:LEU:H	1.72	0.55
1:A:599:TRP:CD1	1:A:779:LEU:HA	2.42	0.55
1:A:938:SER:C	1:A:940:SER:N	2.57	0.55
1:A:976:ILE:HB	1:A:1362:THR:CG2	2.36	0.55
2:B:219:TYR:O	2:B:220:VAL:HG13	2.07	0.55
2:B:756:LEU:HD12	2:B:758:LEU:HG	1.89	0.55
2:B:820:MET:CE	2:B:832:ILE:HD13	2.36	0.55
2:B:918:GLU:OE2	2:B:918:GLU:N	2.39	0.55
1:C:634:CYS:HA	1:C:671:GLU:OE2	2.05	0.55
1:C:653:PHE:CD1	1:C:653:PHE:C	2.80	0.55
1:C:690:TYR:HE1	1:C:696:LYS:CD	2.20	0.55
1:C:938:SER:C	1:C:940:SER:N	2.60	0.55
2:D:1386:MET:HE2	2:D:1472:TYR:OH	2.06	0.55
2:D:339:VAL:HG23	2:D:341:SER:N	2.20	0.55
2:D:603:GLU:C	2:D:605:SER:H	2.10	0.55
2:D:88:GLU:CD	2:D:155:SER:HB2	2.27	0.55
1:A:1019:PHE:CD2	1:A:1020:TYR:N	2.75	0.55
1:A:1488:LEU:O	1:A:1488:LEU:HD12	2.07	0.55
1:A:560:TRP:CE3	1:A:673:LEU:HD22	2.42	0.55
1:A:73:LEU:H	1:A:73:LEU:HD23	1.71	0.55
1:A:984:VAL:HG22	1:A:987:ILE:HD12	1.88	0.55
2:B:384:PHE:CE1	2:B:400:LEU:HG	2.41	0.55
2:B:518:PHE:O	2:B:518:PHE:HD2	1.90	0.55
1:C:1227:PHE:HD2	1:C:1273:TRP:CE2	2.24	0.55
1:C:144:ARG:HD2	1:C:146:TYR:HE1	1.67	0.55
1:C:1403:VAL:HG22	1:C:1476:ARG:HB3	1.89	0.55
1:C:376:LYS:HA	1:C:381:GLN:O	2.05	0.55
1:A:1317:TYR:HD2	1:A:1344:ASP:HB3	1.72	0.55
1:A:1420:SER:O	1:A:1421:HIS:C	2.45	0.55
1:A:54:ILE:HG12	1:A:106:VAL:HG13	1.88	0.55
1:A:127:PHE:CE2	1:A:623:VAL:HG13	2.32	0.55
2:B:216:VAL:O	2:B:216:VAL:CG1	2.54	0.55
2:B:315:TYR:HD1	2:B:315:TYR:O	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:35:THR:HB	2:B:91:ALA:HB2	1.87	0.55
1:C:1507:MET:HG3	1:C:1508:PHE:O	2.07	0.55
1:C:430:VAL:HG22	1:C:455:ILE:HG23	1.88	0.55
1:C:752:LEU:HD12	1:C:752:LEU:C	2.25	0.55
1:C:791:PRO:HG3	1:C:797:TRP:HE1	1.71	0.55
2:D:1528:LEU:HD21	2:D:1531:ILE:HD11	1.89	0.55
2:D:219:TYR:O	2:D:220:VAL:HG13	2.07	0.55
2:D:482:LEU:CD1	2:D:521:VAL:HB	2.36	0.55
2:D:850:LEU:HD13	2:D:882:PHE:CD1	2.42	0.55
2:D:953:ARG:HG2	2:D:954:VAL:H	1.71	0.55
1:A:1549:LYS:HZ2	1:A:1667:PHE:HB3	1.72	0.55
1:A:523:TYR:CE1	2:B:359:PRO:HG2	2.41	0.55
1:A:550:GLN:HG2	1:A:550:GLN:O	2.05	0.55
1:A:539:ARG:NE	1:A:633:GLY:HA3	2.21	0.55
1:A:653:PHE:C	1:A:653:PHE:HD1	2.08	0.55
1:A:862:VAL:HB	1:A:865:ILE:HD11	1.89	0.55
1:A:993:SER:C	1:A:995:GLU:H	2.10	0.55
2:B:963:ILE:CG1	2:B:1325:ILE:HG12	2.37	0.55
1:C:1003:LEU:HD23	1:C:1003:LEU:N	2.22	0.55
1:C:1044:LYS:O	1:C:1047:LYS:HB3	2.07	0.55
1:C:1421:HIS:CD2	1:C:1421:HIS:C	2.78	0.55
1:C:700:TYR:HD2	1:C:701:ASP:N	2.05	0.55
2:D:296:ARG:HG3	2:D:296:ARG:NH1	2.21	0.55
2:D:235:PHE:CE2	2:D:299:PHE:CE2	2.94	0.55
2:D:793:SER:OG	2:D:801:CYS:HB3	2.05	0.55
1:A:1162:VAL:HG22	1:C:1102:ASN:HD22	1.67	0.55
1:A:1431:GLY:HA2	1:A:1483:PHE:CE1	2.41	0.55
1:A:803:GLY:O	1:A:810:CYS:CB	2.55	0.55
2:B:384:PHE:CD1	2:B:400:LEU:HG	2.41	0.55
1:C:296:ILE:HG23	1:C:297:ALA:N	2.21	0.55
1:C:433:PHE:CE1	1:C:452:TYR:HB2	2.42	0.55
1:C:489:LYS:CG	1:C:490:SER:H	2.20	0.55
1:C:115:LYS:CE	1:C:654:LEU:HD11	2.37	0.55
1:C:599:TRP:CD1	1:C:779:LEU:HA	2.42	0.55
2:D:1600:ILE:O	2:D:1602:THR:HG23	2.05	0.55
2:D:476:ILE:HD11	2:D:524:TYR:HB2	1.89	0.55
1:A:1003:LEU:N	1:A:1003:LEU:HD23	2.22	0.55
1:A:1053:MET:HE3	1:A:1086:LEU:HD22	1.89	0.55
1:A:1090:ASN:C	1:A:1092:TYR:H	2.11	0.55
1:A:1252:ALA:O	1:A:1253:TYR:C	2.46	0.55
1:A:331:GLU:HG2	1:A:333:THR:HG23	1.88	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:471:ASP:OD2	1:A:474:LYS:HD2	2.07	0.55
1:A:700:TYR:HD2	1:A:701:ASP:N	2.06	0.55
1:A:977:LEU:C	1:A:977:LEU:HD13	2.27	0.55
2:B:138:THR:O	2:B:139:PRO:C	2.44	0.55
1:C:1090:ASN:C	1:C:1092:TYR:H	2.11	0.55
1:C:1180:LEU:CD2	1:C:1208:ILE:HG12	2.37	0.55
1:C:1268:ASN:N	1:C:1269:PRO:CD	2.70	0.55
1:C:272:ARG:O	1:C:321:LYS:HB2	2.07	0.55
1:C:975:ARG:HG3	1:C:1340:VAL:HB	1.89	0.55
2:D:945:ILE:HD13	2:D:1311:ILE:HB	1.89	0.55
2:D:1447:GLU:HG3	2:D:1447:GLU:O	2.07	0.55
2:D:582:LYS:O	2:D:583:ALA:C	2.45	0.55
2:D:750:ASP:OD1	2:D:752:PRO:HD3	2.07	0.55
2:D:748:ARG:HH12	2:D:784:ILE:HG12	1.72	0.55
1:A:1429:PRO:HB2	1:A:1432:ILE:CG1	2.37	0.54
1:A:221:GLU:HG2	1:A:222:TYR:O	2.07	0.54
1:A:433:PHE:HD1	1:A:433:PHE:N	2.05	0.54
1:A:499:TYR:HE2	1:A:517:LYS:HG3	1.72	0.54
1:A:706:ASN:ND2	1:A:709:GLU:H	2.05	0.54
2:B:762:LEU:HD12	2:B:762:LEU:H	1.71	0.54
2:B:834:ALA:O	2:B:835:ILE:HD13	2.07	0.54
1:C:1164:ILE:O	1:C:1167:ALA:N	2.40	0.54
1:C:136:THR:O	1:C:139:GLN:HB2	2.08	0.54
1:C:238:ILE:HG23	1:C:242:ASN:ND2	2.18	0.54
1:C:457:TYR:C	1:C:457:TYR:HD2	2.09	0.54
1:C:979:VAL:C	1:C:980:LYS:HG2	2.28	0.54
2:D:239:GLY:N	2:D:296:ARG:NH2	2.48	0.54
2:D:574:ARG:HG2	2:D:794:PHE:HB3	1.88	0.54
2:D:849:GLU:OE2	2:D:865:ARG:HD2	2.06	0.54
2:D:891:LEU:CB	2:D:912:LYS:HD3	2.36	0.54
2:D:916:VAL:HG22	2:D:917:PRO:N	2.21	0.54
1:A:1045:LEU:O	1:A:1046:LYS:C	2.45	0.54
1:A:1049:LEU:HD11	1:A:1089:VAL:CG1	2.37	0.54
1:A:1304:VAL:CG1	1:A:1305:LYS:N	2.70	0.54
1:A:1560:ALA:O	1:A:1585:TYR:CD2	2.61	0.54
1:A:1561:TYR:CE1	1:A:1581:LEU:HD21	2.41	0.54
1:A:523:TYR:OH	2:B:359:PRO:HD2	2.06	0.54
1:A:59:TYR:CG	1:A:60:PRO:HD3	2.42	0.54
1:A:791:PRO:HG3	1:A:797:TRP:HE1	1.71	0.54
1:A:805:SER:O	1:A:807:THR:N	2.40	0.54
1:C:1019:PHE:HD2	1:C:1020:TYR:N	2.05	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:331:GLU:HG2	1:C:333:THR:HG23	1.88	0.54
1:C:573:VAL:HG12	1:C:592:MET:HG2	1.88	0.54
1:C:692:HIS:HA	1:C:696:LYS:HD3	1.88	0.54
1:C:993:SER:C	1:C:995:GLU:H	2.11	0.54
2:D:1288:ILE:CD1	2:D:1303:VAL:HG21	2.37	0.54
2:D:1623:LYS:HB3	2:D:1623:LYS:NZ	2.22	0.54
2:D:28:ILE:HG12	2:D:628:LEU:HD13	1.88	0.54
2:D:850:LEU:CG	2:D:851:LEU:N	2.69	0.54
1:A:1190:ILE:HG12	1:A:1253:TYR:CE1	2.42	0.54
1:A:1440:LYS:HD3	1:A:1453:TYR:OH	2.07	0.54
1:A:177:ILE:HG22	1:A:178:ASP:H	1.72	0.54
1:A:60:PRO:CD	1:A:61:ASP:N	2.66	0.54
1:A:970:LYS:O	1:A:971:THR:CG2	2.56	0.54
2:B:1371:TYR:CG	2:B:1377:SER:HB3	2.42	0.54
2:B:1528:LEU:HD13	2:B:1542:MET:CE	2.37	0.54
2:B:302:ARG:HG3	2:B:303:PHE:CD1	2.42	0.54
1:C:864:GLY:HA3	1:C:907:LEU:CD2	2.36	0.54
1:C:888:VAL:CG2	1:C:894:HIS:HB2	2.33	0.54
2:D:1390:PHE:O	2:D:1391:LEU:HD23	2.07	0.54
2:D:816:ILE:HD13	2:D:896:ILE:HG22	1.89	0.54
1:C:1049:LEU:HD11	1:C:1089:VAL:HG13	1.89	0.54
1:C:961:TYR:CE2	1:C:1343:ASN:HA	2.43	0.54
1:C:371:ILE:CG2	1:C:420:PHE:HB2	2.37	0.54
1:A:1084:ARG:CD	1:A:1154:LYS:HE3	2.38	0.54
1:A:1451:THR:O	1:A:1452:ASP:HB2	2.08	0.54
1:A:565:GLU:HG3	1:A:624:PHE:CB	2.37	0.54
2:B:88:GLU:OE1	2:B:155:SER:HB2	2.07	0.54
2:B:481:TYR:CE1	2:B:506:MET:SD	2.94	0.54
1:C:156:LYS:HD2	1:C:156:LYS:C	2.27	0.54
2:D:1475:ASP:N	2:D:1475:ASP:OD1	2.25	0.54
2:D:598:ILE:HD11	2:D:800:ILE:HG21	1.90	0.54
1:A:1106:TRP:HE3	1:A:1107:LEU:HD13	1.73	0.54
1:A:1129:LEU:HD23	1:A:1129:LEU:N	2.22	0.54
1:A:309:GLU:O	1:A:312:TYR:N	2.39	0.54
1:A:443:PRO:HD2	1:A:446:ASN:CB	2.36	0.54
2:B:1288:ILE:CD1	2:B:1303:VAL:HG21	2.38	0.54
2:B:1390:PHE:O	2:B:1391:LEU:HD23	2.08	0.54
2:B:1482:ASN:HB3	2:B:1493:ALA:HB3	1.89	0.54
1:C:1023:HIS:CE1	1:C:1302:LEU:HD11	2.43	0.54
1:C:1127:ILE:HD12	1:C:1127:ILE:N	2.14	0.54
1:C:286:ALA:O	1:C:287:MET:C	2.46	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:947:ARG:O	1:C:949:ILE:HG12	2.07	0.54
1:A:1139:GLU:O	1:A:1140:ASN:C	2.45	0.54
1:A:1227:PHE:HB2	1:A:1251:THR:HG21	1.90	0.54
1:A:1283:GLY:HA3	1:A:1290:THR:HG23	1.88	0.54
1:A:955:ARG:CG	1:A:1350:THR:HG23	2.35	0.54
1:A:1582:LEU:HD12	1:A:1583:ASP:H	1.72	0.54
1:A:174:VAL:CG2	1:A:175:GLU:H	2.17	0.54
2:B:401:ASN:C	2:B:402:ILE:HD13	2.28	0.54
2:B:481:TYR:CE2	2:B:493:GLY:CA	2.89	0.54
1:C:1554:LYS:HE3	1:C:1556:GLU:OE1	2.08	0.54
1:C:1534:GLN:HA	1:C:1608:ASN:HD22	1.73	0.54
1:C:967:LEU:HD12	1:C:968:VAL:H	1.72	0.54
1:C:981:GLY:HA3	1:C:1333:PHE:HB2	1.89	0.54
2:D:322:THR:HG21	2:D:326:SER:HG	1.73	0.54
1:A:1093:VAL:O	1:A:1093:VAL:HG12	2.08	0.54
1:A:133:PRO:HD2	1:A:609:VAL:CG1	2.37	0.54
1:A:639:GLY:H	1:A:645:VAL:HG22	1.73	0.54
2:B:558:MET:HE3	2:B:559:PRO:HD2	1.89	0.54
2:B:965:ILE:HG22	2:B:1323:MET:HB2	1.90	0.54
1:C:1093:VAL:O	1:C:1093:VAL:HG12	2.07	0.54
1:C:1317:TYR:CD2	1:C:1344:ASP:HB3	2.43	0.54
1:C:174:VAL:CG2	1:C:175:GLU:H	2.16	0.54
2:D:142:PRO:HB3	2:D:187:ASN:ND2	2.23	0.54
2:D:88:GLU:OE1	2:D:155:SER:HB2	2.07	0.54
1:A:1033:ILE:CG2	1:A:1034:PHE:CD1	2.91	0.54
1:A:1562:LYS:HD2	1:A:1582:LEU:HD11	1.89	0.54
1:A:371:ILE:HD13	1:A:390:LEU:HD21	1.90	0.54
1:A:483:ASN:ND2	2:B:399:ILE:HB	2.22	0.54
1:A:495:LYS:HE2	1:A:495:LYS:CA	2.38	0.54
1:A:576:SER:CB	1:A:589:SER:H	2.20	0.54
2:B:1284:ARG:HD2	2:B:1285:GLU:N	2.22	0.54
2:B:1623:LYS:HB3	2:B:1623:LYS:NZ	2.23	0.54
2:B:495:GLN:NE2	2:B:496:PRO:HD2	2.23	0.54
2:B:800:ILE:CG2	2:B:801:CYS:N	2.69	0.54
1:A:1163:LYS:NZ	1:C:1109:GLU:HG2	2.23	0.54
1:C:1213:LYS:HG2	1:C:1266:TYR:CE2	2.41	0.54
1:C:1429:PRO:HB2	1:C:1432:ILE:CG1	2.37	0.54
1:C:1560:ALA:HB3	1:C:1585:TYR:HE2	1.72	0.54
1:C:373:VAL:HG11	1:C:435:VAL:HG11	1.88	0.54
1:C:365:PRO:HD2	1:C:464:TYR:CE2	2.42	0.54
1:C:974:LYS:O	1:C:1364:VAL:HG12	2.08	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:129:PHE:HE2	2:D:598:ILE:HG23	1.70	0.54
2:D:519:ARG:NH1	2:D:606:ASP:OD2	2.40	0.54
1:A:1066:TYR:CD1	1:A:1066:TYR:N	2.74	0.54
1:A:1164:ILE:O	1:A:1167:ALA:N	2.41	0.54
1:A:1573:VAL:C	1:A:1603:LYS:HD2	2.27	0.54
1:A:678:THR:HG21	1:A:742:ILE:HB	1.90	0.54
1:A:934:VAL:CG1	1:A:935:LYS:N	2.71	0.54
2:B:1273:LEU:HD12	2:B:1273:LEU:C	2.29	0.54
2:B:501:GLN:CG	2:B:504:VAL:HG23	2.38	0.54
2:B:829:GLN:CG	2:B:1480:LEU:HD13	2.38	0.54
2:B:814:PHE:CZ	2:B:846:VAL:HG21	2.43	0.54
1:C:1008:ALA:O	1:C:1011:GLU:N	2.40	0.54
1:C:1013:MET:SD	1:C:1016:VAL:HG21	2.48	0.54
1:C:1068:VAL:HG13	1:C:1069:TRP:N	2.23	0.54
1:C:1493:PHE:CD1	1:C:1493:PHE:C	2.79	0.54
1:C:576:SER:HB2	1:C:589:SER:N	2.21	0.54
2:D:1284:ARG:HD2	2:D:1285:GLU:N	2.22	0.54
2:D:1623:LYS:NZ	2:D:1623:LYS:CB	2.71	0.54
2:D:353:TYR:HA	2:D:433:ILE:O	2.07	0.54
1:A:961:TYR:CE2	1:A:1343:ASN:HA	2.43	0.53
1:A:1493:PHE:CD1	1:A:1493:PHE:C	2.79	0.53
1:A:1622:LYS:NZ	1:A:1642:LEU:HB3	2.23	0.53
1:A:1629:TYR:O	1:A:1630:ASN:HB2	2.07	0.53
1:A:24:VAL:O	1:A:24:VAL:HG12	2.08	0.53
1:A:228:SER:HB3	1:A:253:ARG:HG2	1.90	0.53
1:A:115:LYS:CE	1:A:654:LEU:HD11	2.38	0.53
1:A:582:TYR:CE2	1:A:817:ALA:HB1	2.43	0.53
1:A:854:GLN:H	1:A:854:GLN:CD	2.11	0.53
2:B:296:ARG:NH1	2:B:296:ARG:HG3	2.24	0.53
2:B:462:VAL:CG1	2:B:506:MET:HE2	2.38	0.53
1:C:1565:ILE:HB	1:C:1614:GLY:H	1.73	0.53
1:C:1582:LEU:HD12	1:C:1583:ASP:H	1.72	0.53
1:C:222:TYR:HD2	1:C:223:VAL:N	2.05	0.53
2:D:138:THR:O	2:D:139:PRO:C	2.43	0.53
2:D:262:PHE:CD1	2:D:282:ARG:HG3	2.43	0.53
2:D:27:LEU:HD13	2:D:43:VAL:HG23	1.90	0.53
1:A:1008:ALA:O	1:A:1011:GLU:N	2.40	0.53
1:A:1110:ASN:O	1:A:1111:TYR:CG	2.62	0.53
1:A:1268:ASN:H	1:A:1268:ASN:ND2	2.05	0.53
1:A:1268:ASN:N	1:A:1269:PRO:CD	2.71	0.53
1:A:1565:ILE:HB	1:A:1614:GLY:H	1.72	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:698:CYS:C	1:A:700:TYR:H	2.12	0.53
1:A:825:LEU:HD12	1:A:844:THR:O	2.08	0.53
1:C:371:ILE:HD13	1:C:390:LEU:HD21	1.90	0.53
1:C:502:LEU:HB2	1:C:541:LEU:CD2	2.39	0.53
1:C:606:ASP:O	1:C:609:VAL:HG23	2.08	0.53
1:C:823:VAL:HG23	1:C:846:TYR:O	2.08	0.53
2:D:829:GLN:HB3	2:D:1471:PHE:HE2	1.74	0.53
2:D:829:GLN:CG	2:D:1480:LEU:HD13	2.38	0.53
2:D:866:TYR:CD2	2:D:866:TYR:C	2.82	0.53
1:C:875:HIS:CB	2:D:901:GLN:NE2	2.72	0.53
1:A:1352:PHE:CD2	1:A:1353:GLY:N	2.76	0.53
1:A:1619:ILE:HG12	1:A:1645:ILE:CD1	2.38	0.53
1:A:177:ILE:HG22	1:A:178:ASP:N	2.22	0.53
1:A:827:MET:SD	1:A:843:GLY:HA3	2.48	0.53
1:A:969:PRO:HG3	1:A:1601:ILE:CD1	2.37	0.53
2:B:806:TYR:C	2:B:806:TYR:CD1	2.81	0.53
2:B:850:LEU:CG	2:B:851:LEU:N	2.70	0.53
1:C:1106:TRP:HE3	1:C:1107:LEU:HD13	1.72	0.53
1:C:1475:VAL:CG2	1:C:1476:ARG:N	2.71	0.53
1:C:422:LEU:HD12	1:C:422:LEU:N	2.22	0.53
1:C:471:ASP:OD2	1:C:474:LYS:HD2	2.08	0.53
2:D:1292:ILE:HD11	2:D:1301:ARG:HE	1.74	0.53
2:D:184:TRP:HB2	2:D:185:PRO:CD	2.39	0.53
1:C:483:ASN:ND2	2:D:399:ILE:HB	2.24	0.53
2:D:556:ILE:H	2:D:556:ILE:CD1	1.98	0.53
2:D:830:VAL:CG2	2:D:831:GLU:N	2.71	0.53
1:A:1244:THR:HG22	1:A:1246:ARG:N	2.23	0.53
1:A:1548:ARG:HH21	1:A:1550:GLN:HE22	1.56	0.53
1:A:371:ILE:HD11	1:A:433:PHE:CD2	2.44	0.53
1:A:906:GLY:O	1:A:908:HIS:NE2	2.41	0.53
1:C:1548:ARG:HH21	1:C:1550:GLN:HE22	1.56	0.53
1:C:269:PHE:HB2	1:C:283:MET:HE3	1.90	0.53
1:C:889:GLU:O	1:C:890:GLY:O	2.27	0.53
1:C:961:TYR:HD1	1:C:961:TYR:O	1.92	0.53
2:D:547:THR:HG22	2:D:548:LEU:N	2.24	0.53
2:D:563:MET:HA	2:D:563:MET:CE	2.38	0.53
1:A:931:PRO:CB	1:A:1366:HIS:CD2	2.91	0.53
2:B:130:ILE:HA	2:B:147:VAL:HG23	1.91	0.53
2:B:261:ALA:CB	2:B:285:ILE:HD11	2.39	0.53
2:B:342:PRO:HB2	2:B:343:TYR:CD1	2.43	0.53
2:B:574:ARG:HG2	2:B:794:PHE:HB3	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:820:MET:HE2	2:B:832:ILE:HD13	1.88	0.53
1:C:1304:VAL:CG1	1:C:1305:LYS:N	2.71	0.53
1:C:1565:ILE:HG22	1:C:1566:THR:H	1.72	0.53
1:C:942:VAL:HG11	1:C:957:LYS:CB	2.38	0.53
2:D:25:TYR:CE2	2:D:113:VAL:HG22	2.43	0.53
2:D:646:GLN:CB	2:D:647:PRO:HD2	2.32	0.53
1:A:1226:ARG:O	1:A:1270:VAL:HG22	2.09	0.53
1:A:1577:TYR:HB2	1:A:1600:PHE:O	2.09	0.53
1:A:433:PHE:N	1:A:433:PHE:CD1	2.75	0.53
1:A:442:LEU:HD23	1:A:443:PRO:CD	2.39	0.53
1:A:678:THR:CG2	1:A:742:ILE:HB	2.39	0.53
2:B:1273:LEU:HD12	2:B:1273:LEU:O	2.09	0.53
2:B:1330:ASN:ND2	2:B:1330:ASN:N	2.56	0.53
2:B:1371:TYR:CD1	2:B:1377:SER:HB3	2.43	0.53
2:B:1482:ASN:H	2:B:1495:GLU:HG2	1.74	0.53
2:B:1609:ARG:NH1	2:B:1609:ARG:CG	2.63	0.53
2:B:315:TYR:C	2:B:315:TYR:HD1	2.12	0.53
1:C:1081:PHE:O	1:C:1084:ARG:N	2.42	0.53
1:C:1533:GLY:O	1:C:1534:GLN:CB	2.56	0.53
1:C:1563:VAL:HG22	1:C:1617:TYR:O	2.08	0.53
1:C:185:PHE:HD1	1:C:186:PRO:HD2	1.74	0.53
1:C:433:PHE:N	1:C:433:PHE:HD1	2.07	0.53
1:C:857:VAL:CG2	1:C:884:VAL:HG21	2.37	0.53
2:D:315:TYR:HD1	2:D:315:TYR:O	1.91	0.53
2:D:481:TYR:CE2	2:D:493:GLY:CA	2.90	0.53
1:A:115:LYS:HB2	1:A:654:LEU:CD1	2.38	0.53
2:B:1284:ARG:HG3	2:B:1286:VAL:N	2.21	0.53
2:B:1528:LEU:HD13	2:B:1542:MET:HE2	1.91	0.53
2:B:1621:PHE:O	2:B:1622:GLN:C	2.47	0.53
2:B:819:GLN:HE21	2:B:819:GLN:HA	1.74	0.53
2:B:88:GLU:CD	2:B:155:SER:HB2	2.29	0.53
1:C:1112:GLN:HB2	1:C:1118:PHE:HE1	1.73	0.53
1:C:1244:THR:HG22	1:C:1246:ARG:N	2.23	0.53
1:C:1279:ARG:NH1	1:C:1280:TYR:CE2	2.77	0.53
1:C:1300:TYR:C	1:C:1300:TYR:CD2	2.82	0.53
1:C:1629:TYR:O	1:C:1630:ASN:HB2	2.09	0.53
1:C:473:HIS:HE1	2:D:455:LYS:NZ	2.07	0.53
2:D:789:VAL:C	2:D:790:LEU:HD12	2.28	0.53
1:A:191:PRO:O	1:A:194:PRO:HD3	2.08	0.53
2:B:105:VAL:HG12	2:B:118:VAL:HA	1.91	0.53
2:B:1446:PHE:CD2	2:B:1448:VAL:HG22	2.44	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:224:PHE:CZ	2:B:329:VAL:HG13	2.44	0.53
2:B:415:THR:O	2:B:425:GLN:NE2	2.42	0.53
1:C:1573:VAL:C	1:C:1603:LYS:HD2	2.29	0.53
1:C:1628:LYS:HB3	1:C:1633:PHE:HD1	1.74	0.53
1:C:25:ILE:HD13	1:C:41:ILE:HB	1.90	0.53
1:C:847:ASN:HD22	1:C:888:VAL:HG13	1.72	0.53
2:D:1301:ARG:HB3	2:D:1301:ARG:HH11	1.74	0.53
2:D:1590:LEU:CD2	2:D:1591:LEU:H	2.09	0.53
2:D:523:TYR:HB3	2:D:533:ALA:HB2	1.91	0.53
2:D:819:GLN:HE21	2:D:819:GLN:HA	1.72	0.53
1:A:1411:SER:H	1:A:1414:GLU:HG3	1.73	0.53
1:A:423:ASN:HB3	2:B:501:GLN:HE22	1.73	0.53
1:A:461:SER:O	1:A:462:GLN:HB2	2.07	0.53
1:A:463:SER:HB3	1:A:491:PRO:HA	1.91	0.53
1:A:125:PHE:CE1	1:A:627:LEU:HD21	2.43	0.53
1:A:970:LYS:C	1:A:971:THR:HG23	2.29	0.53
2:B:224:PHE:CE2	2:B:329:VAL:HG13	2.44	0.53
1:C:1268:ASN:H	1:C:1268:ASN:ND2	2.06	0.53
1:C:495:LYS:CA	1:C:495:LYS:HE2	2.38	0.53
2:D:1305:THR:CG2	2:D:1307:LEU:H	2.20	0.53
2:D:342:PRO:HB2	2:D:343:TYR:CD1	2.43	0.53
2:D:841:ASN:O	2:D:842:GLU:C	2.47	0.53
1:A:1139:GLU:OE1	1:A:1184:SER:HB3	2.09	0.53
1:A:1190:ILE:HG12	1:A:1253:TYR:CD1	2.44	0.53
1:A:371:ILE:CG2	1:A:420:PHE:HB2	2.39	0.53
1:A:520:ASP:N	1:A:520:ASP:OD1	2.41	0.53
1:A:573:VAL:CG1	1:A:592:MET:HG2	2.39	0.53
1:A:576:SER:HB2	1:A:589:SER:N	2.22	0.53
2:B:1456:VAL:HG12	2:B:1456:VAL:O	2.09	0.53
2:B:248:THR:HG22	2:B:289:ASP:OD1	2.09	0.53
2:B:646:GLN:CB	2:B:647:PRO:HD2	2.30	0.53
1:C:1183:GLN:NE2	1:C:1232:LEU:HD22	2.23	0.53
1:C:1264:ILE:O	1:C:1267:VAL:HB	2.09	0.53
1:C:433:PHE:N	1:C:433:PHE:CD1	2.77	0.53
1:C:824:PHE:CE2	1:C:846:TYR:HD1	2.27	0.53
1:C:855:PHE:CD1	1:C:855:PHE:C	2.83	0.53
2:D:1284:ARG:NE	2:D:1285:GLU:H	2.07	0.53
1:A:1191:SER:O	1:A:1194:ALA:HB3	2.08	0.52
1:A:1307:LEU:N	1:A:1307:LEU:HD22	2.24	0.52
1:A:1551:THR:O	1:A:1557:ILE:HG13	2.08	0.52
1:A:1562:LYS:C	1:A:1563:VAL:HG13	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:516:GLU:OE1	1:A:516:GLU:N	2.42	0.52
1:A:598:SER:O	1:A:599:TRP:HD1	1.91	0.52
1:A:706:ASN:HB2	1:A:714:ARG:NH1	2.24	0.52
1:A:779:LEU:O	1:A:781:PRO:HD3	2.09	0.52
2:B:131:GLN:OE1	2:B:146:ARG:NH1	2.41	0.52
2:B:159:LYS:HD3	2:B:180:LEU:HD12	1.91	0.52
2:B:228:LEU:HD22	2:B:247:ILE:HG12	1.91	0.52
1:C:1066:TYR:CD1	1:C:1066:TYR:N	2.75	0.52
1:C:224:LEU:CD2	1:C:225:PRO:HD2	2.28	0.52
1:C:309:GLU:O	1:C:312:TYR:N	2.41	0.52
1:C:308:LYS:HB3	1:C:309:GLU:OE1	2.09	0.52
1:C:23:TYR:CE1	1:C:655:THR:HB	2.43	0.52
1:C:678:THR:HG21	1:C:742:ILE:HB	1.91	0.52
1:C:825:LEU:HD12	1:C:844:THR:O	2.08	0.52
2:D:107:GLN:HG3	2:D:116:GLU:HG3	1.91	0.52
2:D:844:ILE:O	2:D:871:PRO:HA	2.09	0.52
1:A:1022:PHE:O	1:A:1024:TYR:N	2.42	0.52
1:A:1159:CYS:N	1:A:1160:PRO:CD	2.73	0.52
1:A:1562:LYS:HD3	1:A:1648:TRP:HE1	1.74	0.52
1:A:185:PHE:HD1	1:A:186:PRO:HD2	1.73	0.52
1:A:23:TYR:CE1	1:A:655:THR:HB	2.43	0.52
1:A:371:ILE:O	1:A:371:ILE:HG22	2.08	0.52
1:A:433:PHE:CE1	1:A:452:TYR:HB2	2.45	0.52
1:A:535:VAL:HG23	1:A:536:PRO:CD	2.28	0.52
1:A:54:ILE:O	1:A:68:SER:HA	2.09	0.52
1:A:903:LEU:N	1:A:903:LEU:HD22	2.24	0.52
1:A:998:ASN:HB3	1:A:1000:LEU:HG	1.89	0.52
2:B:1443:LEU:CD1	2:B:1443:LEU:N	2.72	0.52
2:B:598:ILE:HD11	2:B:800:ILE:HG21	1.91	0.52
2:B:804:GLU:OE1	2:B:805:PRO:HD2	2.10	0.52
1:C:1268:ASN:HB2	1:C:1269:PRO:HD3	1.91	0.52
1:C:1411:SER:H	1:C:1414:GLU:HG3	1.73	0.52
1:C:1571:GLU:O	1:C:1574:PHE:CD2	2.62	0.52
1:C:501:TYR:HD1	1:C:501:TYR:O	1.91	0.52
1:C:970:LYS:O	1:C:971:THR:CG2	2.57	0.52
2:D:1457:LYS:HG2	2:D:1469:THR:HG1	1.73	0.52
2:D:813:VAL:HG12	2:D:839:TYR:O	2.09	0.52
1:A:1068:VAL:HG21	1:A:1124:TYR:HD1	1.73	0.52
1:A:165:ASP:HB2	1:A:166:PRO:HD2	1.91	0.52
1:A:491:PRO:CG	1:A:494:ASP:CB	2.88	0.52
1:A:824:PHE:CE2	1:A:846:TYR:HD1	2.28	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:840:GLN:NE2	1:A:897:THR:HG21	2.24	0.52
1:A:938:SER:O	1:A:940:SER:N	2.43	0.52
2:B:1527:LYS:HE2	2:B:1578:ASN:OD1	2.09	0.52
2:B:262:PHE:CD1	2:B:282:ARG:HG3	2.44	0.52
2:B:582:LYS:O	2:B:583:ALA:C	2.46	0.52
2:B:813:VAL:HG12	2:B:839:TYR:O	2.08	0.52
2:B:841:ASN:O	2:B:842:GLU:C	2.48	0.52
1:C:1493:PHE:CD1	1:C:1494:THR:N	2.76	0.52
1:C:165:ASP:C	1:C:165:ASP:OD2	2.47	0.52
1:C:307:VAL:O	1:C:308:LYS:O	2.27	0.52
1:C:961:TYR:HB2	1:C:1345:ASP:OD2	2.10	0.52
2:D:762:LEU:HD12	2:D:762:LEU:H	1.74	0.52
1:A:1565:ILE:HG22	1:A:1566:THR:H	1.74	0.52
1:A:560:TRP:CH2	1:A:562:ASN:HB2	2.44	0.52
1:A:606:ASP:O	1:A:609:VAL:HG23	2.09	0.52
1:A:702:GLY:CA	1:A:728:PHE:CD1	2.93	0.52
2:B:1445:HIS:CG	2:B:1446:PHE:N	2.77	0.52
2:B:353:TYR:HA	2:B:433:ILE:O	2.09	0.52
2:B:518:PHE:CD2	2:B:518:PHE:C	2.83	0.52
2:B:829:GLN:HE21	2:B:830:VAL:N	2.07	0.52
2:B:840:VAL:HG12	2:B:841:ASN:H	1.74	0.52
2:B:881:PRO:O	2:B:882:PHE:CD2	2.63	0.52
1:C:1012:LEU:HD13	1:C:1081:PHE:CD2	2.44	0.52
1:C:1161:LEU:O	1:C:1164:ILE:HG12	2.09	0.52
1:C:269:PHE:CG	1:C:301:PHE:CE1	2.97	0.52
1:C:924:VAL:HG21	3:C:2003:NAG:C8	2.38	0.52
2:D:1386:MET:HE2	2:D:1386:MET:HA	1.92	0.52
2:D:1529:LEU:O	2:D:1577:VAL:HG13	2.08	0.52
2:D:766:PRO:HA	2:D:771:ILE:O	2.09	0.52
1:A:1224:ILE:HG22	1:A:1225:TYR:CD2	2.45	0.52
2:B:1326:LEU:HD11	2:B:1328:PHE:CE2	2.44	0.52
2:B:1386:MET:HE2	2:B:1472:TYR:OH	2.09	0.52
2:B:209:ASN:CG	3:B:2001:NAG:C7	2.78	0.52
1:C:1421:HIS:CD2	1:C:1422:ALA:N	2.76	0.52
1:C:191:PRO:HD2	1:C:194:PRO:HB3	1.92	0.52
1:C:560:TRP:CE3	1:C:673:LEU:HD22	2.44	0.52
1:C:96:GLN:HG3	1:C:97:ASN:ND2	2.24	0.52
2:D:1277:ILE:HG22	2:D:1290:TYR:HB2	1.91	0.52
2:D:415:THR:O	2:D:425:GLN:NE2	2.43	0.52
2:D:640:SER:O	2:D:641:ALA:HB2	2.08	0.52
2:D:806:TYR:CD1	2:D:806:TYR:C	2.83	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1300:TYR:CD2	1:A:1300:TYR:C	2.83	0.52
1:A:132:LYS:HZ1	1:A:139:GLN:HE22	1.52	0.52
1:A:1423:VAL:HG11	1:A:1496:TYR:CE1	2.45	0.52
1:A:1590:ALA:HB1	1:A:1635:TYR:CD1	2.44	0.52
1:A:163:PHE:HE2	1:A:201:ILE:HD13	1.74	0.52
1:A:694:VAL:O	1:A:697:LYS:HE3	2.10	0.52
1:A:862:VAL:HB	1:A:865:ILE:HG13	1.92	0.52
1:A:924:VAL:HG21	3:A:2003:NAG:C8	2.38	0.52
2:B:235:PHE:HE2	2:B:299:PHE:CE2	2.28	0.52
2:B:746:ILE:H	2:B:746:ILE:HD13	1.74	0.52
1:C:1031:TRP:CH2	1:C:1042:LYS:HG3	2.45	0.52
1:C:1053:MET:CE	1:C:1089:VAL:HG21	2.39	0.52
1:C:1229:LYS:HZ1	1:C:1240:PRO:HD2	1.74	0.52
1:C:228:SER:HB3	1:C:253:ARG:HG2	1.92	0.52
1:C:238:ILE:HD12	1:C:347:TYR:CE1	2.44	0.52
1:C:998:ASN:HB3	1:C:1000:LEU:HG	1.90	0.52
2:D:1504:GLU:OE2	2:D:1505:ARG:N	2.43	0.52
2:D:409:LEU:C	2:D:409:LEU:HD12	2.30	0.52
1:A:1053:MET:CE	1:A:1089:VAL:HG21	2.38	0.52
1:A:1475:VAL:CG2	1:A:1476:ARG:N	2.72	0.52
1:A:617:LYS:C	1:A:619:PRO:HD2	2.30	0.52
2:B:1290:TYR:CE2	2:B:1301:ARG:HB3	2.45	0.52
2:B:755:TRP:O	2:B:756:LEU:HB3	2.10	0.52
1:C:1023:HIS:O	1:C:1027:THR:HB	2.10	0.52
2:D:127:PHE:O	2:D:149:SER:HA	2.10	0.52
2:D:1354:LEU:HD23	2:D:1354:LEU:O	2.09	0.52
2:D:44:GLU:HG2	2:D:82:LEU:CB	2.36	0.52
2:D:860:SER:OG	2:D:866:TYR:N	2.42	0.52
2:B:1341:ASN:HD22	2:B:1342:LYS:HG2	1.73	0.52
2:B:1480:LEU:HD21	2:B:1483:LYS:NZ	2.25	0.52
2:B:1525:LYS:HD2	2:B:1610:TRP:CH2	2.45	0.52
2:B:822:TYR:O	2:B:914:LYS:HB3	2.10	0.52
1:C:1016:VAL:HG21	1:C:1291:ILE:HD12	1.92	0.52
1:C:1559:TYR:HE1	1:C:1587:THR:HA	1.75	0.52
1:C:267:ILE:CD1	1:C:299:VAL:HG11	2.39	0.52
1:C:365:PRO:CG	1:C:464:TYR:CE2	2.91	0.52
1:C:582:TYR:CE2	1:C:817:ALA:HB1	2.45	0.52
1:C:678:THR:CG2	1:C:742:ILE:HB	2.40	0.52
1:C:698:CYS:C	1:C:700:TYR:H	2.13	0.52
1:C:730:GLU:O	1:C:734:VAL:HG23	2.10	0.52
1:C:840:GLN:NE2	1:C:897:THR:HG21	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:870:SER:C	1:C:872:VAL:H	2.13	0.52
2:D:1386:MET:CE	2:D:1386:MET:HA	2.39	0.52
2:D:1556:PRO:O	2:D:1558:ALA:N	2.43	0.52
2:D:1621:PHE:O	2:D:1622:GLN:C	2.48	0.52
2:D:27:LEU:O	2:D:628:LEU:HD12	2.10	0.52
2:D:59:HIS:HA	2:D:68:LEU:HD22	1.91	0.52
2:D:952:ASP:N	2:D:952:ASP:OD1	2.43	0.52
1:A:111:PHE:CD2	1:A:112:SER:N	2.76	0.52
1:A:156:LYS:C	1:A:156:LYS:HD2	2.29	0.52
1:A:316:GLU:O	1:A:349:LEU:HD21	2.10	0.52
1:A:430:VAL:HG11	1:A:453:ARG:NH2	2.20	0.52
1:A:489:LYS:CG	1:A:490:SER:H	2.22	0.52
2:B:109:THR:HG22	2:B:114:ARG:HB3	1.91	0.52
2:B:1327:THR:HG22	2:B:1328:PHE:N	2.25	0.52
1:C:101:TYR:CE1	1:C:116:ARG:NH2	2.78	0.52
1:C:113:LYS:CG	1:C:114:SER:H	2.19	0.52
1:C:1190:ILE:HG12	1:C:1253:TYR:CD1	2.45	0.52
1:C:1279:ARG:HB2	1:C:1284:PHE:HB2	1.92	0.52
1:C:1560:ALA:O	1:C:1585:TYR:CD2	2.63	0.52
1:C:371:ILE:HD11	1:C:433:PHE:CD2	2.44	0.52
2:D:365:TYR:HD1	2:D:395:THR:HG22	1.75	0.52
2:D:916:VAL:HG22	2:D:917:PRO:O	2.10	0.52
2:B:25:TYR:CE2	2:B:113:VAL:HG22	2.44	0.52
2:B:1556:PRO:O	2:B:1558:ALA:N	2.43	0.52
2:B:44:GLU:HG2	2:B:82:LEU:CB	2.37	0.52
1:C:1128:LYS:HD3	1:C:1414:GLU:OE1	2.10	0.52
1:C:1440:LYS:HD3	1:C:1453:TYR:OH	2.09	0.52
1:C:238:ILE:HB	1:C:347:TYR:CD1	2.45	0.52
1:C:706:ASN:ND2	1:C:709:GLU:H	2.07	0.52
1:C:91:GLN:CA	1:C:91:GLN:OE1	2.54	0.52
1:C:947:ARG:NH1	1:C:1352:PHE:CE2	2.78	0.52
2:D:1525:LYS:HD2	2:D:1610:TRP:CH2	2.45	0.52
2:D:235:PHE:HE2	2:D:299:PHE:CE2	2.28	0.52
2:D:302:ARG:HG3	2:D:303:PHE:CD1	2.45	0.52
2:D:319:THR:HG23	2:D:330:VAL:HG12	1.92	0.52
2:D:348:THR:O	2:D:348:THR:OG1	2.23	0.52
2:D:829:GLN:HE21	2:D:830:VAL:N	2.08	0.52
2:D:829:GLN:HG3	2:D:1480:LEU:HD13	1.92	0.52
1:A:1020:TYR:CE1	1:A:1295:GLU:HG3	2.45	0.51
1:A:144:ARG:HD2	1:A:146:TYR:HE1	1.74	0.51
2:B:69:PHE:CD2	2:B:87:ILE:HG22	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:945:ILE:HD12	2:B:945:ILE:N	2.26	0.51
1:C:1096:ASN:O	1:C:1099:SER:HB3	2.09	0.51
1:C:1190:ILE:HG12	1:C:1253:TYR:CE1	2.45	0.51
1:C:1311:MET:HG2	1:C:1313:ILE:HG12	1.91	0.51
1:C:1564:SER:HB2	1:C:1616:GLN:HG3	1.92	0.51
1:C:81:ASN:CG	1:C:82:SER:H	2.13	0.51
2:D:315:TYR:HD1	2:D:315:TYR:C	2.13	0.51
1:A:1227:PHE:CD2	1:A:1273:TRP:NE1	2.78	0.51
1:A:307:VAL:O	1:A:308:LYS:O	2.27	0.51
1:A:702:GLY:HA3	1:A:728:PHE:CD1	2.45	0.51
1:A:752:LEU:HD12	1:A:752:LEU:C	2.29	0.51
1:A:947:ARG:O	1:A:949:ILE:HG12	2.09	0.51
2:B:234:PHE:HD1	2:B:234:PHE:C	2.14	0.51
2:B:640:SER:O	2:B:641:ALA:CB	2.57	0.51
2:B:69:PHE:CE2	2:B:71:THR:HB	2.45	0.51
2:B:849:GLU:OE2	2:B:865:ARG:HD2	2.10	0.51
1:C:1040:ILE:O	1:C:1043:GLN:HB2	2.10	0.51
1:C:1077:TRP:O	1:C:1080:ALA:HB3	2.10	0.51
1:C:138:ASP:OD1	1:C:192:SER:HA	2.10	0.51
1:C:1423:VAL:HG11	1:C:1496:TYR:CE1	2.45	0.51
1:C:178:ASP:OD2	1:C:179:HIS:N	2.43	0.51
1:C:42:GLN:CG	1:C:43:VAL:N	2.71	0.51
1:C:478:VAL:HG21	1:C:532:GLN:OE1	2.10	0.51
1:C:956:ARG:HG2	1:C:1349:SER:HB3	1.92	0.51
2:D:1273:LEU:HD12	2:D:1273:LEU:O	2.09	0.51
2:D:1330:ASN:ND2	2:D:1330:ASN:N	2.59	0.51
2:D:155:SER:O	2:D:156:LYS:HG2	2.10	0.51
2:D:443:ASN:OD1	2:D:469:ASN:HB3	2.10	0.51
2:D:481:TYR:HE2	2:D:493:GLY:HA3	1.74	0.51
2:D:481:TYR:CB	2:D:520:PHE:HE1	2.16	0.51
2:D:843:ASP:HA	2:D:873:LYS:O	2.10	0.51
2:D:918:GLU:OE2	2:D:918:GLU:N	2.43	0.51
1:A:31:PHE:HB2	1:A:119:ILE:HG22	1.92	0.51
1:A:165:ASP:OD2	1:A:165:ASP:O	2.28	0.51
1:A:191:PRO:HD2	1:A:194:PRO:HB3	1.91	0.51
1:A:870:SER:C	1:A:872:VAL:H	2.14	0.51
2:B:1292:ILE:HD11	2:B:1301:ARG:HE	1.76	0.51
2:B:1367:ILE:HD13	2:B:1456:VAL:HG21	1.92	0.51
2:B:952:ASP:O	2:B:1331:ALA:HA	2.10	0.51
1:C:1024:TYR:C	1:C:1024:TYR:CD2	2.83	0.51
1:C:1031:TRP:CZ2	1:C:1042:LYS:HG3	2.45	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:315:LEU:CD1	1:C:318:LEU:HG	2.40	0.51
1:C:491:PRO:CG	1:C:494:ASP:CB	2.88	0.51
1:C:641:ASN:O	1:C:642:ASN:C	2.49	0.51
1:C:694:VAL:O	1:C:697:LYS:HE3	2.10	0.51
2:D:130:ILE:HA	2:D:147:VAL:HG23	1.92	0.51
2:D:1445:HIS:CG	2:D:1446:PHE:N	2.79	0.51
2:D:1624:LEU:O	2:D:1625:CYS:C	2.49	0.51
1:A:369:TYR:HB3	1:A:422:LEU:CD1	2.41	0.51
2:B:1623:LYS:CB	2:B:1623:LYS:NZ	2.74	0.51
2:B:47:GLY:O	2:B:48:ASP:HB2	2.09	0.51
2:B:252:LEU:HD22	2:B:582:LYS:HB3	1.92	0.51
2:B:814:PHE:HZ	2:B:846:VAL:HG21	1.75	0.51
1:C:1110:ASN:N	1:C:1110:ASN:OD1	2.44	0.51
1:C:1618:LEU:HD13	1:C:1618:LEU:O	2.11	0.51
1:C:594:THR:OG1	1:C:782:ARG:HA	2.11	0.51
1:C:633:GLY:O	1:C:634:CYS:HB2	2.11	0.51
1:C:874:ASP:O	1:C:875:HIS:CG	2.63	0.51
1:C:984:VAL:HG13	1:C:984:VAL:O	2.10	0.51
2:D:1301:ARG:HB3	2:D:1301:ARG:NH1	2.25	0.51
2:D:961:THR:HG22	2:D:1327:THR:CB	2.41	0.51
2:D:1480:LEU:HD21	2:D:1483:LYS:NZ	2.25	0.51
2:D:161:VAL:CG2	2:D:180:LEU:HD21	2.36	0.51
2:D:467:LYS:HG2	2:D:468:GLY:N	2.25	0.51
1:A:1279:ARG:NH1	1:A:1280:TYR:CE2	2.79	0.51
1:A:286:ALA:O	1:A:287:MET:C	2.48	0.51
1:A:486:VAL:HG11	1:A:499:TYR:CE1	2.45	0.51
1:A:478:VAL:HG21	1:A:532:GLN:OE1	2.11	0.51
1:A:730:GLU:O	1:A:734:VAL:HG23	2.10	0.51
1:A:594:THR:OG1	1:A:782:ARG:HA	2.10	0.51
1:A:96:GLN:O	1:A:97:ASN:O	2.29	0.51
2:B:27:LEU:HD13	2:B:43:VAL:HG23	1.91	0.51
2:B:242:ASN:OD1	2:B:295:LYS:HD2	2.10	0.51
2:B:415:THR:O	2:B:425:GLN:CD	2.49	0.51
2:B:481:TYR:HE2	2:B:493:GLY:HA3	1.74	0.51
2:B:523:TYR:CB	2:B:533:ALA:HB2	2.41	0.51
2:B:353:TYR:CD2	2:B:614:GLY:O	2.64	0.51
1:C:1007:SER:OG	1:C:1008:ALA:N	2.40	0.51
1:C:1016:VAL:HG11	1:C:1291:ILE:CG1	2.41	0.51
1:C:1045:LEU:O	1:C:1046:LYS:C	2.47	0.51
1:C:1139:GLU:OE2	1:C:1187:THR:OG1	2.26	0.51
1:C:101:TYR:HE1	1:C:116:ARG:NH2	2.08	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1590:ALA:HB1	1:C:1635:TYR:CD1	2.44	0.51
1:C:145:VAL:CB	1:C:183:ILE:HD12	2.33	0.51
2:D:1548:ILE:HD12	2:D:1636:THR:OG1	2.10	0.51
2:D:210:TYR:CG	2:D:211:THR:N	2.79	0.51
2:D:69:PHE:CE2	2:D:71:THR:HB	2.45	0.51
2:D:800:ILE:CG2	2:D:801:CYS:N	2.72	0.51
2:D:218:LYS:CD	2:D:822:TYR:HE2	2.23	0.51
2:D:840:VAL:HG12	2:D:841:ASN:H	1.75	0.51
2:D:881:PRO:O	2:D:882:PHE:CD2	2.64	0.51
1:A:1110:ASN:OD1	1:A:1110:ASN:N	2.43	0.51
1:A:1279:ARG:HH21	1:A:1362:THR:HG21	1.75	0.51
1:A:1533:GLY:O	1:A:1534:GLN:CB	2.54	0.51
2:B:842:GLU:O	2:B:843:ASP:C	2.48	0.51
1:C:706:ASN:HB2	1:C:714:ARG:NH1	2.25	0.51
1:C:961:TYR:O	1:C:961:TYR:CD1	2.64	0.51
1:C:987:ILE:HG22	1:C:1021:VAL:HG23	1.92	0.51
2:D:257:VAL:HG12	2:D:258:GLU:N	2.25	0.51
2:D:390:THR:HG22	2:D:395:THR:N	2.26	0.51
1:A:1377:PHE:CD2	1:A:1495:VAL:HG22	2.45	0.51
1:A:1381:ILE:HD12	1:A:1493:PHE:HD2	1.76	0.51
1:A:138:ASP:OD1	1:A:192:SER:HA	2.10	0.51
1:A:1568:ILE:HG23	1:A:1577:TYR:CE1	2.41	0.51
1:A:171:VAL:HG22	1:A:1057:MET:HE1	1.92	0.51
2:B:1278:THR:HB	2:B:1314:THR:HB	1.92	0.51
2:B:263:VAL:HG22	2:B:318:VAL:HG23	1.92	0.51
2:B:345:ILE:HG13	2:B:428:LYS:CB	2.40	0.51
2:B:518:PHE:CD2	2:B:518:PHE:O	2.63	0.51
2:B:866:TYR:C	2:B:866:TYR:CD2	2.84	0.51
1:C:33:VAL:HG23	1:C:120:THR:O	2.10	0.51
1:C:1563:VAL:HG12	1:C:1581:LEU:HD23	1.91	0.51
1:C:862:VAL:HB	1:C:865:ILE:HG13	1.92	0.51
1:C:947:ARG:O	1:C:949:ILE:N	2.44	0.51
2:D:922:LYS:HE3	2:D:1329:TYR:OH	2.10	0.51
2:D:198:ARG:HB3	2:D:213:TYR:CE1	2.46	0.51
2:D:251:TYR:CD2	2:D:257:VAL:HG22	2.45	0.51
2:D:347:PHE:O	2:D:348:THR:C	2.49	0.51
1:A:115:LYS:HE2	1:A:654:LEU:HD11	1.93	0.51
1:A:1188:LEU:HD23	1:A:1212:LEU:HA	1.93	0.51
1:A:1421:HIS:CE1	1:A:1498:TYR:CD1	2.98	0.51
1:A:1612:VAL:HB	1:A:1615:ARG:HB3	1.93	0.51
1:A:1628:LYS:HB3	1:A:1633:PHE:HD1	1.76	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:351:PRO:HG2	1:A:352:TYR:HD2	1.67	0.51
2:B:283:ILE:N	2:B:283:ILE:HD12	2.25	0.51
2:B:59:HIS:HA	2:B:68:LEU:HD22	1.92	0.51
1:C:1132:THR:HB	1:C:1134:PRO:HD2	1.93	0.51
1:C:1483:PHE:O	1:C:1485:VAL:HG13	2.11	0.51
1:C:1554:LYS:CG	1:C:1555:PRO:HD2	2.41	0.51
1:C:1616:GLN:NE2	1:C:1648:TRP:CZ3	2.79	0.51
1:C:1560:ALA:HB1	1:C:1620:MET:CG	2.40	0.51
1:C:859:MET:HE1	1:C:898:PHE:CB	2.41	0.51
2:D:197:TRP:HB2	2:D:214:PHE:CD1	2.46	0.51
2:D:248:THR:HG22	2:D:289:ASP:OD1	2.10	0.51
1:A:1150:ILE:HG22	1:A:1151:GLY:N	2.25	0.51
1:A:146:TYR:HD1	1:A:182:ILE:HG23	1.73	0.51
1:A:365:PRO:HD2	1:A:464:TYR:CE2	2.45	0.51
1:A:884:VAL:O	1:A:885:ARG:CB	2.49	0.51
2:B:319:THR:HG23	2:B:330:VAL:HG12	1.93	0.51
2:B:523:TYR:CD1	2:B:523:TYR:C	2.83	0.51
2:B:746:ILE:HD13	2:B:746:ILE:N	2.26	0.51
1:C:1188:LEU:HD23	1:C:1212:LEU:HA	1.93	0.51
1:C:240:TYR:HA	1:C:243:PHE:HB2	1.91	0.51
1:C:357:VAL:O	1:C:359:THR:HG22	2.11	0.51
1:C:369:TYR:HB3	1:C:422:LEU:CD1	2.41	0.51
1:C:477:LEU:HD22	1:C:477:LEU:N	2.26	0.51
1:C:618:LYS:N	1:C:619:PRO:CD	2.73	0.51
1:C:825:LEU:HB2	1:C:845:VAL:HG23	1.92	0.51
2:D:464:PHE:O	2:D:503:LEU:HA	2.10	0.51
2:D:629:THR:HA	2:D:635:ASN:OD1	2.10	0.51
2:D:818:LEU:CD2	2:D:820:MET:HE3	2.38	0.51
2:D:945:ILE:N	2:D:945:ILE:HD12	2.26	0.51
1:A:1534:GLN:HA	1:A:1608:ASN:HD22	1.75	0.51
1:A:25:ILE:HD13	1:A:41:ILE:HB	1.91	0.51
1:A:391:ASN:O	1:A:392:ALA:HB2	2.11	0.51
1:A:961:TYR:O	1:A:961:TYR:HD1	1.94	0.51
2:B:1354:LEU:O	2:B:1354:LEU:HD23	2.11	0.51
2:B:142:PRO:HB3	2:B:187:ASN:HD21	1.76	0.51
2:B:1623:LYS:HA	2:B:1623:LYS:HZ3	1.75	0.51
2:B:161:VAL:CG2	2:B:180:LEU:HD21	2.37	0.51
2:B:164:GLU:HB2	2:B:200:VAL:HG23	1.93	0.51
2:B:345:ILE:HD11	2:B:427:THR:C	2.31	0.51
2:B:78:ALA:C	2:B:80:GLY:H	2.14	0.51
1:C:1279:ARG:NH1	1:C:1280:TYR:CD2	2.79	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:820:PHE:CG	1:C:821:LYS:N	2.79	0.51
1:C:970:LYS:C	1:C:971:THR:HG23	2.30	0.51
1:C:976:ILE:HB	1:C:1362:THR:CG2	2.40	0.51
2:D:242:ASN:OD1	2:D:295:LYS:HD2	2.10	0.51
2:D:924:ILE:HG22	2:D:924:ILE:O	2.11	0.51
1:A:1112:GLN:NE2	1:A:1171:ALA:HB2	2.25	0.50
1:A:518:PHE:O	1:A:520:ASP:N	2.39	0.50
1:A:587:THR:HG22	1:A:789:ALA:HB2	1.92	0.50
2:B:1624:LEU:O	2:B:1625:CYS:C	2.49	0.50
1:C:1019:PHE:CD2	1:C:1020:TYR:N	2.78	0.50
1:C:111:PHE:CD2	1:C:112:SER:N	2.76	0.50
1:C:1139:GLU:O	1:C:1140:ASN:C	2.49	0.50
1:C:1279:ARG:HH21	1:C:1362:THR:HG21	1.75	0.50
2:D:130:ILE:HG23	2:D:147:VAL:HG23	1.93	0.50
2:D:961:THR:HG22	2:D:1327:THR:HA	1.93	0.50
2:D:234:PHE:C	2:D:234:PHE:HD1	2.15	0.50
2:D:866:TYR:OH	2:D:1388:THR:HG21	2.10	0.50
2:D:959:ILE:HG22	2:D:959:ILE:O	2.11	0.50
2:D:964:ILE:HG13	2:D:1302:THR:CG2	2.34	0.50
1:A:1007:SER:OG	1:A:1008:ALA:N	2.39	0.50
1:A:1161:LEU:O	1:A:1164:ILE:HG12	2.12	0.50
1:A:1183:GLN:NE2	1:A:1232:LEU:HD22	2.26	0.50
2:B:189:PRO:C	2:B:191:LEU:N	2.65	0.50
2:B:356:PRO:HD2	2:B:444:TYR:CE2	2.46	0.50
2:B:843:ASP:HA	2:B:873:LYS:O	2.11	0.50
1:C:1110:ASN:O	1:C:1111:TYR:CG	2.63	0.50
1:C:1314:ASP:HA	1:C:1325:ASN:HB2	1.93	0.50
1:C:1429:PRO:O	1:C:1432:ILE:HG12	2.11	0.50
1:C:1500:ARG:C	1:C:1502:ASP:H	2.15	0.50
1:C:584:PRO:HD3	1:C:820:PHE:HB2	1.93	0.50
2:D:1482:ASN:H	2:D:1495:GLU:HG2	1.76	0.50
1:A:136:THR:O	1:A:139:GLN:HB2	2.11	0.50
1:A:1559:TYR:HE1	1:A:1587:THR:HA	1.77	0.50
1:A:238:ILE:HB	1:A:347:TYR:CD1	2.46	0.50
1:A:691:LYS:C	1:A:693:SER:H	2.15	0.50
2:B:130:ILE:HG23	2:B:147:VAL:HG23	1.93	0.50
2:B:1380:THR:HG22	2:B:1381:ILE:H	1.76	0.50
2:B:515:ILE:HG21	2:B:599:TRP:CZ2	2.46	0.50
2:B:949:LYS:O	2:B:950:LEU:HG	2.12	0.50
1:C:931:PRO:CB	1:C:1366:HIS:CD2	2.95	0.50
1:C:146:TYR:CE1	1:C:182:ILE:HG23	2.46	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:504:LEU:HD12	1:C:509:ILE:HA	1.92	0.50
1:C:552:ALA:HB3	1:C:658:ASN:HB3	1.93	0.50
1:C:23:TYR:O	1:C:655:THR:HG21	2.09	0.50
1:C:819:VAL:O	1:C:820:PHE:O	2.29	0.50
2:D:965:ILE:HG22	2:D:1323:MET:HB2	1.94	0.50
2:D:1529:LEU:N	2:D:1529:LEU:HD12	2.27	0.50
2:D:228:LEU:CD2	2:D:247:ILE:HG12	2.41	0.50
2:D:952:ASP:O	2:D:1331:ALA:HA	2.11	0.50
1:A:1421:HIS:NE2	1:A:1498:TYR:CD1	2.80	0.50
1:A:222:TYR:HD2	1:A:223:VAL:N	2.06	0.50
1:A:820:PHE:CG	1:A:821:LYS:N	2.79	0.50
1:A:855:PHE:C	1:A:855:PHE:CD1	2.84	0.50
2:B:1346:ASN:O	2:B:1368:CYS:HB2	2.11	0.50
2:B:1429:LYS:O	2:B:1430:VAL:HG23	2.11	0.50
2:B:235:PHE:HB3	2:B:338:ILE:CG2	2.39	0.50
2:B:421:PRO:HD2	2:B:424:ARG:HG3	1.93	0.50
2:B:519:ARG:CZ	2:B:608:GLY:HA3	2.41	0.50
1:C:191:PRO:O	1:C:194:PRO:HD3	2.11	0.50
1:C:308:LYS:CG	1:C:309:GLU:H	2.22	0.50
1:C:488:PRO:O	1:C:489:LYS:O	2.29	0.50
1:C:790:LEU:HB3	1:C:791:PRO:CD	2.42	0.50
1:C:831:TYR:CZ	1:C:1457:ASP:HB3	2.46	0.50
2:D:345:ILE:HG13	2:D:428:LYS:CB	2.41	0.50
2:D:358:MET:CE	2:D:467:LYS:HD2	2.41	0.50
2:D:253:TYR:HE1	2:D:839:TYR:HE2	1.59	0.50
1:A:178:ASP:OD2	1:A:179:HIS:N	2.45	0.50
1:A:531:THR:HG23	1:A:533:ASN:H	1.77	0.50
1:A:633:GLY:O	1:A:634:CYS:HB2	2.12	0.50
1:A:773:TRP:CZ3	1:A:788:PHE:CE1	2.90	0.50
1:A:947:ARG:O	1:A:949:ILE:N	2.45	0.50
1:A:975:ARG:HG3	1:A:1340:VAL:HB	1.94	0.50
2:B:961:THR:HG22	2:B:1327:THR:CB	2.42	0.50
2:B:1602:THR:H	2:B:1605:THR:HB	1.76	0.50
2:B:259:GLY:HA2	2:B:323:GLU:HB3	1.92	0.50
2:B:347:PHE:O	2:B:348:THR:C	2.49	0.50
2:B:27:LEU:O	2:B:628:LEU:HD12	2.11	0.50
1:A:1162:VAL:N	1:C:1102:ASN:HD21	1.97	0.50
1:C:1434:ALA:HA	1:C:1479:ILE:HG22	1.92	0.50
1:C:60:PRO:CD	1:C:61:ASP:N	2.68	0.50
1:C:792:ASP:OD1	1:C:792:ASP:N	2.45	0.50
2:D:103:TYR:N	2:D:103:TYR:CD2	2.77	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1326:LEU:HD11	2:D:1328:PHE:CE2	2.46	0.50
2:D:356:PRO:HD2	2:D:444:TYR:CE2	2.46	0.50
2:D:421:PRO:HD2	2:D:424:ARG:HG3	1.93	0.50
2:D:512:PRO:O	2:D:515:ILE:HD12	2.11	0.50
1:A:1571:GLU:O	1:A:1574:PHE:CD2	2.64	0.50
1:A:20:GLU:HA	1:A:551:THR:HG22	1.94	0.50
1:A:269:PHE:O	1:A:282:MET:HG2	2.11	0.50
1:A:23:TYR:O	1:A:655:THR:HG21	2.11	0.50
2:B:1482:ASN:HB3	2:B:1493:ALA:CB	2.41	0.50
2:B:481:TYR:CD2	2:B:493:GLY:O	2.64	0.50
2:B:582:LYS:O	2:B:583:ALA:O	2.30	0.50
1:C:1266:TYR:O	1:C:1266:TYR:CD1	2.64	0.50
1:C:1268:ASN:N	1:C:1269:PRO:HD2	2.27	0.50
1:C:573:VAL:CG1	1:C:592:MET:HG2	2.42	0.50
1:C:96:GLN:O	1:C:97:ASN:O	2.30	0.50
2:D:1520:VAL:CG1	2:D:1584:TRP:HD1	2.24	0.50
2:D:345:ILE:HD11	2:D:427:THR:C	2.32	0.50
2:D:523:TYR:CB	2:D:533:ALA:HB2	2.42	0.50
2:D:599:TRP:HA	2:D:599:TRP:CE3	2.45	0.50
2:D:778:PHE:CD2	2:D:778:PHE:N	2.80	0.50
1:A:1279:ARG:NH1	1:A:1280:TYR:CD2	2.80	0.50
1:A:1311:MET:HG2	1:A:1313:ILE:HG12	1.93	0.50
1:A:1378:TYR:O	1:A:1406:ALA:HA	2.12	0.50
1:A:499:TYR:CE2	1:A:517:LYS:HG3	2.47	0.50
1:A:706:ASN:HB2	1:A:714:ARG:HH11	1.77	0.50
2:B:1607:ILE:H	2:B:1607:ILE:CD1	2.05	0.50
2:B:467:LYS:HG2	2:B:468:GLY:N	2.26	0.50
2:B:784:ILE:HD12	2:B:817:ASP:OD1	2.11	0.50
2:B:824:VAL:HG22	2:B:825:VAL:H	1.76	0.50
2:B:947:ALA:HB2	2:B:1309:GLN:HA	1.93	0.50
2:B:954:VAL:CG1	2:B:955:PRO:HD2	2.42	0.50
1:C:1049:LEU:HD11	1:C:1089:VAL:CG1	2.41	0.50
1:C:163:PHE:HE2	1:C:201:ILE:HD13	1.75	0.50
1:C:115:LYS:HE2	1:C:654:LEU:HD11	1.93	0.50
1:C:774:LEU:HG	1:C:788:PHE:CE1	2.46	0.50
1:C:934:VAL:CG1	1:C:935:LYS:N	2.74	0.50
2:D:105:VAL:HG12	2:D:118:VAL:HA	1.93	0.50
2:D:1382:ILE:HB	2:D:1425:ILE:HB	1.94	0.50
2:D:237:ILE:HD11	2:D:309:LEU:HB2	1.92	0.50
2:D:481:TYR:CE1	2:D:506:MET:SD	2.98	0.50
2:D:778:PHE:HD2	2:D:778:PHE:N	2.10	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1023:HIS:CE1	1:A:1302:LEU:HD11	2.47	0.50
1:A:1031:TRP:CH2	1:A:1042:LYS:HG3	2.47	0.50
1:A:987:ILE:CD1	1:A:1294:ILE:HG23	2.42	0.50
1:A:1487:PHE:HD2	1:A:1487:PHE:N	2.05	0.50
1:A:1562:LYS:CD	1:A:1648:TRP:HZ2	2.24	0.50
1:A:477:LEU:N	1:A:477:LEU:HD22	2.27	0.50
2:B:922:LYS:HE3	2:B:1329:TYR:OH	2.11	0.50
2:B:546:GLY:HA3	2:B:570:ASP:OD1	2.10	0.50
1:A:917:TRP:HB3	2:B:558:MET:SD	2.51	0.50
2:B:550:VAL:HG22	2:B:567:LEU:HD21	1.93	0.50
2:B:563:MET:O	2:B:777:SER:HA	2.12	0.50
1:C:115:LYS:HG3	1:C:116:ARG:O	2.12	0.50
1:C:1619:ILE:HG12	1:C:1645:ILE:CD1	2.42	0.50
1:C:237:PHE:HA	1:C:345:ILE:HG23	1.94	0.50
1:C:463:SER:O	1:C:555:VAL:HG21	2.11	0.50
1:C:856:CYS:HB2	2:D:904:LEU:HD21	1.94	0.50
2:D:142:PRO:HB3	2:D:187:ASN:HD21	1.76	0.50
2:D:415:THR:HG23	2:D:426:ALA:O	2.12	0.50
2:D:445:LEU:HD12	2:D:446:HIS:N	2.27	0.50
2:D:469:ASN:C	2:D:469:ASN:ND2	2.65	0.50
2:D:928:VAL:HG23	2:D:1323:MET:HB3	1.93	0.50
2:D:949:LYS:O	2:D:950:LEU:HG	2.11	0.50
1:A:1031:TRP:CZ2	1:A:1042:LYS:HG3	2.46	0.50
1:A:1559:TYR:CE1	1:A:1587:THR:HA	2.47	0.50
1:A:296:ILE:HG23	1:A:297:ALA:N	2.26	0.50
2:B:1284:ARG:NE	2:B:1285:GLU:H	2.09	0.50
2:B:1331:ALA:O	2:B:1332:GLN:CB	2.49	0.50
2:B:142:PRO:HB3	2:B:187:ASN:ND2	2.27	0.50
2:B:1632:SER:O	2:B:1636:THR:HB	2.12	0.50
2:B:870:PHE:HB2	2:B:871:PRO:CD	2.42	0.50
1:C:1019:PHE:CE1	1:C:1088:GLN:HB3	2.47	0.50
1:C:1019:PHE:CZ	1:C:1088:GLN:HB3	2.47	0.50
1:C:1127:ILE:HD13	1:C:1129:LEU:HD21	1.94	0.50
1:C:115:LYS:HB2	1:C:654:LEU:CD1	2.40	0.50
1:C:1227:PHE:CD2	1:C:1273:TRP:CE2	3.00	0.50
1:C:955:ARG:CG	1:C:1350:THR:HG23	2.40	0.50
1:C:1562:LYS:HD3	1:C:1648:TRP:HE1	1.75	0.50
1:C:323:LEU:HD13	1:C:323:LEU:O	2.12	0.50
1:C:936:ARG:HH11	1:C:936:ARG:CG	2.21	0.50
2:D:204:GLU:HG3	2:D:204:GLU:O	2.12	0.50
2:D:586:VAL:HG12	2:D:587:LEU:N	2.26	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:950:LEU:O	2:D:951:ASP:HB2	2.12	0.50
1:A:101:TYR:CE1	1:A:116:ARG:CZ	2.93	0.49
1:A:1271:ILE:HD13	1:A:1300:TYR:CD1	2.47	0.49
1:A:146:TYR:CE1	1:A:182:ILE:HG23	2.46	0.49
1:A:42:GLN:CG	1:A:43:VAL:N	2.75	0.49
1:A:855:PHE:CZ	1:A:886:GLN:HB2	2.47	0.49
2:B:162:ILE:CG2	2:B:202:LYS:HG2	2.42	0.49
2:B:460:LEU:O	2:B:460:LEU:HD23	2.11	0.49
2:B:358:MET:CE	2:B:467:LYS:HD2	2.41	0.49
1:C:1421:HIS:CE1	1:C:1498:TYR:CD1	2.99	0.49
1:C:325:ILE:O	1:C:341:GLU:HB2	2.13	0.49
1:C:824:PHE:O	1:C:845:VAL:HG22	2.12	0.49
1:C:834:VAL:HB	1:C:837:GLU:OE2	2.12	0.49
2:D:1331:ALA:O	2:D:1332:GLN:CB	2.49	0.49
1:A:1024:TYR:CD2	1:A:1024:TYR:C	2.84	0.49
1:A:1007:SER:HA	1:A:1069:TRP:HD1	1.77	0.49
1:A:1279:ARG:HB2	1:A:1284:PHE:HB2	1.94	0.49
1:A:1299:GLU:O	1:A:1303:LEU:HB2	2.12	0.49
1:A:1543:ILE:O	1:A:1547:THR:HG23	2.12	0.49
1:A:1570:VAL:CG2	1:A:1575:VAL:HG22	2.42	0.49
1:A:809:ILE:CG1	1:A:810:CYS:N	2.75	0.49
1:A:854:GLN:O	1:A:854:GLN:OE1	2.30	0.49
2:B:965:ILE:CD1	2:B:1277:ILE:HD13	2.42	0.49
2:B:1508:VAL:HB	2:B:1509:PRO:HD3	1.93	0.49
2:B:184:TRP:HB2	2:B:185:PRO:CD	2.42	0.49
2:B:522:ALA:O	2:B:533:ALA:HB1	2.12	0.49
2:B:519:ARG:NH1	2:B:606:ASP:OD2	2.45	0.49
1:C:1053:MET:HE2	1:C:1089:VAL:CG2	2.41	0.49
1:C:1562:LYS:O	1:C:1563:VAL:CG1	2.60	0.49
1:C:1585:TYR:CE2	1:C:1586:LYS:HB3	2.47	0.49
1:C:231:ILE:HA	1:C:250:ILE:HG22	1.94	0.49
1:C:50:PHE:CD1	1:C:50:PHE:C	2.85	0.49
1:C:54:ILE:O	1:C:68:SER:HA	2.13	0.49
1:C:691:LYS:C	1:C:693:SER:H	2.15	0.49
1:C:805:SER:O	1:C:807:THR:N	2.45	0.49
2:D:1341:ASN:HD22	2:D:1342:LYS:HG2	1.75	0.49
2:D:1482:ASN:HB3	2:D:1493:ALA:HB3	1.94	0.49
2:D:209:ASN:CG	3:D:2001:NAG:C7	2.80	0.49
2:D:447:VAL:HG13	2:D:447:VAL:O	2.12	0.49
2:D:541:LYS:HG3	2:D:543:THR:HG22	1.94	0.49
2:D:546:GLY:HA3	2:D:570:ASP:OD1	2.11	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1102:ASN:HD22	1:C:1162:VAL:HG22	1.75	0.49
1:A:1164:ILE:O	1:A:1165:ASP:C	2.47	0.49
1:A:1213:LYS:CG	1:A:1266:TYR:HE2	2.23	0.49
1:A:1317:TYR:CD2	1:A:1344:ASP:HB3	2.47	0.49
1:A:185:PHE:CD1	1:A:186:PRO:HD2	2.48	0.49
1:A:33:VAL:HA	1:A:87:ILE:HG12	1.95	0.49
1:A:50:PHE:CD1	1:A:50:PHE:C	2.86	0.49
1:A:520:ASP:HB2	2:B:404:LEU:HD13	1.94	0.49
1:A:540:LEU:HD12	1:A:541:LEU:N	2.27	0.49
1:A:639:GLY:H	1:A:645:VAL:CG2	2.25	0.49
1:A:823:VAL:HG23	1:A:846:TYR:O	2.12	0.49
1:A:825:LEU:HB2	1:A:845:VAL:HG23	1.93	0.49
1:A:984:VAL:O	1:A:984:VAL:HG13	2.12	0.49
2:B:1540:TYR:HE1	2:B:1575:LEU:HB2	1.78	0.49
2:B:400:LEU:HB3	2:B:402:ILE:HD11	1.94	0.49
2:B:484:LEU:HD11	2:B:626:LEU:HD11	1.94	0.49
1:C:331:GLU:CG	1:C:333:THR:HG23	2.41	0.49
1:C:361:LEU:H	1:C:361:LEU:HD12	1.77	0.49
1:C:987:ILE:CD1	1:C:1294:ILE:HG23	2.42	0.49
2:D:1327:THR:HG22	2:D:1328:PHE:N	2.27	0.49
2:D:1420:LYS:HB3	2:D:1422:ALA:O	2.12	0.49
2:D:226:VAL:O	2:D:226:VAL:HG12	2.11	0.49
2:D:415:THR:O	2:D:425:GLN:CD	2.51	0.49
2:D:563:MET:CB	2:D:778:PHE:CE2	2.94	0.49
2:D:550:VAL:HG22	2:D:567:LEU:HD21	1.93	0.49
2:D:824:VAL:HG12	2:D:913:LEU:HD21	1.94	0.49
1:A:116:ARG:O	1:A:117:MET:HB3	2.12	0.49
1:A:1268:ASN:HD22	1:A:1268:ASN:H	1.60	0.49
1:A:126:LEU:HD12	1:A:147:SER:HB2	1.93	0.49
2:B:1301:ARG:HB3	2:B:1301:ARG:NH1	2.27	0.49
2:B:1382:ILE:HB	2:B:1425:ILE:HB	1.94	0.49
2:B:1529:LEU:N	2:B:1529:LEU:HD12	2.27	0.49
2:B:435:TYR:CE1	2:B:616:ASN:HA	2.47	0.49
2:B:524:TYR:HE1	2:B:532:VAL:CG1	2.25	0.49
2:B:586:VAL:HG12	2:B:587:LEU:N	2.27	0.49
2:B:825:VAL:HG22	2:B:916:VAL:HG13	1.93	0.49
1:C:1648:TRP:NE1	1:C:1664:LEU:HD22	2.28	0.49
1:C:1549:LYS:HZ2	1:C:1667:PHE:HB3	1.76	0.49
1:C:391:ASN:O	1:C:392:ALA:HB2	2.12	0.49
1:C:820:PHE:O	1:C:821:LYS:CG	2.60	0.49
1:C:834:VAL:HA	1:C:930:VAL:O	2.12	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:864:GLY:HA3	1:C:907:LEU:HD23	1.94	0.49
1:C:59:TYR:CZ	1:C:99:VAL:HG21	2.44	0.49
2:D:1278:THR:HB	2:D:1314:THR:HB	1.94	0.49
2:D:1523:VAL:HG22	2:D:1584:TRP:CB	2.28	0.49
2:D:162:ILE:CG2	2:D:202:LYS:HG2	2.43	0.49
2:D:350:THR:O	2:D:350:THR:HG23	2.11	0.49
2:D:518:PHE:O	2:D:518:PHE:HD2	1.96	0.49
2:D:755:TRP:O	2:D:756:LEU:HB3	2.12	0.49
1:A:100:SER:HB2	1:A:101:TYR:HD2	1.78	0.49
1:A:1104:LEU:O	1:A:1108:VAL:HG12	2.11	0.49
1:A:1128:LYS:O	1:A:1128:LYS:HG3	2.11	0.49
1:A:1487:PHE:O	1:A:1488:LEU:C	2.50	0.49
1:A:475:ALA:HB1	1:A:477:LEU:CD2	2.42	0.49
2:B:930:LEU:HB2	2:B:1321:ALA:HB3	1.93	0.49
2:B:1330:ASN:H	2:B:1330:ASN:HD22	1.60	0.49
2:B:1412:GLU:HB2	2:B:1419:GLN:CG	2.42	0.49
2:B:482:LEU:CD1	2:B:482:LEU:N	2.76	0.49
1:C:100:SER:CB	1:C:101:TYR:HD2	2.25	0.49
1:C:1549:LYS:NZ	1:C:1667:PHE:CB	2.70	0.49
1:C:1559:TYR:CE1	1:C:1587:THR:HA	2.46	0.49
1:C:792:ASP:O	1:C:793:SER:CB	2.60	0.49
2:D:1278:THR:O	2:D:1313:VAL:HA	2.12	0.49
2:D:1345:LEU:HG	2:D:1345:LEU:O	2.13	0.49
2:D:1512:ILE:O	2:D:1516:CYS:HB2	2.12	0.49
2:D:224:PHE:CZ	2:D:329:VAL:HG13	2.47	0.49
2:D:820:MET:HE1	2:D:832:ILE:HD13	1.94	0.49
2:D:825:VAL:HG22	2:D:916:VAL:HG13	1.95	0.49
1:A:1185:THR:OG1	1:A:1231:ASN:HB3	2.12	0.49
1:A:1560:ALA:HB1	1:A:1620:MET:CG	2.42	0.49
1:A:240:TYR:HA	1:A:243:PHE:HB2	1.93	0.49
2:B:778:PHE:CD2	2:B:778:PHE:N	2.81	0.49
1:C:1068:VAL:HG21	1:C:1124:TYR:HD1	1.72	0.49
1:C:1265:ASN:C	1:C:1267:VAL:H	2.16	0.49
1:C:1004:PRO:HG3	1:C:1461:ILE:HD13	1.95	0.49
1:C:1543:ILE:O	1:C:1547:THR:HG23	2.13	0.49
1:C:21:GLN:HE22	1:C:46:TYR:HD2	1.61	0.49
1:C:357:VAL:HG12	1:C:358:ALA:N	2.27	0.49
1:C:431:LEU:O	1:C:431:LEU:HD13	2.11	0.49
1:C:531:THR:HG23	1:C:533:ASN:H	1.78	0.49
1:C:598:SER:O	1:C:599:TRP:HD1	1.95	0.49
1:C:617:LYS:C	1:C:619:PRO:HD2	2.33	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:702:GLY:CA	1:C:728:PHE:CD1	2.95	0.49
2:D:1429:LYS:O	2:D:1430:VAL:HG23	2.13	0.49
2:D:145:TYR:C	2:D:145:TYR:CD1	2.86	0.49
2:D:1507:ASP:OD1	2:D:1509:PRO:HD2	2.12	0.49
1:A:1016:VAL:HG11	1:A:1291:ILE:CG1	2.43	0.49
1:A:1023:HIS:O	1:A:1027:THR:HB	2.12	0.49
1:A:1584:ILE:CG2	1:A:1585:TYR:H	2.04	0.49
1:A:681:LYS:HB2	1:A:738:LEU:HD11	1.95	0.49
1:A:827:MET:HB3	1:A:829:ILE:CD1	2.42	0.49
1:A:946:PRO:HB3	1:A:1352:PHE:O	2.12	0.49
2:B:961:THR:HG22	2:B:1327:THR:HA	1.95	0.49
2:B:40:GLN:O	2:B:489:ILE:HD12	2.12	0.49
2:B:581:ASP:O	2:B:582:LYS:C	2.51	0.49
2:B:61:PHE:CG	2:B:62:PRO:HA	2.47	0.49
2:B:806:TYR:CE1	2:B:807:GLU:O	2.66	0.49
1:C:1252:ALA:O	1:C:1253:TYR:C	2.50	0.49
2:D:1392:PRO:HB2	2:D:1397:LEU:HD22	1.95	0.49
2:D:199:ILE:O	2:D:199:ILE:HG22	2.12	0.49
2:D:353:TYR:CD2	2:D:614:GLY:O	2.66	0.49
2:D:84:THR:N	2:D:85:PRO:HD3	2.27	0.49
2:D:954:VAL:HB	2:D:957:THR:CG2	2.31	0.49
1:A:166:PRO:HB3	1:A:198:MET:H	1.77	0.49
1:A:238:ILE:HD12	1:A:347:TYR:CE1	2.48	0.49
1:A:367:ILE:CD1	1:A:466:TYR:HB3	2.43	0.49
1:A:834:VAL:HB	1:A:837:GLU:OE2	2.13	0.49
1:A:874:ASP:O	1:A:875:HIS:CG	2.66	0.49
2:B:1349:VAL:HA	2:B:1364:MET:O	2.10	0.49
2:B:482:LEU:H	2:B:482:LEU:CD1	2.21	0.49
2:B:795:THR:HG22	2:B:796:PRO:HD2	1.95	0.49
2:B:829:GLN:HG3	2:B:1480:LEU:HD13	1.95	0.49
1:C:128:ILE:HD11	1:C:214:THR:CA	2.43	0.49
1:C:946:PRO:HB3	1:C:1352:PHE:O	2.12	0.49
1:C:1658:GLN:NE2	1:C:1661:LEU:HD12	2.28	0.49
1:C:207:GLU:O	1:C:209:PHE:N	2.45	0.49
1:C:773:TRP:HZ3	1:C:788:PHE:HE1	1.56	0.49
1:C:989:SER:O	1:C:993:SER:CB	2.60	0.49
2:D:137:TYR:CE1	2:D:143:VAL:HG22	2.47	0.49
2:D:597:LYS:NZ	2:D:597:LYS:HB3	2.27	0.49
2:D:61:PHE:CG	2:D:62:PRO:HA	2.47	0.49
2:D:69:PHE:CD2	2:D:69:PHE:C	2.86	0.49
2:D:784:ILE:HD12	2:D:817:ASP:OD1	2.13	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:814:PHE:CZ	2:D:846:VAL:HG21	2.48	0.49
2:D:735:ASN:CB	2:D:869:GLN:HE22	2.25	0.49
2:D:965:ILE:CD1	2:D:1277:ILE:HD13	2.42	0.49
1:A:1109:GLU:HB3	1:A:1110:ASN:OD1	2.11	0.49
1:A:1564:SER:O	1:A:1579:ALA:HB1	2.13	0.49
1:A:1648:TRP:NE1	1:A:1664:LEU:HD22	2.28	0.49
1:A:27:ALA:HB1	1:A:28:PRO:CD	2.43	0.49
2:B:155:SER:O	2:B:156:LYS:HG2	2.13	0.49
2:B:204:GLU:O	2:B:204:GLU:HG3	2.13	0.49
2:B:417:HIS:N	2:B:425:GLN:OE1	2.45	0.49
2:B:437:THR:HG21	2:B:443:ASN:N	2.27	0.49
2:B:481:TYR:C	2:B:481:TYR:CD2	2.85	0.49
2:B:924:ILE:O	2:B:924:ILE:HG22	2.12	0.49
1:C:1008:ALA:O	1:C:1010:ALA:N	2.45	0.49
1:C:111:PHE:CG	1:C:112:SER:N	2.81	0.49
1:C:20:GLU:HA	1:C:551:THR:HG22	1.93	0.49
1:C:222:TYR:HE1	1:C:768:TYR:CB	2.10	0.49
1:C:639:GLY:H	1:C:645:VAL:HG22	1.78	0.49
2:D:109:THR:HG22	2:D:114:ARG:HB3	1.94	0.49
1:A:1088:GLN:O	1:A:1090:ASN:N	2.46	0.49
1:A:1101:CYS:O	1:A:1105:LEU:HD12	2.13	0.49
1:A:1132:THR:HB	1:A:1134:PRO:HD2	1.94	0.49
1:A:1140:ASN:O	1:A:1143:TYR:HB3	2.12	0.49
1:A:1152:ILE:CG2	1:A:1168:LEU:HD21	2.40	0.49
1:A:120:THR:CG2	1:A:122:ASP:H	2.24	0.49
1:A:1268:ASN:HB2	1:A:1269:PRO:HD3	1.95	0.49
1:A:331:GLU:CG	1:A:333:THR:HG23	2.42	0.49
1:A:618:LYS:O	1:A:619:PRO:O	2.31	0.49
1:A:773:TRP:HZ3	1:A:788:PHE:HE1	1.55	0.49
2:B:103:TYR:CD2	2:B:103:TYR:N	2.79	0.49
1:C:1003:LEU:HA	1:C:1004:PRO:HD2	1.64	0.49
1:C:1024:TYR:O	1:C:1025:LEU:C	2.51	0.49
1:C:1271:ILE:HD13	1:C:1300:TYR:CD1	2.47	0.49
1:C:1324:HIS:CD2	1:C:1336:ARG:NH2	2.81	0.49
1:C:1279:ARG:NH2	1:C:1362:THR:HG21	2.28	0.49
1:C:1365:VAL:CG2	1:C:1366:HIS:H	2.23	0.49
1:C:1455:ILE:HD12	1:C:1455:ILE:N	2.27	0.49
2:D:422:ARG:HD3	2:D:422:ARG:N	2.22	0.49
1:A:961:TYR:HB2	1:A:1345:ASP:OD2	2.13	0.48
1:A:1563:VAL:HG12	1:A:1581:LEU:HD23	1.94	0.48
1:A:471:ASP:O	1:A:472:ASN:HB3	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:618:LYS:N	1:A:619:PRO:CD	2.72	0.48
1:A:672:ILE:C	1:A:673:LEU:HG	2.33	0.48
2:B:1301:ARG:HB3	2:B:1301:ARG:HH11	1.78	0.48
2:B:1600:ILE:O	2:B:1602:THR:HG23	2.12	0.48
2:B:421:PRO:O	2:B:424:ARG:HB2	2.13	0.48
2:B:481:TYR:CE2	2:B:493:GLY:C	2.86	0.48
1:C:126:LEU:HD12	1:C:147:SER:HB2	1.94	0.48
1:C:1226:ARG:O	1:C:1270:VAL:HG22	2.13	0.48
1:C:1454:GLN:C	1:C:1455:ILE:HD12	2.33	0.48
1:C:1480:PHE:CD1	1:C:1480:PHE:N	2.81	0.48
1:C:161:LEU:HD11	1:C:185:PHE:CE1	2.47	0.48
2:D:44:GLU:OE2	2:D:523:TYR:OH	2.28	0.48
2:D:58:VAL:HG12	2:D:104:VAL:HG22	1.94	0.48
1:A:1024:TYR:O	1:A:1025:LEU:C	2.51	0.48
1:A:142:LYS:HA	1:A:187:ASP:OD1	2.12	0.48
1:A:1493:PHE:CD1	1:A:1494:THR:N	2.79	0.48
1:A:1563:VAL:HG22	1:A:1617:TYR:O	2.14	0.48
1:A:599:TRP:HE1	1:A:779:LEU:CD1	2.26	0.48
1:A:819:VAL:O	1:A:820:PHE:O	2.30	0.48
2:B:1345:LEU:HG	2:B:1345:LEU:O	2.13	0.48
2:B:378:PRO:HA	2:B:389:THR:HA	1.94	0.48
2:B:438:GLN:CD	2:B:530:GLU:HG3	2.34	0.48
2:B:742:ASP:C	2:B:742:ASP:OD1	2.52	0.48
2:B:818:LEU:CD2	2:B:820:MET:HE3	2.40	0.48
1:C:706:ASN:HB2	1:C:714:ARG:HH11	1.77	0.48
2:D:1528:LEU:HD13	2:D:1542:MET:CE	2.43	0.48
2:D:795:THR:HG22	2:D:796:PRO:HD2	1.95	0.48
2:D:850:LEU:HG	2:D:851:LEU:O	2.13	0.48
1:C:875:HIS:CB	2:D:901:GLN:HE22	2.25	0.48
2:D:913:LEU:HD23	2:D:914:LYS:N	2.28	0.48
1:A:1077:TRP:O	1:A:1080:ALA:HB3	2.13	0.48
1:A:1229:LYS:HZ1	1:A:1240:PRO:HD2	1.78	0.48
1:A:135:TYR:OH	1:A:141:VAL:HG13	2.13	0.48
1:A:1500:ARG:C	1:A:1502:ASP:H	2.17	0.48
1:A:21:GLN:HE22	1:A:46:TYR:HD2	1.61	0.48
1:A:790:LEU:HB3	1:A:791:PRO:CD	2.44	0.48
2:B:44:GLU:OE2	2:B:523:TYR:OH	2.30	0.48
2:B:964:ILE:HG13	2:B:1302:THR:CG2	2.38	0.48
1:C:113:LYS:CG	1:C:114:SER:N	2.74	0.48
1:C:1381:ILE:O	1:C:1382:ASP:CB	2.59	0.48
1:C:1535:MET:HG2	1:C:1608:ASN:O	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:24:VAL:HG12	1:C:24:VAL:O	2.13	0.48
1:C:309:GLU:N	1:C:309:GLU:OE1	2.46	0.48
1:C:367:ILE:CD1	1:C:466:TYR:HB3	2.43	0.48
1:C:956:ARG:HA	1:C:1348:VAL:O	2.12	0.48
1:C:968:VAL:CG2	1:C:971:THR:HG21	2.43	0.48
2:D:1446:PHE:CD2	2:D:1448:VAL:HG22	2.45	0.48
2:D:223:SER:O	2:D:252:LEU:HG	2.13	0.48
2:D:283:ILE:HD12	2:D:283:ILE:N	2.29	0.48
2:D:401:ASN:C	2:D:402:ILE:HD13	2.33	0.48
1:A:1008:ALA:O	1:A:1010:ALA:N	2.46	0.48
1:A:1069:TRP:CZ3	1:A:1451:THR:HG21	2.48	0.48
1:A:1132:THR:HG22	1:A:1133:LEU:N	2.27	0.48
1:A:1450:PHE:HA	1:A:1464:LEU:HB3	1.96	0.48
1:A:968:VAL:CG2	1:A:971:THR:HG21	2.44	0.48
2:B:58:VAL:HG12	2:B:104:VAL:HG22	1.94	0.48
2:B:1424:ILE:CD1	2:B:1424:ILE:N	2.74	0.48
2:B:226:VAL:HG12	2:B:226:VAL:O	2.12	0.48
2:B:350:THR:HG23	2:B:350:THR:O	2.12	0.48
2:B:512:PRO:O	2:B:515:ILE:HD12	2.13	0.48
2:B:842:GLU:O	2:B:844:ILE:HG23	2.14	0.48
1:C:1022:PHE:O	1:C:1024:TYR:N	2.47	0.48
1:C:1127:ILE:HG12	1:C:1143:TYR:CE2	2.48	0.48
1:C:146:TYR:HD1	1:C:182:ILE:HG23	1.75	0.48
1:C:1560:ALA:O	1:C:1561:TYR:HB3	2.13	0.48
1:C:494:ASP:O	1:C:494:ASP:CG	2.52	0.48
1:C:540:LEU:HD12	1:C:541:LEU:N	2.28	0.48
1:C:944:LEU:HD23	1:C:944:LEU:N	2.28	0.48
2:D:1619:GLU:HA	2:D:1622:GLN:NE2	2.27	0.48
2:D:69:PHE:CD2	2:D:87:ILE:HG22	2.49	0.48
2:D:825:VAL:N	2:D:828:GLU:OE1	2.39	0.48
1:A:1279:ARG:NH2	1:A:1362:THR:HG21	2.28	0.48
1:A:1562:LYS:O	1:A:1563:VAL:CG1	2.62	0.48
1:A:1585:TYR:CE2	1:A:1586:LYS:HB3	2.48	0.48
1:A:961:TYR:CD1	1:A:961:TYR:O	2.66	0.48
2:B:1562:GLN:CB	2:B:1598:SER:HB3	2.43	0.48
2:B:235:PHE:CE2	2:B:299:PHE:HE2	2.31	0.48
2:B:816:ILE:CD1	2:B:896:ILE:HG22	2.44	0.48
2:B:830:VAL:CG2	2:B:831:GLU:N	2.72	0.48
1:C:1033:ILE:HG22	1:C:1034:PHE:HD1	1.77	0.48
1:C:1061:ASN:HB3	1:C:1062:ALA:H	1.54	0.48
1:C:1109:GLU:HB3	1:C:1110:ASN:OD1	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1224:ILE:HG22	1:C:1225:TYR:HD2	1.78	0.48
1:C:1227:PHE:CD2	1:C:1273:TRP:NE1	2.80	0.48
1:C:185:PHE:CD1	1:C:186:PRO:HD2	2.48	0.48
1:C:227:PHE:HB2	1:C:338:GLU:HG3	1.94	0.48
1:C:623:VAL:CG1	1:C:624:PHE:N	2.61	0.48
1:C:979:VAL:HG21	1:C:1326:TYR:CZ	2.43	0.48
2:D:543:THR:OG1	2:D:544:CYS:N	2.43	0.48
2:D:91:ALA:HA	2:D:94:VAL:HG23	1.96	0.48
1:A:1314:ASP:HA	1:A:1325:ASN:HB2	1.95	0.48
1:A:308:LYS:HB3	1:A:309:GLU:OE1	2.13	0.48
1:A:463:SER:O	1:A:555:VAL:HG21	2.14	0.48
2:B:129:PHE:HE2	2:B:598:ILE:HG23	1.75	0.48
2:B:422:ARG:HD3	2:B:422:ARG:N	2.23	0.48
2:B:541:LYS:HG3	2:B:543:THR:HG22	1.95	0.48
2:B:69:PHE:C	2:B:69:PHE:CD2	2.87	0.48
2:B:83:VAL:HB	2:B:85:PRO:HD3	1.95	0.48
1:C:544:TYR:HE2	1:C:546:VAL:CG2	2.26	0.48
1:C:125:PHE:CE1	1:C:627:LEU:HD21	2.47	0.48
1:C:950:TYR:HD1	1:C:1268:ASN:OD1	1.95	0.48
2:D:511:THR:H	2:D:514:LEU:CD1	2.26	0.48
2:D:742:ASP:OD1	2:D:742:ASP:C	2.52	0.48
2:D:746:ILE:HD13	2:D:746:ILE:H	1.77	0.48
2:D:947:ALA:HB2	2:D:1309:GLN:HA	1.95	0.48
1:A:1323:LEU:CD1	1:A:1324:HIS:H	2.26	0.48
1:A:251:LYS:HG2	1:A:296:ILE:CD1	2.43	0.48
1:A:794:LEU:N	1:A:794:LEU:HD12	2.28	0.48
1:A:831:TYR:CZ	1:A:1457:ASP:HB3	2.48	0.48
2:B:162:ILE:HG21	2:B:202:LYS:HG2	1.94	0.48
2:B:778:PHE:N	2:B:778:PHE:HD2	2.11	0.48
1:C:1185:THR:OG1	1:C:1231:ASN:HB3	2.13	0.48
1:C:1612:VAL:HB	1:C:1615:ARG:HB3	1.96	0.48
1:C:1675:GLY:O	1:C:1676:CYS:OXT	2.32	0.48
1:C:809:ILE:CG1	1:C:810:CYS:N	2.76	0.48
1:C:855:PHE:CZ	1:C:886:GLN:HB2	2.48	0.48
2:D:640:SER:O	2:D:641:ALA:CB	2.61	0.48
2:D:71:THR:HG23	2:D:72:ARG:N	2.29	0.48
2:D:916:VAL:CG2	2:D:917:PRO:HD2	2.43	0.48
1:A:1143:TYR:O	1:A:1144:LEU:C	2.52	0.48
1:A:115:LYS:HG3	1:A:116:ARG:O	2.14	0.48
1:A:120:THR:HG22	1:A:121:TYR:N	2.29	0.48
1:A:1565:ILE:O	1:A:1566:THR:HG22	2.14	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:534:MET:HB3	1:A:538:SER:OG	2.14	0.48
1:A:641:ASN:O	1:A:642:ASN:C	2.50	0.48
2:B:1300:ALA:O	2:B:1301:ARG:HD2	2.13	0.48
2:B:299:PHE:CE1	2:B:303:PHE:HD2	2.24	0.48
2:B:356:PRO:HD2	2:B:444:TYR:CZ	2.48	0.48
2:B:477:LYS:HD3	2:B:477:LYS:N	2.29	0.48
2:B:84:THR:N	2:B:85:PRO:HD3	2.28	0.48
2:B:860:SER:OG	2:B:866:TYR:N	2.46	0.48
1:C:1020:TYR:CE1	1:C:1295:GLU:HG3	2.48	0.48
1:C:1140:ASN:O	1:C:1143:TYR:HB3	2.14	0.48
1:C:1013:MET:HE2	1:C:1287:THR:HB	1.96	0.48
1:C:1313:ILE:HA	1:C:1313:ILE:HD13	1.68	0.48
1:C:135:TYR:OH	1:C:141:VAL:HG13	2.14	0.48
1:C:1563:VAL:HG12	1:C:1581:LEU:CD2	2.44	0.48
1:C:618:LYS:O	1:C:619:PRO:O	2.32	0.48
2:D:189:PRO:C	2:D:191:LEU:N	2.67	0.48
2:D:214:PHE:CD1	2:D:214:PHE:C	2.86	0.48
2:D:378:PRO:HA	2:D:389:THR:HA	1.95	0.48
1:A:1483:PHE:O	1:A:1485:VAL:HG13	2.14	0.48
1:A:325:ILE:O	1:A:341:GLU:HB2	2.14	0.48
1:A:583:SER:O	1:A:586:GLN:HB3	2.14	0.48
1:A:700:TYR:OH	1:A:757:LEU:HD22	2.14	0.48
2:B:276:ILE:O	2:B:277:PRO:C	2.52	0.48
2:B:365:TYR:HA	2:B:394:GLY:O	2.14	0.48
2:B:455:LYS:O	2:B:458:ASP:HB2	2.14	0.48
2:B:850:LEU:HG	2:B:851:LEU:O	2.14	0.48
2:B:916:VAL:HG22	2:B:917:PRO:O	2.14	0.48
2:B:91:ALA:HA	2:B:94:VAL:HG23	1.96	0.48
2:B:966:GLN:HG3	2:B:966:GLN:O	2.14	0.48
1:C:132:LYS:HZ1	1:C:139:GLN:HE22	1.56	0.48
1:C:166:PRO:HB3	1:C:198:MET:H	1.78	0.48
1:C:25:ILE:N	1:C:655:THR:CG2	2.73	0.48
1:C:700:TYR:OH	1:C:757:LEU:HD22	2.13	0.48
1:C:935:LYS:HD3	1:C:1373:GLU:OE2	2.14	0.48
2:D:421:PRO:O	2:D:424:ARG:HB2	2.14	0.48
1:A:1268:ASN:N	1:A:1269:PRO:HD2	2.29	0.48
1:A:1381:ILE:O	1:A:1382:ASP:CB	2.62	0.48
1:A:1554:LYS:CG	1:A:1555:PRO:HD2	2.43	0.48
1:A:1567:SER:HB3	1:A:1578:LYS:HB2	1.96	0.48
1:A:248:ILE:HD13	1:A:325:ILE:CD1	2.44	0.48
1:A:354:LEU:HD23	1:A:450:GLU:HG3	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:792:ASP:OD1	1:A:792:ASP:N	2.47	0.48
2:B:928:VAL:HG23	2:B:1323:MET:HB3	1.96	0.48
1:C:1076:THR:HG22	1:C:1144:LEU:HD11	1.95	0.48
1:C:1474:CYS:HB3	1:C:1476:ARG:NH1	2.29	0.48
1:C:1567:SER:HB3	1:C:1578:LYS:HB2	1.96	0.48
2:D:1632:SER:O	2:D:1636:THR:HB	2.13	0.48
2:D:236:TYR:C	2:D:238:ASP:N	2.67	0.48
2:D:353:TYR:CD2	2:D:614:GLY:C	2.87	0.48
2:D:438:GLN:CD	2:D:530:GLU:HG3	2.35	0.48
2:D:482:LEU:CD1	2:D:482:LEU:N	2.75	0.48
2:D:746:ILE:HD13	2:D:746:ILE:N	2.29	0.48
1:A:1075:SER:HB2	1:A:1120:GLU:OE1	2.14	0.47
1:A:1143:TYR:O	1:A:1146:ALA:N	2.47	0.47
1:A:1128:LYS:HD3	1:A:1414:GLU:OE1	2.14	0.47
1:A:1532:CYS:SG	1:A:1533:GLY:N	2.87	0.47
1:A:1559:TYR:OH	1:A:1591:VAL:HA	2.14	0.47
1:A:494:ASP:O	1:A:494:ASP:CG	2.52	0.47
1:A:811:VAL:O	1:A:811:VAL:CG1	2.62	0.47
1:A:837:GLU:C	1:A:901:LEU:HD12	2.34	0.47
1:A:934:VAL:O	1:A:935:LYS:HG3	2.13	0.47
2:B:145:TYR:CD1	2:B:145:TYR:C	2.88	0.47
2:B:198:ARG:HB3	2:B:213:TYR:CE1	2.49	0.47
2:B:251:TYR:CD2	2:B:257:VAL:HG22	2.49	0.47
2:B:415:THR:HG23	2:B:426:ALA:O	2.13	0.47
2:B:345:ILE:HG13	2:B:428:LYS:HB2	1.94	0.47
2:B:555:LEU:HG	2:B:555:LEU:H	1.49	0.47
2:B:795:THR:CG2	2:B:796:PRO:HD2	2.45	0.47
1:C:100:SER:HB2	1:C:101:TYR:HD2	1.78	0.47
1:C:1143:TYR:O	1:C:1146:ALA:N	2.47	0.47
1:C:346:LYS:HE3	1:C:348:VAL:HG22	1.96	0.47
1:C:471:ASP:O	1:C:472:ASN:HB3	2.14	0.47
1:C:854:GLN:O	1:C:854:GLN:OE1	2.32	0.47
1:C:963:ILE:HG23	1:C:967:LEU:HD23	1.95	0.47
2:D:1517:GLU:OE2	2:D:1518:THR:HG22	2.13	0.47
2:D:795:THR:CG2	2:D:796:PRO:HD2	2.44	0.47
1:A:100:SER:CB	1:A:101:TYR:HD2	2.27	0.47
1:A:163:PHE:HE1	1:A:188:PHE:CB	2.26	0.47
1:A:270:GLY:HA3	1:A:282:MET:CG	2.43	0.47
1:A:968:VAL:HG23	1:A:971:THR:CG2	2.44	0.47
2:B:1278:THR:O	2:B:1313:VAL:HA	2.13	0.47
2:B:1420:LYS:HB3	2:B:1422:ALA:O	2.14	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:443:ASN:OD1	2:B:469:ASN:HB3	2.14	0.47
2:B:449:ILE:HG23	2:B:449:ILE:O	2.14	0.47
2:B:844:ILE:CD1	2:B:872:ILE:HD11	2.44	0.47
1:C:1041:GLU:O	1:C:1045:LEU:HG	2.14	0.47
1:C:1299:GLU:O	1:C:1303:LEU:HB2	2.13	0.47
1:C:1561:TYR:CE1	1:C:1581:LEU:HD11	2.49	0.47
1:C:289:ASN:OD1	1:C:289:ASN:N	2.46	0.47
1:C:330:ILE:HG22	1:C:337:SER:CB	2.31	0.47
1:C:351:PRO:HG2	1:C:352:TYR:HD2	1.71	0.47
1:C:475:ALA:HB1	1:C:477:LEU:CD2	2.44	0.47
2:D:1382:ILE:HG12	2:D:1427:LEU:HD11	1.95	0.47
2:D:235:PHE:CE2	2:D:299:PHE:HE2	2.32	0.47
2:D:259:GLY:HA2	2:D:323:GLU:HB3	1.94	0.47
2:D:449:ILE:HG23	2:D:449:ILE:O	2.14	0.47
2:D:628:LEU:HB3	2:D:636:THR:HG23	1.96	0.47
2:D:842:GLU:O	2:D:843:ASP:C	2.53	0.47
1:A:1246:ARG:O	1:A:1250:THR:HG23	2.15	0.47
1:A:1271:ILE:CD1	1:A:1300:TYR:CZ	2.97	0.47
1:A:1561:TYR:CE1	1:A:1581:LEU:HD11	2.50	0.47
1:A:600:VAL:CG2	1:A:780:VAL:HG21	2.45	0.47
2:B:1476:LYS:HB3	2:B:1476:LYS:HE3	1.60	0.47
1:C:990:ALA:HB1	1:C:1000:LEU:CD1	2.44	0.47
1:C:1307:LEU:H	1:C:1307:LEU:HD22	1.79	0.47
1:C:1344:ASP:OD1	1:C:1345:ASP:N	2.47	0.47
1:C:333:THR:OG1	1:C:334:GLY:N	2.48	0.47
1:C:560:TRP:CZ3	1:C:562:ASN:HB2	2.49	0.47
1:C:774:LEU:HD12	1:C:799:ILE:HD11	1.97	0.47
2:D:126:SER:OG	2:D:127:PHE:N	2.47	0.47
2:D:1289:ARG:C	2:D:1290:TYR:HD1	2.18	0.47
2:D:139:PRO:HG2	2:D:218:LYS:HE2	1.96	0.47
2:D:1384:ILE:HB	2:D:1423:VAL:HG12	1.96	0.47
2:D:1484:ILE:HG22	2:D:1485:CYS:N	2.29	0.47
2:D:1613:GLU:O	2:D:1616:CYS:CB	2.61	0.47
2:D:1628:PHE:O	2:D:1629:ALA:C	2.52	0.47
2:D:217:ARG:HG2	2:D:218:LYS:N	2.29	0.47
2:D:437:THR:HG21	2:D:443:ASN:N	2.30	0.47
2:D:501:GLN:CG	2:D:504:VAL:HG23	2.43	0.47
2:D:581:ASP:O	2:D:582:LYS:C	2.50	0.47
2:D:953:ARG:HG2	2:D:954:VAL:N	2.29	0.47
1:A:1022:PHE:O	1:A:1023:HIS:C	2.51	0.47
1:A:1139:GLU:OE2	1:A:1187:THR:OG1	2.24	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:237:PHE:HA	1:A:345:ILE:HG23	1.97	0.47
1:A:308:LYS:CG	1:A:309:GLU:H	2.25	0.47
1:A:820:PHE:CE2	1:A:821:LYS:O	2.67	0.47
1:A:864:GLY:HA3	1:A:907:LEU:HD22	1.96	0.47
1:A:859:MET:HE1	1:A:898:PHE:CB	2.44	0.47
2:B:1427:LEU:HD23	2:B:1430:VAL:HG23	1.96	0.47
2:B:26:THR:OG1	2:B:44:GLU:HB2	2.15	0.47
2:B:953:ARG:HG2	2:B:954:VAL:N	2.29	0.47
1:C:1104:LEU:O	1:C:1108:VAL:HG12	2.13	0.47
1:C:975:ARG:HH22	1:C:1346:LEU:HD22	1.79	0.47
1:C:1487:PHE:O	1:C:1488:LEU:C	2.53	0.47
1:C:520:ASP:OD1	1:C:520:ASP:N	2.47	0.47
1:C:705:VAL:HA	1:C:739:ARG:HH12	1.77	0.47
2:D:224:PHE:CE2	2:D:329:VAL:HG13	2.49	0.47
2:D:40:GLN:O	2:D:489:ILE:HD12	2.14	0.47
2:D:481:TYR:CD2	2:D:493:GLY:O	2.67	0.47
2:D:581:ASP:OD2	2:D:785:THR:HG21	2.12	0.47
2:D:940:THR:HG22	2:D:942:LEU:HD22	1.96	0.47
1:A:1016:VAL:HG11	1:A:1291:ILE:CD1	2.45	0.47
1:A:1488:LEU:HD12	1:A:1488:LEU:C	2.35	0.47
1:A:23:TYR:CD1	1:A:23:TYR:C	2.88	0.47
1:A:908:HIS:O	1:A:909:ASN:CB	2.61	0.47
2:B:1517:GLU:OE2	2:B:1518:THR:HG22	2.14	0.47
2:B:192:VAL:CG2	2:B:193:SER:H	2.17	0.47
2:B:584:VAL:HG12	2:B:585:TYR:N	2.29	0.47
2:B:599:TRP:CE3	2:B:599:TRP:HA	2.48	0.47
2:B:825:VAL:N	2:B:828:GLU:OE1	2.39	0.47
2:B:940:THR:HG22	2:B:942:LEU:HD22	1.97	0.47
1:C:1217:LEU:HD13	1:C:1237:SER:HA	1.95	0.47
1:C:1183:GLN:HE22	1:C:1232:LEU:HD22	1.80	0.47
1:C:153:LYS:O	1:C:154:PRO:C	2.53	0.47
1:C:163:PHE:CD2	1:C:201:ILE:HG12	2.49	0.47
1:C:373:VAL:CG2	1:C:418:ALA:HB3	2.43	0.47
1:C:531:THR:O	1:C:534:MET:HG3	2.15	0.47
1:C:706:ASN:HD21	1:C:709:GLU:HB2	1.79	0.47
2:D:203:TYR:O	2:D:204:GLU:C	2.53	0.47
2:D:781:ARG:HD3	2:D:781:ARG:HA	1.58	0.47
2:D:842:GLU:O	2:D:844:ILE:HG23	2.15	0.47
1:A:1040:ILE:O	1:A:1043:GLN:HB2	2.14	0.47
1:A:1102:ASN:HD21	1:C:1162:VAL:N	1.99	0.47
1:A:117:MET:HB2	1:A:118:PRO:HD2	1.97	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:502:LEU:HB2	1:A:541:LEU:CD2	2.45	0.47
1:A:889:GLU:HB2	1:A:892:SER:CB	2.39	0.47
1:A:930:VAL:HA	1:A:931:PRO:HD3	1.78	0.47
2:B:416:ASN:HA	2:B:425:GLN:NE2	2.29	0.47
2:B:436:GLN:O	2:B:437:THR:C	2.53	0.47
2:B:735:ASN:CB	2:B:869:GLN:HE22	2.27	0.47
1:C:958:GLU:HA	1:C:1346:LEU:O	2.14	0.47
1:C:1549:LYS:HZ3	1:C:1549:LYS:HG3	1.57	0.47
1:C:174:VAL:CG2	1:C:175:GLU:N	2.77	0.47
1:C:500:ASN:O	1:C:542:VAL:HA	2.15	0.47
2:D:1581:TYR:HA	2:D:1608:GLU:O	2.15	0.47
2:D:557:GLN:HA	2:D:557:GLN:OE1	2.15	0.47
1:A:1190:ILE:HD11	1:A:1253:TYR:CZ	2.50	0.47
1:A:1482:LEU:HD23	1:A:1482:LEU:O	2.15	0.47
1:A:641:ASN:OD1	1:A:644:ASN:HB2	2.15	0.47
1:A:571:LEU:CD2	1:A:812:ALA:HB2	2.44	0.47
2:B:1370:ARG:HG2	2:B:1371:TYR:O	2.14	0.47
2:B:1623:LYS:CA	2:B:1623:LYS:HZ3	2.28	0.47
2:B:478:TYR:HD1	2:B:478:TYR:O	1.98	0.47
1:C:1320:LYS:HD2	1:C:1321:GLY:N	2.22	0.47
1:C:1559:TYR:OH	1:C:1591:VAL:HA	2.14	0.47
1:C:54:ILE:HG12	1:C:106:VAL:HG13	1.95	0.47
1:C:59:TYR:CD1	1:C:60:PRO:CD	2.97	0.47
1:C:837:GLU:C	1:C:901:LEU:HD12	2.34	0.47
2:D:1509:PRO:O	2:D:1512:ILE:HG13	2.14	0.47
2:D:481:TYR:C	2:D:481:TYR:CD2	2.87	0.47
2:D:545:MET:HG3	2:D:798:LYS:O	2.15	0.47
2:D:63:ARG:HB2	2:D:65:GLN:HG3	1.97	0.47
2:D:916:VAL:CG2	2:D:917:PRO:N	2.78	0.47
1:A:1004:PRO:HG3	1:A:1461:ILE:HD13	1.97	0.47
1:A:1044:LYS:O	1:A:1047:LYS:HB3	2.15	0.47
1:A:1054:LEU:HD22	1:A:1057:MET:CE	2.45	0.47
1:A:950:TYR:HD1	1:A:1268:ASN:OD1	1.98	0.47
1:A:820:PHE:O	1:A:821:LYS:CG	2.62	0.47
1:A:834:VAL:HA	1:A:930:VAL:O	2.15	0.47
2:B:1270:HIS:O	2:B:1270:HIS:CG	2.68	0.47
2:B:236:TYR:C	2:B:238:ASP:N	2.68	0.47
2:B:553:ASP:CG	2:B:555:LEU:HD11	2.34	0.47
2:B:148:PHE:CB	2:B:800:ILE:HD11	2.45	0.47
2:B:964:ILE:HG22	2:B:964:ILE:O	2.15	0.47
1:C:1488:LEU:HD12	1:C:1488:LEU:C	2.35	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1421:HIS:NE2	1:C:1498:TYR:CD1	2.82	0.47
1:C:1548:ARG:HD3	1:C:1548:ARG:H	1.79	0.47
1:C:1565:ILE:O	1:C:1566:THR:HG22	2.14	0.47
1:C:624:PHE:CD1	1:C:625:GLN:N	2.83	0.47
2:D:1296:ASN:O	2:D:1297:ALA:C	2.53	0.47
2:D:1380:THR:HG22	2:D:1381:ILE:H	1.79	0.47
2:D:354:PHE:CE2	2:D:409:LEU:HB2	2.50	0.47
2:D:435:TYR:CE1	2:D:616:ASN:HA	2.50	0.47
2:D:621:PHE:H	2:D:621:PHE:HD2	1.62	0.47
2:D:818:LEU:O	2:D:818:LEU:HG	2.15	0.47
1:A:987:ILE:HG22	1:A:1021:VAL:HG23	1.96	0.47
1:A:1076:THR:HG22	1:A:1144:LEU:HD11	1.97	0.47
1:A:265:VAL:HG23	1:A:292:LEU:H	1.79	0.47
2:B:866:TYR:OH	2:B:1388:THR:HG21	2.15	0.47
2:B:646:GLN:HB3	2:B:647:PRO:CD	2.35	0.47
1:C:1159:CYS:N	1:C:1160:PRO:CD	2.77	0.47
1:C:1209:VAL:HG12	1:C:1210:SER:N	2.30	0.47
1:C:1450:PHE:HA	1:C:1464:LEU:HB3	1.97	0.47
1:C:1475:VAL:HG22	1:C:1476:ARG:N	2.30	0.47
1:C:165:ASP:HB2	1:C:166:PRO:HD2	1.97	0.47
1:C:354:LEU:HA	1:C:374:GLN:O	2.15	0.47
1:C:364:LYS:HE2	1:C:465:LEU:O	2.14	0.47
1:C:549:GLU:CD	1:C:549:GLU:N	2.56	0.47
1:C:599:TRP:HE1	1:C:779:LEU:CD1	2.27	0.47
1:C:794:LEU:HD12	1:C:794:LEU:N	2.30	0.47
2:D:1349:VAL:HA	2:D:1364:MET:O	2.14	0.47
2:D:1402:LYS:HA	2:D:1402:LYS:HD3	1.52	0.47
2:D:1412:GLU:HB2	2:D:1419:GLN:CG	2.45	0.47
2:D:252:LEU:HD22	2:D:582:LYS:HB3	1.97	0.47
2:D:59:HIS:O	2:D:104:VAL:HG23	2.14	0.47
1:A:1454:GLN:C	1:A:1455:ILE:HD12	2.35	0.47
1:A:1548:ARG:HD3	1:A:1548:ARG:H	1.80	0.47
1:A:365:PRO:CG	1:A:464:TYR:CE2	2.97	0.47
1:A:500:ASN:O	1:A:542:VAL:HA	2.15	0.47
2:B:1330:ASN:N	2:B:1330:ASN:HD22	2.12	0.47
2:B:1599:TYR:N	2:B:1599:TYR:HD1	2.13	0.47
2:B:525:GLN:NE2	2:B:528:ASN:H	2.13	0.47
2:B:563:MET:HG3	2:B:780:LEU:CD2	2.43	0.47
1:C:1188:LEU:HD23	1:C:1212:LEU:CD2	2.45	0.47
1:C:1000:LEU:HD22	1:C:1281:GLY:CA	2.45	0.47
1:C:1304:VAL:CG1	1:C:1305:LYS:H	2.27	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1323:LEU:CD1	1:C:1324:HIS:H	2.27	0.47
1:C:238:ILE:HG12	1:C:246:PHE:HE1	1.80	0.47
1:C:25:ILE:HD13	1:C:41:ILE:HG13	1.96	0.47
1:C:968:VAL:HG23	1:C:971:THR:CG2	2.44	0.47
2:D:1506:ILE:HD11	2:D:1628:PHE:CE1	2.50	0.47
2:D:555:LEU:HG	2:D:555:LEU:H	1.48	0.47
2:D:584:VAL:HG12	2:D:585:TYR:N	2.29	0.47
2:D:853:ASN:C	2:D:853:ASN:OD1	2.53	0.47
2:D:745:ILE:HG22	2:D:897:LYS:HD3	1.93	0.47
1:A:1113:LEU:HD23	1:A:1114:ASP:N	2.29	0.47
1:A:1344:ASP:OD1	1:A:1345:ASP:N	2.47	0.47
1:A:136:THR:HG21	1:A:222:TYR:HB2	1.96	0.47
1:A:36:SER:HA	1:A:86:THR:CG2	2.45	0.47
2:B:137:TYR:CE1	2:B:143:VAL:HG22	2.49	0.47
2:B:524:TYR:O	2:B:524:TYR:HD1	1.98	0.47
1:C:1090:ASN:OD1	1:C:1094:GLU:HA	2.15	0.47
1:C:1084:ARG:NE	1:C:1154:LYS:HE3	2.30	0.47
1:C:1268:ASN:H	1:C:1268:ASN:HD22	1.62	0.47
1:C:1584:ILE:HG22	1:C:1586:LYS:H	1.80	0.47
1:C:165:ASP:O	1:C:165:ASP:OD2	2.32	0.47
1:C:558:SER:HB3	1:C:645:VAL:HG13	1.97	0.47
2:D:433:ILE:HG22	2:D:434:ALA:N	2.30	0.47
2:D:478:TYR:HD1	2:D:478:TYR:O	1.98	0.47
2:D:518:PHE:CD2	2:D:518:PHE:C	2.88	0.47
2:D:515:ILE:HG21	2:D:599:TRP:CZ2	2.50	0.47
2:D:78:ALA:C	2:D:80:GLY:H	2.18	0.47
1:A:1026:GLU:HA	1:A:1031:TRP:HE1	1.79	0.46
1:A:1358:THR:HB	1:A:1360:HIS:CE1	2.51	0.46
1:A:1480:PHE:CD1	1:A:1480:PHE:N	2.83	0.46
1:A:163:PHE:CD2	1:A:201:ILE:HG12	2.50	0.46
1:A:367:ILE:HD13	1:A:466:TYR:HD2	1.80	0.46
1:A:604:ALA:HB3	1:A:773:TRP:O	2.14	0.46
1:A:784:LYS:HG2	1:A:785:GLN:N	2.30	0.46
1:A:944:LEU:HD23	1:A:944:LEU:N	2.31	0.46
1:A:960:PRO:HB2	1:A:961:TYR:H	1.59	0.46
2:B:1392:PRO:HB2	2:B:1397:LEU:HD22	1.96	0.46
2:B:322:THR:HG21	2:B:326:SER:HG	1.80	0.46
2:B:253:TYR:HE1	2:B:839:TYR:HE2	1.62	0.46
1:C:1146:ALA:O	1:C:1147:PHE:C	2.53	0.46
1:C:116:ARG:O	1:C:117:MET:HB3	2.15	0.46
1:C:136:THR:HG21	1:C:222:TYR:HB2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1562:LYS:CD	1:C:1648:TRP:HZ2	2.27	0.46
1:C:36:SER:HA	1:C:86:THR:CG2	2.45	0.46
1:C:938:SER:O	1:C:940:SER:N	2.48	0.46
1:C:985:GLY:O	1:C:987:ILE:N	2.48	0.46
2:D:58:VAL:HG12	2:D:104:VAL:CG2	2.45	0.46
2:D:1275:LEU:HA	2:D:1317:GLY:HA3	1.97	0.46
2:D:930:LEU:HB2	2:D:1321:ALA:HB3	1.96	0.46
2:D:919:GLY:HA2	2:D:1331:ALA:O	2.15	0.46
2:D:196:THR:HG23	2:D:215:ASP:OD1	2.16	0.46
2:D:230:PRO:HG3	2:D:333:GLN:HG2	1.97	0.46
2:D:398:LEU:HA	2:D:398:LEU:HD23	1.67	0.46
2:D:522:ALA:O	2:D:533:ALA:HB1	2.15	0.46
2:D:954:VAL:O	2:D:957:THR:HG23	2.16	0.46
1:A:1037:ASP:HA	1:A:1038:PRO:HD3	1.81	0.46
1:A:1180:LEU:HD21	1:A:1208:ILE:HG12	1.95	0.46
1:A:977:LEU:HA	1:A:1361:VAL:HG12	1.97	0.46
1:A:1618:LEU:HD22	1:A:1618:LEU:C	2.35	0.46
1:A:392:ALA:HB2	1:A:433:PHE:CB	2.45	0.46
1:A:888:VAL:CG2	1:A:894:HIS:HB2	2.38	0.46
2:B:919:GLY:HA2	2:B:1331:ALA:O	2.16	0.46
2:B:1606:TRP:O	2:B:1606:TRP:HD1	1.98	0.46
2:B:1635:LEU:O	2:B:1637:GLU:N	2.48	0.46
2:B:464:PHE:O	2:B:503:LEU:HA	2.14	0.46
2:B:133:ASP:HB3	2:B:757:TRP:CZ3	2.51	0.46
1:C:1563:VAL:CG2	1:C:1619:ILE:HD12	2.43	0.46
1:C:145:VAL:O	1:C:183:ILE:HD12	2.15	0.46
1:C:623:VAL:O	1:C:625:GLN:N	2.49	0.46
1:C:692:HIS:O	1:C:692:HIS:CD2	2.68	0.46
1:C:600:VAL:CG2	1:C:780:VAL:HG21	2.45	0.46
2:D:1300:ALA:O	2:D:1301:ARG:HD2	2.15	0.46
2:D:162:ILE:CG2	2:D:162:ILE:O	2.63	0.46
2:D:232:GLU:C	2:D:234:PHE:H	2.19	0.46
2:D:268:LYS:HG3	2:D:273:LYS:HG2	1.97	0.46
2:D:356:PRO:HD2	2:D:444:TYR:CZ	2.50	0.46
1:C:421:VAL:HG11	2:D:505:THR:HG22	1.97	0.46
2:D:519:ARG:CZ	2:D:608:GLY:HA3	2.44	0.46
2:D:857:CYS:HB3	2:D:885:VAL:CG2	2.46	0.46
1:A:1067:SER:HA	1:A:1074:ALA:HA	1.98	0.46
1:A:111:PHE:CG	1:A:112:SER:N	2.82	0.46
1:A:1265:ASN:C	1:A:1267:VAL:H	2.17	0.46
1:A:1556:GLU:HB2	1:A:1622:LYS:HE2	1.96	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1584:ILE:CG2	1:A:1585:TYR:N	2.72	0.46
1:A:346:LYS:HE3	1:A:348:VAL:HG22	1.97	0.46
1:A:774:LEU:HG	1:A:788:PHE:CE1	2.50	0.46
1:A:909:ASN:O	1:A:910:ILE:HG12	2.15	0.46
2:B:1289:ARG:O	2:B:1290:TYR:HD1	1.96	0.46
2:B:1292:ILE:HD12	2:B:1296:ASN:OD1	2.16	0.46
2:B:1296:ASN:O	2:B:1297:ALA:C	2.53	0.46
2:B:1312:THR:HG22	2:B:1312:THR:O	2.14	0.46
2:B:1635:LEU:O	2:B:1636:THR:C	2.53	0.46
2:B:214:PHE:CD1	2:B:214:PHE:C	2.88	0.46
2:B:433:ILE:HG22	2:B:434:ALA:N	2.30	0.46
1:C:1290:THR:O	1:C:1294:ILE:CG1	2.63	0.46
1:C:1413:GLU:HA	1:C:1413:GLU:OE2	2.15	0.46
1:C:1648:TRP:HE1	1:C:1664:LEU:HD22	1.81	0.46
1:C:683:ILE:O	1:C:687:ALA:HB3	2.15	0.46
2:D:162:ILE:HG21	2:D:202:LYS:HG2	1.97	0.46
2:D:757:TRP:O	2:D:758:LEU:HD23	2.16	0.46
1:A:1000:LEU:HD22	1:A:1281:GLY:CA	2.45	0.46
1:A:1041:GLU:O	1:A:1045:LEU:HG	2.16	0.46
1:A:1068:VAL:HG13	1:A:1069:TRP:N	2.27	0.46
1:A:977:LEU:CD2	1:A:1361:VAL:HG13	2.45	0.46
1:A:1479:ILE:CD1	1:A:1479:ILE:N	2.78	0.46
1:A:1587:THR:HB	1:A:1591:VAL:HG13	1.97	0.46
1:A:164:ILE:HG22	1:A:164:ILE:O	2.15	0.46
1:A:353:LYS:CE	1:A:378:SER:HA	2.46	0.46
2:B:237:ILE:HD11	2:B:309:LEU:CB	2.44	0.46
2:B:390:THR:HG22	2:B:394:GLY:C	2.35	0.46
2:B:629:THR:HA	2:B:635:ASN:OD1	2.15	0.46
1:C:1271:ILE:CD1	1:C:1300:TYR:CZ	2.98	0.46
1:C:1602:LYS:HB3	1:C:1639:LEU:CB	2.45	0.46
1:C:466:TYR:CZ	1:C:468:ASP:HB2	2.50	0.46
1:C:700:TYR:CD2	1:C:701:ASP:N	2.83	0.46
1:C:803:GLY:O	1:C:810:CYS:HB2	2.16	0.46
2:D:345:ILE:HG13	2:D:428:LYS:HB2	1.95	0.46
2:D:806:TYR:CE1	2:D:807:GLU:O	2.68	0.46
2:D:824:VAL:HG22	2:D:825:VAL:H	1.79	0.46
1:A:1086:LEU:CD1	1:A:1095:GLN:HG3	2.39	0.46
1:A:1160:PRO:HG2	1:C:1098:ASN:OD1	2.15	0.46
1:A:1188:LEU:HD23	1:A:1212:LEU:CD2	2.45	0.46
1:A:1266:TYR:CD1	1:A:1266:TYR:O	2.69	0.46
1:A:975:ARG:HH22	1:A:1346:LEU:HD22	1.74	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1565:ILE:HD13	1:A:1565:ILE:N	2.30	0.46
1:A:1658:GLN:NE2	1:A:1661:LEU:HD12	2.31	0.46
1:A:288:GLN:O	1:A:289:ASN:C	2.54	0.46
1:A:488:PRO:O	1:A:489:LYS:O	2.33	0.46
1:A:584:PRO:HD3	1:A:820:PHE:HB2	1.97	0.46
2:B:445:LEU:HD12	2:B:446:HIS:N	2.31	0.46
2:B:469:ASN:CG	2:B:472:SER:HB2	2.35	0.46
2:B:853:ASN:C	2:B:853:ASN:OD1	2.54	0.46
2:B:885:VAL:HA	2:B:886:PRO:HD3	1.76	0.46
1:C:267:ILE:CG2	1:C:268:THR:N	2.78	0.46
1:C:902:PRO:C	1:C:903:LEU:HD22	2.36	0.46
2:D:1522:TYR:HB2	2:D:1524:TYR:CE1	2.50	0.46
2:D:1540:TYR:HE1	2:D:1575:LEU:HB2	1.80	0.46
2:D:1591:LEU:CD2	2:D:1591:LEU:C	2.84	0.46
2:D:162:ILE:HG23	2:D:162:ILE:O	2.16	0.46
2:D:820:MET:HA	2:D:821:PRO:HD3	1.78	0.46
1:A:1175:LEU:HB3	1:A:1195:LEU:HD11	1.97	0.46
1:A:955:ARG:HD3	1:A:1351:GLY:O	2.16	0.46
1:A:1474:CYS:HB3	1:A:1476:ARG:NH1	2.31	0.46
1:A:1616:GLN:NE2	1:A:1648:TRP:CZ3	2.84	0.46
1:A:958:GLU:HA	1:A:1346:LEU:O	2.16	0.46
2:B:210:TYR:CG	2:B:211:THR:N	2.83	0.46
2:B:848:VAL:HG22	2:B:898:ALA:CB	2.43	0.46
2:B:916:VAL:HG22	2:B:917:PRO:N	2.30	0.46
1:C:1320:LYS:CG	1:C:1321:GLY:N	2.79	0.46
1:C:1556:GLU:HB2	1:C:1622:LYS:HE2	1.97	0.46
1:C:1622:LYS:HD2	1:C:1642:LEU:HB2	1.97	0.46
1:C:1623:GLU:CB	1:C:1638:PRO:CG	2.91	0.46
1:C:251:LYS:HG2	1:C:296:ILE:CD1	2.45	0.46
1:C:286:ALA:O	1:C:287:MET:O	2.33	0.46
1:C:702:GLY:HA2	1:C:728:PHE:CD1	2.48	0.46
1:C:820:PHE:CE2	1:C:821:LYS:O	2.69	0.46
2:D:1480:LEU:HD12	2:D:1481:LEU:N	2.31	0.46
2:D:1527:LYS:H	2:D:1545:LEU:HD13	1.81	0.46
2:D:1635:LEU:O	2:D:1636:THR:C	2.53	0.46
2:D:531:ILE:O	2:D:617:ASN:ND2	2.48	0.46
2:D:822:TYR:O	2:D:914:LYS:HB3	2.15	0.46
1:A:1088:GLN:C	1:A:1090:ASN:H	2.19	0.46
1:A:259:VAL:HB	1:A:295:GLY:HA2	1.97	0.46
1:A:501:TYR:CD1	1:A:501:TYR:C	2.89	0.46
1:A:59:TYR:CD1	1:A:60:PRO:CD	2.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:642:ASN:HD21	1:A:646:PHE:HE1	1.63	0.46
1:A:990:ALA:HB1	1:A:1000:LEU:CD1	2.46	0.46
2:B:1591:LEU:C	2:B:1591:LEU:CD2	2.84	0.46
2:B:563:MET:HA	2:B:563:MET:CE	2.45	0.46
2:B:63:ARG:HB2	2:B:65:GLN:HG3	1.98	0.46
1:C:100:SER:O	1:C:101:TYR:HB2	2.15	0.46
1:C:1094:GLU:CD	1:C:1094:GLU:H	2.19	0.46
1:C:1159:CYS:O	1:C:1164:ILE:HD11	2.15	0.46
1:C:352:TYR:HE1	1:C:383:VAL:HG21	1.80	0.46
1:C:392:ALA:HB2	1:C:433:PHE:CB	2.45	0.46
1:C:672:ILE:C	1:C:673:LEU:HG	2.36	0.46
1:C:587:THR:HG22	1:C:789:ALA:HB2	1.97	0.46
2:D:133:ASP:OD2	2:D:134:LYS:HG2	2.15	0.46
2:D:1607:ILE:N	2:D:1607:ILE:CD1	2.59	0.46
2:D:263:VAL:HG22	2:D:318:VAL:HG23	1.98	0.46
2:D:485:ASN:C	2:D:487:GLY:H	2.19	0.46
2:D:481:TYR:CE2	2:D:493:GLY:C	2.88	0.46
2:D:503:LEU:C	2:D:503:LEU:HD23	2.36	0.46
2:D:844:ILE:CD1	2:D:872:ILE:HD11	2.46	0.46
1:A:1117:SER:HB3	1:A:1174:PHE:CD2	2.49	0.46
1:A:1323:LEU:O	1:A:1324:HIS:O	2.33	0.46
1:A:956:ARG:HG2	1:A:1349:SER:HB3	1.98	0.46
1:A:1618:LEU:HD22	1:A:1619:ILE:N	2.31	0.46
1:A:1675:GLY:O	1:A:1676:CYS:OXT	2.34	0.46
1:A:23:TYR:HD1	1:A:23:TYR:C	2.18	0.46
1:A:612:VAL:HG12	1:A:612:VAL:O	2.16	0.46
1:A:692:HIS:O	1:A:692:HIS:CD2	2.69	0.46
1:A:694:VAL:HG12	1:A:697:LYS:HE3	1.98	0.46
1:A:985:GLY:O	1:A:987:ILE:N	2.49	0.46
2:B:485:ASN:C	2:B:487:GLY:H	2.18	0.46
1:C:1013:MET:O	1:C:1017:PRO:HD3	2.16	0.46
1:C:1075:SER:HB2	1:C:1120:GLU:OE1	2.16	0.46
1:C:1142:LEU:HD13	1:C:1187:THR:CG2	2.46	0.46
1:C:968:VAL:HG12	1:C:1368:THR:CG2	2.45	0.46
1:C:1499:HIS:C	1:C:1500:ARG:HG3	2.36	0.46
1:C:1631:PHE:N	1:C:1631:PHE:CD2	2.82	0.46
1:C:431:LEU:HD22	1:C:432:GLU:N	2.30	0.46
1:C:486:VAL:O	1:C:486:VAL:HG12	2.15	0.46
2:D:1330:ASN:H	2:D:1330:ASN:HD22	1.64	0.46
2:D:378:PRO:HG3	2:D:389:THR:HG23	1.97	0.46
2:D:482:LEU:HD13	2:D:482:LEU:O	2.16	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:466:VAL:HG12	2:D:524:TYR:CE2	2.50	0.46
2:D:814:PHE:HZ	2:D:846:VAL:HG21	1.81	0.46
1:A:947:ARG:CZ	1:A:1354:SER:HB3	2.46	0.46
1:A:1631:PHE:N	1:A:1631:PHE:CD2	2.80	0.46
1:A:383:VAL:O	1:A:383:VAL:HG22	2.16	0.46
1:A:42:GLN:OE1	1:A:500:ASN:ND2	2.49	0.46
1:A:552:ALA:HB3	1:A:658:ASN:HB3	1.98	0.46
1:A:849:ARG:NH1	1:A:849:ARG:CG	2.76	0.46
1:A:875:HIS:HB3	2:B:901:GLN:HE22	1.81	0.46
1:A:96:GLN:HG3	1:A:97:ASN:H	1.80	0.46
2:B:625:GLY:O	2:B:626:LEU:HG	2.16	0.46
1:C:1570:VAL:CG2	1:C:1575:VAL:HG22	2.46	0.46
1:C:487:THR:HG22	1:C:523:TYR:HB2	1.98	0.46
1:C:691:LYS:O	1:C:693:SER:N	2.49	0.46
1:C:681:LYS:HB2	1:C:738:LEU:HD11	1.96	0.46
2:D:1610:TRP:HA	2:D:1611:PRO:HD2	1.74	0.46
2:D:966:GLN:HG3	2:D:966:GLN:O	2.15	0.46
1:A:1081:PHE:HD1	1:A:1147:PHE:HZ	1.63	0.46
1:A:33:VAL:HG23	1:A:120:THR:O	2.14	0.46
1:A:1183:GLN:HE22	1:A:1232:LEU:HD22	1.81	0.46
1:A:1320:LYS:CG	1:A:1321:GLY:N	2.79	0.46
1:A:1320:LYS:HD2	1:A:1321:GLY:N	2.23	0.46
1:A:153:LYS:O	1:A:154:PRO:C	2.54	0.46
1:A:1563:VAL:HG12	1:A:1581:LEU:CD2	2.46	0.46
1:A:1612:VAL:HB	1:A:1615:ARG:CB	2.46	0.46
1:A:145:VAL:O	1:A:183:ILE:HD12	2.15	0.46
1:A:596:MET:SD	1:A:782:ARG:HG3	2.56	0.46
1:A:709:GLU:HA	1:A:709:GLU:OE1	2.16	0.46
1:A:756:THR:O	1:A:757:LEU:HD23	2.16	0.46
2:B:1407:TYR:O	2:B:1408:ILE:HD13	2.16	0.46
2:B:1448:VAL:O	2:B:1449:GLY:O	2.34	0.46
2:B:1590:LEU:CD2	2:B:1591:LEU:N	2.72	0.46
2:B:1599:TYR:CD1	2:B:1599:TYR:N	2.84	0.46
2:B:1628:PHE:O	2:B:1629:ALA:C	2.54	0.46
2:B:275:SER:C	2:B:277:PRO:HD3	2.36	0.46
2:B:409:LEU:HD12	2:B:409:LEU:C	2.36	0.46
2:B:950:LEU:O	2:B:951:ASP:HB2	2.16	0.46
1:C:1026:GLU:HA	1:C:1031:TRP:HE1	1.80	0.46
1:C:398:ASN:O	1:C:399:GLN:HB2	2.16	0.46
1:C:604:ALA:HB3	1:C:773:TRP:O	2.14	0.46
1:C:565:GLU:HG3	1:C:624:PHE:CG	2.51	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:696:LYS:HZ3	1:C:759:PRO:HG2	1.79	0.46
2:D:164:GLU:HB2	2:D:200:VAL:HG23	1.97	0.46
2:D:365:TYR:HA	2:D:394:GLY:O	2.16	0.46
2:D:361:GLU:HB3	2:D:399:ILE:CD1	2.46	0.46
2:D:833:ARG:HB2	2:D:833:ARG:HE	1.56	0.46
1:A:1037:ASP:O	1:A:1040:ILE:HB	2.15	0.45
1:A:1053:MET:HE3	1:A:1086:LEU:CD2	2.46	0.45
1:A:1304:VAL:CG1	1:A:1305:LYS:H	2.28	0.45
1:A:1365:VAL:CG2	1:A:1366:HIS:H	2.25	0.45
1:A:1365:VAL:CG2	1:A:1366:HIS:N	2.77	0.45
1:A:156:LYS:O	1:A:156:LYS:HG3	2.16	0.45
1:A:1570:VAL:HG22	1:A:1575:VAL:HG13	1.97	0.45
1:A:487:THR:HG22	1:A:523:TYR:HB2	1.98	0.45
1:A:824:PHE:O	1:A:845:VAL:HG22	2.17	0.45
2:B:1382:ILE:HG12	2:B:1427:LEU:HD11	1.96	0.45
2:B:1512:ILE:HG22	2:B:1631:PHE:CE1	2.51	0.45
2:B:257:VAL:HG12	2:B:258:GLU:N	2.30	0.45
2:B:263:VAL:HG13	2:B:318:VAL:HA	1.97	0.45
2:B:415:THR:O	2:B:425:GLN:HB3	2.16	0.45
2:B:511:THR:H	2:B:514:LEU:CD1	2.29	0.45
2:B:916:VAL:CG2	2:B:917:PRO:HD2	2.45	0.45
1:C:1106:TRP:CE3	1:C:1107:LEU:HD13	2.51	0.45
1:C:1151:GLY:O	1:C:1152:ILE:C	2.54	0.45
1:C:1189:ALA:O	1:C:1192:ALA:HB3	2.15	0.45
1:C:1271:ILE:HG21	1:C:1300:TYR:CD1	2.51	0.45
1:C:1532:CYS:SG	1:C:1533:GLY:N	2.89	0.45
1:C:1638:PRO:O	1:C:1639:LEU:HD23	2.16	0.45
1:C:270:GLY:HA3	1:C:282:MET:CG	2.46	0.45
1:C:690:TYR:CZ	1:C:692:HIS:HB2	2.51	0.45
2:D:1292:ILE:HD12	2:D:1296:ASN:OD1	2.16	0.45
2:D:813:VAL:HG12	2:D:840:VAL:HG22	1.98	0.45
1:A:120:THR:HG22	1:A:122:ASP:N	2.27	0.45
1:A:123:ASN:HB3	1:A:209:PHE:CD2	2.51	0.45
1:A:956:ARG:HA	1:A:1348:VAL:O	2.16	0.45
1:A:309:GLU:N	1:A:309:GLU:OE1	2.50	0.45
1:A:706:ASN:HD21	1:A:709:GLU:HB2	1.81	0.45
2:B:108:VAL:O	2:B:114:ARG:HA	2.16	0.45
2:B:924:ILE:HD13	2:B:1329:TYR:HE2	1.82	0.45
2:B:1602:THR:C	2:B:1604:ASN:N	2.69	0.45
2:B:226:VAL:HG21	2:B:320:VAL:HG11	1.98	0.45
2:B:543:THR:OG1	2:B:544:CYS:N	2.42	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:59:HIS:O	2:B:104:VAL:HG23	2.16	0.45
2:B:56:ILE:HG12	2:B:71:THR:O	2.16	0.45
2:B:884:ILE:CG1	2:B:885:VAL:N	2.79	0.45
2:B:96:THR:HB	2:B:123:TYR:OH	2.15	0.45
1:C:161:LEU:HD11	1:C:185:PHE:CD2	2.51	0.45
1:C:232:GLU:HA	1:C:233:PRO:HD3	1.77	0.45
1:C:248:ILE:HD13	1:C:325:ILE:CD1	2.46	0.45
1:C:639:GLY:H	1:C:645:VAL:CG2	2.29	0.45
1:C:702:GLY:CA	1:C:728:PHE:CE1	2.88	0.45
2:D:1407:TYR:O	2:D:1408:ILE:HD13	2.16	0.45
2:D:1480:LEU:HD12	2:D:1481:LEU:O	2.17	0.45
2:D:1528:LEU:HD13	2:D:1542:MET:HE2	1.98	0.45
2:D:130:ILE:HD13	2:D:199:ILE:HG22	1.98	0.45
2:D:553:ASP:CG	2:D:555:LEU:HD11	2.36	0.45
1:A:1061:ASN:HB3	1:A:1062:ALA:H	1.52	0.45
1:A:1103:SER:O	1:A:1106:TRP:N	2.48	0.45
1:A:1404:ALA:HB1	1:A:1493:PHE:HE2	1.74	0.45
1:A:161:LEU:HD11	1:A:185:PHE:CE1	2.51	0.45
1:A:163:PHE:HE1	1:A:188:PHE:HB2	1.81	0.45
1:A:227:PHE:HB2	1:A:338:GLU:HG3	1.98	0.45
1:A:333:THR:OG1	1:A:334:GLY:N	2.49	0.45
1:A:560:TRP:CZ3	1:A:562:ASN:HB2	2.51	0.45
1:A:803:GLY:O	1:A:810:CYS:HB3	2.15	0.45
2:B:1284:ARG:HG3	2:B:1285:GLU:H	1.71	0.45
2:B:1504:GLU:OE2	2:B:1505:ARG:N	2.49	0.45
2:B:1509:PRO:O	2:B:1512:ILE:HG13	2.15	0.45
2:B:164:GLU:HB2	2:B:200:VAL:CG2	2.47	0.45
2:B:353:TYR:CD2	2:B:614:GLY:C	2.89	0.45
2:B:490:PHE:CG	2:B:491:LYS:N	2.83	0.45
2:B:466:VAL:HG12	2:B:524:TYR:CE2	2.51	0.45
2:B:824:VAL:HG22	2:B:825:VAL:N	2.32	0.45
2:B:954:VAL:HG12	2:B:955:PRO:HD2	1.99	0.45
1:C:1088:GLN:O	1:C:1090:ASN:N	2.49	0.45
1:C:101:TYR:CE1	1:C:116:ARG:CZ	2.97	0.45
1:C:120:THR:CG2	1:C:122:ASP:H	2.27	0.45
1:C:1290:THR:O	1:C:1294:ILE:HG12	2.16	0.45
1:C:265:VAL:HG23	1:C:292:LEU:H	1.80	0.45
1:C:641:ASN:OD1	1:C:644:ASN:HB2	2.15	0.45
2:D:1292:ILE:HD11	2:D:1301:ARG:NE	2.30	0.45
2:D:1444:LYS:CE	2:D:1447:GLU:HA	2.43	0.45
2:D:1466:GLU:OE2	2:D:1468:CYS:HB2	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:1526:THR:CG2	2:D:1583:ILE:HG13	2.46	0.45
2:D:198:ARG:HB3	2:D:213:TYR:HE1	1.80	0.45
2:D:228:LEU:HD12	2:D:333:GLN:HB2	1.97	0.45
2:D:484:LEU:HD11	2:D:626:LEU:HD11	1.98	0.45
2:D:563:MET:O	2:D:777:SER:HA	2.16	0.45
1:A:1066:TYR:HD1	1:A:1066:TYR:N	2.13	0.45
1:A:1088:GLN:C	1:A:1090:ASN:N	2.69	0.45
1:A:1099:SER:O	1:A:1100:ILE:C	2.55	0.45
1:A:1233:GLN:O	1:A:1234:HIS:HB3	2.17	0.45
1:A:152:LEU:HD12	1:A:152:LEU:HA	1.81	0.45
1:A:1560:ALA:O	1:A:1561:TYR:HB3	2.16	0.45
1:A:1584:ILE:HG22	1:A:1586:LYS:H	1.82	0.45
1:A:267:ILE:CG2	1:A:268:THR:N	2.79	0.45
1:A:226:HIS:ND1	1:A:336:PHE:CE2	2.85	0.45
1:A:791:PRO:CD	1:A:797:TRP:HE1	2.28	0.45
2:B:963:ILE:CD1	2:B:1311:ILE:HG12	2.45	0.45
2:B:196:THR:HG23	2:B:215:ASP:OD1	2.16	0.45
2:B:203:TYR:O	2:B:204:GLU:C	2.55	0.45
2:B:345:ILE:HD11	2:B:427:THR:N	2.31	0.45
1:C:1128:LYS:HG3	1:C:1128:LYS:O	2.15	0.45
1:C:1152:ILE:CG2	1:C:1168:LEU:HD21	2.41	0.45
1:C:296:ILE:CG2	1:C:297:ALA:N	2.78	0.45
1:C:330:ILE:HG13	1:C:330:ILE:O	2.16	0.45
1:C:934:VAL:O	1:C:935:LYS:HG3	2.16	0.45
1:C:942:VAL:CG2	1:C:1359:VAL:HB	2.47	0.45
2:D:1506:ILE:CD1	2:D:1628:PHE:CD1	2.99	0.45
2:D:183:PHE:N	2:D:183:PHE:HD2	2.13	0.45
2:D:267:VAL:HG13	2:D:313:THR:O	2.16	0.45
2:D:416:ASN:HA	2:D:425:GLN:NE2	2.30	0.45
2:D:464:PHE:HB3	2:D:479:PHE:CE2	2.51	0.45
2:D:445:LEU:HD12	2:D:465:ASN:O	2.17	0.45
2:D:83:VAL:HB	2:D:85:PRO:HD3	1.98	0.45
2:D:964:ILE:O	2:D:964:ILE:HG22	2.17	0.45
1:A:1096:ASN:O	1:A:1099:SER:HB3	2.16	0.45
1:A:363:LEU:HD12	1:A:456:ALA:HA	1.98	0.45
1:A:672:ILE:O	1:A:673:LEU:HG	2.15	0.45
1:A:691:LYS:O	1:A:693:SER:N	2.50	0.45
1:A:820:PHE:CZ	1:A:822:ASP:HB2	2.51	0.45
1:A:902:PRO:C	1:A:903:LEU:HD22	2.37	0.45
2:B:829:GLN:HG2	2:B:1480:LEU:HD13	1.99	0.45
2:B:1527:LYS:O	2:B:1529:LEU:HD12	2.16	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:402:ILE:HA	2:B:403:PRO:HD2	1.76	0.45
1:C:1037:ASP:HA	1:C:1038:PRO:HD3	1.79	0.45
1:C:1054:LEU:HD22	1:C:1057:MET:CE	2.46	0.45
1:C:1079:THR:HG21	1:C:1107:LEU:CD1	2.46	0.45
1:C:1212:LEU:O	1:C:1212:LEU:HD13	2.17	0.45
1:C:365:PRO:CG	1:C:464:TYR:HE2	2.28	0.45
1:C:640:LEU:N	1:C:644:ASN:HB3	2.28	0.45
1:C:908:HIS:O	1:C:909:ASN:CB	2.64	0.45
2:D:1448:VAL:O	2:D:1449:GLY:O	2.34	0.45
2:D:1502:HIS:O	2:D:1503:GLN:HB2	2.16	0.45
1:C:917:TRP:O	2:D:813:VAL:CG2	2.65	0.45
1:C:856:CYS:HB2	2:D:904:LEU:HD11	1.97	0.45
1:A:1112:GLN:HB2	1:A:1118:PHE:CE1	2.49	0.45
1:A:1020:TYR:HE1	1:A:1295:GLU:HG3	1.80	0.45
1:A:1364:VAL:O	1:A:1364:VAL:HG13	2.16	0.45
1:A:1404:ALA:HB1	1:A:1493:PHE:CZ	2.49	0.45
1:A:1455:ILE:N	1:A:1455:ILE:HD12	2.29	0.45
1:A:1549:LYS:HZ3	1:A:1549:LYS:HG3	1.59	0.45
1:A:1627:ILE:O	1:A:1629:TYR:N	2.50	0.45
1:A:357:VAL:HG12	1:A:358:ALA:N	2.31	0.45
1:A:706:ASN:HD22	1:A:709:GLU:H	1.65	0.45
1:A:792:ASP:O	1:A:793:SER:CB	2.63	0.45
1:A:829:ILE:CG1	1:A:925:LYS:HG2	2.41	0.45
2:B:942:LEU:HD13	2:B:1314:THR:HG23	1.98	0.45
2:B:1393:ASP:CB	2:B:1443:LEU:HD11	2.42	0.45
2:B:1500:LEU:CD1	2:B:1500:LEU:C	2.84	0.45
2:B:824:VAL:HG12	2:B:913:LEU:HD21	1.99	0.45
1:C:1552:ALA:HB2	1:C:1620:MET:CE	2.47	0.45
1:C:1581:LEU:HD11	1:C:1598:ILE:HD11	1.96	0.45
1:C:1602:LYS:HB3	1:C:1639:LEU:HB2	1.99	0.45
1:C:1627:ILE:O	1:C:1629:TYR:N	2.50	0.45
1:C:32:ARG:HB2	1:C:35:ALA:HB2	1.98	0.45
1:C:672:ILE:O	1:C:673:LEU:HG	2.16	0.45
1:C:709:GLU:OE1	1:C:709:GLU:HA	2.16	0.45
1:C:773:TRP:NE1	1:C:797:TRP:NE1	2.64	0.45
2:D:1270:HIS:CG	2:D:1270:HIS:O	2.70	0.45
2:D:1508:VAL:HB	2:D:1509:PRO:HD3	1.98	0.45
2:D:243:PHE:CE1	2:D:336:ILE:HG21	2.52	0.45
2:D:525:GLN:NE2	2:D:528:ASN:H	2.14	0.45
1:C:856:CYS:SG	2:D:904:LEU:HD21	2.57	0.45
1:A:1020:TYR:O	1:A:1021:VAL:C	2.54	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1079:THR:HG22	1:A:1107:LEU:HD21	1.99	0.45
1:A:1290:THR:O	1:A:1294:ILE:CG1	2.65	0.45
1:A:1381:ILE:HD13	1:A:1509:TYR:CG	2.52	0.45
1:A:272:ARG:O	1:A:321:LYS:HB2	2.17	0.45
1:A:364:LYS:HE2	1:A:465:LEU:O	2.16	0.45
1:A:531:THR:O	1:A:534:MET:HG3	2.16	0.45
1:A:700:TYR:CD2	1:A:701:ASP:N	2.83	0.45
2:B:323:GLU:C	2:B:323:GLU:OE1	2.55	0.45
2:B:954:VAL:HB	2:B:957:THR:CG2	2.35	0.45
1:C:915:GLU:OE2	2:D:903:ALA:HA	2.17	0.45
2:D:111:PRO:O	2:D:113:VAL:HG23	2.17	0.45
2:D:1523:VAL:O	2:D:1548:ILE:HB	2.17	0.45
2:D:825:VAL:O	2:D:826:LYS:C	2.55	0.45
2:D:848:VAL:HG22	2:D:898:ALA:CB	2.43	0.45
1:A:78:LYS:HD2	1:A:498:HIS:NE2	2.32	0.45
2:B:1290:TYR:CD2	2:B:1301:ARG:HB3	2.51	0.45
2:B:1326:LEU:HD11	2:B:1328:PHE:HE2	1.82	0.45
2:B:1601:ILE:HD12	2:B:1601:ILE:H	1.82	0.45
2:B:1601:ILE:N	2:B:1601:ILE:CD1	2.77	0.45
2:B:183:PHE:HD2	2:B:183:PHE:N	2.15	0.45
2:B:553:ASP:O	2:B:555:LEU:HG	2.17	0.45
2:B:151:ASP:HB2	2:B:794:PHE:HZ	1.82	0.45
2:B:172:LEU:HD23	2:B:966:GLN:NE2	2.31	0.45
1:C:1130:GLN:NE2	1:C:1230:ASP:HB3	2.32	0.45
1:C:1190:ILE:O	1:C:1191:SER:C	2.55	0.45
1:C:1213:LYS:C	1:C:1215:GLU:H	2.20	0.45
1:C:1323:LEU:O	1:C:1324:HIS:O	2.35	0.45
1:C:1565:ILE:N	1:C:1565:ILE:HD13	2.32	0.45
1:C:156:LYS:O	1:C:156:LYS:HG3	2.16	0.45
1:C:142:LYS:HA	1:C:187:ASP:OD1	2.17	0.45
1:C:371:ILE:HG21	1:C:390:LEU:CD2	2.47	0.45
1:C:803:GLY:O	1:C:810:CYS:HB3	2.16	0.45
1:C:889:GLU:HB2	1:C:892:SER:CB	2.38	0.45
2:D:1273:LEU:HB2	2:D:1319:GLY:CA	2.36	0.45
2:D:370:ASP:OD1	2:D:370:ASP:N	2.50	0.45
2:D:417:HIS:N	2:D:425:GLN:OE1	2.48	0.45
1:A:1127:ILE:HG12	1:A:1143:TYR:CE2	2.51	0.45
1:A:1289:ASP:O	1:A:1290:THR:C	2.55	0.45
1:A:1324:HIS:CD2	1:A:1336:ARG:NH2	2.85	0.45
1:A:1562:LYS:HD2	1:A:1648:TRP:CZ2	2.46	0.45
1:A:163:PHE:CE1	1:A:188:PHE:CG	3.04	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:522:SER:HB2	1:A:523:TYR:H	1.60	0.45
1:A:690:TYR:CZ	1:A:692:HIS:HB2	2.52	0.45
1:A:963:ILE:HG23	1:A:967:LEU:HD23	1.97	0.45
2:B:1282:PRO:HD2	2:B:1309:GLN:CD	2.37	0.45
2:B:1294:TYR:O	2:B:1294:TYR:HD2	1.99	0.45
2:B:1540:TYR:CE1	2:B:1575:LEU:HB2	2.51	0.45
2:B:228:LEU:CD2	2:B:247:ILE:HG12	2.47	0.45
2:B:390:THR:HG22	2:B:395:THR:N	2.32	0.45
2:B:545:MET:HG3	2:B:798:LYS:O	2.16	0.45
1:C:1184:SER:O	1:C:1187:THR:HB	2.17	0.45
1:C:1568:ILE:CG2	1:C:1577:TYR:HE1	2.26	0.45
1:C:683:ILE:O	1:C:687:ALA:CB	2.65	0.45
1:C:773:TRP:CZ2	1:C:797:TRP:CD1	3.02	0.45
1:C:862:VAL:HB	1:C:865:ILE:CG1	2.45	0.45
1:C:916:THR:O	1:C:918:PHE:N	2.50	0.45
1:C:829:ILE:CG1	1:C:925:LYS:HG2	2.47	0.45
2:D:1323:MET:HE3	2:D:1325:ILE:HD11	1.97	0.45
2:D:309:LEU:O	2:D:310:VAL:C	2.54	0.45
2:D:455:LYS:O	2:D:458:ASP:HB2	2.17	0.45
2:D:518:PHE:CD2	2:D:518:PHE:O	2.69	0.45
2:D:61:PHE:CE2	2:D:62:PRO:HB3	2.51	0.45
2:D:954:VAL:CG1	2:D:955:PRO:HD2	2.47	0.45
2:D:172:LEU:HD23	2:D:966:GLN:NE2	2.31	0.45
1:A:1184:SER:O	1:A:1187:THR:HB	2.17	0.45
1:A:1245:ALA:HB2	1:A:1285:TYR:HB3	1.98	0.45
1:A:1535:MET:HE2	1:A:1645:ILE:HG21	1.99	0.45
1:A:161:LEU:HD11	1:A:185:PHE:CD2	2.52	0.45
1:A:1623:GLU:CB	1:A:1638:PRO:CG	2.93	0.45
1:A:32:ARG:HB2	1:A:35:ALA:HB2	1.99	0.45
1:A:554:LEU:HA	1:A:554:LEU:HD23	1.67	0.45
1:A:829:ILE:HD12	1:A:829:ILE:N	2.32	0.45
1:A:862:VAL:HG12	1:A:907:LEU:HD21	1.99	0.45
2:B:1623:LYS:HB3	2:B:1623:LYS:HZ2	1.82	0.45
2:B:265:PHE:O	2:B:276:ILE:HG13	2.17	0.45
2:B:348:THR:O	2:B:348:THR:OG1	2.27	0.45
2:B:373:PRO:HB3	2:B:393:ASP:O	2.17	0.45
2:B:78:ALA:O	2:B:80:GLY:N	2.49	0.45
2:B:148:PHE:HB2	2:B:800:ILE:HD11	1.99	0.45
1:C:1243:GLY:O	1:C:1285:TYR:CE2	2.69	0.45
1:C:1525:CYS:N	1:C:1528:VAL:HG13	2.32	0.45
1:C:23:TYR:C	1:C:23:TYR:CD1	2.90	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:259:VAL:HB	1:C:295:GLY:HA2	1.98	0.45
1:C:532:GLN:O	1:C:535:VAL:HG22	2.17	0.45
1:C:694:VAL:HG12	1:C:697:LYS:HE3	1.99	0.45
1:C:87:ILE:HG12	1:C:87:ILE:O	2.16	0.45
2:D:103:TYR:HD2	2:D:103:TYR:N	2.15	0.45
2:D:151:ASP:HB2	2:D:794:PHE:HZ	1.82	0.45
2:D:490:PHE:CG	2:D:491:LYS:N	2.85	0.45
2:D:80:GLY:O	2:D:81:MET:HB2	2.17	0.45
1:A:968:VAL:HG12	1:A:1368:THR:CG2	2.47	0.44
1:A:1638:PRO:O	1:A:1639:LEU:HD23	2.17	0.44
1:A:1641:SER:C	1:A:1643:THR:N	2.71	0.44
1:A:501:TYR:CD1	1:A:501:TYR:O	2.69	0.44
1:A:500:ASN:CB	1:A:543:TYR:HE1	2.10	0.44
1:A:839:ILE:CD1	1:A:1485:VAL:HG12	2.48	0.44
1:A:947:ARG:NH1	1:A:1352:PHE:CE2	2.84	0.44
2:B:1594:LYS:HA	2:B:1594:LYS:HE2	1.97	0.44
2:B:484:LEU:HD11	2:B:626:LEU:CD1	2.47	0.44
2:B:628:LEU:HB3	2:B:636:THR:HG23	1.98	0.44
2:B:829:GLN:CA	2:B:829:GLN:HE21	2.30	0.44
1:C:1061:ASN:HB2	1:C:1065:SER:O	2.17	0.44
1:C:1175:LEU:HB3	1:C:1195:LEU:HD11	1.98	0.44
1:C:120:THR:HG22	1:C:121:TYR:N	2.32	0.44
1:C:1320:LYS:HG2	1:C:1342:LEU:HD12	1.99	0.44
1:C:1564:SER:O	1:C:1579:ALA:HB1	2.17	0.44
1:C:185:PHE:CB	1:C:186:PRO:HD2	2.47	0.44
1:C:701:ASP:N	1:C:701:ASP:OD1	2.50	0.44
2:D:1312:THR:HG22	2:D:1312:THR:O	2.16	0.44
2:D:1387:LEU:O	2:D:1390:PHE:HB2	2.17	0.44
2:D:382:GLU:C	2:D:384:PHE:N	2.71	0.44
2:D:884:ILE:CG1	2:D:885:VAL:N	2.79	0.44
1:A:1084:ARG:NE	1:A:1154:LYS:HE3	2.33	0.44
1:A:1313:ILE:HD13	1:A:1350:THR:HB	1.99	0.44
1:A:1329:THR:OG1	1:A:1331:LYS:HG2	2.18	0.44
1:A:935:LYS:HD3	1:A:1373:GLU:OE2	2.18	0.44
1:A:161:LEU:H	1:A:161:LEU:HD12	1.82	0.44
1:A:1648:TRP:HE1	1:A:1664:LEU:HD22	1.82	0.44
1:A:534:MET:H	1:A:534:MET:HG3	1.56	0.44
2:B:1529:LEU:O	2:B:1577:VAL:HG13	2.16	0.44
2:B:1613:GLU:O	2:B:1616:CYS:CB	2.63	0.44
2:B:71:THR:HG23	2:B:72:ARG:N	2.32	0.44
1:C:23:TYR:HD1	1:C:23:TYR:C	2.20	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:180:ILE:CG2	1:C:599:TRP:CE3	3.00	0.44
1:C:115:LYS:HE3	1:C:654:LEU:HD11	1.99	0.44
1:C:682:LYS:HZ2	1:C:686:ILE:CD1	2.14	0.44
2:D:400:LEU:HB3	2:D:402:ILE:HD11	1.99	0.44
1:A:1209:VAL:HG12	1:A:1210:SER:N	2.32	0.44
1:A:1217:LEU:HD13	1:A:1237:SER:HA	1.99	0.44
1:A:1231:ASN:O	1:A:1234:HIS:O	2.35	0.44
1:A:1377:PHE:CD1	1:A:1408:TYR:HA	2.53	0.44
1:A:539:ARG:NH2	1:A:634:CYS:N	2.52	0.44
1:A:690:TYR:C	1:A:692:HIS:H	2.19	0.44
1:A:961:TYR:HE1	1:A:963:ILE:HG12	1.83	0.44
2:B:130:ILE:HD13	2:B:199:ILE:HG22	1.99	0.44
2:B:1442:ILE:HA	2:B:1443:LEU:HD12	1.99	0.44
2:B:262:PHE:HE1	2:B:282:ARG:CG	2.28	0.44
1:A:875:HIS:HB3	2:B:901:GLN:NE2	2.32	0.44
1:C:1088:GLN:C	1:C:1090:ASN:N	2.71	0.44
1:C:1346:LEU:HA	1:C:1346:LEU:HD12	1.45	0.44
1:C:1366:HIS:N	1:C:1366:HIS:ND1	2.66	0.44
1:C:1381:ILE:HD13	1:C:1509:TYR:CG	2.53	0.44
1:C:1559:TYR:CE1	1:C:1586:LYS:O	2.70	0.44
1:C:1618:LEU:HD22	1:C:1619:ILE:N	2.33	0.44
1:C:571:LEU:CD2	1:C:812:ALA:HB2	2.47	0.44
1:C:577:PRO:CD	1:C:588:VAL:HG23	2.48	0.44
1:C:695:VAL:HG12	1:C:727:ALA:CB	2.47	0.44
1:C:753:HIS:HB3	1:C:754:MET:H	1.43	0.44
1:C:916:THR:C	1:C:918:PHE:N	2.71	0.44
2:D:1442:ILE:HA	2:D:1443:LEU:HD12	2.00	0.44
2:D:226:VAL:CG2	2:D:320:VAL:HG11	2.47	0.44
2:D:32:VAL:HB	2:D:607:PHE:CZ	2.53	0.44
2:D:756:LEU:HD22	2:D:778:PHE:CD1	2.52	0.44
1:A:1274:LEU:O	1:A:1277:GLU:N	2.49	0.44
1:A:1455:ILE:HG22	1:A:1455:ILE:O	2.16	0.44
1:A:207:GLU:O	1:A:209:PHE:N	2.50	0.44
1:A:255:PHE:HD1	1:A:255:PHE:O	2.00	0.44
1:A:565:GLU:CD	1:A:565:GLU:H	2.20	0.44
1:A:591:ASN:C	1:A:592:MET:HG3	2.38	0.44
1:A:623:VAL:O	1:A:625:GLN:N	2.51	0.44
1:A:930:VAL:HG13	1:A:931:PRO:N	2.33	0.44
1:A:970:LYS:C	1:A:971:THR:CG2	2.86	0.44
2:B:1484:ILE:HG22	2:B:1485:CYS:N	2.31	0.44
2:B:1527:LYS:H	2:B:1545:LEU:HD13	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:597:LYS:HB3	2:B:597:LYS:NZ	2.33	0.44
2:B:775:THR:HG22	2:B:776:MET:N	2.32	0.44
1:C:1086:LEU:CD1	1:C:1095:GLN:HG3	2.37	0.44
1:C:1113:LEU:HD23	1:C:1114:ASP:N	2.31	0.44
1:C:1179:THR:HG22	1:C:1180:LEU:HD23	2.00	0.44
1:C:1562:LYS:C	1:C:1563:VAL:CG1	2.85	0.44
1:C:1638:PRO:HB2	1:C:1639:LEU:H	1.48	0.44
1:C:196:TYR:CD2	1:C:196:TYR:N	2.82	0.44
1:C:371:ILE:O	1:C:371:ILE:CG2	2.66	0.44
1:C:412:ARG:HG3	1:C:413:VAL:N	2.32	0.44
1:C:534:MET:HG3	1:C:534:MET:H	1.56	0.44
1:C:961:TYR:HE1	1:C:963:ILE:HG12	1.82	0.44
2:D:1501:ASN:H	2:D:1501:ASN:ND2	2.12	0.44
2:D:319:THR:HG23	2:D:330:VAL:CG1	2.47	0.44
2:D:567:LEU:HD11	2:D:577:LEU:HD21	1.99	0.44
1:A:1019:PHE:CE1	1:A:1088:GLN:HB3	2.53	0.44
1:A:1366:HIS:ND1	1:A:1366:HIS:N	2.65	0.44
1:A:532:GLN:O	1:A:535:VAL:HG13	2.17	0.44
1:A:961:TYR:HE2	1:A:1343:ASN:HA	1.82	0.44
2:B:126:SER:OG	2:B:127:PHE:N	2.49	0.44
2:B:355:LYS:O	2:B:358:MET:HB2	2.17	0.44
2:B:347:PHE:CE1	2:B:430:MET:HG2	2.53	0.44
1:C:1099:SER:O	1:C:1100:ILE:C	2.53	0.44
1:C:234:GLU:HG3	1:C:235:TYR:CE2	2.52	0.44
1:C:255:PHE:HD1	1:C:255:PHE:O	2.00	0.44
1:C:412:ARG:HH12	1:C:472:ASN:HD21	1.64	0.44
1:C:443:PRO:CD	1:C:446:ASN:HB2	2.38	0.44
1:C:518:PHE:O	1:C:520:ASP:N	2.43	0.44
2:D:1623:LYS:HZ3	2:D:1623:LYS:CA	2.30	0.44
2:D:235:PHE:HB3	2:D:338:ILE:CG2	2.46	0.44
2:D:299:PHE:CE1	2:D:303:PHE:HD2	2.27	0.44
2:D:460:LEU:O	2:D:460:LEU:HD23	2.17	0.44
1:A:1494:THR:CB	1:A:1506:THR:HG23	2.24	0.44
1:A:1566:THR:O	1:A:1613:LYS:HE3	2.18	0.44
1:A:286:ALA:O	1:A:287:MET:O	2.35	0.44
1:A:323:LEU:O	1:A:323:LEU:HD13	2.18	0.44
1:A:352:TYR:HE1	1:A:383:VAL:HG21	1.81	0.44
1:A:431:LEU:O	1:A:431:LEU:HD13	2.17	0.44
1:A:466:TYR:CZ	1:A:468:ASP:HB2	2.53	0.44
1:A:631:ASP:C	1:A:633:GLY:H	2.21	0.44
1:A:97:ASN:HA	1:A:98:PRO:HD3	1.83	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:1526:THR:CG2	2:B:1583:ILE:HG13	2.47	0.44
2:B:266:GLY:HA3	2:B:315:TYR:CE1	2.53	0.44
2:B:447:VAL:O	2:B:447:VAL:HG13	2.16	0.44
2:B:61:PHE:CE2	2:B:62:PRO:HB3	2.52	0.44
2:B:913:LEU:HD23	2:B:914:LYS:N	2.33	0.44
1:C:1085:VAL:O	1:C:1089:VAL:CG2	2.63	0.44
1:C:1117:SER:HB3	1:C:1174:PHE:CD2	2.51	0.44
1:C:1379:LEU:HD12	1:C:1505:CYS:SG	2.58	0.44
1:C:1455:ILE:O	1:C:1455:ILE:HG22	2.18	0.44
1:C:1482:LEU:O	1:C:1482:LEU:HD23	2.17	0.44
1:C:1562:LYS:NZ	1:C:1664:LEU:HD23	2.32	0.44
1:C:392:ALA:HB1	1:C:432:GLU:O	2.18	0.44
1:C:180:ILE:HB	1:C:599:TRP:CZ3	2.52	0.44
1:C:690:TYR:C	1:C:692:HIS:H	2.19	0.44
2:D:113:VAL:HG12	2:D:114:ARG:N	2.33	0.44
2:D:1594:LYS:HE2	2:D:1594:LYS:HA	1.99	0.44
2:D:469:ASN:CG	2:D:472:SER:HB2	2.36	0.44
2:D:353:TYR:HB2	2:D:613:SER:HG	1.79	0.44
2:D:133:ASP:HB3	2:D:757:TRP:CZ3	2.53	0.44
2:D:951:ASP:C	2:D:953:ARG:N	2.68	0.44
1:A:1106:TRP:CE3	1:A:1107:LEU:HD13	2.52	0.44
1:A:1079:THR:HG21	1:A:1107:LEU:CD1	2.47	0.44
1:A:1309:LEU:HA	1:A:1309:LEU:HD22	1.77	0.44
1:A:1364:VAL:HG22	1:A:1365:VAL:N	2.32	0.44
1:A:171:VAL:CG1	1:A:172:ASP:N	2.81	0.44
1:A:695:VAL:HG12	1:A:727:ALA:CB	2.47	0.44
1:A:256:TYR:HE2	1:A:826:GLU:OE2	2.00	0.44
1:A:867:THR:O	1:A:868:SER:HB3	2.18	0.44
2:B:58:VAL:HG12	2:B:104:VAL:CG2	2.48	0.44
2:B:138:THR:HB	2:B:141:SER:OG	2.18	0.44
2:B:1466:GLU:HG3	2:B:1468:CYS:H	1.83	0.44
2:B:319:THR:HG23	2:B:330:VAL:CG1	2.48	0.44
2:B:364:VAL:O	2:B:395:THR:HA	2.18	0.44
2:B:134:LYS:HB2	2:B:584:VAL:HG11	2.00	0.44
2:B:951:ASP:C	2:B:953:ARG:N	2.68	0.44
1:C:1066:TYR:O	1:C:1074:ALA:HB1	2.17	0.44
1:C:123:ASN:HB3	1:C:209:PHE:CD2	2.53	0.44
1:C:1386:ILE:HG13	1:C:1387:GLU:N	2.28	0.44
1:C:148:LEU:HA	1:C:148:LEU:HD12	1.79	0.44
1:C:969:PRO:HD3	1:C:1603:LYS:HZ1	1.82	0.44
1:C:820:PHE:CZ	1:C:822:ASP:HB2	2.53	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:33:VAL:HA	1:C:87:ILE:HG12	2.00	0.44
2:D:1602:THR:C	2:D:1604:ASN:N	2.70	0.44
2:D:306:LEU:HD12	2:D:306:LEU:HA	1.82	0.44
2:D:345:ILE:HD11	2:D:427:THR:N	2.32	0.44
2:D:476:ILE:CG1	2:D:524:TYR:CD2	3.01	0.44
1:A:1053:MET:HE3	1:A:1086:LEU:HD13	1.99	0.44
1:A:1084:ARG:HB2	1:A:1151:GLY:HA2	1.99	0.44
1:A:1406:ALA:O	1:A:1472:PHE:HA	2.18	0.44
1:A:1475:VAL:HG22	1:A:1476:ARG:N	2.32	0.44
1:A:1562:LYS:HD3	1:A:1664:LEU:CD2	2.46	0.44
1:A:1622:LYS:HD2	1:A:1642:LEU:HB2	1.98	0.44
1:A:27:ALA:HB2	1:A:39:ILE:HG12	1.99	0.44
1:A:373:VAL:CG2	1:A:418:ALA:HB3	2.47	0.44
1:A:475:ALA:O	1:A:476:LEU:HB2	2.17	0.44
1:A:515:ARG:HG3	1:A:526:ILE:HG23	2.00	0.44
1:A:640:LEU:N	1:A:644:ASN:HB3	2.30	0.44
1:A:87:ILE:HG12	1:A:87:ILE:O	2.18	0.44
2:B:1279:ILE:O	2:B:1287:PRO:HB2	2.18	0.44
2:B:1275:LEU:HA	2:B:1317:GLY:HA3	1.99	0.44
2:B:1391:LEU:HD12	2:B:1417:MET:HE1	2.00	0.44
2:B:1610:TRP:CD1	2:B:1628:PHE:HD2	2.36	0.44
1:C:117:MET:HB2	1:C:118:PRO:HD2	1.99	0.44
1:C:1257:THR:O	1:C:1261:LEU:HG	2.18	0.44
1:C:1013:MET:CE	1:C:1287:THR:HB	2.47	0.44
1:C:269:PHE:O	1:C:282:MET:HG2	2.17	0.44
1:C:914:LEU:HD12	1:C:915:GLU:N	2.32	0.44
2:D:1279:ILE:O	2:D:1287:PRO:HB2	2.18	0.44
2:D:924:ILE:HD13	2:D:1329:TYR:HE2	1.83	0.44
2:D:1466:GLU:HG3	2:D:1468:CYS:H	1.83	0.44
2:D:415:THR:O	2:D:425:GLN:HB3	2.18	0.44
2:D:347:PHE:CE1	2:D:430:MET:HG2	2.53	0.44
2:D:625:GLY:O	2:D:626:LEU:HG	2.17	0.44
2:D:856:PHE:CG	2:D:884:ILE:HD11	2.53	0.44
1:A:110:HIS:ND1	1:A:110:HIS:N	2.65	0.44
1:A:1151:GLY:O	1:A:1152:ILE:C	2.53	0.44
1:A:1183:GLN:NE2	1:A:1183:GLN:O	2.50	0.44
1:A:1247:MET:O	1:A:1248:VAL:C	2.56	0.44
1:A:1285:TYR:O	1:A:1286:SER:O	2.36	0.44
1:A:1559:TYR:CE1	1:A:1586:LYS:O	2.70	0.44
1:A:324:TYR:C	1:A:324:TYR:CD2	2.91	0.44
1:A:476:LEU:HD12	1:A:562:ASN:O	2.18	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:530:VAL:HA	1:A:534:MET:SD	2.58	0.44
1:A:96:GLN:HG3	1:A:97:ASN:N	2.33	0.44
2:B:228:LEU:HD12	2:B:333:GLN:HB2	1.99	0.44
2:B:309:LEU:O	2:B:310:VAL:C	2.57	0.44
2:B:349:LYS:HE2	2:B:365:TYR:CD1	2.53	0.44
1:C:1013:MET:HE3	1:C:1287:THR:O	2.18	0.44
1:C:1056:ILE:O	1:C:1056:ILE:HD13	2.17	0.44
1:C:1066:TYR:HD1	1:C:1066:TYR:N	2.15	0.44
1:C:1079:THR:HG22	1:C:1107:LEU:HD21	2.00	0.44
1:C:164:ILE:HG22	1:C:164:ILE:O	2.16	0.44
1:C:412:ARG:HG3	1:C:413:VAL:H	1.82	0.44
1:C:476:LEU:HD12	1:C:562:ASN:O	2.17	0.44
1:C:96:GLN:HG3	1:C:97:ASN:H	1.81	0.44
2:D:1427:LEU:HD23	2:D:1430:VAL:HG23	1.99	0.44
2:D:1480:LEU:HD12	2:D:1480:LEU:C	2.39	0.44
2:D:1599:TYR:CD1	2:D:1599:TYR:N	2.86	0.44
2:D:263:VAL:HG13	2:D:318:VAL:HA	1.99	0.44
1:A:1562:LYS:NZ	1:A:1664:LEU:HD23	2.32	0.43
1:A:1552:ALA:HB2	1:A:1620:MET:CE	2.48	0.43
1:A:1648:TRP:HE1	1:A:1664:LEU:CD2	2.31	0.43
1:A:284:GLN:O	1:A:285:THR:CB	2.66	0.43
1:A:720:LEU:HB2	1:A:721:GLY:H	1.72	0.43
2:B:1286:VAL:O	2:B:1286:VAL:HG12	2.18	0.43
2:B:1383:ASP:HB3	2:B:1457:LYS:HB2	2.00	0.43
2:B:354:PHE:C	2:B:354:PHE:CD1	2.91	0.43
2:B:387:MET:O	2:B:398:LEU:HD21	2.18	0.43
2:B:581:ASP:OD2	2:B:785:THR:HG21	2.17	0.43
1:C:423:ASN:HB3	2:D:501:GLN:NE2	2.33	0.43
1:C:504:LEU:N	1:C:504:LEU:CD1	2.80	0.43
1:C:695:VAL:HG13	1:C:724:CYS:HA	2.00	0.43
2:D:1438:LEU:N	2:D:1438:LEU:HD13	2.32	0.43
2:D:1482:ASN:HB3	2:D:1493:ALA:CB	2.47	0.43
2:D:1512:ILE:HG23	2:D:1631:PHE:CD1	2.53	0.43
2:D:226:VAL:HG22	2:D:249:ALA:HB2	1.99	0.43
2:D:470:ALA:C	2:D:472:SER:H	2.20	0.43
2:D:558:MET:HB3	2:D:558:MET:HE2	1.70	0.43
2:D:580:VAL:HG12	2:D:581:ASP:N	2.32	0.43
2:D:902:GLU:HG3	2:D:902:GLU:O	2.18	0.43
2:D:916:VAL:CG2	2:D:917:PRO:CD	2.95	0.43
1:A:1118:PHE:CD2	1:A:1148:THR:OG1	2.67	0.43
1:A:1142:LEU:O	1:A:1143:TYR:O	2.36	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1224:ILE:HG22	1:A:1225:TYR:HD2	1.83	0.43
1:A:1267:VAL:O	1:A:1270:VAL:HB	2.17	0.43
1:A:127:PHE:CD1	1:A:127:PHE:N	2.84	0.43
1:A:154:PRO:HB2	1:A:155:ALA:H	1.57	0.43
1:A:1602:LYS:HB3	1:A:1639:LEU:CB	2.48	0.43
1:A:1546:GLU:HG2	1:A:1663:ASN:OD1	2.18	0.43
1:A:578:ASP:O	1:A:579:ALA:O	2.35	0.43
1:A:642:ASN:ND2	1:A:646:PHE:CD1	2.86	0.43
1:A:862:VAL:HB	1:A:865:ILE:CG1	2.47	0.43
1:A:917:TRP:O	2:B:813:VAL:HG22	2.18	0.43
2:B:1296:ASN:HB2	2:B:1299:LEU:HD22	2.00	0.43
2:B:1384:ILE:HB	2:B:1423:VAL:HG12	1.99	0.43
2:B:1520:VAL:CG1	2:B:1584:TRP:HD1	2.29	0.43
2:B:171:ILE:H	2:B:171:ILE:HG13	1.60	0.43
2:B:229:GLN:HA	2:B:230:PRO:HD3	1.81	0.43
2:B:237:ILE:HD11	2:B:309:LEU:HB2	2.00	0.43
2:B:382:GLU:C	2:B:384:PHE:N	2.72	0.43
2:B:410:PRO:CA	2:B:431:THR:HG22	2.44	0.43
2:B:857:CYS:HB3	2:B:885:VAL:CG2	2.48	0.43
1:C:1158:ILE:O	1:C:1158:ILE:HG22	2.17	0.43
1:C:1279:ARG:CD	1:C:1279:ARG:C	2.87	0.43
1:C:1439:LEU:O	1:C:1440:LYS:C	2.57	0.43
1:C:439:ALA:O	1:C:441:ASP:N	2.47	0.43
1:C:494:ASP:OD1	1:C:494:ASP:C	2.57	0.43
1:C:612:VAL:O	1:C:612:VAL:HG12	2.17	0.43
1:C:702:GLY:HA3	1:C:728:PHE:CD1	2.53	0.43
1:C:916:THR:C	1:C:918:PHE:H	2.20	0.43
2:D:1562:GLN:CB	2:D:1598:SER:HB3	2.48	0.43
2:D:462:VAL:CG1	2:D:506:MET:HE2	2.48	0.43
2:D:221:LEU:HD11	2:D:753:LYS:CD	2.48	0.43
2:D:789:VAL:HG23	2:D:806:TYR:O	2.18	0.43
1:A:1127:ILE:HD13	1:A:1129:LEU:HD21	2.00	0.43
1:A:1146:ALA:O	1:A:1147:PHE:C	2.57	0.43
1:A:1320:LYS:HG2	1:A:1342:LEU:HD12	1.99	0.43
1:A:1549:LYS:H	1:A:1549:LYS:HG2	1.49	0.43
1:A:1562:LYS:C	1:A:1563:VAL:CG1	2.86	0.43
1:A:1549:LYS:NZ	1:A:1667:PHE:CD1	2.84	0.43
1:A:223:VAL:O	1:A:225:PRO:HD3	2.18	0.43
1:A:415:ASP:CB	1:A:417:VAL:HB	2.48	0.43
1:A:701:ASP:O	1:A:704:CYS:HB2	2.18	0.43
1:A:847:ASN:HD21	1:A:853:MET:HB2	1.83	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:984:VAL:O	1:A:987:ILE:HB	2.18	0.43
2:B:1482:ASN:C	2:B:1493:ALA:HB3	2.38	0.43
2:B:198:ARG:HB3	2:B:213:TYR:HE1	1.82	0.43
2:B:446:HIS:O	2:B:465:ASN:HB2	2.18	0.43
2:B:567:LEU:HD11	2:B:577:LEU:HD21	1.99	0.43
2:B:856:PHE:CG	2:B:884:ILE:HD11	2.54	0.43
1:C:1231:ASN:O	1:C:1234:HIS:O	2.37	0.43
1:C:1213:LYS:CG	1:C:1266:TYR:HE2	2.29	0.43
1:C:1016:VAL:CG1	1:C:1291:ILE:HG13	2.45	0.43
1:C:1311:MET:HB2	1:C:1311:MET:HE3	1.85	0.43
1:C:1378:TYR:O	1:C:1406:ALA:HA	2.17	0.43
1:C:1562:LYS:HD3	1:C:1664:LEU:CD2	2.47	0.43
1:C:322:TYR:HA	1:C:346:LYS:HA	2.00	0.43
1:C:439:ALA:HA	1:C:440:PRO:HD3	1.79	0.43
1:C:506:LYS:CE	1:C:533:ASN:O	2.65	0.43
2:D:1284:ARG:HG3	2:D:1286:VAL:N	2.24	0.43
2:D:145:TYR:HE2	2:D:165:PHE:CE1	2.35	0.43
2:D:1527:LYS:O	2:D:1529:LEU:HD12	2.18	0.43
2:D:1601:ILE:N	2:D:1601:ILE:CD1	2.81	0.43
2:D:1609:ARG:CG	2:D:1609:ARG:NH1	2.61	0.43
2:D:229:GLN:HA	2:D:230:PRO:HD3	1.83	0.43
2:D:261:ALA:HB3	2:D:285:ILE:HD11	1.99	0.43
2:D:466:VAL:CG1	2:D:524:TYR:HE2	2.31	0.43
2:D:820:MET:HE2	2:D:832:ILE:HD13	1.99	0.43
1:A:1033:ILE:HG22	1:A:1034:PHE:HD1	1.81	0.43
1:A:165:ASP:C	1:A:167:GLU:H	2.20	0.43
1:A:234:GLU:HG3	1:A:235:TYR:CE2	2.54	0.43
1:A:269:PHE:CE1	1:A:287:MET:HB3	2.46	0.43
1:A:424:LEU:N	1:A:424:LEU:HD23	2.32	0.43
1:A:444:GLU:O	1:A:445:GLU:C	2.57	0.43
1:A:989:SER:O	1:A:993:SER:CB	2.64	0.43
2:B:238:ASP:OD1	2:B:238:ASP:O	2.36	0.43
2:B:352:LYS:O	2:B:432:ALA:HB1	2.19	0.43
2:B:148:PHE:CZ	2:B:792:VAL:HG11	2.53	0.43
2:B:919:GLY:CA	2:B:1331:ALA:O	2.66	0.43
1:C:1279:ARG:O	1:C:1280:TYR:C	2.57	0.43
1:C:1358:THR:HB	1:C:1360:HIS:CE1	2.54	0.43
1:C:1500:ARG:C	1:C:1502:ASP:N	2.72	0.43
1:C:467:ILE:HG22	1:C:486:VAL:CG2	2.38	0.43
1:C:476:LEU:HD23	1:C:476:LEU:HA	1.81	0.43
1:C:610:TYR:N	1:C:610:TYR:CD1	2.86	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:949:ILE:O	1:C:949:ILE:CG2	2.67	0.43
2:D:1599:TYR:HD1	2:D:1599:TYR:N	2.16	0.43
2:D:266:GLY:HA3	2:D:315:TYR:CE1	2.54	0.43
2:D:511:THR:H	2:D:514:LEU:HD11	1.83	0.43
2:D:574:ARG:HH21	2:D:759:THR:HG21	1.83	0.43
2:D:735:ASN:OD1	2:D:735:ASN:N	2.52	0.43
2:D:825:VAL:HA	2:D:916:VAL:O	2.19	0.43
1:A:1068:VAL:CG2	1:A:1124:TYR:CD1	2.95	0.43
1:A:1257:THR:O	1:A:1261:LEU:HG	2.18	0.43
1:A:165:ASP:O	1:A:167:GLU:N	2.48	0.43
1:A:371:ILE:HG21	1:A:390:LEU:CD2	2.49	0.43
1:A:565:GLU:HG2	1:A:565:GLU:O	2.18	0.43
1:A:571:LEU:HG	1:A:812:ALA:HB2	2.00	0.43
1:A:565:GLU:HG3	1:A:624:PHE:CG	2.53	0.43
1:A:705:VAL:HA	1:A:739:ARG:HH12	1.83	0.43
1:A:969:PRO:HD3	1:A:1603:LYS:HZ1	1.83	0.43
1:A:970:LYS:O	1:A:971:THR:HG22	2.19	0.43
2:B:464:PHE:HB3	2:B:479:PHE:CE2	2.54	0.43
2:B:80:GLY:O	2:B:81:MET:HB2	2.17	0.43
1:C:1233:GLN:O	1:C:1234:HIS:HB3	2.18	0.43
1:C:1377:PHE:CD1	1:C:1408:TYR:HA	2.53	0.43
1:C:1562:LYS:HD2	1:C:1648:TRP:CZ2	2.48	0.43
1:C:1601:ILE:O	1:C:1638:PRO:O	2.36	0.43
1:C:1660:PHE:HE2	1:C:1664:LEU:CD1	2.26	0.43
1:C:1546:GLU:HG2	1:C:1663:ASN:OD1	2.18	0.43
1:C:190:ILE:CG2	1:C:194:PRO:HG3	2.48	0.43
1:C:520:ASP:HB2	2:D:404:LEU:HD13	2.01	0.43
1:C:561:LEU:HA	1:C:561:LEU:HD23	1.80	0.43
1:C:955:ARG:HG2	1:C:1350:THR:O	2.18	0.43
2:D:436:GLN:O	2:D:437:THR:C	2.56	0.43
1:A:1202:HIS:CG	1:A:1203:PRO:HD2	2.53	0.43
1:A:1264:ILE:HG13	1:A:1264:ILE:H	1.39	0.43
1:A:443:PRO:CD	1:A:446:ASN:HB2	2.41	0.43
2:B:103:TYR:HD2	2:B:103:TYR:N	2.17	0.43
2:B:1502:HIS:O	2:B:1503:GLN:HB2	2.18	0.43
2:B:1548:ILE:CG2	2:B:1635:LEU:HB3	2.48	0.43
2:B:230:PRO:HG3	2:B:333:GLN:HG2	2.01	0.43
2:B:621:PHE:H	2:B:621:PHE:HD2	1.66	0.43
2:B:735:ASN:N	2:B:735:ASN:OD1	2.51	0.43
1:C:1243:GLY:O	1:C:1285:TYR:CZ	2.71	0.43
1:C:1644:TRP:CD1	1:C:1646:GLU:OE1	2.71	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:369:TYR:HA	1:C:370:PRO:HD3	1.88	0.43
1:C:532:GLN:O	1:C:535:VAL:HG13	2.18	0.43
1:C:500:ASN:ND2	1:C:543:TYR:CE1	2.86	0.43
1:C:583:SER:O	1:C:586:GLN:HB3	2.18	0.43
1:C:631:ASP:C	1:C:633:GLY:H	2.22	0.43
1:C:696:LYS:HZ1	1:C:759:PRO:HG2	1.84	0.43
2:D:946:LYS:HA	2:D:1310:ASP:OD1	2.18	0.43
2:D:1512:ILE:HG22	2:D:1631:PHE:CE1	2.53	0.43
2:D:939:GLY:O	2:D:1316:SER:HA	2.18	0.43
1:A:1243:GLY:O	1:A:1285:TYR:CE2	2.72	0.43
1:A:1013:MET:HE3	1:A:1287:THR:O	2.19	0.43
1:A:1381:ILE:HB	1:A:1493:PHE:CE2	2.54	0.43
1:A:1622:LYS:HB2	1:A:1643:THR:HG22	1.99	0.43
1:A:1656:SER:O	1:A:1659:ALA:HB3	2.19	0.43
1:A:651:LEU:HD23	1:A:651:LEU:HA	1.74	0.43
1:A:809:ILE:HG12	1:A:810:CYS:H	1.82	0.43
2:B:129:PHE:CE2	2:B:598:ILE:HD13	2.53	0.43
2:B:1402:LYS:HA	2:B:1402:LYS:HD3	1.53	0.43
2:B:820:MET:HA	2:B:821:PRO:HD3	1.79	0.43
1:C:1589:GLU:HB2	1:C:1590:ALA:H	1.46	0.43
1:C:486:VAL:HG11	1:C:499:TYR:CE1	2.54	0.43
1:C:567:CYS:HB3	1:C:570:GLN:HB3	2.01	0.43
1:C:824:PHE:CD2	1:C:824:PHE:N	2.85	0.43
1:C:827:MET:HB3	1:C:829:ILE:CD1	2.47	0.43
1:C:970:LYS:C	1:C:971:THR:CG2	2.87	0.43
2:D:1330:ASN:N	2:D:1330:ASN:HD22	2.16	0.43
2:D:866:TYR:OH	2:D:1388:THR:CG2	2.67	0.43
2:D:373:PRO:HB3	2:D:393:ASP:O	2.19	0.43
2:D:387:MET:O	2:D:398:LEU:HD21	2.18	0.43
2:D:859:ALA:O	2:D:866:TYR:HB2	2.19	0.43
1:A:1013:MET:O	1:A:1017:PRO:HD3	2.18	0.43
1:A:1212:LEU:O	1:A:1215:GLU:HB2	2.18	0.43
1:A:1637:TYR:HA	1:A:1638:PRO:HD3	1.86	0.43
1:A:163:PHE:CE1	1:A:188:PHE:CD1	3.06	0.43
1:A:342:ILE:HA	1:A:343:PRO:HD3	1.74	0.43
1:A:367:ILE:O	1:A:368:PRO:C	2.57	0.43
1:A:494:ASP:C	1:A:494:ASP:OD1	2.57	0.43
1:A:884:VAL:CG1	1:A:886:GLN:CG	2.90	0.43
2:B:1387:LEU:O	2:B:1390:PHE:HB2	2.18	0.43
2:B:1390:PHE:CD1	2:B:1442:ILE:HG13	2.54	0.43
2:B:445:LEU:HD12	2:B:465:ASN:O	2.19	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:885:VAL:HG23	2:B:887:LEU:CD2	2.48	0.43
1:C:1067:SER:HA	1:C:1074:ALA:HA	2.01	0.43
1:C:1120:GLU:OE2	1:C:1121:ASN:N	2.52	0.43
1:C:1127:ILE:HG13	1:C:1143:TYR:CE2	2.44	0.43
1:C:1142:LEU:O	1:C:1143:TYR:O	2.37	0.43
1:C:1159:CYS:O	1:C:1161:LEU:N	2.42	0.43
1:C:1168:LEU:HD23	1:C:1168:LEU:N	2.32	0.43
1:C:27:ALA:HB2	1:C:39:ILE:HG12	2.01	0.43
1:C:226:HIS:ND1	1:C:336:PHE:CE2	2.86	0.43
1:C:383:VAL:O	1:C:383:VAL:HG22	2.18	0.43
1:C:354:LEU:HD23	1:C:450:GLU:HG3	2.01	0.43
1:C:599:TRP:HE1	1:C:779:LEU:CB	2.32	0.43
1:C:867:THR:O	1:C:868:SER:HB3	2.19	0.43
2:D:1296:ASN:HB2	2:D:1299:LEU:HD22	2.01	0.43
2:D:963:ILE:CD1	2:D:1311:ILE:HG12	2.49	0.43
2:D:261:ALA:N	2:D:285:ILE:CD1	2.82	0.43
2:D:338:ILE:C	2:D:339:VAL:CG1	2.87	0.43
2:D:829:GLN:CA	2:D:829:GLN:HE21	2.31	0.43
1:A:1148:THR:O	1:A:1149:VAL:C	2.57	0.43
1:A:128:ILE:HD11	1:A:214:THR:CA	2.49	0.43
1:A:1650:ARG:N	1:A:1650:ARG:HD2	2.27	0.43
1:A:222:TYR:HE1	1:A:768:TYR:CB	2.13	0.43
1:A:624:PHE:CD1	1:A:625:GLN:N	2.85	0.43
2:B:946:LYS:HA	2:B:1310:ASP:OD1	2.18	0.43
2:B:1391:LEU:HD12	2:B:1417:MET:CE	2.49	0.43
2:B:1556:PRO:C	2:B:1558:ALA:N	2.72	0.43
2:B:145:TYR:HE2	2:B:165:PHE:CE1	2.37	0.43
2:B:378:PRO:HG3	2:B:389:THR:HG23	2.00	0.43
2:B:485:ASN:O	2:B:486:LYS:HB2	2.18	0.43
2:B:511:THR:O	2:B:513:ASP:N	2.52	0.43
2:B:32:VAL:HB	2:B:607:PHE:CZ	2.54	0.43
2:B:646:GLN:O	2:B:647:PRO:C	2.57	0.43
2:B:755:TRP:O	2:B:756:LEU:CB	2.66	0.43
2:B:847:ARG:CZ	2:B:867:ARG:NH1	2.82	0.43
2:B:745:ILE:HG22	2:B:897:LYS:HD3	1.97	0.43
2:B:902:GLU:O	2:B:903:ALA:HB2	2.19	0.43
1:C:1022:PHE:O	1:C:1023:HIS:C	2.57	0.43
1:C:1132:THR:HG22	1:C:1133:LEU:N	2.31	0.43
1:C:156:LYS:C	1:C:156:LYS:CD	2.87	0.43
1:C:223:VAL:O	1:C:225:PRO:HD3	2.19	0.43
1:C:552:ALA:O	1:C:658:ASN:ND2	2.52	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:593:ALA:O	1:C:594:THR:HG23	2.17	0.43
1:C:756:THR:O	1:C:757:LEU:HD23	2.19	0.43
1:C:804:ILE:O	1:C:804:ILE:HG13	2.19	0.43
1:C:971:THR:O	1:C:972:GLU:C	2.57	0.43
2:D:1326:LEU:HD11	2:D:1328:PHE:HE2	1.84	0.43
2:D:276:ILE:O	2:D:277:PRO:C	2.57	0.43
1:C:421:VAL:HG23	2:D:507:ASN:ND2	2.33	0.43
2:D:578:VAL:HG13	2:D:578:VAL:O	2.18	0.43
2:D:923:SER:O	2:D:924:ILE:HD12	2.18	0.43
2:D:946:LYS:N	2:D:946:LYS:HD3	2.34	0.43
1:A:101:TYR:N	1:A:101:TYR:CD2	2.87	0.43
1:A:1162:VAL:HG11	1:C:1064:TYR:HE2	1.83	0.43
1:A:1153:ARG:NH2	1:A:1168:LEU:HD13	2.34	0.43
1:A:1638:PRO:O	1:A:1639:LEU:HB2	2.19	0.43
1:A:1638:PRO:HB2	1:A:1639:LEU:H	1.48	0.43
1:A:354:LEU:HA	1:A:374:GLN:O	2.19	0.43
1:A:412:ARG:HG3	1:A:413:VAL:N	2.34	0.43
1:A:495:LYS:HA	1:A:495:LYS:HD3	1.59	0.43
1:A:504:LEU:HD12	1:A:509:ILE:CA	2.48	0.43
2:B:355:LYS:HA	2:B:356:PRO:HD3	1.91	0.43
2:B:466:VAL:CG1	2:B:524:TYR:HE2	2.32	0.43
2:B:756:LEU:HD22	2:B:778:PHE:CD1	2.53	0.43
2:B:788:VAL:HG22	2:B:807:GLU:HG2	2.01	0.43
1:C:101:TYR:N	1:C:101:TYR:CD2	2.87	0.43
1:C:1155:ALA:O	1:C:1158:ILE:HG13	2.19	0.43
1:C:1298:THR:O	1:C:1301:SER:N	2.52	0.43
1:C:1365:VAL:CG2	1:C:1366:HIS:N	2.75	0.43
1:C:1455:ILE:CD1	1:C:1455:ILE:N	2.82	0.43
1:C:1664:LEU:HD23	1:C:1664:LEU:O	2.19	0.43
1:C:25:ILE:HD13	1:C:41:ILE:CG1	2.49	0.43
1:C:553:GLU:HA	1:C:553:GLU:OE1	2.19	0.43
1:C:74:SER:HA	1:C:79:PHE:HE1	1.84	0.43
1:C:773:TRP:CZ3	1:C:788:PHE:CE1	2.92	0.43
2:D:1525:LYS:HD2	2:D:1610:TRP:CZ2	2.53	0.43
2:D:202:LYS:CG	2:D:203:TYR:N	2.82	0.43
2:D:262:PHE:HE1	2:D:282:ARG:CG	2.29	0.43
2:D:646:GLN:HB3	2:D:647:PRO:CD	2.37	0.43
2:D:74:ASP:OD1	2:D:74:ASP:N	2.52	0.43
2:D:96:THR:HB	2:D:123:TYR:OH	2.18	0.43
1:A:196:TYR:CD2	1:A:196:TYR:N	2.85	0.42
1:A:27:ALA:HB1	1:A:28:PRO:HD2	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:HG3	1:A:413:VAL:H	1.84	0.42
1:A:587:THR:CG2	1:A:789:ALA:HB2	2.49	0.42
1:A:33:VAL:HA	1:A:87:ILE:CG1	2.49	0.42
1:A:916:THR:O	1:A:918:PHE:N	2.52	0.42
2:B:1466:GLU:OE2	2:B:1468:CYS:HB2	2.19	0.42
2:B:1505:ARG:NH1	2:B:1627:ASP:OD1	2.51	0.42
2:B:1562:GLN:HB2	2:B:1598:SER:HB3	2.00	0.42
2:B:531:ILE:O	2:B:617:ASN:ND2	2.51	0.42
2:B:748:ARG:NH1	2:B:784:ILE:HG12	2.33	0.42
1:C:1007:SER:HA	1:C:1069:TRP:HD1	1.83	0.42
1:C:1213:LYS:HE2	1:C:1266:TYR:CE2	2.54	0.42
1:C:1648:TRP:HE1	1:C:1664:LEU:CD2	2.32	0.42
1:C:348:VAL:HG12	1:C:350:SER:H	1.84	0.42
1:C:473:HIS:HE1	2:D:455:LYS:HZ3	1.67	0.42
1:C:49:ALA:HB2	1:C:74:SER:HB2	2.01	0.42
1:C:503:ILE:HD11	1:C:528:ILE:HG21	2.01	0.42
1:C:554:LEU:HD23	1:C:554:LEU:HA	1.60	0.42
2:D:952:ASP:O	2:D:1331:ALA:HB1	2.19	0.42
2:D:449:ILE:HD13	2:D:462:VAL:CG2	2.45	0.42
2:D:567:LEU:HD23	2:D:567:LEU:HA	1.55	0.42
2:D:580:VAL:CG1	2:D:581:ASP:N	2.81	0.42
2:D:824:VAL:HG22	2:D:825:VAL:N	2.34	0.42
1:A:1022:PHE:O	1:A:1025:LEU:N	2.52	0.42
1:A:1060:ARG:CG	1:A:1061:ASN:N	2.82	0.42
1:A:1090:ASN:C	1:A:1092:TYR:N	2.72	0.42
1:A:1226:ARG:HD3	1:A:1266:TYR:CE1	2.54	0.42
1:A:1279:ARG:O	1:A:1280:TYR:C	2.56	0.42
1:A:1413:GLU:OE2	1:A:1413:GLU:HA	2.19	0.42
1:A:153:LYS:O	1:A:154:PRO:O	2.37	0.42
1:A:171:VAL:HG22	1:A:1057:MET:CE	2.49	0.42
1:A:847:ASN:ND2	1:A:853:MET:HB2	2.34	0.42
2:B:350:THR:HA	2:B:351:PRO:HD3	1.88	0.42
2:B:511:THR:OG1	2:B:512:PRO:HD2	2.18	0.42
2:B:946:LYS:N	2:B:946:LYS:HD3	2.34	0.42
1:C:110:HIS:N	1:C:110:HIS:ND1	2.66	0.42
1:C:1143:TYR:O	1:C:1144:LEU:C	2.56	0.42
1:C:1118:PHE:HE2	1:C:1148:THR:HG1	1.57	0.42
1:C:1255:LEU:C	1:C:1255:LEU:HD12	2.40	0.42
1:C:1324:HIS:CG	1:C:1336:ARG:NH2	2.87	0.42
1:C:1467:ILE:HA	1:C:1468:PRO:HD3	1.78	0.42
1:C:1570:VAL:HG22	1:C:1575:VAL:HG13	2.00	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:363:LEU:HD12	1:C:456:ALA:HA	2.00	0.42
1:C:620:LEU:HG	1:C:620:LEU:H	1.60	0.42
1:C:784:LYS:HG2	1:C:785:GLN:N	2.33	0.42
1:C:862:VAL:HG12	1:C:907:LEU:HD21	2.01	0.42
1:C:961:TYR:HE2	1:C:1343:ASN:HA	1.83	0.42
2:D:129:PHE:CE2	2:D:598:ILE:HD13	2.54	0.42
2:D:919:GLY:CA	2:D:1331:ALA:O	2.67	0.42
2:D:275:SER:C	2:D:277:PRO:HD3	2.39	0.42
2:D:358:MET:HE3	2:D:358:MET:HB2	1.95	0.42
2:D:553:ASP:O	2:D:555:LEU:HG	2.19	0.42
2:D:811:MET:HG3	2:D:812:LYS:N	2.34	0.42
2:D:942:LEU:HD13	2:D:1314:THR:HG23	2.01	0.42
2:D:943:GLU:HB2	2:D:1313:VAL:HG23	2.01	0.42
1:A:1086:LEU:O	1:A:1087:GLY:C	2.57	0.42
1:A:1094:GLU:H	1:A:1094:GLU:CD	2.22	0.42
1:A:1179:THR:HG22	1:A:1180:LEU:HD23	2.01	0.42
1:A:1189:ALA:O	1:A:1192:ALA:HB3	2.19	0.42
1:A:1226:ARG:HD2	1:A:1270:VAL:CG2	2.50	0.42
1:A:1370:THR:O	1:A:1371:SER:C	2.56	0.42
1:A:847:ASN:ND2	1:A:853:MET:CB	2.83	0.42
1:A:914:LEU:HD12	1:A:915:GLU:N	2.34	0.42
1:A:832:SER:HA	1:A:928:ARG:HB3	2.02	0.42
2:B:111:PRO:O	2:B:113:VAL:HG23	2.19	0.42
2:B:113:VAL:HG12	2:B:114:ARG:N	2.34	0.42
2:B:1273:LEU:HB2	2:B:1319:GLY:CA	2.36	0.42
2:B:1506:ILE:HD11	2:B:1628:PHE:CE1	2.54	0.42
2:B:1548:ILE:HD12	2:B:1636:THR:OG1	2.18	0.42
2:B:336:ILE:HD13	2:B:336:ILE:HA	1.78	0.42
2:B:358:MET:HB2	2:B:358:MET:HE3	1.99	0.42
2:B:775:THR:HG22	2:B:776:MET:H	1.84	0.42
2:B:218:LYS:CD	2:B:822:TYR:HE2	2.31	0.42
1:C:1068:VAL:CG2	1:C:1124:TYR:CD1	2.94	0.42
1:C:1020:TYR:HE1	1:C:1295:GLU:HG3	1.84	0.42
1:C:1381:ILE:CG1	1:C:1382:ASP:N	2.81	0.42
1:C:144:ARG:HD2	1:C:146:TYR:CZ	2.54	0.42
1:C:1641:SER:C	1:C:1643:THR:N	2.73	0.42
1:C:1658:GLN:HA	1:C:1661:LEU:HB2	2.01	0.42
1:C:499:TYR:HE2	1:C:517:LYS:HG3	1.84	0.42
1:C:534:MET:HB3	1:C:538:SER:OG	2.19	0.42
1:C:584:PRO:CB	1:C:792:ASP:HA	2.37	0.42
1:C:827:MET:HB3	1:C:829:ILE:HD13	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:870:SER:N	1:C:871:PRO:HD3	2.33	0.42
2:D:1305:THR:HG23	2:D:1307:LEU:N	2.30	0.42
2:D:138:THR:HG22	2:D:139:PRO:O	2.18	0.42
2:D:477:LYS:HD3	2:D:477:LYS:H	1.84	0.42
2:D:64:LYS:HG3	2:D:64:LYS:O	2.20	0.42
2:D:69:PHE:HE2	2:D:71:THR:HB	1.84	0.42
2:D:788:VAL:HG22	2:D:807:GLU:HG2	2.01	0.42
1:A:1013:MET:HA	1:A:1016:VAL:HG23	2.00	0.42
1:A:1027:THR:HG21	1:A:1302:LEU:HD13	2.02	0.42
1:A:54:ILE:CG1	1:A:106:VAL:HG13	2.49	0.42
1:A:1664:LEU:O	1:A:1664:LEU:HD23	2.19	0.42
1:A:774:LEU:HD12	1:A:799:ILE:HD11	2.02	0.42
2:B:1305:THR:HG23	2:B:1306:LYS:N	2.34	0.42
2:B:1525:LYS:HD2	2:B:1610:TRP:CZ2	2.54	0.42
2:B:449:ILE:HD13	2:B:462:VAL:CG2	2.46	0.42
2:B:491:LYS:HB3	2:B:491:LYS:HE2	1.71	0.42
2:B:830:VAL:HG23	2:B:831:GLU:N	2.34	0.42
2:B:933:ARG:HH11	2:B:933:ARG:HG3	1.84	0.42
1:C:1088:GLN:C	1:C:1090:ASN:H	2.22	0.42
1:C:1280:TYR:O	1:C:1280:TYR:CG	2.72	0.42
1:C:1027:THR:HG21	1:C:1302:LEU:HD13	2.01	0.42
1:C:1307:LEU:HD22	1:C:1307:LEU:N	2.33	0.42
1:C:1439:LEU:HD23	1:C:1439:LEU:HA	1.61	0.42
1:C:1545:ALA:HB2	1:C:1660:PHE:CE1	2.54	0.42
1:C:1585:TYR:CE1	1:C:1671:ILE:HG12	2.51	0.42
1:C:27:ALA:HB1	1:C:28:PRO:CD	2.50	0.42
1:C:395:ILE:CG1	1:C:430:VAL:HB	2.50	0.42
1:C:424:LEU:HD23	1:C:424:LEU:N	2.34	0.42
1:C:774:LEU:HG	1:C:788:PHE:HE1	1.84	0.42
1:C:780:VAL:HA	1:C:781:PRO:HD3	1.85	0.42
2:D:102:GLN:C	2:D:103:TYR:HD2	2.22	0.42
2:D:1370:ARG:HG2	2:D:1371:TYR:O	2.19	0.42
2:D:415:THR:O	2:D:415:THR:OG1	2.34	0.42
2:D:829:GLN:HG2	2:D:1480:LEU:HD13	2.01	0.42
1:A:1091:LYS:H	1:A:1091:LYS:HG3	1.39	0.42
1:A:1016:VAL:CG2	1:A:1291:ILE:HD12	2.49	0.42
1:A:532:GLN:O	1:A:535:VAL:HG22	2.20	0.42
1:A:610:TYR:CD1	1:A:610:TYR:N	2.86	0.42
2:B:1292:ILE:HD11	2:B:1301:ARG:NE	2.32	0.42
2:B:1506:ILE:CD1	2:B:1628:PHE:CD1	3.03	0.42
2:B:1525:LYS:HD2	2:B:1610:TRP:CZ3	2.54	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:354:PHE:O	2:B:434:ALA:HA	2.19	0.42
2:B:558:MET:HE2	2:B:558:MET:HB3	1.64	0.42
2:B:567:LEU:HD23	2:B:567:LEU:HA	1.52	0.42
2:B:780:LEU:HD22	2:B:780:LEU:HA	1.83	0.42
1:C:1083:LEU:CD1	1:C:1104:LEU:HD23	2.49	0.42
1:C:1101:CYS:O	1:C:1105:LEU:HD12	2.20	0.42
1:C:1183:GLN:NE2	1:C:1183:GLN:O	2.53	0.42
1:C:196:TYR:H	1:C:196:TYR:HD2	1.64	0.42
1:C:444:GLU:O	1:C:445:GLU:C	2.57	0.42
1:C:256:TYR:HE2	1:C:826:GLU:OE2	2.02	0.42
1:C:85:LEU:N	1:C:85:LEU:CD2	2.79	0.42
2:D:108:VAL:O	2:D:114:ARG:HA	2.18	0.42
2:D:1385:SER:OG	2:D:1455:SER:N	2.47	0.42
2:D:1606:TRP:O	2:D:1606:TRP:HD1	2.03	0.42
2:D:1635:LEU:O	2:D:1637:GLU:N	2.52	0.42
2:D:485:ASN:O	2:D:486:LYS:HB2	2.18	0.42
2:D:524:TYR:HE1	2:D:532:VAL:CG1	2.29	0.42
2:D:859:ALA:HB1	2:D:866:TYR:CD1	2.55	0.42
1:A:1581:LEU:HD11	1:A:1598:ILE:HD11	1.99	0.42
1:A:185:PHE:CB	1:A:186:PRO:HD2	2.49	0.42
1:A:438:ASP:HA	1:A:447:GLN:NE2	2.35	0.42
1:A:501:TYR:HD1	1:A:501:TYR:C	2.21	0.42
1:A:626:PHE:O	1:A:628:GLU:N	2.52	0.42
1:A:689:LYS:O	1:A:691:LYS:N	2.52	0.42
2:B:232:GLU:C	2:B:234:PHE:H	2.22	0.42
2:B:490:PHE:C	2:B:490:PHE:CD1	2.91	0.42
1:C:1037:ASP:O	1:C:1040:ILE:HB	2.19	0.42
1:C:1618:LEU:C	1:C:1618:LEU:HD22	2.40	0.42
1:C:487:THR:HA	1:C:488:PRO:HD3	1.81	0.42
1:C:516:GLU:N	1:C:516:GLU:CD	2.70	0.42
1:C:715:ALA:O	1:C:718:ILE:HG13	2.20	0.42
1:C:829:ILE:HA	1:C:830:PRO:HD3	1.84	0.42
1:C:839:ILE:CD1	1:C:1485:VAL:HG12	2.50	0.42
1:C:946:PRO:HB2	1:C:947:ARG:H	1.52	0.42
2:D:1367:ILE:HD13	2:D:1456:VAL:CG2	2.49	0.42
2:D:1540:TYR:CE1	2:D:1575:LEU:HB2	2.54	0.42
2:D:263:VAL:HG23	2:D:283:ILE:CD1	2.48	0.42
1:C:849:ARG:NH2	2:D:556:ILE:O	2.52	0.42
1:A:1025:LEU:HD23	1:A:1025:LEU:HA	1.72	0.42
1:A:1208:ILE:HG22	1:A:1208:ILE:O	2.19	0.42
1:A:1255:LEU:C	1:A:1255:LEU:HD12	2.39	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1311:MET:HE3	1:A:1311:MET:HB2	1.88	0.42
1:A:1504:GLN:HG3	1:A:1505:CYS:N	2.35	0.42
1:A:1602:LYS:HB3	1:A:1639:LEU:HB2	2.02	0.42
1:A:1652:THR:HB	1:A:1653:THR:H	1.73	0.42
2:B:219:TYR:CD1	2:B:220:VAL:N	2.86	0.42
2:B:229:GLN:OE1	2:B:229:GLN:HA	2.19	0.42
2:B:29:THR:CB	2:B:30:PRO:CD	2.97	0.42
2:B:263:VAL:CG1	2:B:318:VAL:HG23	2.50	0.42
2:B:236:TYR:CZ	2:B:424:ARG:HD2	2.54	0.42
2:B:480:THR:OG1	2:B:494:ARG:NE	2.51	0.42
1:C:1364:VAL:HG22	1:C:1365:VAL:N	2.35	0.42
1:C:1549:LYS:H	1:C:1549:LYS:HG2	1.51	0.42
1:C:1658:GLN:N	1:C:1658:GLN:HE21	2.17	0.42
1:C:1549:LYS:NZ	1:C:1667:PHE:CD1	2.85	0.42
1:C:269:PHE:CE1	1:C:287:MET:HB3	2.47	0.42
1:C:365:PRO:CD	1:C:464:TYR:CE2	3.03	0.42
1:C:864:GLY:HA3	1:C:907:LEU:HD22	2.01	0.42
2:D:1438:LEU:HD22	2:D:1438:LEU:C	2.39	0.42
2:D:524:TYR:HD1	2:D:524:TYR:O	2.03	0.42
2:D:848:VAL:HG12	2:D:848:VAL:O	2.18	0.42
2:D:916:VAL:HG23	2:D:917:PRO:CD	2.48	0.42
1:A:162:THR:HG21	1:A:204:LYS:CE	2.40	0.42
1:A:386:VAL:HA	1:A:387:PRO:HD3	1.89	0.42
1:A:391:ASN:HD21	1:A:406:PRO:HG3	1.84	0.42
1:A:25:ILE:HD13	1:A:41:ILE:HG13	2.01	0.42
1:A:517:LYS:HG2	1:A:518:PHE:H	1.85	0.42
1:A:544:TYR:HE2	1:A:546:VAL:CG2	2.33	0.42
1:A:549:GLU:CD	1:A:549:GLU:N	2.57	0.42
1:A:594:THR:OG1	1:A:782:ARG:CA	2.67	0.42
1:A:786:LEU:N	1:A:786:LEU:HD23	2.30	0.42
2:B:1323:MET:HE3	2:B:1325:ILE:HD11	2.02	0.42
2:B:1623:LYS:HD2	2:B:1623:LYS:N	2.31	0.42
2:B:350:THR:CG2	2:B:350:THR:O	2.68	0.42
2:B:398:LEU:HA	2:B:398:LEU:HD23	1.68	0.42
2:B:438:GLN:HB2	2:B:617:ASN:HD21	1.83	0.42
2:B:476:ILE:HD11	2:B:524:TYR:CB	2.49	0.42
2:B:69:PHE:HE2	2:B:71:THR:HB	1.85	0.42
2:B:742:ASP:OD1	2:B:743:SER:N	2.53	0.42
2:B:847:ARG:HG3	2:B:869:GLN:CG	2.50	0.42
2:B:954:VAL:O	2:B:957:THR:HG23	2.20	0.42
1:C:1043:GLN:O	1:C:1044:LYS:C	2.58	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1103:SER:O	1:C:1106:TRP:N	2.50	0.42
1:C:1148:THR:O	1:C:1149:VAL:C	2.56	0.42
1:C:31:PHE:O	1:C:119:ILE:HA	2.19	0.42
1:C:1381:ILE:HB	1:C:1493:PHE:CE2	2.55	0.42
1:C:1587:THR:HB	1:C:1591:VAL:HG13	2.01	0.42
1:C:639:GLY:H	1:C:645:VAL:HA	1.84	0.42
1:C:571:LEU:HD22	1:C:803:GLY:HA3	2.02	0.42
2:D:1286:VAL:O	2:D:1286:VAL:HG12	2.20	0.42
2:D:1371:TYR:HB2	2:D:1377:SER:HB3	2.02	0.42
2:D:164:GLU:HB2	2:D:200:VAL:CG2	2.50	0.42
2:D:146:ARG:HA	2:D:183:PHE:CE2	2.54	0.42
2:D:264:LEU:HB2	2:D:280:LEU:HB2	2.02	0.42
2:D:354:PHE:O	2:D:434:ALA:HA	2.19	0.42
2:D:819:GLN:NE2	2:D:819:GLN:CA	2.82	0.42
1:A:1243:GLY:O	1:A:1285:TYR:CZ	2.73	0.42
1:A:1587:THR:HB	1:A:1591:VAL:CG2	2.48	0.42
1:A:1545:ALA:HB2	1:A:1660:PHE:CE1	2.55	0.42
1:A:831:TYR:O	1:A:928:ARG:CB	2.67	0.42
1:A:870:SER:N	1:A:871:PRO:HD3	2.33	0.42
2:B:102:GLN:C	2:B:103:TYR:HD2	2.23	0.42
2:B:1349:VAL:CG2	2:B:1363:LEU:HD12	2.50	0.42
2:B:1397:LEU:HA	2:B:1397:LEU:HD12	1.75	0.42
2:B:370:ASP:N	2:B:370:ASP:OD1	2.52	0.42
2:B:818:LEU:HD23	2:B:911:LYS:CD	2.44	0.42
2:B:963:ILE:O	2:B:963:ILE:HG22	2.20	0.42
1:C:1020:TYR:O	1:C:1021:VAL:C	2.59	0.42
1:C:1060:ARG:CG	1:C:1061:ASN:N	2.83	0.42
1:C:1091:LYS:HG3	1:C:1091:LYS:H	1.43	0.42
1:C:1212:LEU:O	1:C:1215:GLU:HB2	2.20	0.42
1:C:1279:ARG:CZ	1:C:1280:TYR:CD2	3.03	0.42
1:C:1545:ALA:CB	1:C:1660:PHE:CE1	3.03	0.42
1:C:1636:ILE:O	1:C:1636:ILE:CG2	2.68	0.42
1:C:20:GLU:O	1:C:20:GLU:CG	2.61	0.42
1:C:565:GLU:HG2	1:C:565:GLU:O	2.20	0.42
1:C:621:GLU:HG3	1:C:621:GLU:H	1.74	0.42
1:C:949:ILE:C	1:C:950:TYR:CG	2.93	0.42
2:D:1294:TYR:O	2:D:1294:TYR:HD2	2.02	0.42
2:D:1378:THR:O	2:D:1379:MET:C	2.58	0.42
2:D:1424:ILE:CD1	2:D:1424:ILE:N	2.76	0.42
2:D:1602:THR:H	2:D:1605:THR:HB	1.85	0.42
2:D:296:ARG:NH1	2:D:296:ARG:CG	2.83	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:435:TYR:OH	2:D:617:ASN:HB3	2.20	0.42
2:D:646:GLN:O	2:D:647:PRO:C	2.59	0.42
2:D:739:PHE:CE1	2:D:901:GLN:HB2	2.55	0.42
2:D:830:VAL:HG23	2:D:831:GLU:N	2.34	0.42
2:D:860:SER:OG	2:D:866:TYR:HB3	2.20	0.42
2:D:857:CYS:HB3	2:D:885:VAL:HG22	2.01	0.42
1:A:1212:LEU:HD13	1:A:1228:TRP:NE1	2.35	0.42
1:A:144:ARG:HD2	1:A:146:TYR:CZ	2.55	0.42
1:A:21:GLN:HB3	1:A:44:TYR:O	2.20	0.42
1:A:289:ASN:N	1:A:289:ASN:OD1	2.52	0.42
1:A:296:ILE:CG2	1:A:297:ALA:N	2.82	0.42
1:A:371:ILE:CG2	1:A:371:ILE:O	2.67	0.42
1:A:472:ASN:O	1:A:473:HIS:CB	2.67	0.42
1:A:663:GLN:O	1:A:664:GLU:HB2	2.20	0.42
1:A:721:GLY:C	1:A:723:ARG:N	2.73	0.42
1:A:780:VAL:HA	1:A:781:PRO:HD3	1.85	0.42
1:A:827:MET:HB3	1:A:829:ILE:HD13	2.01	0.42
2:B:1385:SER:OG	2:B:1455:SER:N	2.46	0.42
2:B:825:VAL:O	2:B:826:LYS:C	2.58	0.42
2:B:829:GLN:HE21	2:B:829:GLN:C	2.23	0.42
1:C:1153:ARG:NH2	1:C:1168:LEU:HD13	2.35	0.42
1:C:1016:VAL:HG11	1:C:1291:ILE:CD1	2.50	0.42
1:C:654:LEU:HA	1:C:654:LEU:HD23	1.58	0.42
1:C:96:GLN:HG3	1:C:97:ASN:N	2.35	0.42
2:D:1275:LEU:HD13	2:D:1321:ALA:HB2	2.02	0.42
2:D:1606:TRP:C	2:D:1606:TRP:HD1	2.22	0.42
2:D:171:ILE:HG13	2:D:171:ILE:H	1.59	0.42
2:D:76:ASN:CB	2:D:77:PRO:HD2	2.44	0.42
1:A:1061:ASN:HB2	1:A:1065:SER:O	2.20	0.41
1:A:1641:SER:O	1:A:1643:THR:HG23	2.20	0.41
1:A:222:TYR:CD2	1:A:222:TYR:C	2.94	0.41
1:A:354:LEU:N	1:A:354:LEU:CD2	2.83	0.41
1:A:654:LEU:C	1:A:655:THR:HG23	2.40	0.41
1:A:773:TRP:CZ3	1:A:774:LEU:HB2	2.55	0.41
1:A:606:ASP:HB2	1:A:797:TRP:HZ3	1.85	0.41
1:A:901:LEU:HA	1:A:902:PRO:HD3	1.78	0.41
2:B:138:THR:HG22	2:B:139:PRO:O	2.20	0.41
2:B:1457:LYS:HG2	2:B:1469:THR:HG1	1.83	0.41
2:B:343:TYR:HE1	2:B:420:LEU:HD11	1.84	0.41
2:B:415:THR:OG1	2:B:415:THR:O	2.35	0.41
2:B:352:LYS:HG3	2:B:430:MET:HE1	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:438:GLN:O	2:B:439:GLY:C	2.58	0.41
2:B:748:ARG:NH1	2:B:784:ILE:HG23	2.35	0.41
2:B:811:MET:HG3	2:B:812:LYS:N	2.34	0.41
2:B:36:ASP:OD1	2:B:90:PRO:HA	2.19	0.41
1:C:1133:LEU:N	1:C:1133:LEU:HD12	2.32	0.41
1:C:1313:ILE:HD13	1:C:1350:THR:HB	2.01	0.41
1:C:135:TYR:CE1	1:C:141:VAL:HG13	2.51	0.41
1:C:1435:ASN:O	1:C:1436:GLU:C	2.58	0.41
1:C:163:PHE:HE1	1:C:188:PHE:HB2	1.85	0.41
1:C:387:PRO:HG2	1:C:438:ASP:O	2.20	0.41
1:C:501:TYR:CD1	1:C:501:TYR:C	2.93	0.41
1:C:504:LEU:HD13	1:C:504:LEU:N	2.35	0.41
1:C:700:TYR:CZ	1:C:757:LEU:HD22	2.55	0.41
1:C:754:MET:HE1	1:C:756:THR:HA	2.02	0.41
1:C:594:THR:OG1	1:C:782:ARG:CA	2.68	0.41
1:C:829:ILE:HD12	1:C:829:ILE:N	2.34	0.41
2:D:1301:ARG:CB	2:D:1301:ARG:HH11	2.32	0.41
2:D:1380:THR:HG23	2:D:1460:SER:HA	2.01	0.41
2:D:265:PHE:O	2:D:276:ILE:HG13	2.19	0.41
2:D:756:LEU:CD2	2:D:778:PHE:CE1	3.03	0.41
1:A:1003:LEU:HA	1:A:1004:PRO:HD2	1.64	0.41
1:A:1060:ARG:CG	1:A:1061:ASN:H	2.33	0.41
1:A:1271:ILE:O	1:A:1272:LYS:C	2.57	0.41
1:A:1439:LEU:HA	1:A:1439:LEU:HD23	1.58	0.41
1:A:1500:ARG:C	1:A:1502:ASP:N	2.73	0.41
1:A:1545:ALA:CB	1:A:1660:PHE:CE1	3.03	0.41
1:A:1584:ILE:O	1:A:1585:TYR:CB	2.68	0.41
1:A:1641:SER:O	1:A:1642:LEU:HB2	2.20	0.41
1:A:240:TYR:CD2	1:A:240:TYR:C	2.89	0.41
1:A:518:PHE:HD2	1:A:524:GLN:NE2	2.17	0.41
1:A:621:GLU:HG3	1:A:621:GLU:H	1.73	0.41
1:A:683:ILE:O	1:A:687:ALA:HB3	2.20	0.41
1:A:804:ILE:O	1:A:804:ILE:HG13	2.21	0.41
1:A:824:PHE:N	1:A:824:PHE:CD2	2.82	0.41
1:A:971:THR:O	1:A:972:GLU:C	2.58	0.41
2:B:1412:GLU:HB2	2:B:1419:GLN:HB2	2.01	0.41
2:B:1445:HIS:CG	2:B:1446:PHE:H	2.37	0.41
2:B:1498:SER:O	2:B:1573:LEU:CD2	2.68	0.41
2:B:264:LEU:HB2	2:B:280:LEU:HB2	2.01	0.41
2:B:27:LEU:HD11	2:B:29:THR:HG22	2.03	0.41
2:B:267:VAL:HG13	2:B:313:THR:O	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:127:PHE:N	1:C:127:PHE:CD1	2.87	0.41
1:C:1320:LYS:CG	1:C:1321:GLY:H	2.34	0.41
1:C:1329:THR:OG1	1:C:1331:LYS:HG2	2.21	0.41
1:C:269:PHE:HB2	1:C:283:MET:CE	2.50	0.41
1:C:405:ASP:OD1	1:C:405:ASP:N	2.52	0.41
1:C:565:GLU:H	1:C:565:GLU:CD	2.22	0.41
1:C:591:ASN:C	1:C:592:MET:HG3	2.40	0.41
1:C:791:PRO:CD	1:C:797:TRP:HE1	2.32	0.41
2:D:1466:GLU:CD	2:D:1468:CYS:HB2	2.41	0.41
2:D:214:PHE:C	2:D:214:PHE:HD1	2.22	0.41
1:A:1158:ILE:O	1:A:1158:ILE:HG22	2.19	0.41
1:A:1336:ARG:HA	1:A:1337:PRO:HD3	1.95	0.41
1:A:222:TYR:HH	1:A:224:LEU:HD23	1.83	0.41
1:A:700:TYR:CZ	1:A:757:LEU:HD22	2.55	0.41
1:A:701:ASP:OD1	1:A:701:ASP:N	2.51	0.41
2:B:1408:ILE:HD11	2:B:1425:ILE:CG1	2.44	0.41
1:C:1053:MET:HE1	1:C:1085:VAL:CG1	2.50	0.41
1:C:1081:PHE:HD1	1:C:1147:PHE:HZ	1.68	0.41
1:C:1226:ARG:HD2	1:C:1270:VAL:CG2	2.51	0.41
1:C:977:LEU:CD2	1:C:1361:VAL:HG13	2.50	0.41
1:C:24:VAL:HG11	1:C:543:TYR:HE2	1.83	0.41
1:C:423:ASN:OD1	2:D:504:VAL:HG22	2.19	0.41
1:C:545:ILE:HG12	1:C:545:ILE:H	1.65	0.41
1:C:984:VAL:O	1:C:987:ILE:HB	2.19	0.41
2:D:1275:LEU:HD21	2:D:1319:GLY:C	2.39	0.41
2:D:1407:TYR:CD2	2:D:1407:TYR:C	2.92	0.41
2:D:219:TYR:CD1	2:D:220:VAL:N	2.86	0.41
2:D:41:ILE:O	2:D:85:PRO:HD2	2.20	0.41
2:D:454:ILE:HD12	2:D:538:VAL:HG11	2.02	0.41
2:D:818:LEU:HD23	2:D:911:LYS:CD	2.47	0.41
2:D:923:SER:C	2:D:924:ILE:HD12	2.41	0.41
1:A:1019:PHE:CZ	1:A:1088:GLN:HB3	2.56	0.41
1:A:124:GLY:C	1:A:125:PHE:CG	2.93	0.41
1:A:1013:MET:HE2	1:A:1287:THR:HB	2.02	0.41
1:A:330:ILE:HG13	1:A:330:ILE:O	2.20	0.41
1:A:40:VAL:HA	1:A:82:SER:HB3	2.02	0.41
1:A:931:PRO:HG2	1:A:1366:HIS:NE2	2.36	0.41
1:A:987:ILE:HG22	1:A:988:LEU:N	2.34	0.41
2:B:1275:LEU:HD13	2:B:1321:ALA:HB2	2.02	0.41
2:B:1277:ILE:HG22	2:B:1290:TYR:HB2	2.02	0.41
2:B:148:PHE:CZ	2:B:792:VAL:CG1	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:412:ARG:CD	2:B:458:ASP:OD1	2.66	0.41
1:C:1020:TYR:CZ	1:C:1295:GLU:HB2	2.55	0.41
1:C:1364:VAL:HG13	1:C:1364:VAL:O	2.19	0.41
1:C:1381:ILE:HD12	1:C:1493:PHE:HD2	1.85	0.41
1:C:1587:THR:HB	1:C:1591:VAL:CG2	2.50	0.41
1:C:404:LEU:HA	1:C:404:LEU:HD22	1.85	0.41
1:C:915:GLU:HB3	2:D:905:TRP:CZ2	2.55	0.41
2:D:1610:TRP:CG	2:D:1628:PHE:CD2	3.07	0.41
2:D:302:ARG:HG3	2:D:303:PHE:CE1	2.56	0.41
2:D:339:VAL:HG23	2:D:340:ALA:N	2.35	0.41
2:D:438:GLN:HB2	2:D:617:ASN:HD21	1.84	0.41
1:A:1525:CYS:N	1:A:1528:VAL:HG13	2.36	0.41
1:A:1660:PHE:HE2	1:A:1664:LEU:CD1	2.28	0.41
1:A:431:LEU:HD22	1:A:432:GLU:N	2.35	0.41
1:A:36:SER:HA	1:A:86:THR:HG22	2.02	0.41
1:A:979:VAL:HG21	1:A:1326:TYR:CZ	2.49	0.41
2:B:939:GLY:O	2:B:1316:SER:HA	2.21	0.41
2:B:133:ASP:OD2	2:B:134:LYS:HG2	2.19	0.41
2:B:330:VAL:HG23	2:B:330:VAL:O	2.20	0.41
2:B:339:VAL:HG23	2:B:340:ALA:N	2.35	0.41
2:B:762:LEU:N	2:B:762:LEU:CD1	2.82	0.41
2:B:41:ILE:O	2:B:85:PRO:HD2	2.20	0.41
1:C:1025:LEU:HD23	1:C:1025:LEU:HA	1.75	0.41
1:C:1208:ILE:HG22	1:C:1208:ILE:O	2.21	0.41
1:C:24:VAL:HG11	1:C:543:TYR:CZ	2.56	0.41
1:C:288:GLN:O	1:C:289:ASN:C	2.57	0.41
1:C:654:LEU:C	1:C:655:THR:HG23	2.40	0.41
1:C:74:SER:HA	1:C:79:PHE:CE1	2.56	0.41
1:C:960:PRO:HB2	1:C:961:TYR:H	1.62	0.41
1:C:961:TYR:CE1	1:C:963:ILE:HG12	2.55	0.41
2:D:1282:PRO:HD2	2:D:1309:GLN:CD	2.40	0.41
2:D:1349:VAL:CG2	2:D:1363:LEU:HD12	2.50	0.41
2:D:1528:LEU:HD12	2:D:1541:VAL:O	2.20	0.41
2:D:1556:PRO:C	2:D:1558:ALA:N	2.73	0.41
2:D:511:THR:OG1	2:D:512:PRO:HD2	2.20	0.41
2:D:885:VAL:HA	2:D:886:PRO:HD3	1.75	0.41
2:D:902:GLU:O	2:D:903:ALA:HB2	2.20	0.41
1:A:1026:GLU:OE1	1:A:1031:TRP:NE1	2.53	0.41
1:A:1328:MET:HE2	1:A:1328:MET:HB2	1.88	0.41
1:A:1455:ILE:N	1:A:1455:ILE:CD1	2.84	0.41
1:A:24:VAL:CG1	1:A:24:VAL:O	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:558:SER:HB3	1:A:645:VAL:HG13	2.03	0.41
1:A:59:TYR:N	1:A:60:PRO:CD	2.84	0.41
1:A:775:TRP:CD1	1:A:775:TRP:O	2.74	0.41
1:A:829:ILE:HG12	1:A:925:LYS:CG	2.45	0.41
2:B:1606:TRP:O	2:B:1606:TRP:CD1	2.74	0.41
1:A:470:THR:CG2	2:B:450:THR:HG22	2.40	0.41
2:B:789:VAL:C	2:B:790:LEU:HD12	2.41	0.41
1:C:1180:LEU:HD21	1:C:1208:ILE:HG12	2.01	0.41
1:C:1226:ARG:HD2	1:C:1270:VAL:HG23	2.02	0.41
1:C:938:SER:OG	1:C:1284:PHE:CZ	2.74	0.41
1:C:1560:ALA:HA	1:C:1620:MET:HA	2.03	0.41
1:C:1616:GLN:CD	1:C:1648:TRP:CZ3	2.94	0.41
1:C:163:PHE:HE1	1:C:188:PHE:CB	2.33	0.41
1:C:342:ILE:HA	1:C:343:PRO:HD3	1.73	0.41
1:C:361:LEU:CD1	1:C:361:LEU:N	2.83	0.41
1:C:501:TYR:CE1	1:C:512:PHE:C	2.94	0.41
2:D:104:VAL:CG2	2:D:105:VAL:H	2.30	0.41
2:D:1277:ILE:HG12	2:D:1278:THR:N	2.36	0.41
2:D:1445:HIS:CG	2:D:1446:PHE:H	2.38	0.41
2:D:1512:ILE:CG2	2:D:1631:PHE:CD1	3.03	0.41
2:D:466:VAL:CG1	2:D:524:TYR:CE2	3.04	0.41
1:A:1133:LEU:HD12	1:A:1133:LEU:N	2.34	0.41
1:A:1161:LEU:N	1:A:1161:LEU:HD22	2.35	0.41
1:A:1212:LEU:CD1	1:A:1228:TRP:NE1	2.83	0.41
1:A:354:LEU:H	1:A:354:LEU:HD23	1.85	0.41
1:A:484:ILE:HG21	1:A:528:ILE:HD11	2.03	0.41
1:A:626:PHE:C	1:A:628:GLU:H	2.23	0.41
1:A:81:ASN:CG	1:A:82:SER:N	2.72	0.41
2:B:1277:ILE:HG12	2:B:1278:THR:N	2.35	0.41
2:B:1444:LYS:CE	2:B:1447:GLU:HA	2.45	0.41
2:B:1522:TYR:HB2	2:B:1524:TYR:CE1	2.55	0.41
2:B:1581:TYR:HA	2:B:1608:GLU:O	2.20	0.41
2:B:756:LEU:CD2	2:B:778:PHE:CE1	3.03	0.41
2:B:857:CYS:O	2:B:885:VAL:HG22	2.20	0.41
2:B:923:SER:O	2:B:924:ILE:HD12	2.20	0.41
1:A:1162:VAL:HG11	1:C:1064:TYR:CE2	2.56	0.41
1:C:1090:ASN:C	1:C:1092:TYR:N	2.71	0.41
1:C:1566:THR:O	1:C:1613:LYS:HE3	2.20	0.41
1:C:78:LYS:HD2	1:C:498:HIS:NE2	2.35	0.41
1:C:97:ASN:HA	1:C:98:PRO:HD3	1.84	0.41
2:D:25:TYR:CZ	2:D:113:VAL:HG22	2.55	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:285:ILE:O	2:D:286:ILE:HD13	2.20	0.41
2:D:323:GLU:C	2:D:323:GLU:OE1	2.59	0.41
2:D:338:ILE:C	2:D:339:VAL:HG13	2.41	0.41
2:D:34:ARG:HH11	2:D:34:ARG:HG2	1.85	0.41
2:D:512:PRO:HA	2:D:515:ILE:HD12	2.03	0.41
2:D:593:ILE:HG12	2:D:593:ILE:O	2.10	0.41
2:D:621:PHE:CD2	2:D:621:PHE:N	2.86	0.41
2:D:56:ILE:HG12	2:D:71:THR:O	2.20	0.41
1:A:108:SER:HG	1:A:111:PHE:C	2.24	0.41
1:A:1313:ILE:HA	1:A:1313:ILE:HD13	1.67	0.41
1:A:1346:LEU:HD12	1:A:1346:LEU:HA	1.46	0.41
1:A:1428:LEU:HD11	1:A:1434:ALA:HB2	2.03	0.41
1:A:1537:GLU:O	1:A:1539:LEU:N	2.54	0.41
1:A:1574:PHE:HA	1:A:1603:LYS:HD2	2.02	0.41
1:A:1667:PHE:CD2	1:A:1667:PHE:N	2.88	0.41
1:A:179:HIS:C	1:A:180:ILE:HG12	2.40	0.41
1:A:690:TYR:CG	1:A:690:TYR:O	2.73	0.41
1:A:77:ASN:C	1:A:79:PHE:N	2.73	0.41
1:A:571:LEU:HD22	1:A:803:GLY:HA3	2.03	0.41
1:A:888:VAL:O	1:A:888:VAL:HG13	2.20	0.41
1:A:899:THR:C	1:A:900:VAL:HG13	2.41	0.41
1:A:91:GLN:CA	1:A:91:GLN:OE1	2.58	0.41
2:B:952:ASP:O	2:B:1331:ALA:HB1	2.21	0.41
2:B:1623:LYS:HD2	2:B:1623:LYS:HA	1.66	0.41
2:B:143:VAL:HG23	2:B:188:LEU:HD11	2.01	0.41
2:B:306:LEU:HA	2:B:306:LEU:HD12	1.83	0.41
2:B:386:SER:O	2:B:398:LEU:HD11	2.21	0.41
2:B:470:ALA:C	2:B:472:SER:H	2.23	0.41
2:B:557:GLN:HA	2:B:557:GLN:OE1	2.19	0.41
2:B:783:SER:HB2	2:B:787:TRP:CZ2	2.55	0.41
1:A:917:TRP:O	2:B:813:VAL:CG2	2.69	0.41
2:B:819:GLN:CA	2:B:819:GLN:NE2	2.84	0.41
2:B:891:LEU:HB2	2:B:912:LYS:CE	2.51	0.41
2:B:952:ASP:O	2:B:1331:ALA:CA	2.68	0.41
1:C:1013:MET:HA	1:C:1016:VAL:HG23	2.02	0.41
1:C:1022:PHE:O	1:C:1025:LEU:N	2.54	0.41
1:C:1108:VAL:HG21	1:C:1167:ALA:HB2	2.02	0.41
1:C:1133:LEU:H	1:C:1133:LEU:CD1	2.31	0.41
1:C:1232:LEU:HD12	1:C:1233:GLN:H	1.86	0.41
1:C:42:GLN:OE1	1:C:500:ASN:ND2	2.53	0.41
2:D:1393:ASP:CB	2:D:1443:LEU:HD11	2.44	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:229:GLN:HA	2:D:229:GLN:OE1	2.20	0.41
2:D:247:ILE:HD11	2:D:318:VAL:CG2	2.48	0.41
2:D:383:ALA:C	2:D:384:PHE:CD2	2.94	0.41
2:D:438:GLN:O	2:D:439:GLY:C	2.59	0.41
2:D:839:TYR:HD1	2:D:839:TYR:HA	1.65	0.41
2:D:952:ASP:O	2:D:1331:ALA:CA	2.69	0.41
1:A:101:TYR:O	1:A:102:VAL:HG23	2.21	0.41
1:A:1108:VAL:H	1:A:1108:VAL:HG12	1.60	0.41
1:A:31:PHE:O	1:A:119:ILE:HA	2.21	0.41
1:A:1279:ARG:CZ	1:A:1280:TYR:CD2	3.04	0.41
1:A:1320:LYS:CG	1:A:1321:GLY:H	2.34	0.41
1:A:1541:LEU:HD21	1:A:1543:ILE:HD12	2.03	0.41
1:A:176:GLU:HB2	1:A:185:PHE:CE1	2.56	0.41
1:A:539:ARG:HH21	1:A:634:CYS:H	1.59	0.41
2:B:1610:TRP:CG	2:B:1628:PHE:CD2	3.08	0.41
2:B:383:ALA:C	2:B:384:PHE:CD2	2.94	0.41
2:B:518:PHE:HE2	2:B:538:VAL:CG2	2.33	0.41
2:B:74:ASP:OD1	2:B:74:ASP:N	2.54	0.41
2:B:757:TRP:C	2:B:758:LEU:HD23	2.41	0.41
2:B:866:TYR:OH	2:B:1388:THR:CG2	2.69	0.41
1:C:124:GLY:C	1:C:125:PHE:CG	2.94	0.41
1:C:20:GLU:CB	1:C:551:THR:HG22	2.51	0.41
1:C:599:TRP:HE1	1:C:779:LEU:HB2	1.86	0.41
1:C:811:VAL:CG1	1:C:811:VAL:O	2.64	0.41
2:D:350:THR:O	2:D:350:THR:CG2	2.69	0.41
2:D:36:ASP:O	2:D:154:THR:HG22	2.20	0.41
2:D:407:GLN:HA	2:D:407:GLN:HE21	1.84	0.41
2:D:954:VAL:HG12	2:D:955:PRO:HD2	2.03	0.41
1:A:1213:LYS:HE2	1:A:1266:TYR:CE2	2.56	0.41
1:A:1271:ILE:HG21	1:A:1300:TYR:CD1	2.55	0.41
1:A:1280:TYR:CG	1:A:1280:TYR:O	2.74	0.41
1:A:382:LEU:HA	1:A:382:LEU:HD23	1.87	0.41
1:A:476:LEU:HA	1:A:476:LEU:HD23	1.78	0.41
1:A:541:LEU:HB2	1:A:557:ASP:O	2.20	0.41
1:A:599:TRP:HE1	1:A:779:LEU:CB	2.34	0.41
1:A:695:VAL:HG13	1:A:724:CYS:HA	2.02	0.41
2:B:1380:THR:HG23	2:B:1460:SER:HA	2.02	0.41
2:B:144:LEU:HD23	2:B:144:LEU:N	2.34	0.41
2:B:440:GLY:O	2:B:441:SER:C	2.60	0.41
2:B:514:LEU:HG	2:B:514:LEU:H	1.73	0.41
2:B:739:PHE:CE1	2:B:901:GLN:HB2	2.56	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1213:LYS:C	1:C:1215:GLU:N	2.73	0.41
1:C:501:TYR:CD1	1:C:501:TYR:O	2.73	0.41
1:C:515:ARG:HG3	1:C:526:ILE:HG23	2.03	0.41
1:C:663:GLN:O	1:C:664:GLU:HB2	2.21	0.41
1:C:682:LYS:HZ3	1:C:686:ILE:HD11	1.77	0.41
1:C:721:GLY:C	1:C:723:ARG:N	2.73	0.41
2:D:1632:SER:O	2:D:1636:THR:CB	2.68	0.41
2:D:226:VAL:HG21	2:D:320:VAL:CG1	2.51	0.41
2:D:238:ASP:O	2:D:238:ASP:OD1	2.39	0.41
2:D:355:LYS:HA	2:D:356:PRO:HD3	1.91	0.41
2:D:148:PHE:HB2	2:D:800:ILE:HD11	2.02	0.41
1:A:1013:MET:HA	1:A:1016:VAL:CG2	2.51	0.41
1:A:1159:CYS:O	1:A:1164:ILE:HD11	2.21	0.41
1:A:1426:ILE:HG22	1:A:1426:ILE:O	2.20	0.41
1:A:1379:LEU:HD12	1:A:1505:CYS:SG	2.61	0.41
1:A:1538:GLU:O	1:A:1539:LEU:C	2.59	0.41
1:A:1658:GLN:N	1:A:1658:GLN:HE21	2.17	0.41
1:A:269:PHE:HB2	1:A:283:MET:CE	2.50	0.41
1:A:392:ALA:HB1	1:A:432:GLU:O	2.21	0.41
1:A:510:ILE:HD12	1:A:533:ASN:HB2	2.02	0.41
1:A:543:TYR:H	1:A:543:TYR:HD1	1.68	0.41
1:A:567:CYS:HB3	1:A:570:GLN:HB3	2.03	0.41
2:B:943:GLU:HB2	2:B:1313:VAL:HG23	2.03	0.41
2:B:1407:TYR:CD2	2:B:1407:TYR:C	2.94	0.41
2:B:1501:ASN:H	2:B:1501:ASN:ND2	2.16	0.41
2:B:1575:LEU:N	2:B:1575:LEU:CD2	2.84	0.41
2:B:217:ARG:HG2	2:B:218:LYS:N	2.33	0.41
2:B:243:PHE:CE1	2:B:336:ILE:HG21	2.56	0.41
2:B:76:ASN:CB	2:B:77:PRO:HD2	2.44	0.41
1:C:1277:GLU:O	1:C:1278:GLN:C	2.58	0.41
1:C:1570:VAL:HG22	1:C:1575:VAL:HA	2.02	0.41
1:C:367:ILE:HD13	1:C:466:TYR:HD2	1.83	0.41
1:C:367:ILE:O	1:C:368:PRO:C	2.58	0.41
1:C:38:ASN:ND2	1:C:509:ILE:O	2.51	0.41
1:C:501:TYR:HE1	1:C:512:PHE:C	2.25	0.41
1:C:77:ASN:C	1:C:79:PHE:N	2.73	0.41
1:C:859:MET:HE1	1:C:898:PHE:HB3	2.02	0.41
1:C:970:LYS:O	1:C:971:THR:HG22	2.21	0.41
2:D:147:VAL:CG1	2:D:147:VAL:O	2.68	0.41
2:D:1519:ASN:O	2:D:1520:VAL:CG2	2.69	0.41
2:D:295:LYS:HD2	2:D:295:LYS:HA	1.87	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:D:860:SER:OG	2:D:866:TYR:CB	2.69	0.41
2:D:885:VAL:HG23	2:D:887:LEU:CD2	2.49	0.41
1:A:1020:TYR:CZ	1:A:1295:GLU:HB2	2.55	0.40
1:A:99:VAL:HG13	1:A:119:ILE:HD11	2.03	0.40
1:A:1226:ARG:HD2	1:A:1270:VAL:HG23	2.03	0.40
1:A:1568:ILE:CG2	1:A:1577:TYR:HE1	2.30	0.40
1:A:1625:LEU:O	1:A:1627:ILE:HG23	2.20	0.40
1:A:40:VAL:CG2	1:A:41:ILE:N	2.84	0.40
1:A:463:SER:CB	1:A:491:PRO:HA	2.51	0.40
1:A:60:PRO:HD2	1:A:61:ASP:N	2.17	0.40
1:A:862:VAL:CG1	1:A:907:LEU:HD21	2.50	0.40
1:A:949:ILE:CG2	1:A:949:ILE:O	2.69	0.40
2:B:1371:TYR:HB2	2:B:1377:SER:HB3	2.03	0.40
2:B:1414:ASP:O	2:B:1415:ASN:C	2.58	0.40
2:B:146:ARG:HA	2:B:183:PHE:CE2	2.56	0.40
2:B:402:ILE:N	2:B:402:ILE:HD13	2.36	0.40
1:C:1202:HIS:CG	1:C:1203:PRO:HD2	2.56	0.40
1:C:1245:ALA:HB2	1:C:1285:TYR:HB3	2.02	0.40
1:C:1406:ALA:O	1:C:1472:PHE:HA	2.21	0.40
1:C:1541:LEU:HD21	1:C:1543:ILE:HD12	2.03	0.40
1:C:163:PHE:CE2	1:C:201:ILE:HG12	2.56	0.40
1:C:355:ASN:ND2	1:C:355:ASN:N	2.67	0.40
1:C:518:PHE:HD2	1:C:524:GLN:NE2	2.19	0.40
1:C:651:LEU:HD23	1:C:651:LEU:HA	1.76	0.40
1:C:758:LEU:CB	1:C:759:PRO:HD2	2.50	0.40
1:C:832:SER:HA	1:C:928:ARG:HB3	2.03	0.40
1:C:36:SER:HA	1:C:86:THR:HG22	2.03	0.40
2:D:1289:ARG:C	2:D:1290:TYR:CD1	2.94	0.40
2:D:1369:THR:OG1	2:D:1370:ARG:N	2.54	0.40
2:D:1459:TYR:HB3	2:D:1466:GLU:HB3	2.03	0.40
2:D:148:PHE:CZ	2:D:792:VAL:HG11	2.55	0.40
2:D:386:SER:O	2:D:398:LEU:HD11	2.21	0.40
2:D:466:VAL:HG12	2:D:524:TYR:HE2	1.86	0.40
2:D:857:CYS:O	2:D:885:VAL:HG22	2.21	0.40
2:D:889:GLN:C	2:D:889:GLN:HE21	2.24	0.40
1:A:1127:ILE:HD12	1:A:1127:ILE:N	2.15	0.40
1:A:1161:LEU:HA	1:A:1161:LEU:HD13	1.85	0.40
1:A:1168:LEU:HA	1:A:1168:LEU:HD22	1.77	0.40
1:A:1217:LEU:HD12	1:A:1227:PHE:HE1	1.86	0.40
1:A:1277:GLU:O	1:A:1278:GLN:C	2.58	0.40
1:A:1439:LEU:O	1:A:1440:LYS:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1580:THR:HG23	1:A:1597:GLU:OE2	2.21	0.40
1:A:327:VAL:HG12	1:A:328:THR:N	2.36	0.40
1:A:330:ILE:HG22	1:A:337:SER:CB	2.38	0.40
1:A:354:LEU:CD2	1:A:450:GLU:HG3	2.51	0.40
1:A:404:LEU:HD22	1:A:404:LEU:HA	1.85	0.40
1:A:577:PRO:CD	1:A:588:VAL:HG23	2.51	0.40
1:A:700:TYR:HD1	1:A:758:LEU:HD12	1.86	0.40
1:A:800:GLN:HE21	1:A:800:GLN:HB2	1.69	0.40
1:A:885:ARG:HA	1:A:885:ARG:HD3	1.88	0.40
1:A:916:THR:C	1:A:918:PHE:H	2.25	0.40
1:A:934:VAL:HG13	1:A:935:LYS:N	2.36	0.40
2:B:354:PHE:CE2	2:B:409:LEU:HB2	2.57	0.40
1:C:1226:ARG:NE	1:C:1266:TYR:CE1	2.89	0.40
1:C:1226:ARG:HD3	1:C:1266:TYR:CE1	2.56	0.40
1:C:1285:TYR:O	1:C:1286:SER:O	2.39	0.40
1:C:1562:LYS:HB2	1:C:1583:ASP:O	2.21	0.40
1:C:196:TYR:CE1	1:C:221:GLU:CB	3.03	0.40
1:C:459:SER:OG	1:C:461:SER:HB3	2.22	0.40
1:C:577:PRO:HD2	1:C:588:VAL:HG23	2.02	0.40
1:C:23:TYR:C	1:C:655:THR:HG21	2.40	0.40
1:C:773:TRP:CZ3	1:C:774:LEU:HB2	2.54	0.40
1:C:953:ILE:HD12	1:C:955:ARG:HH21	1.87	0.40
2:D:1635:LEU:HD23	2:D:1635:LEU:HA	1.83	0.40
2:D:167:THR:HG23	2:D:171:ILE:N	2.37	0.40
2:D:354:PHE:CD1	2:D:354:PHE:C	2.93	0.40
2:D:484:LEU:HD11	2:D:626:LEU:CD1	2.51	0.40
2:D:511:THR:O	2:D:513:ASP:N	2.54	0.40
2:D:41:ILE:HG23	2:D:87:ILE:HD11	2.04	0.40
1:A:1043:GLN:O	1:A:1044:LYS:C	2.59	0.40
1:A:1083:LEU:CD2	1:A:1104:LEU:CD2	2.99	0.40
1:A:1091:LYS:HB2	1:A:1091:LYS:NZ	2.37	0.40
1:A:1127:ILE:HG13	1:A:1143:TYR:CE2	2.45	0.40
1:A:113:LYS:CG	1:A:114:SER:N	2.69	0.40
1:A:1467:ILE:HA	1:A:1468:PRO:HD3	1.78	0.40
1:A:575:LEU:HD23	1:A:590:LEU:HD13	2.04	0.40
1:A:115:LYS:HE3	1:A:654:LEU:HD11	2.02	0.40
1:A:49:ALA:HB2	1:A:74:SER:HB2	2.03	0.40
1:A:754:MET:HE1	1:A:756:THR:HA	2.03	0.40
1:A:942:VAL:CG2	1:A:1359:VAL:HB	2.52	0.40
1:A:942:VAL:HG11	1:A:957:LYS:HG2	2.03	0.40
1:A:961:TYR:CE1	1:A:963:ILE:HG12	2.56	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:89:ILE:CD1	2:B:121:LEU:HD11	2.52	0.40
2:B:1619:GLU:HA	2:B:1622:GLN:NE2	2.36	0.40
2:B:495:GLN:OE1	2:B:506:MET:HB2	2.22	0.40
2:B:580:VAL:CG1	2:B:581:ASP:N	2.84	0.40
2:B:825:VAL:HA	2:B:916:VAL:O	2.22	0.40
1:C:1054:LEU:O	1:C:1057:MET:HB2	2.21	0.40
1:C:1289:ASP:O	1:C:1290:THR:C	2.60	0.40
1:C:141:VAL:HG23	1:C:188:PHE:O	2.21	0.40
1:C:1432:ILE:N	1:C:1432:ILE:HD13	2.35	0.40
1:C:1560:ALA:O	1:C:1561:TYR:CB	2.69	0.40
1:C:1568:ILE:HD11	1:C:1613:LYS:HB2	2.03	0.40
1:C:1573:VAL:HG12	1:C:1603:LYS:CB	2.50	0.40
1:C:1578:LYS:HD3	1:C:1578:LYS:HA	1.87	0.40
1:C:1622:LYS:HB2	1:C:1643:THR:HG22	2.02	0.40
1:C:29:LYS:HB3	1:C:29:LYS:HE3	1.88	0.40
1:C:354:LEU:H	1:C:354:LEU:HD23	1.86	0.40
2:D:1273:LEU:HD13	2:D:1275:LEU:HG	2.04	0.40
2:D:27:LEU:HD11	2:D:29:THR:HG22	2.03	0.40
2:D:341:SER:HA	2:D:342:PRO:HD3	1.82	0.40
2:D:364:VAL:O	2:D:395:THR:HA	2.21	0.40
2:D:536:VAL:HG22	2:D:537:TRP:N	2.37	0.40
2:D:742:ASP:OD1	2:D:743:SER:N	2.55	0.40
1:A:1499:HIS:C	1:A:1500:ARG:HG3	2.42	0.40
1:A:156:LYS:CD	1:A:156:LYS:C	2.89	0.40
1:A:238:ILE:HG12	1:A:246:PHE:HE1	1.84	0.40
1:A:336:PHE:HB3	1:A:337:SER:H	1.76	0.40
1:A:500:ASN:CB	1:A:543:TYR:CD1	2.94	0.40
2:B:1327:THR:CG2	2:B:1328:PHE:N	2.84	0.40
2:B:1569:CYS:O	2:B:1570:GLN:C	2.59	0.40
2:B:202:LYS:CG	2:B:203:TYR:N	2.84	0.40
2:B:296:ARG:NH1	2:B:296:ARG:CG	2.85	0.40
2:B:302:ARG:HG3	2:B:303:PHE:CE1	2.56	0.40
2:B:511:THR:H	2:B:514:LEU:HD11	1.87	0.40
2:B:574:ARG:HH21	2:B:759:THR:HG21	1.87	0.40
2:B:151:ASP:HB2	2:B:794:PHE:CZ	2.56	0.40
2:B:41:ILE:HG23	2:B:87:ILE:HD11	2.04	0.40
2:B:884:ILE:HG21	2:B:884:ILE:HD13	1.84	0.40
1:C:1016:VAL:N	1:C:1017:PRO:HD2	2.33	0.40
1:A:1305:LYS:CB	1:C:116:ARG:HH21	2.35	0.40
1:C:1244:THR:O	1:C:1248:VAL:HG23	2.22	0.40
1:C:1267:VAL:O	1:C:1270:VAL:HB	2.20	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:1304:VAL:HG12	1:C:1305:LYS:H	1.83	0.40
1:C:1347:ILE:HG22	1:C:1347:ILE:O	2.20	0.40
1:C:1616:GLN:HB2	1:C:1648:TRP:O	2.21	0.40
1:C:308:LYS:HA	1:C:313:TYR:O	2.21	0.40
1:C:350:SER:OG	1:C:352:TYR:O	2.40	0.40
1:C:398:ASN:O	1:C:399:GLN:CB	2.69	0.40
1:C:689:LYS:O	1:C:691:LYS:N	2.52	0.40
1:C:775:TRP:CD1	1:C:775:TRP:O	2.75	0.40
2:D:1391:LEU:HD12	2:D:1417:MET:CE	2.52	0.40
2:D:151:ASP:HB2	2:D:794:PHE:CZ	2.57	0.40
2:D:1506:ILE:CD1	2:D:1628:PHE:CE1	3.05	0.40
2:D:343:TYR:HE1	2:D:420:LEU:HD11	1.85	0.40
2:D:42:LEU:HD22	2:D:492:VAL:HG21	2.04	0.40
2:D:824:VAL:CG1	2:D:913:LEU:HD21	2.51	0.40
2:D:895:GLU:HA	2:D:909:VAL:O	2.21	0.40
2:D:965:ILE:HD12	2:D:1277:ILE:HD13	2.03	0.40
1:A:1151:GLY:O	1:A:1154:LYS:N	2.52	0.40
1:A:1274:LEU:HD23	1:A:1274:LEU:HA	1.84	0.40
1:A:1324:HIS:CG	1:A:1336:ARG:NH2	2.89	0.40
1:A:1381:ILE:HB	1:A:1493:PHE:CD2	2.57	0.40
1:A:1003:LEU:HD12	1:A:1498:TYR:CE2	2.56	0.40
1:A:1560:ALA:HA	1:A:1620:MET:HA	2.04	0.40
1:A:449:ARG:O	1:A:450:GLU:HG2	2.21	0.40
1:A:545:ILE:HG12	1:A:545:ILE:H	1.63	0.40
1:A:40:VAL:HB	1:A:82:SER:HB3	2.02	0.40
1:A:945:ASP:OD1	1:A:945:ASP:C	2.59	0.40
1:A:970:LYS:O	1:A:971:THR:HG23	2.21	0.40
2:B:1459:TYR:HB3	2:B:1466:GLU:HB3	2.03	0.40
2:B:1498:SER:O	2:B:1573:LEU:HD21	2.22	0.40
2:B:295:LYS:HA	2:B:295:LYS:HD2	1.89	0.40
2:B:376:HIS:HA	2:B:389:THR:HG22	2.04	0.40
2:B:60:ASP:N	2:B:68:LEU:HD21	2.37	0.40
2:B:902:GLU:HG3	2:B:902:GLU:O	2.22	0.40
1:C:1226:ARG:NH1	1:C:1266:TYR:CE1	2.86	0.40
1:C:1386:ILE:HG22	1:C:1399:TYR:HB2	2.03	0.40
1:C:1538:GLU:O	1:C:1539:LEU:C	2.60	0.40
1:C:1570:VAL:C	1:C:1571:GLU:HG3	2.42	0.40
1:C:1612:VAL:HB	1:C:1615:ARG:CB	2.51	0.40
1:C:1646:GLU:OE2	1:C:1660:PHE:HZ	2.04	0.40
1:C:23:TYR:CE1	1:C:655:THR:CB	3.05	0.40
1:C:240:TYR:CD2	1:C:240:TYR:C	2.92	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:C:324:TYR:C	1:C:324:TYR:CD2	2.95	0.40
1:C:436:LYS:HA	1:C:448:ALA:O	2.22	0.40
1:C:495:LYS:HD3	1:C:495:LYS:HA	1.57	0.40
1:C:61:ASP:O	1:C:62:LYS:HB2	2.22	0.40
1:C:970:LYS:O	1:C:971:THR:HG23	2.22	0.40
2:D:1623:LYS:HD2	2:D:1623:LYS:N	2.36	0.40
2:D:405:ASN:N	2:D:405:ASN:OD1	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	1617/1676 (96%)	1173 (72%)	292 (18%)	152 (9%)	0	12
1	C	1617/1676 (96%)	1179 (73%)	288 (18%)	150 (9%)	0	12
2	B	1215/1642 (74%)	998 (82%)	161 (13%)	56 (5%)	2	24
2	D	1215/1642 (74%)	995 (82%)	162 (13%)	58 (5%)	2	23
All	All	5664/6636 (85%)	4345 (77%)	903 (16%)	416 (7%)	1	16

All (416) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	48	GLU
1	A	60	PRO
1	A	89	PRO
1	A	96	GLN
1	A	97	ASN
1	A	154	PRO
1	A	155	ALA
1	A	181	GLY

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Mol	Chain	Res	Type
1	A	208	ASP
1	A	255	PHE
1	A	285	THR
1	A	287	MET
1	A	308	LYS
1	A	309	GLU
1	A	312	TYR
1	A	489	LYS
1	A	490	SER
1	A	519	SER
1	A	522	SER
1	A	579	ALA
1	A	619	PRO
1	A	621	GLU
1	A	656	ASN
1	A	692	HIS
1	A	754	MET
1	A	759	PRO
1	A	793	SER
1	A	873	ILE
1	A	884	VAL
1	A	885	ARG
1	A	931	PRO
1	A	946	PRO
1	A	948	GLY
1	A	960	PRO
1	A	1091	LYS
1	A	1143	TYR
1	A	1284	PHE
1	A	1286	SER
1	A	1352	PHE
1	A	1386	ILE
1	A	1452	ASP
1	A	1534	GLN
1	A	1584	ILE
1	A	1585	TYR
1	A	1589	GLU
1	A	1628	LYS
1	A	1638	PRO
1	A	1639	LEU
1	A	1651	ASP
1	A	1654	CYS

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Mol	Chain	Res	Type
1	A	1674	ASN
2	B	48	ASP
2	B	207	PRO
2	B	220	VAL
2	B	349	LYS
2	B	418	GLY
2	B	490	PHE
2	B	545	MET
2	B	583	ALA
2	B	641	ALA
2	B	643	LYS
2	B	647	PRO
2	B	736	GLU
2	B	937	VAL
2	B	1297	ALA
2	B	1449	GLY
2	B	1529	LEU
2	B	1597	ILE
1	C	48	GLU
1	C	60	PRO
1	C	89	PRO
1	C	96	GLN
1	C	97	ASN
1	C	154	PRO
1	C	155	ALA
1	C	181	GLY
1	C	208	ASP
1	C	255	PHE
1	C	285	THR
1	C	287	MET
1	C	308	LYS
1	C	309	GLU
1	C	312	TYR
1	C	489	LYS
1	C	490	SER
1	C	522	SER
1	C	616	ALA
1	C	621	GLU
1	C	656	ASN
1	C	692	HIS
1	C	754	MET
1	C	759	PRO

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Mol	Chain	Res	Type
1	C	793	SER
1	C	820	PHE
1	C	873	ILE
1	C	884	VAL
1	C	885	ARG
1	C	931	PRO
1	C	946	PRO
1	C	948	GLY
1	C	960	PRO
1	C	1091	LYS
1	C	1143	TYR
1	C	1284	PHE
1	C	1286	SER
1	C	1352	PHE
1	C	1386	ILE
1	C	1452	ASP
1	C	1534	GLN
1	C	1584	ILE
1	C	1585	TYR
1	C	1589	GLU
1	C	1628	LYS
1	C	1638	PRO
1	C	1639	LEU
1	C	1651	ASP
1	C	1654	CYS
1	C	1674	ASN
2	D	48	ASP
2	D	220	VAL
2	D	348	THR
2	D	349	LYS
2	D	418	GLY
2	D	490	PHE
2	D	545	MET
2	D	583	ALA
2	D	641	ALA
2	D	643	LYS
2	D	647	PRO
2	D	736	GLU
2	D	937	VAL
2	D	1297	ALA
2	D	1449	GLY
2	D	1529	LEU

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Mol	Chain	Res	Type
2	D	1597	ILE
1	A	459	SER
1	A	474	LYS
1	A	475	ALA
1	A	552	ALA
1	A	569	ASN
1	A	616	ALA
1	A	623	VAL
1	A	627	LEU
1	A	638	GLY
1	A	664	GLU
1	A	806	ASN
1	A	820	PHE
1	A	889	GLU
1	A	890	GLY
1	A	939	TYR
1	A	981	GLY
1	A	998	ASN
1	A	1001	THR
1	A	1004	PRO
1	A	1009	GLU
1	A	1096	ASN
1	A	1122	SER
1	A	1140	ASN
1	A	1238	SER
1	A	1321	GLY
1	A	1324	HIS
1	A	1334	LEU
1	A	1382	ASP
1	A	1421	HIS
1	A	1471	ASP
1	A	1538	GLU
1	A	1590	ALA
2	B	237	ILE
2	B	348	THR
2	B	604	LYS
2	B	842	GLU
2	B	862	LYS
2	B	873	LYS
2	B	1319	GLY
2	B	1379	MET
2	B	1503	GLN

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Mol	Chain	Res	Type
2	B	1558	ALA
2	B	1570	GLN
1	C	305	THR
1	C	459	SER
1	C	474	LYS
1	C	519	SER
1	C	552	ALA
1	C	569	ASN
1	C	579	ALA
1	C	619	PRO
1	C	623	VAL
1	C	627	LEU
1	C	634	CYS
1	C	638	GLY
1	C	664	GLU
1	C	889	GLU
1	C	890	GLY
1	C	981	GLY
1	C	994	GLN
1	C	998	ASN
1	C	1001	THR
1	C	1004	PRO
1	C	1009	GLU
1	C	1096	ASN
1	C	1140	ASN
1	C	1238	SER
1	C	1321	GLY
1	C	1324	HIS
1	C	1334	LEU
1	C	1382	ASP
1	C	1421	HIS
1	C	1471	ASP
1	C	1538	GLU
1	C	1590	ALA
1	C	1609	ALA
2	D	142	PRO
2	D	207	PRO
2	D	237	ILE
2	D	470	ALA
2	D	604	LYS
2	D	842	GLU
2	D	873	LYS

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Mol	Chain	Res	Type
2	D	1319	GLY
2	D	1379	MET
2	D	1503	GLN
2	D	1558	ALA
2	D	1570	GLN
1	A	209	PHE
1	A	286	ALA
1	A	289	ASN
1	A	305	THR
1	A	440	PRO
1	A	441	ASP
1	A	472	ASN
1	A	624	PHE
1	A	634	CYS
1	A	657	ALA
1	A	791	PRO
1	A	821	LYS
1	A	823	VAL
1	A	849	ARG
1	A	938	SER
1	A	994	GLN
1	A	1194	ALA
1	A	1196	SER
1	A	1539	LEU
1	A	1588	GLY
1	A	1609	ALA
1	A	1632	SER
1	A	1652	THR
2	B	142	PRO
2	B	435	TYR
2	B	470	ALA
2	B	613	SER
2	B	780	LEU
2	B	1340	CYS
2	B	1497	CYS
2	B	1557	ARG
1	C	167	GLU
1	C	440	PRO
1	C	441	ASP
1	C	472	ASN
1	C	475	ALA
1	C	488	PRO

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Mol	Chain	Res	Type
1	C	520	ASP
1	C	624	PHE
1	C	657	ALA
1	C	760	VAL
1	C	791	PRO
1	C	806	ASN
1	C	821	LYS
1	C	823	VAL
1	C	849	ARG
1	C	938	SER
1	C	939	TYR
1	C	1122	SER
1	C	1194	ALA
1	C	1196	SER
1	C	1539	LEU
1	C	1632	SER
1	C	1652	THR
2	D	326	SER
2	D	435	TYR
2	D	613	SER
2	D	780	LEU
2	D	862	LYS
2	D	1340	CYS
2	D	1497	CYS
2	D	1557	ARG
1	A	234	GLU
1	A	256	TYR
1	A	520	ASP
1	A	667	GLU
1	A	690	TYR
1	A	760	VAL
1	A	882	LYS
1	A	909	ASN
1	A	988	LEU
1	A	1139	GLU
1	A	1150	ILE
1	A	1513	ASN
1	A	1540	ASP
1	A	1573	VAL
1	A	1655	SER
2	B	81	MET
2	B	277	PRO

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Mol	Chain	Res	Type
2	B	326	SER
2	B	959	ILE
2	B	1447	GLU
2	B	1501	ASN
1	C	94	GLY
1	C	256	TYR
1	C	286	ALA
1	C	289	ASN
1	C	337	SER
1	C	667	GLU
1	C	690	TYR
1	C	909	ASN
1	C	987	ILE
1	C	988	LEU
1	C	997	ILE
1	C	1098	ASN
1	C	1139	GLU
1	C	1540	ASP
1	C	1573	VAL
1	C	1588	GLY
1	C	1655	SER
2	D	81	MET
2	D	277	PRO
2	D	471	ASN
2	D	821	PRO
2	D	959	ILE
2	D	1298	LEU
2	D	1332	GLN
2	D	1447	GLU
2	D	1501	ASN
2	D	1553	ASP
2	D	1560	THR
1	A	94	GLY
1	A	101	TYR
1	A	167	GLU
1	A	186	PRO
1	A	274	ASP
1	A	291	MET
1	A	337	SER
1	A	488	PRO
1	A	576	SER
1	A	737	GLN

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Mol	Chain	Res	Type
1	A	753	HIS
1	A	987	ILE
1	A	997	ILE
1	A	1098	ASN
1	A	1134	PRO
1	A	1160	PRO
1	A	1272	LYS
1	A	1675	GLY
2	B	471	ASN
2	B	950	LEU
2	B	1332	GLN
2	B	1556	PRO
2	B	1639	GLY
1	C	101	TYR
1	C	186	PRO
1	C	234	GLU
1	C	291	MET
1	C	576	SER
1	C	753	HIS
1	C	882	LYS
1	C	1023	HIS
1	C	1134	PRO
1	C	1150	ILE
1	C	1513	ASN
1	C	1675	GLY
2	D	1556	PRO
2	D	1592	PRO
1	A	633	GLY
1	A	986	GLU
1	A	1002	HIS
1	A	1022	PHE
1	A	1243	GLY
2	B	560	GLY
2	B	1514	LYS
2	B	1592	PRO
1	C	274	ASP
1	C	970	LYS
1	C	1272	LYS
2	D	49	SER
2	D	950	LEU
2	B	821	PRO
1	C	633	GLY

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Mol	Chain	Res	Type
1	C	1160	PRO
1	C	1243	GLY
1	C	1649	PRO
2	D	560	GLY
1	A	166	PRO
1	A	1649	PRO
2	B	339	VAL
1	C	510	ILE
1	C	1671	ILE
2	D	339	VAL
2	D	403	PRO
1	A	93	PRO
1	A	171	VAL
1	A	999	ILE
1	A	1671	ILE
2	B	79	GLY
2	B	403	PRO
2	B	512	PRO
2	B	559	PRO
1	C	93	PRO
1	C	166	PRO
1	C	171	VAL
2	D	79	GLY
2	D	512	PRO
2	D	584	VAL
1	A	137	PRO
1	A	168	GLY
1	C	168	GLY
1	C	999	ILE
1	C	1239	VAL

### 5.3.2 Protein sidechains ⓘ

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	1446/1484 (97%)	1108 (77%)	338 (23%)	<b>1</b> <b>5</b>

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	C	1446/1484 (97%)	1109 (77%)	337 (23%)	1	5
2	B	1093/1435 (76%)	845 (77%)	248 (23%)	1	6
2	D	1093/1435 (76%)	845 (77%)	248 (23%)	1	6
All	All	5078/5838 (87%)	3907 (77%)	1171 (23%)	1	5

All (1171) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	21	GLN
1	A	22	THR
1	A	23	TYR
1	A	24	VAL
1	A	26	SER
1	A	38	ASN
1	A	40	VAL
1	A	41	ILE
1	A	47	THR
1	A	55	SER
1	A	63	LYS
1	A	64	PHE
1	A	67	SER
1	A	71	VAL
1	A	73	LEU
1	A	87	ILE
1	A	89	PRO
1	A	91	GLN
1	A	99	VAL
1	A	104	LEU
1	A	106	VAL
1	A	110	HIS
1	A	125	PHE
1	A	126	LEU
1	A	131	ASP
1	A	136	THR
1	A	144	ARG
1	A	148	LEU
1	A	156	LYS
1	A	157	ARG
1	A	158	GLU
1	A	161	LEU
1	A	162	THR

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Mol	Chain	Res	Type
1	A	167	GLU
1	A	169	SER
1	A	171	VAL
1	A	176	GLU
1	A	182	ILE
1	A	183	ILE
1	A	200	THR
1	A	208	ASP
1	A	211	THR
1	A	212	THR
1	A	214	THR
1	A	222	TYR
1	A	224	LEU
1	A	228	SER
1	A	230	SER
1	A	232	GLU
1	A	240	TYR
1	A	241	LYS
1	A	242	ASN
1	A	249	THR
1	A	261	THR
1	A	268	THR
1	A	279	GLN
1	A	287	MET
1	A	288	GLN
1	A	289	ASN
1	A	291	MET
1	A	292	LEU
1	A	296	ILE
1	A	310	LEU
1	A	315	LEU
1	A	321	LYS
1	A	322	TYR
1	A	323	LEU
1	A	324	TYR
1	A	328	THR
1	A	333	THR
1	A	337	SER
1	A	353	LYS
1	A	354	LEU
1	A	355	ASN
1	A	363	LEU

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Mol	Chain	Res	Type
1	A	371	ILE
1	A	373	VAL
1	A	375	VAL
1	A	383	VAL
1	A	389	THR
1	A	390	LEU
1	A	394	THR
1	A	396	ASP
1	A	400	GLU
1	A	402	SER
1	A	404	LEU
1	A	407	SER
1	A	412	ARG
1	A	414	ASP
1	A	419	SER
1	A	422	LEU
1	A	431	LEU
1	A	433	PHE
1	A	441	ASP
1	A	442	LEU
1	A	457	TYR
1	A	458	SER
1	A	460	LEU
1	A	467	ILE
1	A	469	TRP
1	A	471	ASP
1	A	474	LYS
1	A	477	LEU
1	A	492	TYR
1	A	495	LYS
1	A	497	THR
1	A	498	HIS
1	A	501	TYR
1	A	504	LEU
1	A	506	LYS
1	A	509	ILE
1	A	516	GLU
1	A	522	SER
1	A	526	ILE
1	A	534	MET
1	A	535	VAL
1	A	540	LEU

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Mol	Chain	Res	Type
1	A	541	LEU
1	A	543	TYR
1	A	545	ILE
1	A	547	THR
1	A	549	GLU
1	A	550	GLN
1	A	555	VAL
1	A	558	SER
1	A	559	VAL
1	A	563	ILE
1	A	565	GLU
1	A	569	ASN
1	A	573	VAL
1	A	580	ASP
1	A	587	THR
1	A	596	MET
1	A	597	ASP
1	A	599	TRP
1	A	605	VAL
1	A	613	GLN
1	A	614	ARG
1	A	618	LYS
1	A	621	GLU
1	A	625	GLN
1	A	627	LEU
1	A	640	LEU
1	A	642	ASN
1	A	644	ASN
1	A	652	THR
1	A	653	PHE
1	A	663	GLN
1	A	664	GLU
1	A	667	GLU
1	A	672	ILE
1	A	692	HIS
1	A	697	LYS
1	A	699	CYS
1	A	704	CYS
1	A	710	THR
1	A	713	GLN
1	A	720	LEU
1	A	732	CYS

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Mol	Chain	Res	Type
1	A	753	HIS
1	A	754	MET
1	A	756	THR
1	A	758	LEU
1	A	766	ARG
1	A	767	SER
1	A	774	LEU
1	A	777	VAL
1	A	782	ARG
1	A	787	GLN
1	A	788	PHE
1	A	793	SER
1	A	795	THR
1	A	797	TRP
1	A	800	GLN
1	A	811	VAL
1	A	824	PHE
1	A	825	LEU
1	A	838	GLN
1	A	845	VAL
1	A	849	ARG
1	A	850	THR
1	A	854	GLN
1	A	856	CYS
1	A	857	VAL
1	A	859	MET
1	A	865	ILE
1	A	867	THR
1	A	876	GLN
1	A	887	LYS
1	A	895	LEU
1	A	896	VAL
1	A	899	THR
1	A	901	LEU
1	A	912	PHE
1	A	914	LEU
1	A	915	GLU
1	A	923	LEU
1	A	928	ARG
1	A	935	LYS
1	A	936	ARG
1	A	940	SER

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Mol	Chain	Res	Type
1	A	944	LEU
1	A	947	ARG
1	A	952	THR
1	A	953	ILE
1	A	955	ARG
1	A	967	LEU
1	A	972	GLU
1	A	975	ARG
1	A	977	LEU
1	A	983	LEU
1	A	984	VAL
1	A	988	LEU
1	A	1001	THR
1	A	1002	HIS
1	A	1003	LEU
1	A	1007	SER
1	A	1011	GLU
1	A	1013	MET
1	A	1014	SER
1	A	1018	VAL
1	A	1033	ILE
1	A	1055	SER
1	A	1056	ILE
1	A	1070	LYS
1	A	1078	LEU
1	A	1084	ARG
1	A	1089	VAL
1	A	1091	LYS
1	A	1098	ASN
1	A	1105	LEU
1	A	1107	LEU
1	A	1108	VAL
1	A	1110	ASN
1	A	1113	LEU
1	A	1127	ILE
1	A	1128	LYS
1	A	1129	LEU
1	A	1140	ASN
1	A	1141	SER
1	A	1164	ILE
1	A	1166	THR
1	A	1168	LEU

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Mol	Chain	Res	Type
1	A	1175	LEU
1	A	1180	LEU
1	A	1183	GLN
1	A	1185	THR
1	A	1196	SER
1	A	1200	LYS
1	A	1201	THR
1	A	1209	VAL
1	A	1212	LEU
1	A	1218	VAL
1	A	1227	PHE
1	A	1231	ASN
1	A	1236	ASP
1	A	1246	ARG
1	A	1259	LEU
1	A	1264	ILE
1	A	1279	ARG
1	A	1280	TYR
1	A	1301	SER
1	A	1302	LEU
1	A	1303	LEU
1	A	1306	GLN
1	A	1307	LEU
1	A	1308	ARG
1	A	1309	LEU
1	A	1311	MET
1	A	1313	ILE
1	A	1323	LEU
1	A	1326	TYR
1	A	1330	ASP
1	A	1331	LYS
1	A	1333	PHE
1	A	1334	LEU
1	A	1336	ARG
1	A	1338	VAL
1	A	1341	LEU
1	A	1346	LEU
1	A	1356	LEU
1	A	1361	VAL
1	A	1363	THR
1	A	1366	HIS
1	A	1367	LYS

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Mol	Chain	Res	Type
1	A	1372	GLU
1	A	1374	VAL
1	A	1375	CYS
1	A	1397	SER
1	A	1423	VAL
1	A	1433	SER
1	A	1450	PHE
1	A	1454	GLN
1	A	1464	LEU
1	A	1470	SER
1	A	1474	CYS
1	A	1475	VAL
1	A	1476	ARG
1	A	1479	ILE
1	A	1480	PHE
1	A	1483	PHE
1	A	1487	PHE
1	A	1488	LEU
1	A	1492	THR
1	A	1493	PHE
1	A	1494	THR
1	A	1500	ARG
1	A	1503	LYS
1	A	1504	GLN
1	A	1506	THR
1	A	1507	MET
1	A	1512	SER
1	A	1535	MET
1	A	1542	THR
1	A	1544	SER
1	A	1548	ARG
1	A	1549	LYS
1	A	1553	CYS
1	A	1566	THR
1	A	1577	TYR
1	A	1580	THR
1	A	1581	LEU
1	A	1585	TYR
1	A	1598	ILE
1	A	1602	LYS
1	A	1605	THR
1	A	1606	CYS

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Mol	Chain	Res	Type
1	A	1618	LEU
1	A	1626	GLN
1	A	1627	ILE
1	A	1631	PHE
1	A	1636	ILE
1	A	1639	LEU
1	A	1650	ARG
1	A	1651	ASP
1	A	1652	THR
1	A	1655	SER
1	A	1663	ASN
2	B	29	THR
2	B	40	GLN
2	B	43	VAL
2	B	54	LEU
2	B	56	ILE
2	B	58	VAL
2	B	68	LEU
2	B	71	THR
2	B	74	ASP
2	B	82	LEU
2	B	86	THR
2	B	87	ILE
2	B	100	GLN
2	B	105	VAL
2	B	106	VAL
2	B	108	VAL
2	B	114	ARG
2	B	119	VAL
2	B	120	LEU
2	B	124	GLN
2	B	144	LEU
2	B	147	VAL
2	B	161	VAL
2	B	167	THR
2	B	171	ILE
2	B	175	SER
2	B	176	ASN
2	B	177	SER
2	B	179	ASP
2	B	183	PHE
2	B	190	ASP

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Mol	Chain	Res	Type
2	B	191	LEU
2	B	196	THR
2	B	198	ARG
2	B	202	LYS
2	B	208	GLU
2	B	214	PHE
2	B	216	VAL
2	B	217	ARG
2	B	219	TYR
2	B	220	VAL
2	B	221	LEU
2	B	223	SER
2	B	231	SER
2	B	234	PHE
2	B	243	PHE
2	B	258	GLU
2	B	263	VAL
2	B	264	LEU
2	B	278	ASP
2	B	280	LEU
2	B	285	ILE
2	B	291	LYS
2	B	296	ARG
2	B	297	ASP
2	B	298	THR
2	B	299	PHE
2	B	301	SER
2	B	306	LEU
2	B	315	TYR
2	B	317	SER
2	B	323	GLU
2	B	327	ASP
2	B	328	MET
2	B	341	SER
2	B	344	GLN
2	B	345	ILE
2	B	348	THR
2	B	349	LYS
2	B	358	MET
2	B	379	VAL
2	B	382	GLU
2	B	386	SER

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Mol	Chain	Res	Type
2	B	389	THR
2	B	390	THR
2	B	398	LEU
2	B	400	LEU
2	B	404	LEU
2	B	414	ARG
2	B	416	ASN
2	B	422	ARG
2	B	427	THR
2	B	433	ILE
2	B	435	TYR
2	B	437	THR
2	B	449	ILE
2	B	460	LEU
2	B	465	ASN
2	B	466	VAL
2	B	469	ASN
2	B	472	SER
2	B	473	LEU
2	B	481	TYR
2	B	482	LEU
2	B	483	ILE
2	B	490	PHE
2	B	497	ARG
2	B	504	VAL
2	B	505	THR
2	B	511	THR
2	B	513	ASP
2	B	518	PHE
2	B	520	PHE
2	B	521	VAL
2	B	523	TYR
2	B	524	TYR
2	B	525	GLN
2	B	526	VAL
2	B	531	ILE
2	B	532	VAL
2	B	543	THR
2	B	544	CYS
2	B	555	LEU
2	B	556	ILE
2	B	558	MET

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Mol	Chain	Res	Type
2	B	563	MET
2	B	567	LEU
2	B	586	VAL
2	B	588	ASN
2	B	593	ILE
2	B	597	LYS
2	B	598	ILE
2	B	602	ILE
2	B	606	ASP
2	B	613	SER
2	B	615	GLN
2	B	629	THR
2	B	638	GLN
2	B	735	ASN
2	B	742	ASP
2	B	745	ILE
2	B	746	ILE
2	B	747	SER
2	B	764	GLU
2	B	769	GLN
2	B	773	SER
2	B	778	PHE
2	B	780	LEU
2	B	784	ILE
2	B	789	VAL
2	B	800	ILE
2	B	813	VAL
2	B	816	ILE
2	B	817	ASP
2	B	819	GLN
2	B	829	GLN
2	B	830	VAL
2	B	836	LEU
2	B	840	VAL
2	B	851	LEU
2	B	857	CYS
2	B	868	GLN
2	B	870	PHE
2	B	872	ILE
2	B	873	LYS
2	B	884	ILE
2	B	887	LEU

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Mol	Chain	Res	Type
2	B	889	GLN
2	B	891	LEU
2	B	918	GLU
2	B	920	VAL
2	B	925	VAL
2	B	926	THR
2	B	946	LYS
2	B	948	ARG
2	B	949	LYS
2	B	952	ASP
2	B	963	ILE
2	B	964	ILE
2	B	1273	LEU
2	B	1274	ASN
2	B	1278	THR
2	B	1279	ILE
2	B	1281	LEU
2	B	1291	ARG
2	B	1292	ILE
2	B	1301	ARG
2	B	1304	GLU
2	B	1305	THR
2	B	1308	ASN
2	B	1313	VAL
2	B	1322	THR
2	B	1324	THR
2	B	1329	TYR
2	B	1330	ASN
2	B	1332	GLN
2	B	1344	HIS
2	B	1345	LEU
2	B	1346	ASN
2	B	1350	GLU
2	B	1351	ASN
2	B	1364	MET
2	B	1365	LEU
2	B	1372	LEU
2	B	1378	THR
2	B	1380	THR
2	B	1388	THR
2	B	1396	ASP
2	B	1398	THR

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Mol	Chain	Res	Type
2	B	1401	SER
2	B	1406	ARG
2	B	1423	VAL
2	B	1424	ILE
2	B	1427	LEU
2	B	1429	LYS
2	B	1431	SER
2	B	1433	SER
2	B	1437	CYS
2	B	1438	LEU
2	B	1439	HIS
2	B	1442	ILE
2	B	1443	LEU
2	B	1448	VAL
2	B	1450	PHE
2	B	1451	ILE
2	B	1456	VAL
2	B	1464	LEU
2	B	1475	ASP
2	B	1480	LEU
2	B	1481	LEU
2	B	1490	CYS
2	B	1492	CYS
2	B	1495	GLU
2	B	1496	THR
2	B	1497	CYS
2	B	1500	LEU
2	B	1502	HIS
2	B	1504	GLU
2	B	1511	GLN
2	B	1516	CYS
2	B	1519	ASN
2	B	1526	THR
2	B	1535	ASP
2	B	1561	HIS
2	B	1566	GLN
2	B	1571	GLU
2	B	1582	LEU
2	B	1583	ILE
2	B	1584	TRP
2	B	1594	LYS
2	B	1598	SER

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Mol	Chain	Res	Type
2	B	1599	TYR
2	B	1604	ASN
2	B	1606	TRP
2	B	1607	ILE
2	B	1609	ARG
2	B	1622	GLN
2	B	1623	LYS
1	C	21	GLN
1	C	22	THR
1	C	23	TYR
1	C	24	VAL
1	C	26	SER
1	C	38	ASN
1	C	40	VAL
1	C	41	ILE
1	C	47	THR
1	C	55	SER
1	C	63	LYS
1	C	64	PHE
1	C	67	SER
1	C	71	VAL
1	C	73	LEU
1	C	85	LEU
1	C	87	ILE
1	C	91	GLN
1	C	99	VAL
1	C	104	LEU
1	C	106	VAL
1	C	110	HIS
1	C	125	PHE
1	C	126	LEU
1	C	131	ASP
1	C	136	THR
1	C	143	VAL
1	C	144	ARG
1	C	148	LEU
1	C	156	LYS
1	C	157	ARG
1	C	158	GLU
1	C	161	LEU
1	C	162	THR
1	C	164	ILE

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Mol	Chain	Res	Type
1	C	167	GLU
1	C	169	SER
1	C	176	GLU
1	C	182	ILE
1	C	183	ILE
1	C	200	THR
1	C	208	ASP
1	C	211	THR
1	C	212	THR
1	C	214	THR
1	C	222	TYR
1	C	224	LEU
1	C	228	SER
1	C	230	SER
1	C	232	GLU
1	C	240	TYR
1	C	241	LYS
1	C	242	ASN
1	C	249	THR
1	C	261	THR
1	C	268	THR
1	C	279	GLN
1	C	287	MET
1	C	288	GLN
1	C	289	ASN
1	C	291	MET
1	C	292	LEU
1	C	296	ILE
1	C	310	LEU
1	C	315	LEU
1	C	322	TYR
1	C	323	LEU
1	C	324	TYR
1	C	328	THR
1	C	333	THR
1	C	337	SER
1	C	354	LEU
1	C	355	ASN
1	C	363	LEU
1	C	371	ILE
1	C	373	VAL
1	C	375	VAL

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Mol	Chain	Res	Type
1	C	383	VAL
1	C	389	THR
1	C	390	LEU
1	C	394	THR
1	C	396	ASP
1	C	400	GLU
1	C	404	LEU
1	C	407	SER
1	C	412	ARG
1	C	414	ASP
1	C	419	SER
1	C	422	LEU
1	C	431	LEU
1	C	433	PHE
1	C	441	ASP
1	C	442	LEU
1	C	457	TYR
1	C	458	SER
1	C	460	LEU
1	C	467	ILE
1	C	469	TRP
1	C	471	ASP
1	C	474	LYS
1	C	477	LEU
1	C	492	TYR
1	C	495	LYS
1	C	497	THR
1	C	498	HIS
1	C	501	TYR
1	C	504	LEU
1	C	506	LYS
1	C	509	ILE
1	C	516	GLU
1	C	522	SER
1	C	526	ILE
1	C	535	VAL
1	C	540	LEU
1	C	541	LEU
1	C	543	TYR
1	C	544	TYR
1	C	545	ILE
1	C	547	THR

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Mol	Chain	Res	Type
1	C	549	GLU
1	C	550	GLN
1	C	555	VAL
1	C	558	SER
1	C	559	VAL
1	C	563	ILE
1	C	565	GLU
1	C	569	ASN
1	C	573	VAL
1	C	580	ASP
1	C	587	THR
1	C	596	MET
1	C	597	ASP
1	C	599	TRP
1	C	605	VAL
1	C	613	GLN
1	C	614	ARG
1	C	618	LYS
1	C	621	GLU
1	C	625	GLN
1	C	627	LEU
1	C	640	LEU
1	C	642	ASN
1	C	644	ASN
1	C	652	THR
1	C	653	PHE
1	C	663	GLN
1	C	664	GLU
1	C	667	GLU
1	C	672	ILE
1	C	692	HIS
1	C	697	LYS
1	C	699	CYS
1	C	701	ASP
1	C	710	THR
1	C	713	GLN
1	C	720	LEU
1	C	732	CYS
1	C	753	HIS
1	C	754	MET
1	C	756	THR
1	C	758	LEU

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Mol	Chain	Res	Type
1	C	766	ARG
1	C	767	SER
1	C	774	LEU
1	C	777	VAL
1	C	782	ARG
1	C	787	GLN
1	C	788	PHE
1	C	793	SER
1	C	795	THR
1	C	797	TRP
1	C	800	GLN
1	C	811	VAL
1	C	824	PHE
1	C	825	LEU
1	C	838	GLN
1	C	845	VAL
1	C	849	ARG
1	C	850	THR
1	C	854	GLN
1	C	856	CYS
1	C	857	VAL
1	C	859	MET
1	C	865	ILE
1	C	867	THR
1	C	876	GLN
1	C	887	LYS
1	C	895	LEU
1	C	896	VAL
1	C	899	THR
1	C	901	LEU
1	C	912	PHE
1	C	914	LEU
1	C	915	GLU
1	C	923	LEU
1	C	928	ARG
1	C	935	LYS
1	C	936	ARG
1	C	940	SER
1	C	944	LEU
1	C	947	ARG
1	C	952	THR
1	C	953	ILE

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Mol	Chain	Res	Type
1	C	955	ARG
1	C	967	LEU
1	C	972	GLU
1	C	975	ARG
1	C	977	LEU
1	C	983	LEU
1	C	984	VAL
1	C	988	LEU
1	C	1001	THR
1	C	1002	HIS
1	C	1003	LEU
1	C	1007	SER
1	C	1011	GLU
1	C	1013	MET
1	C	1014	SER
1	C	1033	ILE
1	C	1055	SER
1	C	1056	ILE
1	C	1070	LYS
1	C	1078	LEU
1	C	1084	ARG
1	C	1089	VAL
1	C	1091	LYS
1	C	1098	ASN
1	C	1105	LEU
1	C	1107	LEU
1	C	1108	VAL
1	C	1110	ASN
1	C	1113	LEU
1	C	1127	ILE
1	C	1128	LYS
1	C	1129	LEU
1	C	1140	ASN
1	C	1141	SER
1	C	1164	ILE
1	C	1166	THR
1	C	1168	LEU
1	C	1175	LEU
1	C	1180	LEU
1	C	1183	GLN
1	C	1185	THR
1	C	1196	SER

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Mol	Chain	Res	Type
1	C	1200	LYS
1	C	1201	THR
1	C	1209	VAL
1	C	1212	LEU
1	C	1218	VAL
1	C	1227	PHE
1	C	1231	ASN
1	C	1236	ASP
1	C	1246	ARG
1	C	1259	LEU
1	C	1264	ILE
1	C	1279	ARG
1	C	1280	TYR
1	C	1301	SER
1	C	1302	LEU
1	C	1303	LEU
1	C	1306	GLN
1	C	1307	LEU
1	C	1308	ARG
1	C	1309	LEU
1	C	1311	MET
1	C	1323	LEU
1	C	1326	TYR
1	C	1330	ASP
1	C	1331	LYS
1	C	1332	ASN
1	C	1333	PHE
1	C	1334	LEU
1	C	1336	ARG
1	C	1338	VAL
1	C	1341	LEU
1	C	1346	LEU
1	C	1356	LEU
1	C	1358	THR
1	C	1361	VAL
1	C	1363	THR
1	C	1366	HIS
1	C	1367	LYS
1	C	1372	GLU
1	C	1374	VAL
1	C	1375	CYS
1	C	1397	SER

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Mol	Chain	Res	Type
1	C	1423	VAL
1	C	1433	SER
1	C	1450	PHE
1	C	1454	GLN
1	C	1464	LEU
1	C	1470	SER
1	C	1474	CYS
1	C	1475	VAL
1	C	1476	ARG
1	C	1479	ILE
1	C	1480	PHE
1	C	1483	PHE
1	C	1487	PHE
1	C	1488	LEU
1	C	1492	THR
1	C	1493	PHE
1	C	1494	THR
1	C	1500	ARG
1	C	1503	LYS
1	C	1504	GLN
1	C	1506	THR
1	C	1507	MET
1	C	1512	SER
1	C	1535	MET
1	C	1542	THR
1	C	1544	SER
1	C	1548	ARG
1	C	1549	LYS
1	C	1553	CYS
1	C	1566	THR
1	C	1577	TYR
1	C	1580	THR
1	C	1581	LEU
1	C	1585	TYR
1	C	1598	ILE
1	C	1602	LYS
1	C	1605	THR
1	C	1606	CYS
1	C	1616	GLN
1	C	1618	LEU
1	C	1626	GLN
1	C	1627	ILE

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Mol	Chain	Res	Type
1	C	1631	PHE
1	C	1636	ILE
1	C	1639	LEU
1	C	1650	ARG
1	C	1651	ASP
1	C	1652	THR
1	C	1655	SER
1	C	1663	ASN
2	D	29	THR
2	D	40	GLN
2	D	43	VAL
2	D	54	LEU
2	D	56	ILE
2	D	58	VAL
2	D	68	LEU
2	D	71	THR
2	D	74	ASP
2	D	82	LEU
2	D	86	THR
2	D	87	ILE
2	D	100	GLN
2	D	105	VAL
2	D	106	VAL
2	D	108	VAL
2	D	114	ARG
2	D	119	VAL
2	D	120	LEU
2	D	124	GLN
2	D	144	LEU
2	D	147	VAL
2	D	167	THR
2	D	171	ILE
2	D	175	SER
2	D	176	ASN
2	D	177	SER
2	D	179	ASP
2	D	183	PHE
2	D	190	ASP
2	D	191	LEU
2	D	196	THR
2	D	198	ARG
2	D	202	LYS

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Mol	Chain	Res	Type
2	D	208	GLU
2	D	214	PHE
2	D	216	VAL
2	D	217	ARG
2	D	219	TYR
2	D	220	VAL
2	D	221	LEU
2	D	223	SER
2	D	226	VAL
2	D	231	SER
2	D	234	PHE
2	D	243	PHE
2	D	258	GLU
2	D	263	VAL
2	D	264	LEU
2	D	278	ASP
2	D	280	LEU
2	D	285	ILE
2	D	291	LYS
2	D	296	ARG
2	D	297	ASP
2	D	298	THR
2	D	299	PHE
2	D	301	SER
2	D	306	LEU
2	D	315	TYR
2	D	317	SER
2	D	323	GLU
2	D	327	ASP
2	D	328	MET
2	D	344	GLN
2	D	345	ILE
2	D	348	THR
2	D	349	LYS
2	D	358	MET
2	D	368	ASN
2	D	379	VAL
2	D	382	GLU
2	D	386	SER
2	D	389	THR
2	D	390	THR
2	D	398	LEU

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Mol	Chain	Res	Type
2	D	400	LEU
2	D	404	LEU
2	D	414	ARG
2	D	416	ASN
2	D	422	ARG
2	D	427	THR
2	D	433	ILE
2	D	435	TYR
2	D	437	THR
2	D	449	ILE
2	D	460	LEU
2	D	466	VAL
2	D	469	ASN
2	D	472	SER
2	D	473	LEU
2	D	481	TYR
2	D	482	LEU
2	D	483	ILE
2	D	490	PHE
2	D	497	ARG
2	D	504	VAL
2	D	505	THR
2	D	511	THR
2	D	513	ASP
2	D	518	PHE
2	D	520	PHE
2	D	521	VAL
2	D	523	TYR
2	D	524	TYR
2	D	525	GLN
2	D	526	VAL
2	D	531	ILE
2	D	532	VAL
2	D	543	THR
2	D	544	CYS
2	D	555	LEU
2	D	556	ILE
2	D	558	MET
2	D	563	MET
2	D	567	LEU
2	D	586	VAL
2	D	588	ASN

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Mol	Chain	Res	Type
2	D	593	ILE
2	D	597	LYS
2	D	598	ILE
2	D	602	ILE
2	D	613	SER
2	D	615	GLN
2	D	629	THR
2	D	638	GLN
2	D	735	ASN
2	D	742	ASP
2	D	745	ILE
2	D	746	ILE
2	D	747	SER
2	D	764	GLU
2	D	769	GLN
2	D	773	SER
2	D	778	PHE
2	D	780	LEU
2	D	784	ILE
2	D	789	VAL
2	D	800	ILE
2	D	812	LYS
2	D	813	VAL
2	D	816	ILE
2	D	817	ASP
2	D	819	GLN
2	D	829	GLN
2	D	830	VAL
2	D	836	LEU
2	D	840	VAL
2	D	851	LEU
2	D	857	CYS
2	D	866	TYR
2	D	868	GLN
2	D	870	PHE
2	D	872	ILE
2	D	873	LYS
2	D	881	PRO
2	D	884	ILE
2	D	889	GLN
2	D	891	LEU
2	D	918	GLU

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Mol	Chain	Res	Type
2	D	920	VAL
2	D	925	VAL
2	D	926	THR
2	D	946	LYS
2	D	948	ARG
2	D	949	LYS
2	D	952	ASP
2	D	963	ILE
2	D	964	ILE
2	D	1273	LEU
2	D	1274	ASN
2	D	1278	THR
2	D	1279	ILE
2	D	1281	LEU
2	D	1291	ARG
2	D	1292	ILE
2	D	1301	ARG
2	D	1304	GLU
2	D	1305	THR
2	D	1308	ASN
2	D	1313	VAL
2	D	1322	THR
2	D	1324	THR
2	D	1330	ASN
2	D	1332	GLN
2	D	1344	HIS
2	D	1345	LEU
2	D	1346	ASN
2	D	1349	VAL
2	D	1350	GLU
2	D	1351	ASN
2	D	1365	LEU
2	D	1372	LEU
2	D	1378	THR
2	D	1380	THR
2	D	1388	THR
2	D	1396	ASP
2	D	1398	THR
2	D	1401	SER
2	D	1406	ARG
2	D	1423	VAL
2	D	1424	ILE

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Mol	Chain	Res	Type
2	D	1427	LEU
2	D	1429	LYS
2	D	1431	SER
2	D	1433	SER
2	D	1437	CYS
2	D	1438	LEU
2	D	1439	HIS
2	D	1442	ILE
2	D	1443	LEU
2	D	1448	VAL
2	D	1450	PHE
2	D	1451	ILE
2	D	1456	VAL
2	D	1464	LEU
2	D	1475	ASP
2	D	1480	LEU
2	D	1481	LEU
2	D	1490	CYS
2	D	1492	CYS
2	D	1495	GLU
2	D	1496	THR
2	D	1497	CYS
2	D	1500	LEU
2	D	1502	HIS
2	D	1504	GLU
2	D	1511	GLN
2	D	1516	CYS
2	D	1519	ASN
2	D	1526	THR
2	D	1535	ASP
2	D	1561	HIS
2	D	1566	GLN
2	D	1571	GLU
2	D	1582	LEU
2	D	1583	ILE
2	D	1584	TRP
2	D	1594	LYS
2	D	1598	SER
2	D	1599	TYR
2	D	1604	ASN
2	D	1606	TRP
2	D	1607	ILE

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Mol	Chain	Res	Type
2	D	1609	ARG
2	D	1614	ASP
2	D	1622	GLN
2	D	1623	LYS

Some sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (139) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	80	GLN
1	A	97	ASN
1	A	139	GLN
1	A	242	ASN
1	A	257	ASN
1	A	288	GLN
1	A	298	GLN
1	A	355	ASN
1	A	391	ASN
1	A	472	ASN
1	A	473	HIS
1	A	483	ASN
1	A	550	GLN
1	A	569	ASN
1	A	613	GLN
1	A	692	HIS
1	A	706	ASN
1	A	785	GLN
1	A	787	GLN
1	A	800	GLN
1	A	854	GLN
1	A	875	HIS
1	A	876	GLN
1	A	894	HIS
1	A	1023	HIS
1	A	1029	ASN
1	A	1102	ASN
1	A	1112	GLN
1	A	1183	GLN
1	A	1234	HIS
1	A	1241	ASN
1	A	1268	ASN
1	A	1343	ASN
1	A	1366	HIS

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Mol	Chain	Res	Type
1	A	1550	GLN
1	A	1608	ASN
1	A	1658	GLN
2	B	40	GLN
2	B	65	GLN
2	B	124	GLN
2	B	152	HIS
2	B	176	ASN
2	B	187	ASN
2	B	312	HIS
2	B	333	GLN
2	B	337	HIS
2	B	344	GLN
2	B	417	HIS
2	B	469	ASN
2	B	525	GLN
2	B	528	ASN
2	B	588	ASN
2	B	615	GLN
2	B	735	ASN
2	B	769	GLN
2	B	819	GLN
2	B	829	GLN
2	B	869	GLN
2	B	889	GLN
2	B	901	GLN
2	B	921	GLN
2	B	1330	ASN
2	B	1341	ASN
2	B	1419	GLN
2	B	1473	HIS
2	B	1482	ASN
2	B	1501	ASN
2	B	1503	GLN
2	B	1562	GLN
2	B	1566	GLN
1	C	80	GLN
1	C	97	ASN
1	C	139	GLN
1	C	242	ASN
1	C	257	ASN
1	C	298	GLN

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Mol	Chain	Res	Type
1	C	355	ASN
1	C	391	ASN
1	C	472	ASN
1	C	473	HIS
1	C	483	ASN
1	C	550	GLN
1	C	569	ASN
1	C	613	GLN
1	C	692	HIS
1	C	706	ASN
1	C	785	GLN
1	C	787	GLN
1	C	800	GLN
1	C	854	GLN
1	C	875	HIS
1	C	876	GLN
1	C	894	HIS
1	C	1023	HIS
1	C	1029	ASN
1	C	1102	ASN
1	C	1112	GLN
1	C	1183	GLN
1	C	1234	HIS
1	C	1241	ASN
1	C	1268	ASN
1	C	1324	HIS
1	C	1366	HIS
1	C	1550	GLN
1	C	1608	ASN
1	C	1658	GLN
2	D	40	GLN
2	D	65	GLN
2	D	124	GLN
2	D	152	HIS
2	D	176	ASN
2	D	187	ASN
2	D	312	HIS
2	D	333	GLN
2	D	337	HIS
2	D	344	GLN
2	D	417	HIS
2	D	507	ASN

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Mol	Chain	Res	Type
2	D	525	GLN
2	D	528	ASN
2	D	588	ASN
2	D	615	GLN
2	D	735	ASN
2	D	769	GLN
2	D	819	GLN
2	D	829	GLN
2	D	869	GLN
2	D	889	GLN
2	D	901	GLN
2	D	921	GLN
2	D	1330	ASN
2	D	1341	ASN
2	D	1419	GLN
2	D	1473	HIS
2	D	1482	ASN
2	D	1501	ASN
2	D	1503	GLN
2	D	1562	GLN
2	D	1566	GLN

### 5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

### 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

### 5.6 Ligand geometry [i](#)

6 ligands 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
3	NAG	B	2001	2	14,14,15	0.81	1 (7%)	17,19,21	2.07	3 (17%)
3	NAG	D	2002	2	14,14,15	0.92	0	17,19,21	1.16	1 (5%)
3	NAG	C	2003	1	14,14,15	0.58	0	17,19,21	2.21	4 (23%)
3	NAG	A	2003	1	14,14,15	0.60	0	17,19,21	2.19	4 (23%)
3	NAG	D	2001	2	14,14,15	0.74	0	17,19,21	2.16	4 (23%)
3	NAG	B	2002	2	14,14,15	0.92	0	17,19,21	1.16	1 (5%)

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
3	NAG	B	2001	2	-	2/6/23/26	0/1/1/1
3	NAG	D	2002	2	-	0/6/23/26	0/1/1/1
3	NAG	C	2003	1	-	3/6/23/26	0/1/1/1
3	NAG	A	2003	1	-	3/6/23/26	0/1/1/1
3	NAG	D	2001	2	-	2/6/23/26	0/1/1/1
3	NAG	B	2002	2	-	0/6/23/26	0/1/1/1

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
3	B	2001	NAG	C1-C2	2.16	1.55	1.52

All (17) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	D	2001	NAG	C1-O5-C5	6.57	121.10	112.19
3	B	2001	NAG	C1-O5-C5	6.17	120.56	112.19
3	A	2003	NAG	C1-O5-C5	5.70	119.91	112.19
3	C	2003	NAG	C1-O5-C5	5.67	119.87	112.19
3	C	2003	NAG	C4-C3-C2	4.36	117.41	111.02
3	A	2003	NAG	C4-C3-C2	4.24	117.23	111.02
3	B	2001	NAG	O5-C1-C2	3.91	117.46	111.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	B	2002	NAG	O5-C1-C2	-3.70	105.45	111.29
3	D	2002	NAG	O5-C1-C2	-3.68	105.48	111.29
3	D	2001	NAG	O5-C1-C2	3.63	117.02	111.29
3	C	2003	NAG	C1-C2-N2	-3.17	105.07	110.49
3	A	2003	NAG	C1-C2-N2	-3.07	105.25	110.49
3	A	2003	NAG	C3-C4-C5	2.99	115.56	110.24
3	C	2003	NAG	C3-C4-C5	2.95	115.50	110.24
3	D	2001	NAG	C2-N2-C7	-2.57	119.24	122.90
3	B	2001	NAG	C2-N2-C7	-2.38	119.52	122.90
3	D	2001	NAG	O5-C5-C6	2.08	110.46	107.20

There are no chirality outliers.

All (10) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
3	B	2001	NAG	C8-C7-N2-C2
3	B	2001	NAG	O7-C7-N2-C2
3	C	2003	NAG	C3-C2-N2-C7
3	C	2003	NAG	C8-C7-N2-C2
3	C	2003	NAG	O7-C7-N2-C2
3	A	2003	NAG	C3-C2-N2-C7
3	A	2003	NAG	C8-C7-N2-C2
3	A	2003	NAG	O7-C7-N2-C2
3	D	2001	NAG	C8-C7-N2-C2
3	D	2001	NAG	O7-C7-N2-C2

There are no ring outliers.

4 monomers are involved in 6 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
3	B	2001	NAG	1	0
3	C	2003	NAG	2	0
3	A	2003	NAG	2	0
3	D	2001	NAG	1	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 [i](#)

### 6.1 Protein, DNA and RNA chains [i](#)

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<sup>th</sup> 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 <sup>2</sup> )	Q<0.9
1	A	1627/1676 (97%)	0.03	37 (2%) 60 51	90, 187, 312, 465	0
1	C	1627/1676 (97%)	0.01	31 (1%) 66 58	97, 186, 299, 486	0
2	B	1225/1642 (74%)	-0.01	25 (2%) 65 56	107, 174, 261, 395	0
2	D	1225/1642 (74%)	-0.01	18 (1%) 73 64	114, 181, 263, 371	0
All	All	5704/6636 (85%)	0.01	111 (1%) 66 58	90, 183, 291, 486	0

All (111) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
2	D	1355	ASN	5.3
1	A	1650	ARG	5.2
1	A	1622	LYS	4.9
2	B	155	SER	4.8
1	C	1676	CYS	4.8
2	B	156	LYS	4.8
1	A	1676	CYS	4.7
1	A	1585	TYR	4.6
2	D	155	SER	4.3
2	B	111	PRO	4.2
1	A	94	GLY	4.2
1	C	1622	LYS	4.1
1	C	317	ASP	4.1
2	D	154	THR	3.8
1	C	858	LYS	3.6
1	C	1534	GLN	3.5
1	A	1592	ALA	3.4
1	C	240	TYR	3.4
2	B	735	ASN	3.4
1	C	271	ILE	3.3
1	C	882	LYS	3.3

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Mol	Chain	Res	Type	RSRZ
1	A	1537	GLU	3.2
2	B	154	THR	3.1
2	B	157	MET	3.1
2	B	1355	ASN	3.0
1	A	1526	LYS	3.0
1	C	1526	LYS	3.0
1	A	273	GLU	3.0
2	D	1360	LYS	3.0
2	B	74	ASP	3.0
1	A	1597	GLU	3.0
1	A	1651	ASP	3.0
1	A	314	SER	2.9
1	C	1550	GLN	2.9
2	D	156	LYS	2.9
1	C	874	ASP	2.9
2	D	120	LEU	2.8
1	C	315	LEU	2.8
2	B	93	GLU	2.8
1	A	882	LYS	2.8
1	A	95	GLY	2.8
2	B	123	TYR	2.8
2	B	1353	HIS	2.7
1	A	1525	CYS	2.7
1	A	1598	ILE	2.7
1	C	272	ARG	2.7
1	C	94	GLY	2.6
2	D	735	ASN	2.6
2	B	95	SER	2.6
1	C	318	LEU	2.6
2	D	641	ALA	2.5
1	A	1590	ALA	2.5
2	B	424	ARG	2.5
2	B	1360	LYS	2.5
1	A	1588	GLY	2.5
2	B	1533	GLU	2.5
1	A	311	SER	2.5
1	C	93	PRO	2.5
1	A	1649	PRO	2.4
1	A	661	ASP	2.4
1	A	1572	ASN	2.4
1	A	1635	TYR	2.4
1	C	1551	THR	2.4

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Mol	Chain	Res	Type	RSRZ
1	A	1586	LYS	2.4
1	A	283	MET	2.4
2	D	157	MET	2.4
2	D	98	SER	2.4
1	A	1587	THR	2.4
1	A	1674	ASN	2.4
1	C	246	PHE	2.3
2	D	1354	LEU	2.3
1	C	301	PHE	2.3
2	D	65	GLN	2.3
1	A	1534	GLN	2.3
1	A	855	PHE	2.2
1	C	270	GLY	2.2
2	B	1495	GLU	2.2
1	C	1623	GLU	2.2
2	B	1374	GLU	2.2
1	C	273	GLU	2.2
1	C	857	VAL	2.2
2	B	902	GLU	2.2
2	B	52	LYS	2.2
2	B	237	ILE	2.2
1	A	313	TYR	2.2
1	C	1585	TYR	2.2
2	B	1532	GLU	2.2
1	C	321	LYS	2.1
1	A	1544	SER	2.1
1	C	1675	GLY	2.1
2	B	1466	GLU	2.1
1	A	281	GLU	2.1
1	A	348	VAL	2.1
2	B	1376	ASP	2.1
2	D	52	LYS	2.1
1	A	1579	ALA	2.1
2	D	308	GLU	2.1
2	B	153	ASN	2.1
1	C	887	LYS	2.1
1	C	1611	LEU	2.1
1	A	1620	MET	2.1
2	D	66	LYS	2.1
2	D	648	ALA	2.1
1	C	913	SER	2.1
2	B	67	THR	2.1

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Mol	Chain	Res	Type	RSRZ
2	D	99	ARG	2.0
1	A	1557	ILE	2.0
1	C	1609	ALA	2.0
2	D	158	ASN	2.0
1	C	1177	GLU	2.0
1	A	887	LYS	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](#)

There are no monosaccharides in this entry.

## 6.4 Ligands [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. The B-factors column lists the minimum, median, 95<sup>th</sup> 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	B-factors( $\text{\AA}^2$ )	Q<0.9
3	NAG	B	2002	14/15	0.45	0.44	321,327,336,339	0
3	NAG	A	2003	14/15	0.64	0.38	284,286,289,289	0
3	NAG	C	2003	14/15	0.72	0.34	260,272,284,287	0
3	NAG	D	2002	14/15	0.74	0.47	289,293,305,308	0
3	NAG	B	2001	14/15	0.78	0.26	275,285,305,313	0
3	NAG	D	2001	14/15	0.80	0.31	285,296,309,310	0

## 6.5 Other polymers [i](#)

There are no such residues in this entry.