



Full wwPDB X-ray Structure Validation Report ⓘ

Mar 9, 2026 – 05:42 AM UTC

PDB ID : 3G61 / pdb_00003g61
Title : Structure of P-glycoprotein Reveals a Molecular Basis for Poly-Specific Drug Binding
Authors : Aller, S.G.; Yu, J.; Ward, A.; Weng, Y.; Chittaboina, S.; Zhuo, R.; Harrell, P.M.; Trinh, Y.T.; Zhang, Q.; Urbatsch, I.L.; Chang, G.
Deposited on : 2009-02-05
Resolution : 4.35 Å(reported)

This is a Full wwPDB X-ray Structure Validation Report for a publicly released PDB entry.

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

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

with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

MolProbity	:	4-5-2 with Phenix2.0
Mogul	:	2022.3.0, CSD as543be (2022)
Xtriage (Phenix)	:	2.0
EDS	:	3.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
CCP4	:	9.0.010 (Gargrove)
Density-Fitness	:	1.0.12
Ideal geometry (proteins)	:	Engh & Huber (2001)
Ideal geometry (DNA, RNA)	:	Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP)	:	2.49

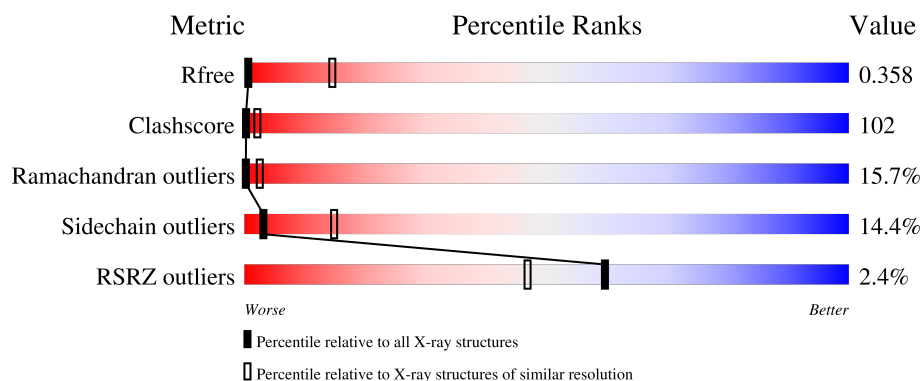
1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

X-RAY DIFFRACTION

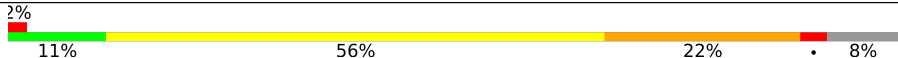
The reported resolution of this entry is 4.35 Å.

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}	180053	1059 (4.76-3.90)
Clashscore	190562	1105 (4.76-3.90)
Ramachandran outliers	187476	1007 (4.76-3.90)
Sidechain outliers	187428	1022 (4.80-3.88)
RSRZ outliers	180081	1056 (4.76-3.90)

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 of the lower bar indicate the fraction of residues that contain outliers for ≥ 3 , 2, 1 and 0 types of geometric quality criteria respectively. A grey segment represents the fraction of residues that are not modelled. The numeric value for each fraction is indicated below the corresponding segment, with a dot representing fractions $\leq 5\%$. 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	1284	
1	B	1284	

2 Entry composition [i](#)

There are 2 unique types of molecules in this entry. The entry contains 18448 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.

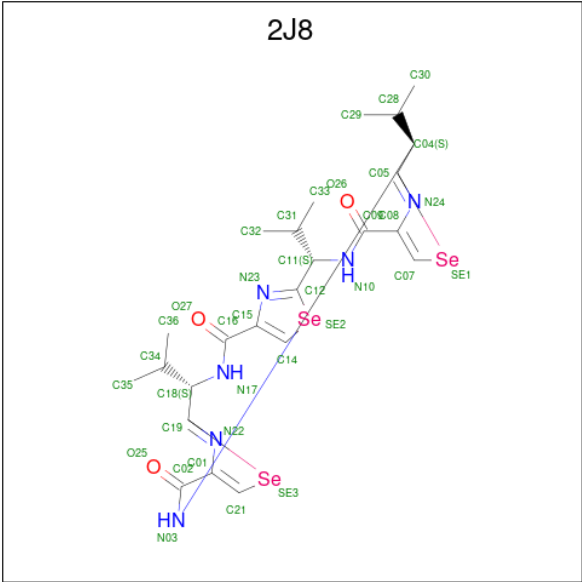
- Molecule 1 is a protein called Multidrug resistance protein 1a.

Mol	Chain	Residues	Atoms					ZeroOcc	AltConf	Trace
1	A	1182	Total	C	N	O	S	0	0	0
			9171	5895	1552	1686	38			
1	B	1182	Total	C	N	O	S	0	0	0
			9171	5895	1552	1686	38			

There are 16 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
A	1277	TYR	-	expression tag	UNP Q5I1Y5
A	1278	VAL	-	expression tag	UNP Q5I1Y5
A	1279	HIS	-	expression tag	UNP Q5I1Y5
A	1280	HIS	-	expression tag	UNP Q5I1Y5
A	1281	HIS	-	expression tag	UNP Q5I1Y5
A	1282	HIS	-	expression tag	UNP Q5I1Y5
A	1283	HIS	-	expression tag	UNP Q5I1Y5
A	1284	HIS	-	expression tag	UNP Q5I1Y5
B	1277	TYR	-	expression tag	UNP Q5I1Y5
B	1278	VAL	-	expression tag	UNP Q5I1Y5
B	1279	HIS	-	expression tag	UNP Q5I1Y5
B	1280	HIS	-	expression tag	UNP Q5I1Y5
B	1281	HIS	-	expression tag	UNP Q5I1Y5
B	1282	HIS	-	expression tag	UNP Q5I1Y5
B	1283	HIS	-	expression tag	UNP Q5I1Y5
B	1284	HIS	-	expression tag	UNP Q5I1Y5

- Molecule 2 is (4S,11S,18S)-4,11,18-tri(propan-2-yl)-6,13,20-triseleno-3,10,17,22,23,24-hexaazatetracyclo[17.2.1.1.5,8.1.12,15]tetracos-1(21),5(24),7,12(23),14,19(22)-hexaene-2,9,16-tri-one (CCD ID: 2J8) (formula: C₂₄H₃₀N₆O₃Se₃).

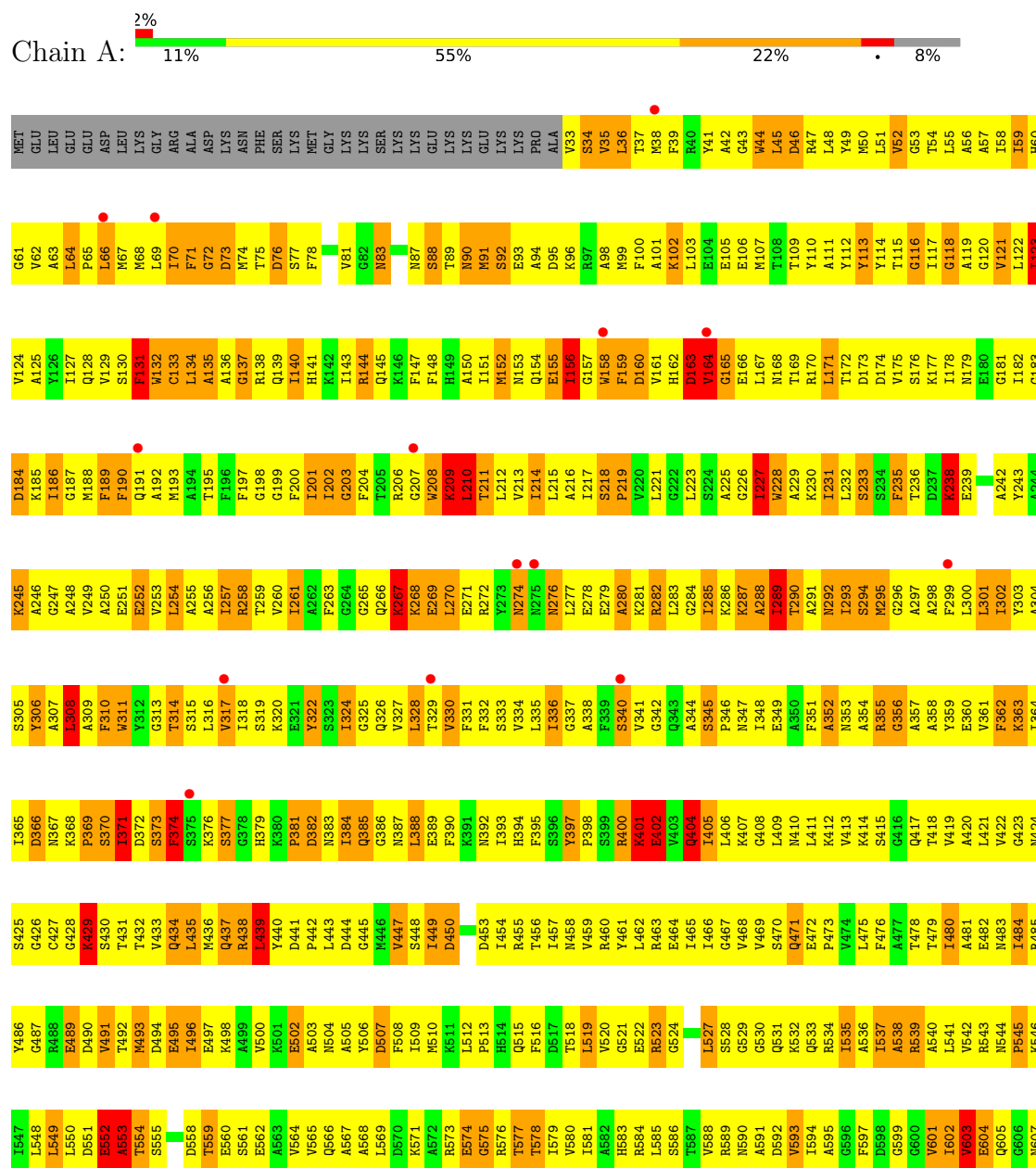


Mol	Chain	Residues	Atoms					ZeroOcc	AltConf
2	A	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		
2	A	1	Total	C	N	O	Se	0	0
			17	11	3	1	2		
2	B	1	Total	C	N	O	Se	0	0
			36	24	6	3	3		
2	B	1	Total	C	N	O	Se	0	0
			17	11	3	1	2		

3 Residue-property plots

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

- Molecule 1: Multidrug resistance protein 1a





A976	A977	A978	A979	A980	A981	A982	A983	A984	A985	A986	A987	A988	A989	A990	A991	A992	A993	A994	A995	A996	A997	A998	A999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																								
L853	L854	L855	L856	L857	L858	L859	L860	L861	L862	L863	L864	L865	L866	L867	L868	L869	L870	L871	L872	L873	L874	L875	L876	L877	L878	L879	L880	L881	L882	L883	L884	L885	L886	L887	L888	L889	L890	L891	L892	L893	L894	L895	L896	L897	L898	L899	L900	L901	L902	L903	L904	L905	L906	L907	L908	L909	L910	L911	L912	L913	L914	L915	L916	L917	L918	L919	L920	L921	L922	L923	L924	L925	L926	L927	L928	L929	L930	L931	L932	L933	L934	L935	L936	L937	L938	L939	L940	L941	L942	L943	L944	L945	L946	L947	L948	L949	L950	L951	L952	L953	L954	L955	L956	L957	L958	L959	L960	L961	L962	L963	L964	L965	L966	L967	L968	L969	L970	L971	L972	L973	L974	L975	L976	L977	L978	L979	L980	L981	L982	L983	L984	L985	L986	L987	L988	L989	L990	L991	L992	L993	L994	L995	L996	L997	L998	L999	A1000	A1001	A1002	A1003	A1004	A1005	A1006	A1007	A1008	A1009	A1010	A1011	A1012	A1013	A1014	A1015	A1016	A1017	A1018	A1019	A1020	A1021	A1022	A1023	A1024	A1025	A1026	A1027	A1028	A1029	A1030	A1031	A1032	A1033	A1034	A1035	A1036	A1037	A1038																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																																													
V732	V733	V734	V735	V736	V737	V738	V739	V740	V741	V742	V743	V744	V745	V746	V747	V748	V749	V750	V751	V752	V753	V754	V755	V756	V757	V758	V759	V760	V761	V762	V763	V764	V765	V766	V767	V768	V769	V770	V771	V772	V773	V774	V775	V776	V777	V778	V779	V780	V781	V782	V783	V784	V785	V786	V787	V788	V789	V790	V791	V792	V793	V794	V795	V796	V797	V798	V799	V800	V801	V802	V803	V804	V805	V806	V807	V808	V809	V810	V811	V812	V813	V814	V815	V816	V817	V818	V819	V820	V821	V822	V823	V824	V825	V826	V827	V828	V829	V830	V831	V832	V833	V834	V835	V836	V837	V838	V839	V840	V841	V842	V843	V844	V845	V846	V847	V848	V849	V850	V851	V852	V853	V854	V855	V856	V857	V858	V859	V860	V861	V862	V863	V864	V865	V866	V867	V868	V869	V870	V871	V872	V873	V874	V875	V876	V877	V878	V879	V880	V881	V882	V883	V884	V885	V886	V887	V888	V889	V890	V891	V892	V893	V894	V895	V896	V897	V898	V899	V900	V901	V902	V903	V904	V905	V906	V907	V908	V909	V910	V911	V912	V913	V914	V915	V916	V917	V918	V919	V920	V921	V922	V923	V924	V925	V926	V927	V928	V929	V930	V931	V932	V933	V934	V935	V936	V937	V938	V939	V940	V941	V942	V943	V944	V945	V946	V947	V948	V949	V950	V951	V952	V953	V954	V955	V956	V957	V958	V959	V960	V961	V962	V963	V964	V965	V966	V967	V968	V969	V970	V971	V972	V973	V974	V975	V976	V977	V978	V979	V980	V981	V982	V983	V984	V985	V986	V987	V988	V989	V990	V991	V992	V993	V994	V995	V996	V997	V998	V999	S1000	S1001	S1002	S1003	S1004	S1005	S1006	S1007	S1008	S1009	S1010	S1011	S1012	S1013	S1014	S1015	S1016	S1017	S1018	S1019	S1020	S1021	S1022	S1023	S1024	S1025	S1026	S1027	S1028	S1029	S1030	S1031	S1032	S1033	S1034	S1035	S1036	S1037	S1038	S1039	S1040	S1041	S1042	S1043	S1044	S1045	S1046	S1047	S1048	S1049	S1050	S1051	S1052	S1053	S1054	S1055	S1056	S1057	S1058	S1059	S1060	S1061	S1062	S1063	S1064	S1065	S1066	S1067	S1068	S1069	S1070	S1071	S1072	S1073	S1074	S1075	S1076	S1077	S1078	S1079	S1080	S1081	S1082	S1083	S1084	S1085	S1086	S1087	S1088	S1089	S1090	S1091	S1092	S1093	S1094	S1095	S1096	S1097	S1098	S1099	S1100	S1101	S1102	S1103	S1104	S1105	S1106	S1107	S1108	S1109	S1110	S1111	S1112	S1113	S1114	S1115	S1116	S1117	S1118	S1119	S1120	S1121	S1122	S1123	S1124	S1125	S1126	S1127	S1128	S1129	S1130	S1131	S1132	S1133	S1134	S1135	S1136	S1137	S1138	S1139	S1140	S1141	S1142	S1143	S1144	S1145	S1146	S1147	S1148	S1149	S1150	S1151	S1152	S1153	S1154	S1155	S1156	S1157	S1158	S1159	S1160	S1161	S1162	S1163	S1164	S1165	S1166	S1167	S1168	S1169	S1170	S1171	S1172	S1173	S1174	S1175	S1176	S1177	S1178	S1179	S1180	S1181	S1182	S1183	S1184	S1185	S1186	S1187	S1188	S1189	S1190	S1191	S1192	S1193	S1194	S1195	S1196	S1197	S1198	S1199	S1200	S1201	S1202	S1203	S1204	S1205	S1206	S1207	S1208	S1209	S1210	S1211	S1212	S1213	S1214	S1215	S1216	S1217	S1218	S1219	S1220	S1221	S1222	S1223	S1224	S1225	S1226	S1227	S1228	S1229	S1230	S1231	S1232	S1233	S1234	S1235	S1236	S1237	S1238	S1239	S1240	S1241	S1242	S1243	S1244	S1245	S1246	S1247	S1248	S1249	S1250	S1251	S1252	S1253	S1254	S1255	S1256	S1257	S1258	S1259	S1260	S1261	S1262	S1263	S1264	S1265	S1266	S1267	S1268	S1269	S1270	S1271	S1272	S1273	S1274	S1275	S1276	S1277	S1278	S1279	S1280	S1281	S1282	S1283	S1284	S1285	S1286	S1287	S1288	S1289	S1290	S1291	S1292	S1293	S1294	S1295	S1296	S1297	S1298	S1299	S1300	S1301	S1302	S1303	S1304	S1305	S1306	S1307	S1308	S1309	S1310	S1311	S1312	S1313	S1314	S1315	S1316	S1317	S1318	S1319	S1320	S1321	S1322	S1323	S1324	S1325	S1326	S1327	S1328	S1329	S1330	S1331	S1332	S1333	S1334	S1335	S1336	S1337	S1338	S1339	S1340	S1341	S1342	S1343	S1344	S1345	S1346	S1347	S1348	S1349	S1350	S1351	S1352	S1353	S1354	S1355	S1356	S1357	S1358	S1359	S1360	S1361	S1362	S1363	S1364	S1365	S1366	S1367	S1368	S1369	S1370	S1371	S1372	S1373	S1374	S1375	S1376	S1377	S1378	S1379	S1380	S1381	S1382	S1383	S1384	S1385	S1386	S1387	S1388	S1389	S1390	S1391	S1392	S1393	S1394	S1395	S1396	S1397	S1398	S1399	S1400	S1401	S1402	S1403	S1404	S1405	S1406	S1407	S1408	S1409	S1410	S1411	S1412	S1413	S1414	S1415	S1416	S1417	S1418	S1419	S1420	S1421	S1422	S1423	S1424	S1425	S1426	S1427	S1428	S1429	S1430	S1431	S1432	S1433	S1434	S1435	S1436	S1437	S1438	S1439	S1440	S1441	S1442	S1443	S1444	S1445	S1446	S1447	S1448	S1449	S1450	S1451	S1452	S1453	S1454	S1455	S1456	S1457	S1458	S1459	S1460	S1461	S1462	S1463	S1464	S1465	S1466	S1467	S1468	S1469	S1470	S1471	S1472	S1473	S1474	S1475	S1476	S1477	S1478	S1479	S1480	S1481	S1482	S1483	S1484	S1485	S1486	S1487	S1488	S1489	S1490	S1491	S1492	S1493	S1494	S1495	S1496	S1497	S1498	S1499	S1500	S1501	S1502	S1503	S1504	S1505	S1506	S1507	S1508	S1509	S1510	S1511	S1512	S1513	S1514	S1515	S1516	S1517	S1518	S1519	S1520	S1521	S1522	S1523	S1524	S1525	S1526	S1527	S1528	S1529	S1530	S1531	S1532	S1533	S1534	S1535	S1536	S1537	S1538	S1539	S1540	S1541	S1542	S1543	S1544	S1545	S1546	S1547	S1548	S1549	S1550	S1551	S1552	S1553	S1554	S1555	S1556	S1557	S1558	S1559	S1560	S1561	S1562	S1563	S1564	S1565	S1566	S1567	S1568	S1569	S1570	S1571	S1572	S1573	S1574	S1575	S1576	S1577	S1578	S1579	S1580	S1581	S1582	S1583	S1584	S1585	S1586	S1587	S1588	S1589	S1590	S1591	S1592	S1593	S1594	S1595	S1596	S1597	S1598	S1599	S1600	S1601	S1602	S1603	S1604	S1605	S1606	S1607	S1608	S1609	S1610	S1611	S1612	S1613	S1614	S1615	S1616	S1617	S1618	S1619	S1620	S1621	S1622	S1623	S1624	S1625	S1626	S1627	S1628	S1629	S1630	S1631	S1632	S1633	S1634	S1635	S1636	S1637	S1638	S1639	S1640	S1641	S1642	S1643	S1644	S1645	S1646	S1647	S1648	S1649	S1650	S1651	S1652	S1653	S1654	S1655	S1656	S1657	S1658	S1659	S1660	S1661	S1662	S1663	S1664	S1665	S1666	S1667	S1668	S1669	S1670	S1671	S1672	S1673	S1674	S1675	S1676	S1677	S1678	S1679	S1680	S1681	S1682	S1683	S1684	S1685	S1686	S1687	S1688	S1689	S1690	S1691	S1692	S1693	S1694	S1695	S1696	S1697	S1698	S1699	S1700	S1701	S1702	S1703	S1704	S1705	S1706	S1707	S1708	S1709	S1710	S1711	S1712	S1713	S1714	S1715	S1716	S1717	S1718	S1719	S1720	S1721	S1722	S1723	S1724	S1725	S1726	S1727	S1728	S1729	S1730	S1731	S1732	S1733	S1734	S1735	S1736	S1737	S1738	S1739	S1740	S1741	S1742	S1743	S1744	S1745	S1746	S1747	S1748	S1749	S1750	S1751	S1752	S1753	S1754	S1755	S1756	S1757	S1758	S1759	S1760	S1761	S1762	S1763	S1764	S1765	S1766	S1767	S1768	S1769	S1770	S1771	S1772	S1773	S1774	S1775	S1776	S1777	S1778	S1779	S1780	S1781	S1782	S1783	S1784	S1785	S1786	S1787	S1788	S1789	S1790	S1791	S1792	S1793	S1></

HIS	R1221	K1160	L1100	M1039
HIS	T1222	Y1161	N1101	Y1040
	C1223		V1102	P1041
	I1224	R1164	Q1103	T1042
	V1225	G1165	W1104	R1043
	I1226	G1166	L1105	P1044
	A1227	D1167	R1106	S1045
	H1228	K1168	A1107	I1046
	R1229	G1169	Q1108	P1047
	L1230	T1170	L1109	V1048
	S1231	Q1171	G1110	L1049
	T1232	L1172	I1111	Q1050
	I1233	S1173	W1112	G1051
	Q1234	G1174	S1113	L1052
	M1235	G1175	E1114	S1053
	A1236	Q1176	E1115	L1054
		K1177	P1116	E1055
		Q1178	I1117	V1056
	I1239	R1179	L1118	K1057
	V1240	I1180	F1119	K1058
	V1241	A1181	D1120	G1059
	I1242	I1182	C1121	Q1060
	Q1243	A1183	S1122	T1061
	M1244	R1184	I1123	L1062
	G1245	A1185	A1124	A1063
	K1246	L1186	E1125	L1064
	V1247	V1187	N1126	V1065
	K1248	R1188	I1127	G1066
	E1249	Q1189	A1128	S1067
	H1250	P1190	Y1129	S1068
	G1251	H1191	G1130	G1069
	T1252	I1192	D1131	G1070
	H1253	L1193	N1132	G1071
	Q1254	L1194	S1133	K1072
	Q1255	L1195	R1134	
	L1256	D1196	V1135	V1075
	L1257	E1197	V1136	V1076
	A1258	A1198	S1137	Q1077
	Q1259	T1199	Y1138	L1078
	K1260	S1200	E1139	L1079
	G1261	L1201	A1140	E1080
	Y1263	L1202	I1141	R1081
	I1262	D1203	V1142	F1082
	F1264	T1204	R1143	Y1083
	S1265	E1205	A1144	D1084
	M1266	S1206	A1145	P1085
	V1267	E1207	K1146	M1086
		K1208	E1147	A1087
	Q1270	V1209	A1148	G1088
	A1271	V1210	N1149	S1089
GLY		Q1211	I1150	V1090
ALA		E1212	H1151	F1091
LYS		A1213	Q1152	L1092
ARG		L1214	F1153	D1093
SER		D1215	I1154	G1094
TYR		K1216	D1155	K1095
VAL		A1217	S1156	E1096
HIS		R1218	L1157	I1097
HIS		E1219	P1158	K1098
HIS		G1220	D1159	Q1099

4 Data and refinement statistics

Property	Value	Source
Space group	P 21 21 21	Depositor
Cell constants a, b, c, α , β , γ	97.74Å 114.98Å 375.81Å 90.00° 90.00° 90.00°	Depositor
Resolution (Å)	19.95 – 4.35 19.95 – 4.35	Depositor EDS
% Data completeness (in resolution range)	93.3 (19.95-4.35) 92.1 (19.95-4.35)	Depositor EDS
R_{merge}	(Not available)	Depositor
R_{sym}	(Not available)	Depositor
$\langle I/\sigma(I) \rangle$ ¹	4.03 (at 4.36Å)	Xtriage
Refinement program	CNS	Depositor
R, R_{free}	0.308 , 0.356 0.312 , 0.358	Depositor DCC
R_{free} test set	2807 reflections (9.92%)	wwPDB-VP
Wilson B-factor (Å ²)	195.7	Xtriage
Anisotropy	0.362	Xtriage
Bulk solvent k_{sol} (e/Å ³), B_{sol} (Å ²)	0.17 , 50.2	EDS
L-test for twinning ²	$\langle L \rangle = 0.47$, $\langle L^2 \rangle = 0.30$	Xtriage
Estimated twinning fraction	No twinning to report.	Xtriage
F_o, F_c correlation	0.91	EDS
Total number of atoms	18448	wwPDB-VP
Average B, all atoms (Å ²)	182.0	wwPDB-VP

Xtriage's analysis on translational NCS is as follows: *The largest off-origin peak in the Patterson function is 2.34% of the height of the origin peak. No significant pseudotranslation is detected.*

¹Intensities estimated from amplitudes.

²Theoretical 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 [i](#)

5.1 Standard geometry [i](#)

Bond lengths and bond angles in the following residue types are not validated in this section: 2J8

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	0.56	1/9339 (0.0%)	1.13	95/12626 (0.8%)
1	B	0.54	0/9339	1.11	97/12626 (0.8%)
All	All	0.55	1/18678 (0.0%)	1.12	192/25252 (0.8%)

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

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

All (1) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
1	A	1204	THR	CA-CB	6.34	1.64	1.53

All (192) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	370	SER	N-CA-C	12.90	138.27	110.80
1	A	450	ASP	N-CA-C	-12.66	89.26	108.00
1	A	64	LEU	CA-C-N	-11.59	106.21	118.85
1	A	64	LEU	C-N-CA	-11.59	106.21	118.85
1	B	64	LEU	CA-C-N	-11.51	106.31	118.85
1	B	64	LEU	C-N-CA	-11.51	106.31	118.85
1	A	804	LYS	N-CA-C	-10.80	98.37	112.41
1	A	374	PHE	N-CA-C	10.64	133.47	110.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1159	ASP	N-CA-C	-10.57	88.29	110.80
1	A	345	SER	CA-C-N	-10.54	108.28	119.24
1	A	345	SER	C-N-CA	-10.54	108.28	119.24
1	B	804	LYS	N-CA-C	-10.24	97.43	111.87
1	A	163	ASP	N-CA-C	-9.82	98.88	113.61
1	B	345	SER	CA-C-N	-9.81	108.77	118.97
1	B	345	SER	C-N-CA	-9.81	108.77	118.97
1	B	852	GLN	N-CA-C	-9.81	96.55	111.56
1	A	1098	LYS	N-CA-C	-9.75	90.04	110.80
1	A	159	PHE	N-CA-C	-9.60	98.98	112.13
1	A	211	THR	N-CA-C	-9.39	100.92	112.38
1	A	1159	ASP	N-CA-C	-9.31	90.98	110.80
1	B	159	PHE	N-CA-C	-9.22	99.50	112.13
1	B	211	THR	N-CA-C	-9.12	101.25	112.38
1	A	708	VAL	N-CA-C	-9.06	100.29	110.62
1	B	980	GLY	N-CA-C	-8.68	102.31	112.73
1	A	293	ILE	N-CA-C	-8.66	100.26	113.16
1	A	267	LYS	N-CA-C	8.61	129.13	110.80
1	B	292	ASN	N-CA-C	-8.50	102.69	113.23
1	A	164	VAL	N-CA-C	8.47	126.95	109.34
1	A	480	ILE	N-CA-C	-8.46	102.58	110.53
1	B	293	ILE	N-CA-C	-8.44	100.59	113.16
1	A	980	GLY	N-CA-C	-8.40	102.65	112.73
1	B	268	LYS	N-CA-C	-8.38	100.65	112.13
1	B	708	VAL	N-CA-C	-8.28	101.18	110.62
1	B	902	THR	N-CA-C	-8.21	102.21	112.72
1	A	503	ALA	N-CA-C	-8.13	103.45	112.72
1	A	294	SER	N-CA-C	-8.11	103.38	113.28
1	A	66	LEU	N-CA-C	-8.02	101.63	111.33
1	B	66	LEU	N-CA-C	-8.01	101.64	111.33
1	A	902	THR	N-CA-C	-8.00	102.48	112.72
1	B	503	ALA	N-CA-C	-7.99	103.61	112.72
1	A	1017	TYR	N-CA-C	7.86	127.55	110.80
1	B	450	ASP	N-CA-C	-7.85	95.56	108.67
1	B	1098	LYS	N-CA-C	-7.82	94.14	110.80
1	A	123	ILE	N-CA-C	7.82	117.88	110.30
1	A	292	ASN	N-CA-C	-7.76	103.61	113.23
1	A	822	LYS	N-CA-C	-7.74	101.97	111.33
1	A	922	ILE	CA-C-N	-7.70	110.21	119.84
1	A	922	ILE	C-N-CA	-7.70	110.21	119.84
1	B	267	LYS	N-CA-C	7.66	127.12	110.80
1	B	480	ILE	N-CA-C	-7.50	103.22	110.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	268	LYS	N-CA-C	-7.47	101.42	111.96
1	B	922	ILE	CA-C-N	-7.44	110.53	119.84
1	B	922	ILE	C-N-CA	-7.44	110.53	119.84
1	B	294	SER	N-CA-C	-7.44	104.20	113.28
1	B	123	ILE	N-CA-C	7.38	117.46	110.30
1	B	164	VAL	N-CA-C	7.37	124.68	109.34
1	B	165	GLY	N-CA-C	-7.35	95.76	113.18
1	A	554	THR	N-CA-C	-7.34	102.24	112.45
1	A	972	LEU	N-CA-C	-7.34	103.59	112.54
1	B	743	THR	N-CA-C	-7.31	103.31	111.71
1	B	739	GLY	CA-C-N	7.30	127.90	120.38
1	B	739	GLY	C-N-CA	7.30	127.90	120.38
1	B	822	LYS	N-CA-C	-7.22	102.59	111.33
1	A	290	THR	N-CA-C	-7.18	104.39	113.01
1	B	1142	VAL	N-CA-C	-7.15	103.56	110.42
1	B	87	ASN	N-CA-C	-7.14	103.11	111.03
1	B	362	PHE	N-CA-C	-7.06	103.33	112.23
1	B	290	THR	N-CA-C	-7.06	104.54	113.01
1	A	695	ARG	N-CA-C	-7.05	103.59	111.28
1	A	743	THR	N-CA-C	-7.01	103.65	111.71
1	A	1142	VAL	N-CA-C	-6.96	103.73	110.42
1	B	210	LEU	N-CA-C	-6.92	103.17	111.69
1	A	165	GLY	N-CA-C	-6.91	96.79	113.18
1	B	972	LEU	N-CA-C	-6.88	104.15	112.54
1	A	739	GLY	CA-C-N	6.82	127.41	120.38
1	A	739	GLY	C-N-CA	6.82	127.41	120.38
1	B	1191	HIS	N-CA-C	-6.80	103.41	113.61
1	A	1191	HIS	N-CA-C	-6.76	103.48	113.61
1	A	818	ALA	N-CA-C	-6.74	103.85	111.07
1	A	362	PHE	N-CA-C	-6.72	103.76	112.23
1	A	699	LEU	N-CA-C	-6.70	103.23	111.33
1	B	233	SER	N-CA-C	-6.66	104.09	111.82
1	A	87	ASN	N-CA-C	-6.63	103.67	111.03
1	A	925	ARG	N-CA-C	-6.57	104.12	111.28
1	B	502	GLU	N-CA-C	-6.56	105.43	113.50
1	A	233	SER	N-CA-C	-6.56	104.21	111.82
1	B	721	GLN	CA-C-N	-6.52	111.89	119.32
1	B	721	GLN	C-N-CA	-6.52	111.89	119.32
1	B	340	SER	N-CA-C	-6.49	104.21	111.28
1	A	1016	SER	N-CA-C	6.48	118.14	111.14
1	B	853	LEU	N-CA-C	-6.46	103.86	111.03
1	B	818	ALA	N-CA-C	-6.42	104.19	111.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	575	GLY	N-CA-C	-6.42	97.97	113.18
1	A	164	VAL	CB-CA-C	-6.41	100.77	111.29
1	A	740	PRO	N-CA-C	6.41	118.52	110.70
1	A	721	GLN	CA-C-N	-6.41	112.02	119.32
1	A	721	GLN	C-N-CA	-6.41	112.02	119.32
1	B	699	LEU	N-CA-C	-6.38	104.33	111.28
1	B	740	PRO	N-CA-C	6.38	118.48	110.70
1	B	301	LEU	N-CA-C	-6.34	104.00	111.03
1	A	372	ASP	N-CA-C	-6.31	105.44	113.02
1	B	88	SER	N-CA-C	6.30	124.23	110.80
1	B	383	ASN	N-CA-C	6.30	120.69	113.19
1	A	88	SER	N-CA-C	6.21	124.04	110.80
1	A	553	ALA	N-CA-C	6.17	123.93	110.80
1	B	925	ARG	N-CA-C	-6.16	104.56	111.28
1	A	502	GLU	N-CA-C	-6.15	105.94	113.50
1	B	1107	ALA	N-CA-C	-6.12	103.93	111.40
1	A	689	PRO	N-CA-C	6.12	118.17	110.70
1	A	1079	LEU	N-CA-C	-6.06	104.59	111.07
1	A	301	LEU	N-CA-C	-6.04	104.33	111.03
1	A	1080	GLU	N-CA-C	-6.04	105.63	112.87
1	A	1082	PHE	N-CA-C	-6.01	105.44	112.89
1	B	690	PRO	N-CA-C	6.00	122.05	113.47
1	A	235	PHE	N-CA-C	-5.98	104.10	111.33
1	B	46	ASP	N-CA-C	-5.96	104.48	110.97
1	B	1082	PHE	N-CA-C	-5.93	105.53	112.89
1	A	288	ALA	N-CA-C	-5.91	104.78	112.23
1	B	163	ASP	N-CA-C	-5.91	104.74	113.61
1	B	964	LEU	N-CA-C	5.91	117.52	110.19
1	B	575	GLY	N-CA-C	-5.90	99.21	113.18
1	B	235	PHE	N-CA-C	-5.88	104.22	111.33
1	B	385	GLN	N-CA-C	5.88	123.31	110.80
1	A	289	ILE	N-CA-C	-5.87	105.02	110.53
1	A	1107	ALA	N-CA-C	-5.86	104.25	111.40
1	A	210	LEU	N-CA-C	-5.85	104.31	112.45
1	A	377	SER	N-CA-C	5.85	116.66	108.00
1	B	377	SER	N-CA-C	5.78	123.10	110.80
1	A	552	GLU	CB-CA-C	-5.74	98.99	110.42
1	B	1079	LEU	N-CA-C	-5.74	104.93	111.07
1	B	1013	GLU	N-CA-C	5.73	123.00	110.80
1	B	973	VAL	N-CA-C	-5.72	105.15	110.53
1	B	288	ALA	N-CA-C	-5.71	105.04	112.23
1	A	311	TRP	N-CA-C	5.69	118.22	111.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	A	340	SER	N-CA-C	-5.65	105.12	111.28
1	A	1204	THR	N-CA-C	5.61	122.74	110.80
1	A	964	LEU	N-CA-C	5.59	117.12	110.19
1	B	289	ILE	N-CA-C	-5.58	105.28	110.53
1	A	319	SER	N-CA-C	-5.58	105.52	112.93
1	B	311	TRP	N-CA-C	5.55	118.05	111.33
1	B	1080	GLU	N-CA-C	-5.55	106.21	112.87
1	B	963	GLN	N-CA-C	5.54	122.60	110.80
1	A	603	VAL	N-CA-C	5.46	120.69	109.34
1	A	1042	THR	N-CA-C	-5.45	99.19	110.80
1	B	182	ILE	N-CA-C	5.45	115.65	110.42
1	A	401	LYS	N-CA-C	5.43	117.90	111.33
1	B	979	PHE	N-CA-C	-5.42	105.45	111.36
1	B	1206	SER	CB-CA-C	5.42	121.21	110.42
1	B	36	LEU	N-CA-C	5.42	116.99	111.14
1	B	1181	ALA	N-CA-C	-5.40	104.79	111.33
1	B	363	LYS	N-CA-C	-5.40	105.47	111.36
1	A	1097	ILE	N-CA-C	-5.37	99.87	107.98
1	A	437	GLN	N-CA-C	-5.35	106.62	112.72
1	A	801	ASP	N-CA-C	-5.34	105.45	111.28
1	A	363	LYS	N-CA-C	-5.34	105.54	111.36
1	B	370	SER	CB-CA-C	-5.32	99.84	110.42
1	A	963	GLN	N-CA-C	5.31	122.10	110.80
1	B	485	ARG	N-CA-C	-5.30	104.75	111.11
1	A	46	ASP	N-CA-C	-5.30	105.19	110.97
1	A	1204	THR	N-CA-CB	-5.29	101.54	110.49
1	B	861	VAL	CA-C-N	-5.29	113.23	119.84
1	B	861	VAL	C-N-CA	-5.29	113.23	119.84
1	B	92	SER	N-CA-C	-5.28	106.90	113.55
1	B	1042	THR	N-CA-C	-5.27	99.56	110.80
1	B	376	LYS	N-CA-C	5.27	116.78	107.61
1	A	36	LEU	N-CA-C	5.24	116.80	111.14
1	B	603	VAL	N-CA-C	5.23	120.22	109.34
1	A	1011	THR	N-CA-C	-5.22	98.28	109.81
1	A	377	SER	CB-CA-C	-5.21	109.05	116.34
1	B	851	TRP	CB-CA-C	-5.21	100.06	110.42
1	A	92	SER	N-CA-C	-5.19	107.01	113.55
1	A	1157	LEU	CA-C-N	5.19	126.33	119.84
1	A	1157	LEU	C-N-CA	5.19	126.33	119.84
1	B	164	VAL	CB-CA-C	-5.18	102.80	111.29
1	B	1206	SER	N-CA-C	-5.14	99.85	110.80
1	B	1157	LEU	CA-C-N	5.14	126.26	119.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	B	1157	LEU	C-N-CA	5.14	126.26	119.84
1	A	979	PHE	N-CA-C	-5.12	105.78	111.36
1	B	695	ARG	N-CA-C	-5.12	105.59	111.07
1	B	319	SER	N-CA-C	-5.12	106.12	112.93
1	B	578	THR	N-CA-C	5.12	116.76	109.14
1	B	69	LEU	N-CA-C	-5.10	105.61	111.07
1	B	184	ASP	N-CA-C	-5.10	105.16	111.33
1	A	238	LYS	N-CA-C	-5.09	105.86	111.71
1	B	238	LYS	N-CA-C	-5.08	105.87	111.71
1	A	184	ASP	N-CA-C	-5.06	105.21	111.33
1	B	466	ILE	N-CA-C	5.06	114.03	106.85
1	A	1202	LEU	N-CA-C	5.04	115.19	108.23
1	B	296	GLY	N-CA-C	-5.04	106.56	113.27
1	A	287	LYS	N-CA-C	-5.04	105.44	112.45
1	A	371	ILE	CB-CA-C	-5.02	103.06	111.29
1	A	1181	ALA	N-CA-C	-5.01	105.26	111.33

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	916	TYR	Sidechain
1	B	916	TYR	Sidechain

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	9171	0	9344	1916	0
1	B	9171	0	9344	1904	0
2	A	53	0	36	5	0
2	B	53	0	36	20	0
All	All	18448	0	18760	3810	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 102.

All (3810) close contacts within the same asymmetric unit are listed below, sorted by their clash

magnitude.

Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:718:GLY:O	1:B:722:PRO:HD2	1.44	1.17
1:A:718:GLY:O	1:A:722:PRO:HD2	1.43	1.15
1:B:858:LEU:O	1:B:862:PRO:HD2	1.47	1.15
1:A:195:THR:HB	1:A:340:SER:HB2	1.27	1.14
1:B:35:VAL:HG23	1:B:36:LEU:H	1.13	1.11
1:A:858:LEU:O	1:A:862:PRO:HD2	1.50	1.09
1:B:195:THR:HB	1:B:340:SER:HB2	1.30	1.09
1:A:35:VAL:HG23	1:A:36:LEU:H	1.14	1.08
1:B:1011:THR:H	1:B:1012:PRO:HD2	1.16	1.07
1:B:711:ILE:HD11	1:B:832:ILE:HG21	1.37	1.06
1:B:691:ALA:HA	1:B:1002:SER:OG	1.55	1.06
1:A:523:ARG:HD3	1:A:524:GLY:H	1.20	1.05
1:A:711:ILE:HD11	1:A:832:ILE:HG21	1.39	1.05
1:A:61:GLY:O	1:A:65:PRO:HD2	1.56	1.04
1:B:61:GLY:O	1:B:65:PRO:HD2	1.56	1.04
1:B:851:TRP:HA	1:B:854:THR:HB	1.38	1.04
1:A:387:ASN:HD22	1:A:414:LYS:HA	1.21	1.04
1:B:1063:ALA:HB3	1:B:1239:ILE:HA	1.37	1.04
1:A:826:GLY:HA2	1:A:829:LEU:HD12	1.39	1.03
1:B:387:ASN:HD22	1:B:414:LYS:HA	1.23	1.03
1:B:523:ARG:HD3	1:B:524:GLY:H	1.19	1.03
1:A:253:VAL:HB	1:A:1119:PHE:HE1	1.17	1.03
1:A:853:LEU:HD22	1:A:853:LEU:H	1.20	1.03
1:B:1039:ASN:HB2	1:B:1047:PRO:HA	1.39	1.03
1:B:766:PHE:HA	1:B:769:GLN:HE21	1.24	1.02
1:A:1039:ASN:HB2	1:A:1047:PRO:HA	1.38	1.01
1:A:1018:SER:O	1:A:1101:ASN:HB2	1.59	1.01
1:B:959:LEU:HD22	1:B:964:LEU:HB2	1.41	1.01
1:A:1144:ALA:HA	1:A:1186:LEU:HD11	1.43	1.01
1:A:1063:ALA:HB3	1:A:1239:ILE:HA	1.39	1.00
1:B:1090:VAL:HG13	1:B:1097:ILE:HB	1.40	1.00
1:A:384:ILE:HG22	1:A:385:GLN:H	1.24	1.00
1:B:826:GLY:HA2	1:B:829:LEU:HD12	1.40	0.99
1:A:766:PHE:HA	1:A:769:GLN:HE21	1.25	0.99
1:A:1090:VAL:HG13	1:A:1097:ILE:HB	1.40	0.99
1:A:158:TRP:HE1	1:A:900:PHE:CB	1.75	0.99
1:B:897:ILE:HG13	1:B:898:GLU:H	1.26	0.99
1:B:1144:ALA:HA	1:B:1186:LEU:HD11	1.42	0.98
1:B:1036:VAL:HB	1:B:1052:LEU:HB3	1.45	0.98
1:A:1218:ARG:HH22	1:A:1235:ASN:HD22	1.10	0.98
1:B:67:MET:HE2	1:B:117:ILE:HG21	1.45	0.97

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:429:LYS:HD3	1:A:429:LYS:H	1.27	0.97
1:A:1022:LEU:HG	1:A:1104:TRP:NE1	1.80	0.97
1:B:1218:ARG:HH22	1:B:1235:ASN:HD22	1.10	0.96
1:A:373:SER:O	1:A:374:PHE:HB2	1.62	0.96
1:A:1036:VAL:HB	1:A:1052:LEU:HB3	1.44	0.95
1:A:394:HIS:HA	1:A:406:LEU:O	1.66	0.95
1:B:339:PHE:CE2	2:B:6003:2J8:SE3	2.69	0.95
1:B:978:VAL:HG21	2:B:6003:2J8:H30	1.46	0.95
1:A:996:LYS:H	1:A:996:LYS:HD3	1.30	0.95
1:B:1011:THR:H	1:B:1012:PRO:CD	1.79	0.95
1:B:339:PHE:CZ	2:B:6003:2J8:SE3	2.69	0.94
1:A:897:ILE:HG13	1:A:898:GLU:H	1.29	0.94
1:A:67:MET:HE2	1:A:117:ILE:HG21	1.45	0.94
1:B:523:ARG:CD	1:B:524:GLY:H	1.79	0.94
1:B:919:SER:O	1:B:923:PRO:HD2	1.67	0.94
1:A:616:GLY:O	1:A:620:LYS:HB2	1.66	0.94
1:B:996:LYS:H	1:B:996:LYS:HD3	1.30	0.94
1:A:1013:GLU:O	1:A:1014:ILE:HG23	1.68	0.93
1:B:394:HIS:HA	1:B:406:LEU:O	1.69	0.93
1:A:798:SER:OG	1:A:1041:PRO:HG2	1.69	0.93
1:A:158:TRP:HE1	1:A:900:PHE:HB3	1.31	0.92
1:B:318:ILE:HD11	1:B:325:GLY:N	1.83	0.92
1:A:797:VAL:HG21	1:A:1013:GLU:HG3	1.49	0.92
1:A:800:PHE:O	1:A:803:PRO:HD3	1.70	0.92
1:B:797:VAL:HG12	1:B:798:SER:H	1.35	0.92
1:B:795:GLN:HA	1:B:1012:PRO:HG3	1.52	0.92
1:B:1216:LYS:HA	1:B:1216:LYS:HE2	1.52	0.92
1:A:686:GLU:HG2	1:A:813:ARG:HH22	1.33	0.92
1:B:118:GLY:O	1:B:121:VAL:HG22	1.70	0.92
1:B:616:GLY:O	1:B:620:LYS:HB2	1.68	0.92
1:A:919:SER:O	1:A:923:PRO:HD2	1.70	0.91
1:A:964:LEU:HD13	1:A:965:MET:N	1.84	0.91
1:B:484:ILE:HG21	1:B:496:ILE:HD12	1.51	0.91
1:A:118:GLY:O	1:A:121:VAL:HG22	1.70	0.91
1:A:253:VAL:HB	1:A:1119:PHE:CE1	2.06	0.91
1:A:484:ILE:HG21	1:A:496:ILE:HD12	1.51	0.91
1:B:964:LEU:HD13	1:B:965:MET:N	1.85	0.91
1:B:690:PRO:HG2	1:B:1006:ARG:NH2	1.85	0.91
1:A:523:ARG:CD	1:A:524:GLY:H	1.83	0.91
1:B:202:ILE:HD12	1:B:203:GLY:N	1.86	0.91
1:B:318:ILE:HD13	1:B:327:VAL:HG13	1.54	0.90

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:892:ILE:HB	1:B:916:TYR:HE1	1.37	0.90
1:B:155:GLU:O	1:B:157:GLY:N	2.03	0.90
1:A:155:GLU:O	1:A:157:GLY:N	2.05	0.90
1:B:1202:LEU:HD21	1:B:1206:SER:HB3	1.54	0.90
1:B:907:THR:C	1:B:908:ARG:HE	1.79	0.90
1:B:1091:PHE:HE1	1:B:1096:GLU:HG2	1.37	0.90
1:B:318:ILE:HD11	1:B:324:ILE:HG12	1.54	0.89
1:A:892:ILE:HB	1:A:916:TYR:HE1	1.37	0.89
1:B:202:ILE:HD12	1:B:203:GLY:H	1.36	0.89
1:A:278:GLU:O	1:A:282:ARG:HG2	1.71	0.89
1:A:907:THR:C	1:A:908:ARG:HE	1.80	0.89
1:B:816:ASN:O	1:B:820:GLN:HG2	1.71	0.89
1:A:270:LEU:HD23	1:A:270:LEU:H	1.36	0.89
1:A:816:ASN:O	1:A:820:GLN:HG2	1.72	0.88
1:A:72:GLY:HA2	1:A:326:GLN:NE2	1.88	0.88
1:B:270:LEU:HD23	1:B:270:LEU:H	1.35	0.88
1:B:278:GLU:O	1:B:282:ARG:HG2	1.73	0.88
1:A:292:ASN:HA	1:A:295:MET:HB2	1.55	0.88
1:A:267:LYS:N	1:A:270:LEU:HD21	1.89	0.88
1:B:207:GLY:HA3	1:B:211:THR:HB	1.54	0.88
1:B:384:ILE:HG22	1:B:385:GLN:H	1.36	0.88
1:B:889:SER:HA	1:B:892:ILE:HD11	1.56	0.88
1:A:318:ILE:HD11	1:A:325:GLY:H	1.39	0.87
1:B:386:GLY:HA3	1:B:450:ASP:HA	1.54	0.87
1:A:34:SER:O	1:A:38:MET:HB2	1.74	0.87
1:A:478:THR:HG22	1:A:479:THR:H	1.39	0.87
1:A:1216:LYS:HE2	1:A:1216:LYS:HA	1.54	0.87
1:A:122:LEU:HD12	1:A:939:SER:HB2	1.56	0.87
1:A:1179:ARG:HH21	1:A:1209:VAL:HG11	1.39	0.87
1:B:64:LEU:O	1:B:67:MET:HB3	1.74	0.87
1:B:72:GLY:HA2	1:B:326:GLN:NE2	1.90	0.87
1:B:209:LYS:O	1:B:212:LEU:HB3	1.72	0.87
1:A:1261:GLY:H	1:A:1264:PHE:HB3	1.38	0.87
1:A:202:ILE:HD12	1:A:203:GLY:H	1.39	0.87
1:A:603:VAL:HG23	1:A:604:GLU:H	1.40	0.87
1:A:202:ILE:HD12	1:A:203:GLY:N	1.88	0.87
1:A:360:GLU:HA	1:A:363:LYS:HE2	1.56	0.87
1:B:267:LYS:N	1:B:270:LEU:HD21	1.89	0.87
1:A:1091:PHE:HE1	1:A:1096:GLU:HG2	1.37	0.86
1:B:34:SER:O	1:B:38:MET:HB2	1.74	0.86
1:B:379:HIS:O	1:B:381:PRO:HD3	1.75	0.86

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1179:ARG:HH21	1:B:1209:VAL:HG11	1.39	0.86
1:B:1128:ALA:HB2	1:B:1141:ILE:HG21	1.57	0.86
1:B:1261:GLY:H	1:B:1264:PHE:HB3	1.38	0.86
1:B:603:VAL:HG23	1:B:604:GLU:H	1.39	0.86
1:B:1020:GLN:HG2	1:B:1021:GLY:H	1.41	0.86
1:A:1202:LEU:HG	1:A:1203:ASP:H	1.41	0.86
1:B:964:LEU:HD13	1:B:965:MET:H	1.39	0.86
1:B:379:HIS:HB3	1:B:457:ILE:HA	1.58	0.86
1:A:1128:ALA:HB2	1:A:1141:ILE:HG21	1.58	0.86
1:B:853:LEU:HD22	1:B:853:LEU:H	1.39	0.85
1:A:49:TYR:OH	1:A:130:SER:HB2	1.76	0.85
1:A:1202:LEU:HD21	1:A:1206:SER:HB3	1.59	0.85
1:A:697:LEU:O	1:A:700:ASN:HB3	1.76	0.85
1:B:49:TYR:OH	1:B:130:SER:HB2	1.76	0.85
1:A:64:LEU:O	1:A:67:MET:HB3	1.76	0.85
1:B:742:GLU:O	1:B:746:GLN:HG2	1.77	0.85
1:A:386:GLY:HA3	1:A:450:ASP:HA	1.59	0.84
1:A:889:SER:HA	1:A:892:ILE:HD11	1.58	0.84
1:B:210:LEU:HG	1:B:322:TYR:CD2	2.12	0.84
1:B:278:GLU:C	1:B:282:ARG:HG2	2.03	0.84
1:B:800:PHE:O	1:B:803:PRO:HD3	1.78	0.84
1:A:35:VAL:HG23	1:A:36:LEU:N	1.93	0.84
1:B:974:PHE:HB2	2:B:6004:2J8:SE2	2.26	0.84
1:B:292:ASN:HA	1:B:295:MET:HB2	1.58	0.84
1:A:791:SER:HA	1:A:1010:LYS:HE2	1.59	0.84
1:A:694:TRP:O	1:A:697:LEU:HG	1.77	0.84
1:B:478:THR:HG22	1:B:479:THR:H	1.41	0.84
1:B:360:GLU:HA	1:B:363:LYS:HE2	1.58	0.84
1:A:964:LEU:HD13	1:A:965:MET:H	1.37	0.83
1:B:986:GLN:HE22	2:B:6003:2J8:H31	1.41	0.83
1:B:697:LEU:O	1:B:700:ASN:HB3	1.78	0.83
1:A:136:ALA:HB2	1:A:182:ILE:HB	1.61	0.83
1:B:267:LYS:HB3	1:B:790:LYS:HE3	1.59	0.83
1:B:1197:GLU:HG2	1:B:1227:ALA:HA	1.60	0.83
1:B:164:VAL:HG12	1:B:164:VAL:O	1.76	0.83
1:B:324:ILE:HG13	1:B:326:GLN:HB3	1.61	0.83
1:B:811:THR:O	1:B:814:LEU:HB2	1.79	0.83
1:A:158:TRP:HA	1:A:162:HIS:HD2	1.42	0.83
1:A:689:PRO:HB2	1:A:690:PRO:HD3	1.61	0.83
1:B:374:PHE:HE1	1:B:376:LYS:HB2	1.43	0.83
1:B:552:GLU:O	1:B:554:THR:N	2.11	0.83

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:278:GLU:C	1:A:282:ARG:HG2	2.03	0.83
1:A:185:LYS:HZ2	1:A:186:ILE:N	1.77	0.83
1:A:801:ASP:HB3	1:A:1083:TYR:OH	1.78	0.83
1:B:1202:LEU:HG	1:B:1203:ASP:H	1.42	0.83
1:B:375:SER:C	1:B:376:LYS:HD2	2.04	0.82
1:A:204:PHE:HA	1:A:211:THR:HG21	1.58	0.82
1:A:742:GLU:O	1:A:746:GLN:HG2	1.77	0.82
1:A:1120:ASP:HB3	1:A:1168:LYS:HA	1.61	0.82
1:A:969:ASN:HA	1:A:972:LEU:HD13	1.62	0.82
1:B:942:GLN:O	1:B:945:MET:HB3	1.80	0.82
1:A:1197:GLU:HG2	1:A:1227:ALA:HA	1.60	0.82
1:B:226:GLY:O	1:B:230:LYS:HG2	1.80	0.82
1:B:128:GLN:O	1:B:131:PHE:HB3	1.80	0.82
1:A:859:ALA:O	1:A:863:ILE:HG13	1.80	0.81
1:A:713:CYS:CB	1:A:768:LEU:HD11	2.11	0.81
1:A:812:THR:HG22	1:A:816:ASN:HD22	1.44	0.81
1:A:853:LEU:HG	1:A:973:VAL:HG22	1.62	0.81
1:B:136:ALA:HB2	1:B:182:ILE:HB	1.62	0.81
1:B:401:LYS:H	1:B:401:LYS:HD2	1.45	0.81
1:A:401:LYS:H	1:A:401:LYS:HD2	1.45	0.81
1:A:762:SER:HA	1:A:765:THR:HG22	1.60	0.81
1:A:226:GLY:O	1:A:230:LYS:HG2	1.80	0.81
1:B:286:LYS:HA	1:B:289:ILE:HB	1.62	0.81
1:A:39:PHE:CE2	1:A:355:ARG:HA	2.16	0.81
1:B:713:CYS:CB	1:B:768:LEU:HD11	2.10	0.81
1:B:766:PHE:O	1:B:769:GLN:HG2	1.80	0.81
1:A:289:ILE:O	1:A:293:ILE:HG12	1.80	0.81
1:B:158:TRP:HA	1:B:162:HIS:HD2	1.45	0.81
1:B:324:ILE:HG13	1:B:326:GLN:CB	2.10	0.81
1:B:762:SER:HA	1:B:765:THR:HG22	1.61	0.81
1:A:183:GLY:O	1:A:186:ILE:HG13	1.81	0.81
1:A:942:GLN:O	1:A:945:MET:HB3	1.81	0.81
1:B:35:VAL:HG12	1:B:359:TYR:CE2	2.15	0.81
1:B:429:LYS:H	1:B:429:LYS:HD3	1.45	0.81
1:B:694:TRP:O	1:B:697:LEU:HG	1.80	0.81
1:A:212:LEU:HA	1:A:215:LEU:HG	1.63	0.80
1:B:982:MET:HG3	2:B:6003:2J8:H33	1.63	0.80
1:A:1181:ALA:O	1:A:1184:ARG:HB3	1.81	0.80
1:A:110:TYR:HA	1:A:113:TYR:HD2	1.46	0.80
1:A:363:LYS:O	1:A:367:ASN:HB3	1.81	0.80
1:B:183:GLY:O	1:B:186:ILE:HG13	1.80	0.80

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1120:ASP:HB3	1:B:1168:LYS:HA	1.63	0.80
1:A:168:ASN:HB3	1:A:897:ILE:CD1	2.10	0.80
1:A:527:LEU:HD23	1:A:527:LEU:H	1.46	0.80
1:B:61:GLY:O	1:B:65:PRO:CD	2.29	0.80
1:B:318:ILE:HD11	1:B:325:GLY:H	1.45	0.80
1:B:363:LYS:O	1:B:367:ASN:HB3	1.82	0.80
1:A:286:LYS:HA	1:A:289:ILE:HB	1.62	0.80
1:B:39:PHE:CE2	1:B:355:ARG:HA	2.17	0.80
1:A:857:LEU:HD11	1:A:977:ILE:HG12	1.64	0.80
1:A:1092:LEU:HB3	1:A:1097:ILE:HD11	1.64	0.80
1:A:35:VAL:HG12	1:A:359:TYR:CE2	2.15	0.79
1:A:291:ALA:HA	1:A:294:SER:HB2	1.64	0.79
1:A:61:GLY:O	1:A:65:PRO:CD	2.30	0.79
1:A:766:PHE:O	1:A:769:GLN:HG2	1.82	0.79
1:A:958:TYR:O	1:A:966:THR:HG21	1.83	0.79
1:B:35:VAL:HG23	1:B:36:LEU:N	1.92	0.79
1:B:100:PHE:HB2	1:B:961:THR:HG23	1.64	0.79
1:B:257:ILE:O	1:B:260:VAL:HB	1.83	0.79
1:B:812:THR:HG22	1:B:816:ASN:HD22	1.44	0.79
1:B:889:SER:O	1:B:892:ILE:HG13	1.80	0.79
1:A:969:ASN:HD22	1:A:970:VAL:N	1.79	0.79
1:A:207:GLY:HA3	1:A:211:THR:H	1.48	0.79
1:A:834:GLN:HB3	1:A:986:GLN:HG2	1.65	0.79
1:B:820:GLN:HG3	1:B:1000:SER:CB	2.12	0.79
1:A:140:ILE:HG13	1:A:179:ASN:HD22	1.46	0.79
1:A:257:ILE:O	1:A:260:VAL:HB	1.83	0.79
1:B:969:ASN:HA	1:B:972:LEU:HD13	1.63	0.79
1:B:339:PHE:CE1	2:B:6003:2J8:SE3	2.86	0.79
1:B:1181:ALA:O	1:B:1184:ARG:HB3	1.83	0.79
1:A:512:LEU:HD12	1:A:513:PRO:HD2	1.65	0.79
1:A:756:LEU:HD12	1:A:757:ILE:N	1.98	0.79
1:B:110:TYR:HA	1:B:113:TYR:HD2	1.47	0.79
1:B:289:ILE:O	1:B:293:ILE:HG12	1.81	0.79
1:B:339:PHE:CD2	2:B:6003:2J8:SE3	2.86	0.79
1:B:1092:LEU:HB3	1:B:1097:ILE:HD11	1.64	0.79
1:B:102:LYS:HA	1:B:102:LYS:HE3	1.65	0.78
1:B:727:ILE:HG21	1:B:754:LEU:HG	1.64	0.78
1:A:852:GLN:HB2	1:A:853:LEU:HD22	1.65	0.78
1:A:1154:ILE:HD13	1:A:1161:TYR:CE2	2.19	0.78
1:B:834:GLN:HB3	1:B:986:GLN:HG2	1.66	0.78
1:A:727:ILE:HG21	1:A:754:LEU:HG	1.63	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:770:GLY:HA2	1:A:773:PHE:CZ	2.19	0.78
1:A:811:THR:O	1:A:814:LEU:HB2	1.84	0.78
1:A:902:THR:C	1:A:904:VAL:H	1.90	0.78
1:A:992:PRO:HB2	1:A:996:LYS:NZ	1.98	0.78
1:A:102:LYS:HA	1:A:102:LYS:HE3	1.65	0.78
1:A:574:GLU:HG3	1:A:574:GLU:O	1.84	0.78
1:A:797:VAL:HG12	1:A:798:SER:H	1.48	0.78
1:B:239:GLU:HG3	1:B:288:ALA:CB	2.13	0.78
1:A:467:GLY:HA3	1:A:545:PRO:HG3	1.64	0.78
1:B:314:THR:HG23	1:B:327:VAL:HG21	1.66	0.78
1:B:467:GLY:HA3	1:B:545:PRO:HG3	1.66	0.78
1:B:756:LEU:HD12	1:B:757:ILE:N	1.99	0.78
1:A:47:ARG:O	1:A:50:MET:HB3	1.83	0.78
1:A:1145:ALA:CB	1:A:1154:ILE:HD12	2.14	0.78
1:B:263:PHE:HE1	1:B:1129:TYR:HB3	1.49	0.78
1:B:770:GLY:HA2	1:B:773:PHE:CZ	2.19	0.78
1:A:420:ALA:C	1:A:421:LEU:HD12	2.09	0.78
1:B:117:ILE:O	1:B:121:VAL:HG13	1.83	0.78
1:B:969:ASN:HD22	1:B:970:VAL:N	1.80	0.78
1:B:992:PRO:HB2	1:B:996:LYS:NZ	1.98	0.78
1:A:128:GLN:O	1:A:131:PHE:HB3	1.84	0.78
1:A:239:GLU:HG3	1:A:288:ALA:CB	2.14	0.78
1:A:892:ILE:HB	1:A:916:TYR:CE1	2.19	0.78
1:B:1183:ALA:O	1:B:1187:VAL:HB	1.84	0.78
1:B:140:ILE:HG13	1:B:179:ASN:HD22	1.46	0.77
1:B:512:LEU:HD12	1:B:513:PRO:HD2	1.65	0.77
1:B:1010:LYS:H	1:B:1010:LYS:HD2	1.49	0.77
1:B:892:ILE:HB	1:B:916:TYR:CE1	2.18	0.77
1:A:889:SER:O	1:A:892:ILE:HG13	1.83	0.77
1:B:210:LEU:HD23	1:B:317:VAL:HG11	1.65	0.77
1:B:527:LEU:HD23	1:B:527:LEU:H	1.47	0.77
1:A:303:TYR:O	1:A:306:TYR:HB3	1.84	0.77
1:B:291:ALA:HA	1:B:294:SER:HB2	1.65	0.77
1:B:303:TYR:O	1:B:306:TYR:HB3	1.84	0.77
1:A:692:SER:OG	1:A:696:ILE:HG23	1.84	0.77
1:B:449:ILE:HD13	1:B:450:ASP:N	1.99	0.77
1:B:523:ARG:HD3	1:B:524:GLY:N	1.99	0.77
1:B:1120:ASP:HA	1:B:1165:VAL:CG2	2.15	0.77
1:B:1158:PRO:O	1:B:1159:ASP:HB2	1.85	0.77
1:A:573:ARG:HD2	1:A:578:THR:HG21	1.67	0.77
1:A:1120:ASP:HA	1:A:1165:VAL:CG2	2.14	0.77

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:185:LYS:HZ2	1:B:186:ILE:N	1.80	0.77
1:B:574:GLU:O	1:B:574:GLU:HG3	1.85	0.77
1:A:210:LEU:HD23	1:A:317:VAL:HG11	1.65	0.77
1:A:1159:ASP:O	1:A:1160:LYS:HG3	1.84	0.77
1:A:385:GLN:HE21	1:A:386:GLY:H	1.33	0.77
1:B:693:PHE:H	1:B:693:PHE:HD2	1.31	0.77
1:B:1023:LYS:HB3	1:B:1026:MET:HG2	1.65	0.77
1:B:1120:ASP:HA	1:B:1165:VAL:HG21	1.67	0.77
1:A:164:VAL:O	1:A:164:VAL:HG12	1.84	0.76
1:A:1120:ASP:HA	1:A:1165:VAL:HG21	1.67	0.76
1:B:713:CYS:HB3	1:B:768:LEU:HD11	1.67	0.76
1:A:117:ILE:O	1:A:121:VAL:HG13	1.85	0.76
1:B:321:GLU:O	1:B:323:SER:N	2.17	0.76
1:B:1167:ASP:O	1:B:1168:LYS:HB2	1.85	0.76
1:A:361:VAL:O	1:A:365:ILE:HD12	1.85	0.76
1:A:820:GLN:HG3	1:A:1000:SER:CB	2.14	0.76
1:A:238:LYS:NZ	1:A:242:ALA:HB2	2.00	0.76
1:A:806:THR:O	1:A:810:LEU:HG	1.86	0.76
1:B:212:LEU:HA	1:B:215:LEU:HG	1.65	0.76
1:A:178:ILE:HG12	1:A:358:ALA:CB	2.14	0.76
1:A:1183:ALA:O	1:A:1187:VAL:HB	1.86	0.76
1:A:713:CYS:HB3	1:A:768:LEU:HD11	1.68	0.76
1:B:306:TYR:O	1:B:310:PHE:HB2	1.86	0.76
1:B:1010:LYS:O	1:B:1011:THR:HG23	1.85	0.76
1:B:178:ILE:HG12	1:B:358:ALA:CB	2.15	0.76
1:B:731:VAL:HG22	1:B:750:LEU:HB3	1.68	0.76
1:A:900:PHE:C	1:A:902:THR:H	1.93	0.75
1:A:1039:ASN:CB	1:A:1047:PRO:HA	2.16	0.75
1:B:385:GLN:HE21	1:B:386:GLY:H	1.34	0.75
1:B:902:THR:C	1:B:904:VAL:H	1.91	0.75
1:A:207:GLY:HA3	1:A:211:THR:HB	1.67	0.75
1:B:68:MET:HE2	1:B:68:MET:HA	1.69	0.75
1:A:50:MET:HG3	1:A:131:PHE:CZ	2.22	0.75
1:A:306:TYR:O	1:A:310:PHE:HB2	1.85	0.75
1:B:238:LYS:NZ	1:B:242:ALA:HB2	2.01	0.75
1:B:362:PHE:HA	1:B:365:ILE:HD12	1.68	0.75
1:A:158:TRP:NE1	1:A:900:PHE:CB	2.50	0.75
1:A:552:GLU:O	1:A:554:THR:N	2.20	0.75
1:A:1179:ARG:NH2	1:A:1209:VAL:HG11	2.01	0.75
1:B:272:ARG:O	1:B:276:ASN:HB2	1.87	0.75
1:B:302:ILE:O	1:B:305:SER:HB3	1.85	0.75

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:859:ALA:O	1:B:863:ILE:HG13	1.85	0.75
1:A:324:ILE:HG13	1:A:326:GLN:CB	2.16	0.75
1:A:731:VAL:HG22	1:A:750:LEU:HB3	1.67	0.75
1:B:64:LEU:HD11	1:B:945:MET:HE2	1.67	0.75
1:B:133:CYS:O	1:B:134:LEU:C	2.30	0.75
1:B:384:ILE:HG22	1:B:385:GLN:N	2.01	0.75
1:A:467:GLY:CA	1:A:545:PRO:HG3	2.16	0.75
1:A:780:LEU:O	1:A:784:LEU:HD23	1.87	0.75
1:B:573:ARG:HD2	1:B:578:THR:HG21	1.67	0.75
1:B:849:TYR:HB3	1:B:854:THR:OG1	1.87	0.75
1:B:900:PHE:C	1:B:902:THR:H	1.94	0.75
1:B:970:VAL:O	1:B:973:VAL:HB	1.87	0.75
1:A:484:ILE:HG23	1:A:542:VAL:HG21	1.68	0.74
1:A:531:GLN:O	1:A:534:ARG:HB2	1.87	0.74
1:A:945:MET:SD	1:A:946:TYR:N	2.60	0.74
1:B:261:ILE:C	1:B:263:PHE:H	1.95	0.74
1:A:68:MET:HA	1:A:68:MET:HE2	1.68	0.74
1:A:519:LEU:H	1:A:519:LEU:HD13	1.52	0.74
1:B:118:GLY:HA3	1:B:946:TYR:CE2	2.22	0.74
1:B:1020:GLN:HG2	1:B:1021:GLY:N	2.00	0.74
1:A:387:ASN:ND2	1:A:414:LYS:HA	2.01	0.74
1:A:927:ALA:HA	1:A:930:LYS:HE3	1.69	0.74
1:B:47:ARG:O	1:B:50:MET:HB3	1.86	0.74
1:A:156:ILE:N	1:A:156:ILE:HD12	2.02	0.74
1:B:531:GLN:O	1:B:534:ARG:HB2	1.87	0.74
1:B:537:ILE:O	1:B:538:ALA:C	2.30	0.74
1:B:945:MET:SD	1:B:946:TYR:N	2.60	0.74
1:A:589:ARG:O	1:A:591:ALA:N	2.17	0.74
1:A:695:ARG:O	1:A:699:LEU:HD23	1.87	0.74
1:A:718:GLY:O	1:A:722:PRO:CD	2.31	0.74
1:B:902:THR:C	1:B:904:VAL:N	2.39	0.74
1:A:155:GLU:HB3	1:A:156:ILE:HD12	1.68	0.74
1:A:1167:ASP:O	1:A:1168:LYS:HB2	1.86	0.74
1:B:704:TRP:CZ2	1:B:707:PHE:HB2	2.22	0.74
1:A:1026:MET:HE3	1:A:1095:LYS:HD3	1.69	0.74
1:B:239:GLU:HB3	1:B:285:ILE:HG12	1.69	0.74
1:B:991:ALA:HB1	1:B:992:PRO:HD2	1.70	0.74
1:B:1122:SER:HA	1:B:1164:ARG:HA	1.69	0.74
1:A:307:ALA:CB	1:A:754:LEU:HD22	2.17	0.74
1:A:902:THR:C	1:A:904:VAL:N	2.38	0.74
1:A:1081:ARG:NH2	1:A:1098:LYS:O	2.20	0.74

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:195:THR:CB	1:A:340:SER:HB2	2.15	0.74
1:A:791:SER:N	1:A:794:ARG:HH21	1.86	0.74
1:B:484:ILE:HG23	1:B:542:VAL:HG21	1.68	0.74
1:B:420:ALA:C	1:B:421:LEU:HD12	2.12	0.73
1:A:302:ILE:O	1:A:305:SER:HB3	1.88	0.73
1:A:523:ARG:HD3	1:A:524:GLY:N	2.00	0.73
1:B:780:LEU:O	1:B:784:LEU:HD23	1.88	0.73
1:A:588:VAL:O	1:A:591:ALA:HB2	1.88	0.73
1:B:155:GLU:HB3	1:B:156:ILE:HD12	1.71	0.73
1:B:387:ASN:ND2	1:B:414:LYS:HA	2.03	0.73
1:A:133:CYS:O	1:A:134:LEU:C	2.29	0.73
1:B:50:MET:HG3	1:B:131:PHE:CZ	2.22	0.73
1:B:543:ARG:NH1	1:B:905:SER:HB3	2.02	0.73
1:A:1091:PHE:CE1	1:A:1096:GLU:HG2	2.22	0.73
1:B:215:LEU:O	1:B:219:PRO:HD2	1.88	0.73
1:B:1179:ARG:NH2	1:B:1209:VAL:HG11	2.02	0.73
1:A:225:ALA:HA	1:A:302:ILE:HD12	1.70	0.73
1:A:1053:SER:C	1:A:1054:LEU:HD22	2.13	0.73
1:B:695:ARG:O	1:B:699:LEU:HD23	1.88	0.73
1:A:35:VAL:CG2	1:A:36:LEU:H	1.98	0.73
1:A:704:TRP:CZ2	1:A:707:PHE:HB2	2.23	0.73
1:A:960:VAL:HG12	1:A:966:THR:OG1	1.87	0.73
1:B:878:GLN:O	1:B:882:ASP:HB2	1.88	0.73
1:B:1053:SER:C	1:B:1054:LEU:HD22	2.13	0.73
1:A:537:ILE:O	1:A:538:ALA:C	2.30	0.73
1:A:834:GLN:HG3	1:A:835:ASN:N	2.04	0.73
1:B:163:ASP:HB2	1:B:166:GLU:HB3	1.69	0.73
1:B:467:GLY:CA	1:B:545:PRO:HG3	2.19	0.73
1:B:233:SER:O	1:B:236:THR:HB	1.89	0.73
1:A:158:TRP:NE1	1:A:900:PHE:HB2	2.04	0.72
1:A:272:ARG:O	1:A:276:ASN:HB2	1.88	0.72
1:A:611:LEU:HD23	1:A:618:TYR:HB2	1.71	0.72
1:A:1022:LEU:HG	1:A:1104:TRP:CE2	2.23	0.72
1:A:1037:VAL:HG12	1:A:1051:GLY:H	1.53	0.72
1:B:419:VAL:HG23	1:B:593:VAL:HG13	1.71	0.72
1:B:791:SER:O	1:B:795:GLN:HB2	1.89	0.72
1:B:846:SER:O	1:B:849:TYR:HB2	1.89	0.72
1:B:927:ALA:HA	1:B:930:LYS:HE3	1.70	0.72
1:B:1076:VAL:HG13	1:B:1194:LEU:HD13	1.70	0.72
1:A:254:LEU:HD22	1:A:254:LEU:N	2.04	0.72
1:A:991:ALA:HB1	1:A:992:PRO:HD2	1.69	0.72

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:254:LEU:HD22	1:B:254:LEU:N	2.04	0.72
1:A:233:SER:O	1:A:236:THR:HB	1.89	0.72
1:A:1037:VAL:HG21	1:A:1087:ALA:HB3	1.71	0.72
1:B:213:VAL:O	1:B:217:ILE:HG12	1.89	0.72
1:B:484:ILE:CG2	1:B:496:ILE:HD12	2.19	0.72
1:A:1076:VAL:HG13	1:A:1194:LEU:HD13	1.70	0.72
1:A:168:ASN:HB3	1:A:897:ILE:HD13	1.69	0.72
1:A:550:LEU:HB2	1:A:580:VAL:HG23	1.72	0.72
1:B:797:VAL:O	1:B:799:TRP:N	2.23	0.72
1:A:913:GLU:OE2	1:A:913:GLU:HA	1.89	0.72
1:B:740:PRO:HG2	1:B:741:PRO:HD3	1.70	0.72
1:B:1091:PHE:CE1	1:B:1096:GLU:HG2	2.22	0.72
1:A:1080:GLU:OE2	1:A:1109:LEU:HD12	1.90	0.72
1:B:156:ILE:HD12	1:B:156:ILE:N	2.04	0.72
1:B:519:LEU:HD13	1:B:519:LEU:H	1.52	0.72
1:B:589:ARG:O	1:B:591:ALA:N	2.20	0.72
1:B:766:PHE:HA	1:B:769:GLN:NE2	2.04	0.72
1:B:888:GLY:O	1:B:892:ILE:HG12	1.90	0.72
1:B:1037:VAL:HG12	1:B:1051:GLY:H	1.54	0.72
1:B:1147:GLU:HB3	1:B:1186:LEU:HD22	1.71	0.72
1:A:970:VAL:O	1:A:973:VAL:HB	1.88	0.72
1:A:1012:PRO:O	1:A:1013:GLU:HB2	1.89	0.72
1:A:1150:ILE:O	1:A:1154:ILE:HG13	1.88	0.72
1:B:86:LYS:HG2	1:B:738:GLY:O	1.89	0.72
1:A:202:ILE:HG12	1:A:333:SER:OG	1.89	0.72
1:A:471:GLN:HA	1:A:553:ALA:HA	1.72	0.72
1:B:202:ILE:HG12	1:B:333:SER:OG	1.90	0.72
1:A:215:LEU:O	1:A:219:PRO:HD2	1.90	0.72
1:A:324:ILE:HG13	1:A:326:GLN:HB3	1.72	0.72
1:A:385:GLN:NE2	1:A:386:GLY:H	1.87	0.72
1:A:534:ARG:NH2	1:A:564:VAL:HG11	2.05	0.72
1:A:711:ILE:O	1:A:715:ILE:HG12	1.90	0.72
1:A:1040:TYR:O	1:A:1042:THR:HG22	1.89	0.72
1:B:1229:ARG:C	1:B:1231:SER:H	1.98	0.72
1:A:178:ILE:HG12	1:A:358:ALA:HB2	1.72	0.71
1:A:922:ILE:HB	1:A:923:PRO:HD3	1.71	0.71
1:B:225:ALA:HA	1:B:302:ILE:HD12	1.71	0.71
1:B:588:VAL:O	1:B:591:ALA:HB2	1.90	0.71
1:B:1076:VAL:HG13	1:B:1194:LEU:HD22	1.72	0.71
1:A:318:ILE:HD11	1:A:325:GLY:N	2.05	0.71
1:A:878:GLN:O	1:A:882:ASP:HB2	1.89	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:453:ASP:HB3	1:B:456:THR:HG23	1.72	0.71
1:B:1037:VAL:HG21	1:B:1087:ALA:HB3	1.72	0.71
1:A:846:SER:O	1:A:849:TYR:HB2	1.91	0.71
1:A:1014:ILE:HD13	1:A:1106:ARG:NH1	2.05	0.71
1:B:267:LYS:H	1:B:270:LEU:HD21	1.52	0.71
1:B:711:ILE:O	1:B:715:ILE:HG12	1.89	0.71
1:B:718:GLY:O	1:B:722:PRO:CD	2.32	0.71
1:B:806:THR:O	1:B:810:LEU:HG	1.90	0.71
1:B:850:GLY:C	1:B:852:GLN:H	1.98	0.71
1:A:246:ALA:HB1	1:A:277:LEU:HB3	1.72	0.71
1:A:265:GLY:HA2	1:A:793:LEU:HD21	1.72	0.71
1:A:1014:ILE:HD13	1:A:1106:ARG:HH12	1.55	0.71
1:B:447:VAL:HG13	1:B:454:ILE:CG2	2.21	0.71
1:B:970:VAL:HG23	1:B:971:LEU:HD22	1.72	0.71
1:A:78:PHE:HZ	1:A:967:PHE:O	1.74	0.71
1:A:740:PRO:HG2	1:A:741:PRO:HD3	1.70	0.71
1:A:786:TYR:HE2	1:A:790:LYS:HZ3	1.38	0.71
1:A:791:SER:O	1:A:795:GLN:HB2	1.90	0.71
1:A:888:GLY:O	1:A:892:ILE:HG12	1.91	0.71
1:A:1039:ASN:HB2	1:A:1047:PRO:CA	2.19	0.71
1:B:908:ARG:O	1:B:909:GLU:C	2.34	0.71
1:B:1037:VAL:CG2	1:B:1087:ALA:HB3	2.21	0.71
1:B:1260:LYS:HD2	1:B:1260:LYS:H	1.55	0.71
1:A:59:ILE:HD11	1:A:124:VAL:HG11	1.73	0.71
1:A:453:ASP:HB3	1:A:456:THR:HG23	1.71	0.71
1:A:1145:ALA:HB2	1:A:1154:ILE:HD12	1.71	0.71
1:A:1229:ARG:C	1:A:1231:SER:H	1.99	0.71
1:B:58:ILE:HG13	1:B:193:MET:HG3	1.73	0.71
1:B:534:ARG:NH2	1:B:564:VAL:HG11	2.05	0.71
1:B:1079:LEU:HD23	1:B:1194:LEU:HD11	1.73	0.71
1:A:163:ASP:HB2	1:A:166:GLU:HB3	1.73	0.71
1:A:970:VAL:HG23	1:A:971:LEU:HD22	1.73	0.71
1:B:246:ALA:HB1	1:B:277:LEU:HB3	1.71	0.71
1:B:897:ILE:HG13	1:B:898:GLU:N	2.01	0.71
1:A:158:TRP:CZ2	1:A:900:PHE:HB2	2.26	0.71
1:A:429:LYS:HD3	1:A:429:LYS:N	2.05	0.71
1:B:279:GLU:HG2	1:B:782:LYS:HZ2	1.54	0.71
1:B:386:GLY:CA	1:B:450:ASP:HA	2.21	0.71
1:B:429:LYS:HD3	1:B:429:LYS:N	2.06	0.71
1:B:550:LEU:HB2	1:B:580:VAL:HG23	1.72	0.71
1:B:1036:VAL:HG11	1:B:1052:LEU:HD23	1.73	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:213:VAL:O	1:A:217:ILE:HG12	1.91	0.71
1:A:419:VAL:HG23	1:A:593:VAL:HG13	1.71	0.71
1:A:484:ILE:CG2	1:A:496:ILE:HD12	2.19	0.71
1:B:35:VAL:CG2	1:B:36:LEU:H	1.97	0.71
1:B:1039:ASN:CB	1:B:1047:PRO:HA	2.16	0.71
1:A:68:MET:O	1:A:71:PHE:HB3	1.91	0.70
1:A:174:ASP:O	1:A:178:ILE:HG13	1.91	0.70
1:A:1037:VAL:CG2	1:A:1087:ALA:HB3	2.21	0.70
1:B:245:LYS:HZ1	1:B:245:LYS:HA	1.56	0.70
1:B:318:ILE:CD1	1:B:325:GLY:H	2.03	0.70
1:B:409:LEU:CD2	1:B:602:ILE:HB	2.21	0.70
1:A:35:VAL:CG2	1:A:355:ARG:HH21	2.05	0.70
1:A:261:ILE:C	1:A:263:PHE:H	1.98	0.70
1:B:611:LEU:HD23	1:B:618:TYR:HB2	1.72	0.70
1:A:1019:THR:OG1	1:A:1101:ASN:HA	1.91	0.70
1:A:1036:VAL:HG11	1:A:1052:LEU:HD23	1.73	0.70
1:B:385:GLN:NE2	1:B:386:GLY:H	1.89	0.70
1:B:791:SER:N	1:B:794:ARG:HH21	1.89	0.70
1:A:979:PHE:O	1:A:982:MET:HB3	1.91	0.70
1:A:1076:VAL:HG13	1:A:1194:LEU:HD22	1.72	0.70
1:B:304:ALA:HB2	1:B:758:LEU:HD23	1.72	0.70
1:B:607:ASN:HB3	1:B:610:GLU:OE2	1.92	0.70
1:B:834:GLN:HG3	1:B:835:ASN:N	2.05	0.70
1:A:811:THR:HA	1:A:814:LEU:HD23	1.73	0.70
1:A:834:GLN:HG3	1:A:835:ASN:H	1.56	0.70
1:A:1122:SER:HA	1:A:1164:ARG:HA	1.72	0.70
1:B:1040:TYR:O	1:B:1042:THR:HG22	1.91	0.70
1:B:1202:LEU:HD21	1:B:1206:SER:CB	2.20	0.70
1:A:285:ILE:O	1:A:289:ILE:HG12	1.91	0.70
1:A:449:ILE:HD13	1:A:450:ASP:N	2.06	0.70
1:A:324:ILE:CG1	1:A:326:GLN:H	2.05	0.70
1:B:1036:VAL:CB	1:B:1052:LEU:HB3	2.22	0.70
1:B:1080:GLU:OE2	1:B:1109:LEU:HD12	1.90	0.70
1:B:374:PHE:HD1	1:B:375:SER:H	1.40	0.70
1:B:392:ASN:O	1:B:445:GLY:HA3	1.92	0.70
1:A:527:LEU:HD23	1:A:527:LEU:N	2.06	0.70
1:A:618:TYR:O	1:A:622:VAL:HG23	1.91	0.70
1:B:35:VAL:CG2	1:B:355:ARG:HH21	2.05	0.70
1:B:834:GLN:HG3	1:B:835:ASN:H	1.57	0.70
1:A:60:HIS:O	1:A:63:ALA:HB3	1.92	0.69
1:A:354:ALA:O	1:A:358:ALA:HB3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1147:GLU:HB3	1:A:1186:LEU:HD22	1.73	0.69
1:A:1178:GLN:O	1:A:1181:ALA:HB3	1.92	0.69
1:B:318:ILE:CD1	1:B:324:ILE:HG12	2.20	0.69
1:A:423:GLY:HA2	1:A:597:PHE:O	1.93	0.69
1:A:589:ARG:C	1:A:591:ALA:H	2.00	0.69
1:A:607:ASN:HB3	1:A:610:GLU:OE2	1.92	0.69
1:B:297:ALA:O	1:B:301:LEU:HB2	1.92	0.69
1:A:218:SER:HB2	1:A:219:PRO:CD	2.22	0.69
1:A:727:ILE:O	1:A:731:VAL:HG23	1.92	0.69
1:B:178:ILE:HG12	1:B:358:ALA:HB2	1.72	0.69
1:B:232:LEU:HB2	1:B:295:MET:SD	2.32	0.69
1:B:285:ILE:O	1:B:289:ILE:HG12	1.91	0.69
1:B:322:TYR:CZ	1:B:324:ILE:HD12	2.27	0.69
1:A:257:ILE:HD13	1:A:257:ILE:C	2.17	0.69
1:B:99:MET:HB3	1:B:960:VAL:O	1.92	0.69
1:B:295:MET:HA	1:B:295:MET:HE3	1.74	0.69
1:B:409:LEU:HD13	1:B:410:ASN:N	2.08	0.69
1:B:819:ALA:O	1:B:822:LYS:HB3	1.91	0.69
1:B:913:GLU:HA	1:B:913:GLU:OE2	1.92	0.69
1:A:467:GLY:N	1:A:545:PRO:HG3	2.08	0.69
1:A:883:LYS:HA	1:A:886:LEU:HG	1.73	0.69
1:B:207:GLY:HA3	1:B:211:THR:N	2.08	0.69
1:B:218:SER:HB2	1:B:219:PRO:CD	2.22	0.69
1:A:58:ILE:HG13	1:A:193:MET:HG3	1.74	0.69
1:A:138:ARG:NH2	1:B:515:GLN:HE21	1.91	0.69
1:A:406:LEU:HD11	1:A:432:THR:CG2	2.23	0.69
1:A:857:LEU:HD13	1:A:976:ALA:HB3	1.74	0.69
1:B:913:GLU:HA	1:B:916:TYR:HD2	1.58	0.69
1:A:125:ALA:O	1:A:129:VAL:HG23	1.93	0.69
1:A:204:PHE:CA	1:A:211:THR:HG21	2.21	0.69
1:A:232:LEU:HB2	1:A:295:MET:SD	2.32	0.69
1:A:447:VAL:HG13	1:A:454:ILE:CG2	2.22	0.69
1:B:354:ALA:O	1:B:358:ALA:HB3	1.93	0.69
1:A:45:LEU:HD22	1:A:45:LEU:H	1.57	0.69
1:A:388:LEU:HB2	1:A:413:VAL:HG12	1.73	0.69
1:A:409:LEU:CD2	1:A:602:ILE:HB	2.22	0.69
1:A:409:LEU:HD13	1:A:410:ASN:N	2.08	0.69
1:A:1079:LEU:HD23	1:A:1194:LEU:HD11	1.73	0.69
1:B:35:VAL:O	1:B:39:PHE:HB2	1.92	0.69
1:B:59:ILE:HD11	1:B:124:VAL:HG11	1.73	0.69
1:B:60:HIS:O	1:B:63:ALA:HB3	1.92	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:SER:HB2	1:B:219:PRO:HD3	1.75	0.69
1:B:527:LEU:HD23	1:B:527:LEU:N	2.07	0.69
1:B:849:TYR:HD1	1:B:854:THR:HA	1.58	0.69
1:B:883:LYS:HA	1:B:886:LEU:HG	1.74	0.69
1:B:1142:VAL:O	1:B:1146:LYS:HG2	1.92	0.69
1:A:219:PRO:O	1:A:223:LEU:HG	1.91	0.69
1:A:585:LEU:HD12	1:A:618:TYR:HE1	1.56	0.69
1:B:585:LEU:HD12	1:B:618:TYR:HE1	1.56	0.69
1:B:972:LEU:O	1:B:975:SER:HB2	1.93	0.69
1:A:519:LEU:HD13	1:A:519:LEU:N	2.07	0.69
1:A:267:LYS:H	1:A:270:LEU:HD21	1.56	0.68
1:A:482:GLU:O	1:A:485:ARG:N	2.26	0.68
1:B:121:VAL:HG23	1:B:122:LEU:N	2.08	0.68
1:B:324:ILE:CG1	1:B:326:GLN:H	2.05	0.68
1:A:354:ALA:O	1:A:358:ALA:CB	2.41	0.68
1:A:791:SER:HB3	1:A:1010:LYS:HG2	1.75	0.68
1:B:615:LYS:HA	1:B:619:PHE:CD2	2.28	0.68
1:A:282:ARG:HB3	1:A:778:GLU:HG2	1.74	0.68
1:A:389:GLU:HB2	1:A:448:SER:HB3	1.75	0.68
1:A:1243:GLN:O	1:A:1246:LYS:HD2	1.93	0.68
1:B:857:LEU:CD1	1:B:976:ALA:HB3	2.23	0.68
1:A:158:TRP:HE1	1:A:900:PHE:HB2	1.55	0.68
1:A:819:ALA:O	1:A:822:LYS:HB3	1.94	0.68
1:A:1137:SER:OG	1:A:1140:GLU:HB2	1.93	0.68
1:A:1158:PRO:O	1:A:1159:ASP:HB2	1.94	0.68
1:B:389:GLU:HB2	1:B:448:SER:HB3	1.74	0.68
1:A:210:LEU:HG	1:A:322:TYR:CD2	2.29	0.68
1:A:217:ILE:HG13	1:A:218:SER:N	2.08	0.68
1:A:615:LYS:HA	1:A:619:PHE:CD2	2.28	0.68
1:A:972:LEU:O	1:A:975:SER:HB2	1.93	0.68
1:B:90:ASN:HB2	1:B:91:MET:HE3	1.75	0.68
1:B:310:PHE:CE2	1:B:331:PHE:HB3	2.28	0.68
1:B:910:GLN:O	1:B:911:LYS:C	2.37	0.68
1:B:1166:GLY:O	1:B:1167:ASP:HB3	1.93	0.68
1:A:297:ALA:O	1:A:301:LEU:HB2	1.93	0.68
1:A:362:PHE:HA	1:A:365:ILE:HD12	1.75	0.68
1:A:36:LEU:HD12	1:A:37:THR:N	2.07	0.68
1:A:585:LEU:HD22	1:A:585:LEU:H	1.59	0.68
1:A:1036:VAL:CB	1:A:1052:LEU:HB3	2.22	0.68
1:A:1142:VAL:O	1:A:1146:LYS:HG2	1.94	0.68
1:A:1166:GLY:O	1:A:1167:ASP:HB3	1.93	0.68

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:388:LEU:HB2	1:B:413:VAL:HG12	1.75	0.68
1:B:979:PHE:O	1:B:982:MET:HB3	1.94	0.68
1:B:1102:VAL:HG13	1:B:1103:GLN:H	1.59	0.68
1:A:256:ALA:O	1:A:260:VAL:HG23	1.94	0.68
1:B:548:LEU:C	1:B:549:LEU:HD12	2.19	0.68
1:B:1037:VAL:HG22	1:B:1087:ALA:O	1.93	0.68
1:B:1137:SER:OG	1:B:1140:GLU:HB2	1.94	0.68
1:A:443:LEU:HD23	1:A:443:LEU:O	1.93	0.68
1:A:908:ARG:O	1:A:909:GLU:C	2.34	0.68
1:B:1032:GLN:HE21	1:B:1055:GLU:CG	2.07	0.68
1:B:1243:GLN:O	1:B:1246:LYS:HD2	1.94	0.68
1:A:697:LEU:HB3	1:A:828:ARG:NH2	2.09	0.68
1:A:826:GLY:O	1:A:829:LEU:HB2	1.94	0.68
1:A:911:LYS:O	1:A:914:THR:HB	1.94	0.68
1:B:519:LEU:HD13	1:B:519:LEU:N	2.09	0.68
1:B:922:ILE:HB	1:B:923:PRO:HD3	1.75	0.68
1:B:1039:ASN:HB2	1:B:1047:PRO:CA	2.20	0.68
1:A:315:SER:OG	1:A:747:ASN:HB3	1.95	0.67
1:B:45:LEU:HD22	1:B:45:LEU:H	1.57	0.67
1:B:36:LEU:HD12	1:B:37:THR:N	2.08	0.67
1:B:357:ALA:O	1:B:361:VAL:HG22	1.95	0.67
1:A:91:MET:HB2	1:A:94:ALA:HB3	1.76	0.67
1:A:288:ALA:HA	1:A:291:ALA:HB3	1.75	0.67
1:B:315:SER:CB	1:B:747:ASN:HD22	2.08	0.67
1:B:354:ALA:O	1:B:358:ALA:CB	2.42	0.67
1:B:390:PHE:HB2	1:B:411:LEU:O	1.94	0.67
1:B:401:LYS:H	1:B:401:LYS:CD	2.06	0.67
1:B:433:VAL:HG13	1:B:549:LEU:HD23	1.74	0.67
1:B:534:ARG:HH21	1:B:564:VAL:HG11	1.60	0.67
1:B:697:LEU:HB3	1:B:828:ARG:NH2	2.09	0.67
1:A:78:PHE:CZ	1:A:967:PHE:O	2.48	0.67
1:A:218:SER:HB2	1:A:219:PRO:HD3	1.75	0.67
1:A:295:MET:HE3	1:A:295:MET:HA	1.75	0.67
1:A:314:THR:O	1:A:318:ILE:HG22	1.94	0.67
1:B:91:MET:HB2	1:B:94:ALA:HB3	1.75	0.67
1:B:99:MET:HB2	1:B:961:THR:O	1.95	0.67
1:B:187:GLY:O	1:B:190:PHE:HB3	1.94	0.67
1:B:286:LYS:HE2	1:B:778:GLU:HG2	1.77	0.67
1:B:919:SER:O	1:B:923:PRO:CD	2.42	0.67
1:A:552:GLU:O	1:A:555:SER:N	2.25	0.67
1:A:1037:VAL:HG22	1:A:1087:ALA:O	1.94	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:286:LYS:HG2	1:B:778:GLU:HG3	1.75	0.67
1:B:207:GLY:HA3	1:B:211:THR:H	1.59	0.67
1:B:338:ALA:O	1:B:341:VAL:HB	1.94	0.67
1:B:482:GLU:O	1:B:485:ARG:N	2.27	0.67
1:A:141:HIS:O	1:A:144:ARG:HB3	1.95	0.67
1:A:696:ILE:HD13	1:A:998:THR:HG23	1.75	0.67
1:A:1114:GLN:HE22	1:A:1200:SER:HB2	1.58	0.67
1:B:68:MET:O	1:B:71:PHE:HB3	1.94	0.67
1:B:811:THR:HA	1:B:814:LEU:HD23	1.75	0.67
1:B:1019:THR:HG22	1:B:1100:LEU:HD12	1.76	0.67
1:A:35:VAL:O	1:A:39:PHE:HB2	1.94	0.67
1:A:933:VAL:O	1:A:934:PHE:C	2.38	0.67
1:B:55:LEU:O	1:B:59:ILE:HG23	1.95	0.67
1:B:1137:SER:HB3	1:B:1140:GLU:CB	2.25	0.67
1:B:441:ASP:CG	1:B:442:PRO:HD2	2.20	0.67
1:B:696:ILE:HD13	1:B:998:THR:HG23	1.75	0.67
1:A:74:MET:SD	1:A:953:PHE:CE1	2.88	0.67
1:A:318:ILE:HG23	1:A:735:PHE:CE2	2.29	0.67
1:A:1137:SER:HB3	1:A:1140:GLU:CB	2.24	0.67
1:B:618:TYR:O	1:B:622:VAL:HG23	1.94	0.67
1:B:799:TRP:HA	1:B:799:TRP:HE3	1.60	0.67
1:B:909:GLU:O	1:B:912:PHE:HB2	1.95	0.67
1:A:138:ARG:NH2	1:B:515:GLN:NE2	2.42	0.66
1:A:910:GLN:O	1:A:911:LYS:C	2.38	0.66
1:B:98:ALA:O	1:B:102:LYS:HG2	1.95	0.66
1:B:210:LEU:HG	1:B:322:TYR:HD2	1.58	0.66
1:B:773:PHE:O	1:B:776:ALA:HB3	1.95	0.66
1:B:1063:ALA:HA	1:B:1225:VAL:HG13	1.77	0.66
1:A:214:ILE:HG12	1:A:331:PHE:CE1	2.30	0.66
1:A:386:GLY:CA	1:A:450:ASP:HA	2.24	0.66
1:A:901:ARG:HD3	1:A:901:ARG:H	1.59	0.66
1:A:992:PRO:C	1:A:994:TYR:H	2.03	0.66
1:A:1032:GLN:HE21	1:A:1055:GLU:CG	2.07	0.66
1:A:1154:ILE:HD13	1:A:1161:TYR:HE2	1.58	0.66
1:B:125:ALA:O	1:B:129:VAL:HG23	1.94	0.66
1:A:35:VAL:HG21	1:A:355:ARG:HH21	1.60	0.66
1:A:548:LEU:C	1:A:549:LEU:HD12	2.19	0.66
1:A:1260:LYS:H	1:A:1260:LYS:HD2	1.59	0.66
1:B:122:LEU:HD12	1:B:939:SER:HB2	1.77	0.66
1:B:164:VAL:O	1:B:164:VAL:CG1	2.43	0.66
1:B:414:LYS:HB2	1:B:417:GLN:OE1	1.96	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:447:VAL:HG13	1:B:454:ILE:HG22	1.77	0.66
1:B:589:ARG:C	1:B:591:ALA:H	2.02	0.66
1:B:851:TRP:HA	1:B:854:THR:CB	2.21	0.66
1:B:978:VAL:HG22	2:B:6003:2J8:H29	1.77	0.66
1:A:175:VAL:HG13	1:A:176:SER:N	2.10	0.66
1:A:238:LYS:HZ2	1:A:242:ALA:HB2	1.58	0.66
1:A:357:ALA:O	1:A:361:VAL:HG22	1.94	0.66
1:A:441:ASP:CG	1:A:442:PRO:HD2	2.21	0.66
1:A:1001:ALA:O	1:A:1005:ILE:HG13	1.94	0.66
1:A:212:LEU:HA	1:A:215:LEU:CG	2.26	0.66
1:A:318:ILE:HG23	1:A:735:PHE:CZ	2.30	0.66
1:B:207:GLY:HA3	1:B:211:THR:CB	2.24	0.66
1:B:238:LYS:HZ3	1:B:242:ALA:HB2	1.57	0.66
1:A:121:VAL:HG23	1:A:122:LEU:N	2.09	0.66
1:A:900:PHE:O	1:A:902:THR:N	2.21	0.66
1:B:256:ALA:O	1:B:260:VAL:HG23	1.95	0.66
1:A:401:LYS:H	1:A:401:LYS:CD	2.07	0.66
1:A:534:ARG:HH21	1:A:564:VAL:HG11	1.60	0.66
1:A:790:LYS:HB3	1:A:794:ARG:NH2	2.10	0.66
1:B:219:PRO:O	1:B:223:LEU:HG	1.96	0.66
1:B:257:ILE:C	1:B:257:ILE:HD13	2.21	0.66
1:B:288:ALA:HA	1:B:291:ALA:HB3	1.78	0.66
1:B:318:ILE:HD13	1:B:327:VAL:CG1	2.25	0.66
1:B:443:LEU:O	1:B:443:LEU:HD23	1.96	0.66
1:B:458:ASN:ND2	1:B:459:VAL:N	2.44	0.66
1:B:468:VAL:HG22	1:B:549:LEU:HD13	1.78	0.66
1:A:239:GLU:HB3	1:A:285:ILE:HG12	1.78	0.66
1:A:282:ARG:O	1:A:286:LYS:HD3	1.96	0.66
1:A:909:GLU:O	1:A:912:PHE:HB2	1.96	0.66
1:B:207:GLY:CA	1:B:211:THR:HB	2.24	0.66
1:B:1179:ARG:HA	1:B:1182:ILE:HG13	1.77	0.66
1:B:1184:ARG:O	1:B:1187:VAL:HG12	1.95	0.66
1:A:414:LYS:HB2	1:A:417:GLN:OE1	1.95	0.66
1:B:985:GLY:HA3	2:B:6003:2J8:H32A	1.76	0.66
1:A:458:ASN:ND2	1:A:459:VAL:N	2.44	0.66
1:B:68:MET:SD	1:B:332:PHE:HE1	2.18	0.66
1:B:147:PHE:CD2	1:B:365:ILE:HG12	2.31	0.66
1:B:217:ILE:HG13	1:B:218:SER:N	2.11	0.66
1:B:465:ILE:O	1:B:545:PRO:HB2	1.96	0.66
1:B:697:LEU:HD12	1:B:698:LYS:N	2.11	0.66
1:B:1042:THR:C	1:B:1044:PRO:HD2	2.21	0.66

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:447:VAL:HG13	1:A:454:ILE:HG22	1.78	0.65
1:A:468:VAL:HG22	1:A:549:LEU:HD13	1.77	0.65
1:B:141:HIS:O	1:B:144:ARG:HB3	1.96	0.65
1:B:467:GLY:N	1:B:545:PRO:HG3	2.11	0.65
1:A:98:ALA:O	1:A:102:LYS:HG2	1.96	0.65
1:A:158:TRP:CE2	1:A:900:PHE:HB2	2.31	0.65
1:A:214:ILE:HD11	1:A:330:VAL:HB	1.78	0.65
1:A:1137:SER:CB	1:A:1140:GLU:HB2	2.26	0.65
1:A:324:ILE:HG13	1:A:326:GLN:H	1.61	0.65
1:A:438:ARG:HB2	1:A:462:LEU:HD21	1.78	0.65
1:A:892:ILE:CB	1:A:916:TYR:HE1	2.09	0.65
1:A:1042:THR:C	1:A:1044:PRO:HD2	2.22	0.65
1:B:379:HIS:CD2	1:B:380:LYS:H	2.14	0.65
1:B:972:LEU:N	1:B:972:LEU:HD12	2.12	0.65
1:B:1144:ALA:HA	1:B:1186:LEU:CD1	2.23	0.65
1:A:889:SER:OG	1:A:919:SER:HB2	1.96	0.65
1:B:286:LYS:HE2	1:B:778:GLU:CG	2.26	0.65
1:B:585:LEU:H	1:B:585:LEU:HD22	1.61	0.65
1:B:790:LYS:HB3	1:B:794:ARG:NH2	2.11	0.65
1:B:799:TRP:HA	1:B:799:TRP:CE3	2.28	0.65
1:A:148:PHE:HD2	1:A:913:GLU:OE2	1.79	0.65
1:A:462:LEU:O	1:A:466:ILE:HD13	1.96	0.65
1:A:533:GLN:NE2	1:A:553:ALA:HB1	2.11	0.65
1:B:1063:ALA:HB2	1:B:1236:ALA:HB1	1.79	0.65
1:A:43:GLY:HA3	1:A:46:ASP:HB2	1.79	0.65
1:A:55:LEU:O	1:A:59:ILE:HG23	1.97	0.65
1:A:207:GLY:HA3	1:A:211:THR:N	2.11	0.65
1:A:857:LEU:CD1	1:A:977:ILE:HG12	2.25	0.65
1:B:727:ILE:O	1:B:731:VAL:HG23	1.96	0.65
1:A:68:MET:SD	1:A:332:PHE:HE1	2.19	0.65
1:A:338:ALA:O	1:A:341:VAL:HB	1.95	0.65
1:A:799:TRP:HA	1:A:799:TRP:CE3	2.29	0.65
1:A:799:TRP:HA	1:A:799:TRP:HE3	1.60	0.65
1:A:919:SER:O	1:A:923:PRO:CD	2.45	0.65
1:A:1106:ARG:O	1:A:1109:LEU:HD22	1.96	0.65
1:B:158:TRP:CZ2	1:B:900:PHE:HB2	2.32	0.65
1:B:536:ALA:O	1:B:539:ARG:HB3	1.97	0.65
1:B:1114:GLN:HE22	1:B:1200:SER:HB2	1.61	0.65
1:A:322:TYR:CZ	1:A:324:ILE:CD1	2.80	0.65
1:A:564:VAL:O	1:A:567:ALA:HB3	1.96	0.65
1:A:697:LEU:HD12	1:A:698:LYS:N	2.11	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1063:ALA:HA	1:A:1225:VAL:HG13	1.79	0.65
1:B:211:THR:O	1:B:215:LEU:HG	1.97	0.65
1:B:1036:VAL:HB	1:B:1052:LEU:CB	2.24	0.65
1:A:90:ASN:HB2	1:A:91:MET:HE3	1.77	0.65
1:A:837:ALA:HB1	1:A:982:MET:HE1	1.79	0.65
1:A:1195:LEU:HD23	1:A:1214:LEU:HD11	1.79	0.65
1:B:288:ALA:O	1:B:291:ALA:HB3	1.97	0.65
1:B:769:GLN:HG3	1:B:773:PHE:HE2	1.62	0.65
1:B:1138:TYR:O	1:B:1142:VAL:HG23	1.97	0.65
1:A:315:SER:HA	1:A:747:ASN:HD22	1.61	0.65
1:A:388:LEU:HD13	1:A:413:VAL:HG13	1.79	0.65
1:A:465:ILE:C	1:A:466:ILE:HD12	2.22	0.65
1:A:883:LYS:O	1:A:887:GLU:HB2	1.97	0.65
1:B:1137:SER:CB	1:B:1140:GLU:HB2	2.26	0.65
1:A:834:GLN:O	1:A:837:ALA:HB3	1.96	0.64
1:A:857:LEU:HG	1:A:977:ILE:CD1	2.27	0.64
1:A:972:LEU:HD12	1:A:972:LEU:N	2.13	0.64
1:A:1179:ARG:HA	1:A:1182:ILE:HG13	1.78	0.64
1:B:198:GLY:O	1:B:202:ILE:HG13	1.97	0.64
1:B:324:ILE:HG12	1:B:326:GLN:H	1.61	0.64
1:B:361:VAL:O	1:B:365:ILE:HD12	1.96	0.64
1:B:847:LEU:C	1:B:849:TYR:H	2.04	0.64
1:B:879:ALA:O	1:B:883:LYS:HG2	1.97	0.64
1:A:371:ILE:CG2	1:A:371:ILE:O	2.45	0.64
1:A:549:LEU:HD12	1:A:549:LEU:N	2.13	0.64
1:A:722:PRO:HG2	1:A:841:THR:CB	2.27	0.64
1:A:1023:LYS:HG3	1:A:1026:MET:HG3	1.80	0.64
1:A:1102:VAL:HG13	1:A:1103:GLN:H	1.61	0.64
1:B:690:PRO:HG2	1:B:1006:ARG:HH22	1.60	0.64
1:B:762:SER:O	1:B:765:THR:HG22	1.96	0.64
1:B:838:ASN:ND2	1:B:979:PHE:HB3	2.11	0.64
1:B:845:ILE:HA	1:B:848:ILE:HG22	1.78	0.64
1:B:892:ILE:CB	1:B:916:TYR:HE1	2.09	0.64
1:A:762:SER:O	1:A:765:THR:HG22	1.97	0.64
1:B:107:MET:HA	1:B:110:TYR:HD2	1.62	0.64
1:B:174:ASP:O	1:B:178:ILE:HG13	1.97	0.64
1:B:857:LEU:HD12	1:B:973:VAL:HG13	1.79	0.64
1:B:1128:ALA:CB	1:B:1136:VAL:HG13	2.27	0.64
1:A:390:PHE:HB2	1:A:411:LEU:O	1.98	0.64
1:B:339:PHE:CE1	2:B:6003:2J8:C21	2.81	0.64
1:B:465:ILE:C	1:B:466:ILE:HD12	2.22	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:478:THR:HG21	1:B:482:GLU:HG3	1.80	0.64
1:B:692:SER:HB2	1:B:695:ARG:HB3	1.78	0.64
1:B:837:ALA:HB1	1:B:982:MET:HE1	1.78	0.64
1:B:857:LEU:HD11	1:B:976:ALA:HB3	1.79	0.64
1:B:911:LYS:O	1:B:914:THR:HB	1.97	0.64
1:A:288:ALA:O	1:A:291:ALA:HB3	1.98	0.64
1:A:308:LEU:HA	1:A:751:PHE:CE2	2.32	0.64
1:A:419:VAL:O	1:A:579:ILE:HA	1.96	0.64
1:A:688:VAL:HG22	1:A:1003:HIS:CE1	2.33	0.64
1:A:827:SER:O	1:A:828:ARG:C	2.41	0.64
1:A:1116:PRO:HB3	1:A:1178:GLN:OE1	1.97	0.64
1:A:1199:THR:CG2	1:A:1210:VAL:HG11	2.28	0.64
1:B:58:ILE:HD12	1:B:58:ILE:H	1.63	0.64
1:B:458:ASN:ND2	1:B:459:VAL:H	1.94	0.64
1:B:762:SER:CA	1:B:765:THR:HG22	2.28	0.64
1:B:883:LYS:O	1:B:887:GLU:HB2	1.96	0.64
1:B:1195:LEU:HD23	1:B:1214:LEU:HD11	1.79	0.64
1:B:1205:GLU:HA	1:B:1208:LYS:HB3	1.80	0.64
1:A:158:TRP:HA	1:A:162:HIS:CD2	2.30	0.64
1:A:198:GLY:O	1:A:202:ILE:HG13	1.98	0.64
1:A:536:ALA:O	1:A:539:ARG:HB3	1.98	0.64
1:A:1138:TYR:O	1:A:1142:VAL:HG23	1.97	0.64
1:B:359:TYR:HA	1:B:362:PHE:HB3	1.80	0.64
1:B:438:ARG:HB2	1:B:462:LEU:HD21	1.78	0.64
1:B:889:SER:OG	1:B:919:SER:HB2	1.97	0.64
1:B:901:ARG:H	1:B:901:ARG:HD3	1.60	0.64
1:B:1116:PRO:HB3	1:B:1178:GLN:OE1	1.97	0.64
1:A:211:THR:O	1:A:215:LEU:HG	1.98	0.64
1:A:267:LYS:HA	1:A:270:LEU:HD11	1.79	0.64
1:A:292:ASN:CA	1:A:295:MET:HB2	2.26	0.64
1:A:838:ASN:ND2	1:A:979:PHE:HB3	2.12	0.64
1:A:894:THR:O	1:A:895:GLU:C	2.41	0.64
1:A:1020:GLN:NE2	1:A:1022:LEU:H	1.95	0.64
1:B:76:ASP:OD1	1:B:326:GLN:HB2	1.98	0.64
1:B:423:GLY:HA2	1:B:597:PHE:O	1.98	0.64
1:B:478:THR:CG2	1:B:482:GLU:HG3	2.28	0.64
1:A:147:PHE:CD2	1:A:365:ILE:HG12	2.33	0.64
1:A:279:GLU:HG2	1:A:782:LYS:NZ	2.13	0.64
1:A:458:ASN:ND2	1:A:459:VAL:H	1.96	0.64
1:A:996:LYS:H	1:A:996:LYS:CD	2.08	0.64
1:A:1081:ARG:CZ	1:A:1098:LYS:O	2.46	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1159:ASP:O	1:B:1160:LYS:HG3	1.98	0.64
1:A:585:LEU:O	1:A:588:VAL:HB	1.97	0.64
1:B:175:VAL:HG13	1:B:176:SER:N	2.13	0.64
1:B:1178:GLN:O	1:B:1181:ALA:HB3	1.97	0.64
1:A:59:ILE:CD1	1:A:124:VAL:HG11	2.28	0.64
1:A:392:ASN:O	1:A:445:GLY:HA3	1.98	0.64
1:A:465:ILE:O	1:A:545:PRO:HB2	1.98	0.64
1:A:1128:ALA:CB	1:A:1136:VAL:HG13	2.27	0.64
1:B:322:TYR:CZ	1:B:324:ILE:CD1	2.81	0.64
1:B:464:GLU:HA	1:B:543:ARG:NH2	2.12	0.64
1:B:750:LEU:O	1:B:753:LEU:HB3	1.98	0.64
1:B:834:GLN:O	1:B:837:ALA:HB3	1.97	0.64
1:B:853:LEU:HD22	1:B:853:LEU:N	2.12	0.64
1:B:1192:ILE:HD13	1:B:1193:LEU:N	2.12	0.64
1:A:913:GLU:HA	1:A:916:TYR:HD2	1.62	0.63
1:A:1184:ARG:O	1:A:1187:VAL:HG12	1.98	0.63
1:B:59:ILE:CD1	1:B:124:VAL:HG11	2.28	0.63
1:B:458:ASN:HD22	1:B:459:VAL:H	1.46	0.63
1:A:478:THR:CG2	1:A:482:GLU:HG3	2.28	0.63
1:A:762:SER:HA	1:A:765:THR:CG2	2.29	0.63
1:A:795:GLN:HE21	1:A:796:ASP:N	1.96	0.63
1:A:879:ALA:O	1:A:883:LYS:HG2	1.98	0.63
1:A:891:LYS:O	1:A:894:THR:HB	1.98	0.63
1:B:212:LEU:HA	1:B:215:LEU:CG	2.28	0.63
1:B:239:GLU:HB3	1:B:285:ILE:CG1	2.28	0.63
1:B:564:VAL:O	1:B:567:ALA:HB3	1.99	0.63
1:B:891:LYS:O	1:B:894:THR:HB	1.99	0.63
1:A:118:GLY:O	1:A:119:ALA:C	2.42	0.63
1:A:478:THR:HG21	1:A:482:GLU:HG3	1.80	0.63
1:B:133:CYS:SG	1:B:931:ALA:HA	2.39	0.63
1:A:212:LEU:HD12	1:A:215:LEU:HB2	1.80	0.63
1:A:267:LYS:HG2	1:A:793:LEU:HG	1.79	0.63
1:B:263:PHE:CE1	1:B:1129:TYR:HB3	2.32	0.63
1:A:239:GLU:HB3	1:A:285:ILE:CG1	2.28	0.63
1:A:458:ASN:HD22	1:A:459:VAL:H	1.47	0.63
1:A:471:GLN:O	1:A:473:PRO:HD3	1.98	0.63
1:A:492:THR:HG22	1:A:494:ASP:H	1.63	0.63
1:A:933:VAL:O	1:A:936:ILE:HG22	1.99	0.63
1:A:1009:GLU:C	1:A:1010:LYS:HG3	2.23	0.63
1:A:1014:ILE:O	1:A:1014:ILE:HD12	1.98	0.63
1:B:341:VAL:O	1:B:344:ALA:HB3	1.99	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:933:VAL:O	1:B:936:ILE:HG22	1.98	0.63
1:B:933:VAL:O	1:B:934:PHE:C	2.39	0.63
1:A:245:LYS:HA	1:A:245:LYS:HZ1	1.64	0.63
1:B:35:VAL:HG21	1:B:355:ARG:HH21	1.60	0.63
1:B:43:GLY:HA3	1:B:46:ASP:HB2	1.80	0.63
1:B:1092:LEU:HD13	1:B:1100:LEU:HD21	1.81	0.63
1:A:164:VAL:O	1:A:164:VAL:CG1	2.47	0.63
1:A:187:GLY:O	1:A:190:PHE:HB3	1.98	0.63
1:A:762:SER:CA	1:A:765:THR:HG22	2.28	0.63
1:B:296:GLY:O	1:B:300:LEU:HG	1.97	0.63
1:B:1102:VAL:HG13	1:B:1103:GLN:N	2.14	0.63
1:B:1199:THR:CG2	1:B:1210:VAL:HG11	2.28	0.63
1:A:107:MET:HA	1:A:110:TYR:HD2	1.62	0.63
1:A:172:THR:O	1:A:175:VAL:HG12	1.99	0.63
1:A:296:GLY:O	1:A:300:LEU:HG	1.99	0.63
1:A:855:LEU:O	1:A:858:LEU:HG	1.99	0.63
1:A:1036:VAL:HB	1:A:1052:LEU:CB	2.24	0.63
1:B:147:PHE:O	1:B:151:ILE:HG13	1.99	0.63
1:B:204:PHE:HA	1:B:211:THR:HG21	1.80	0.63
1:B:282:ARG:O	1:B:286:LYS:HD3	1.99	0.63
1:B:462:LEU:O	1:B:466:ILE:HD13	1.99	0.63
1:B:339:PHE:CD1	2:B:6003:2J8:SE3	3.02	0.63
1:B:785:ARG:HH21	1:B:815:ALA:HA	1.63	0.63
1:B:1106:ARG:O	1:B:1109:LEU:HD22	1.99	0.63
1:A:58:ILE:H	1:A:58:ILE:HD12	1.64	0.62
1:A:374:PHE:CE2	1:A:376:LYS:HB3	2.34	0.62
1:A:540:ALA:O	1:A:543:ARG:HB3	1.98	0.62
1:B:59:ILE:CG1	1:B:124:VAL:HG11	2.29	0.62
1:B:195:THR:CB	1:B:340:SER:HB2	2.18	0.62
1:B:217:ILE:HD11	1:B:331:PHE:HE2	1.64	0.62
1:B:471:GLN:HA	1:B:553:ALA:HA	1.79	0.62
1:B:722:PRO:HG2	1:B:841:THR:CB	2.29	0.62
1:B:943:ALA:O	1:B:947:PHE:HB2	1.99	0.62
1:A:214:ILE:HG12	1:A:331:PHE:CZ	2.34	0.62
1:A:315:SER:HA	1:A:747:ASN:ND2	2.14	0.62
1:A:847:LEU:C	1:A:849:TYR:H	2.05	0.62
1:A:943:ALA:O	1:A:947:PHE:HB2	1.99	0.62
1:A:1005:ILE:O	1:A:1008:ILE:HG22	1.99	0.62
1:A:1063:ALA:HB2	1:A:1236:ALA:HB1	1.80	0.62
1:B:318:ILE:CD1	1:B:327:VAL:HG13	2.29	0.62
1:B:894:THR:O	1:B:897:ILE:HG13	1.99	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:769:GLN:HG3	1:A:773:PHE:HE2	1.63	0.62
1:A:785:ARG:HH21	1:A:815:ALA:HA	1.64	0.62
1:A:1095:LYS:H	1:A:1095:LYS:HD2	1.64	0.62
1:B:864:ILE:HD12	1:B:865:ALA:N	2.14	0.62
1:A:548:LEU:HD23	1:A:549:LEU:N	2.14	0.62
1:A:1109:LEU:O	1:A:1109:LEU:HD23	1.99	0.62
1:B:118:GLY:O	1:B:119:ALA:C	2.42	0.62
1:B:123:ILE:O	1:B:127:ILE:HG12	2.00	0.62
1:B:858:LEU:HD12	1:B:859:ALA:N	2.14	0.62
1:A:59:ILE:CG1	1:A:124:VAL:HG11	2.29	0.62
1:A:310:PHE:CE2	1:A:331:PHE:HB3	2.35	0.62
1:A:462:LEU:HD12	1:A:466:ILE:HD13	1.80	0.62
1:A:894:THR:O	1:A:897:ILE:HG13	1.99	0.62
1:A:1097:ILE:HG23	1:A:1105:LEU:HD22	1.81	0.62
1:A:1261:GLY:H	1:A:1264:PHE:CB	2.11	0.62
1:B:221:LEU:HD11	1:B:309:ALA:HB3	1.79	0.62
1:B:371:ILE:C	1:B:373:SER:H	2.08	0.62
1:B:1011:THR:N	1:B:1012:PRO:CD	2.56	0.62
1:B:1097:ILE:HG23	1:B:1105:LEU:HD22	1.82	0.62
1:A:76:ASP:OD1	1:A:326:GLN:HB2	1.99	0.62
1:A:144:ARG:NH1	1:A:175:VAL:HG11	2.15	0.62
1:A:155:GLU:CB	1:A:156:ILE:HD12	2.30	0.62
1:A:286:LYS:O	1:A:290:THR:HG23	1.99	0.62
1:A:359:TYR:HA	1:A:362:PHE:HB3	1.80	0.62
1:A:1102:VAL:HG13	1:A:1103:GLN:N	2.14	0.62
1:B:209:LYS:C	1:B:212:LEU:HB3	2.25	0.62
1:B:304:ALA:CB	1:B:758:LEU:HD23	2.29	0.62
1:B:549:LEU:HD12	1:B:549:LEU:N	2.13	0.62
1:B:1026:MET:HG3	1:B:1026:MET:O	1.99	0.62
1:A:175:VAL:HG13	1:A:176:SER:H	1.64	0.62
1:A:1144:ALA:HA	1:A:1186:LEU:CD1	2.23	0.62
1:A:1192:ILE:HD13	1:A:1193:LEU:N	2.15	0.62
1:A:750:LEU:O	1:A:753:LEU:HB3	1.99	0.62
1:A:864:ILE:HD12	1:A:865:ALA:N	2.14	0.62
1:A:1129:TYR:CD2	1:A:1184:ARG:HG3	2.35	0.62
1:B:419:VAL:O	1:B:579:ILE:HA	1.99	0.62
1:B:502:GLU:OE1	1:B:541:LEU:HD11	2.00	0.62
1:A:64:LEU:HD11	1:A:945:MET:HE2	1.82	0.62
1:A:502:GLU:OE1	1:A:541:LEU:HD11	2.00	0.62
1:A:1218:ARG:HH22	1:A:1235:ASN:ND2	1.90	0.62
1:B:144:ARG:NH1	1:B:175:VAL:HG11	2.15	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:215:LEU:C	1:B:219:PRO:HD2	2.25	0.62
1:B:411:LEU:HD23	1:B:412:LYS:N	2.15	0.62
1:B:462:LEU:HD12	1:B:466:ILE:HD13	1.80	0.62
1:B:585:LEU:O	1:B:588:VAL:HB	1.99	0.62
1:B:900:PHE:O	1:B:903:VAL:HG12	1.99	0.62
1:A:123:ILE:O	1:A:127:ILE:HG12	1.99	0.62
1:A:221:LEU:HD11	1:A:309:ALA:HB3	1.81	0.62
1:A:257:ILE:HG21	1:A:800:PHE:HB3	1.81	0.62
1:A:298:ALA:O	1:A:302:ILE:HG13	1.99	0.62
1:A:429:LYS:H	1:A:429:LYS:CD	2.09	0.62
1:A:978:VAL:CG2	2:A:6001:2J8:H29	2.30	0.62
1:B:548:LEU:HD23	1:B:549:LEU:N	2.13	0.62
1:B:559:THR:O	1:B:562:GLU:HB3	2.00	0.62
1:B:971:LEU:O	1:B:974:PHE:HB3	1.99	0.62
1:B:1063:ALA:HB2	1:B:1236:ALA:CB	2.30	0.62
1:A:254:LEU:HD22	1:A:254:LEU:H	1.64	0.61
1:A:360:GLU:HA	1:A:363:LYS:CE	2.29	0.61
1:A:379:HIS:HB3	1:A:457:ILE:HA	1.80	0.61
1:A:883:LYS:HD3	1:A:886:LEU:HD21	1.82	0.61
1:A:902:THR:O	1:A:904:VAL:N	2.33	0.61
1:A:959:LEU:HD22	1:A:964:LEU:HG	1.81	0.61
1:B:254:LEU:HD22	1:B:254:LEU:H	1.63	0.61
1:B:314:THR:O	1:B:315:SER:C	2.43	0.61
1:B:904:VAL:HG13	1:B:905:SER:N	2.15	0.61
1:B:996:LYS:H	1:B:996:LYS:CD	2.08	0.61
1:B:1150:ILE:O	1:B:1154:ILE:HG13	2.00	0.61
1:A:341:VAL:O	1:A:344:ALA:HB3	2.00	0.61
1:B:339:PHE:CG	2:B:6003:2J8:SE3	3.03	0.61
1:A:853:LEU:O	1:A:854:THR:C	2.44	0.61
1:A:1058:LYS:O	1:A:1060:GLN:HG3	2.00	0.61
1:A:1260:LYS:HD2	1:A:1260:LYS:N	2.16	0.61
1:B:1208:LYS:C	1:B:1208:LYS:HD3	2.25	0.61
1:A:858:LEU:HD12	1:A:859:ALA:N	2.15	0.61
1:A:1063:ALA:HB2	1:A:1236:ALA:CB	2.30	0.61
1:A:1092:LEU:HD13	1:A:1100:LEU:HD21	1.81	0.61
1:B:172:THR:O	1:B:175:VAL:HG12	2.00	0.61
1:B:795:GLN:HE21	1:B:796:ASP:N	1.98	0.61
1:B:1001:ALA:O	1:B:1005:ILE:HG13	2.00	0.61
1:B:1260:LYS:HD2	1:B:1260:LYS:N	2.15	0.61
1:A:810:LEU:O	1:A:813:ARG:HB2	1.99	0.61
1:A:1205:GLU:HA	1:A:1208:LYS:HB3	1.81	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1252:THR:HG23	1:A:1255:GLN:HB2	1.82	0.61
1:B:267:LYS:HA	1:B:270:LEU:HD11	1.83	0.61
1:B:292:ASN:CA	1:B:295:MET:HB2	2.29	0.61
1:B:388:LEU:HD13	1:B:413:VAL:HG13	1.81	0.61
1:B:691:ALA:HA	1:B:1002:SER:HG	1.65	0.61
1:B:1095:LYS:H	1:B:1095:LYS:HD2	1.64	0.61
1:A:515:GLN:HE21	1:B:138:ARG:NH2	1.98	0.61
1:A:722:PRO:HA	1:A:979:PHE:CZ	2.35	0.61
1:A:927:ALA:HA	1:A:930:LYS:CE	2.30	0.61
1:A:1139:GLU:CD	1:A:1139:GLU:H	2.09	0.61
1:B:509:ILE:HD12	1:B:510:MET:N	2.15	0.61
1:B:1129:TYR:CD2	1:B:1184:ARG:HG3	2.35	0.61
1:A:39:PHE:HE2	1:A:358:ALA:HB3	1.65	0.61
1:B:982:MET:HA	2:B:6003:2J8:H32	1.83	0.61
1:A:265:GLY:CA	1:A:793:LEU:HD21	2.31	0.61
1:A:706:TYR:CD1	1:A:706:TYR:C	2.78	0.61
1:A:720:LEU:O	1:A:723:ALA:HB3	2.00	0.61
1:A:845:ILE:HA	1:A:848:ILE:HG22	1.81	0.61
1:A:857:LEU:HG	1:A:977:ILE:HD11	1.83	0.61
1:A:1090:VAL:HG13	1:A:1097:ILE:CB	2.25	0.61
1:B:265:GLY:C	1:B:267:LYS:HG3	2.26	0.61
1:B:810:LEU:O	1:B:813:ARG:HB2	2.00	0.61
1:B:1113:SER:HA	1:B:1196:ASP:HB3	1.83	0.61
1:A:773:PHE:CD1	1:A:774:GLY:N	2.68	0.61
1:A:1023:LYS:NZ	1:A:1023:LYS:HB3	2.16	0.61
1:A:1202:LEU:CG	1:A:1203:ASP:H	2.11	0.61
1:A:1248:LYS:HG2	1:A:1262:ILE:HD12	1.83	0.61
1:B:883:LYS:HD3	1:B:886:LEU:HD21	1.82	0.61
1:A:303:TYR:CZ	2:A:6001:2J8:SE1	3.04	0.61
1:A:509:ILE:HD12	1:A:510:MET:N	2.15	0.61
1:A:766:PHE:HA	1:A:769:GLN:NE2	2.06	0.61
1:B:170:ARG:HB2	1:B:174:ASP:OD1	2.01	0.61
1:B:203:GLY:C	1:B:211:THR:OG1	2.43	0.61
1:B:212:LEU:HD12	1:B:215:LEU:HB2	1.82	0.61
1:B:720:LEU:HD11	1:B:758:LEU:HA	1.83	0.61
1:A:185:LYS:O	1:A:186:ILE:C	2.44	0.60
1:A:756:LEU:HD12	1:A:757:ILE:HG12	1.83	0.60
1:B:168:ASN:O	1:B:171:LEU:HB3	2.01	0.60
1:B:253:VAL:C	1:B:254:LEU:HD13	2.26	0.60
1:B:383:ASN:O	1:B:384:ILE:C	2.44	0.60
1:B:1252:THR:HG23	1:B:1255:GLN:HB2	1.82	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:170:ARG:HB2	1:A:174:ASP:OD1	2.00	0.60
1:A:238:LYS:HD3	1:A:238:LYS:C	2.26	0.60
1:A:253:VAL:C	1:A:254:LEU:HD13	2.27	0.60
1:A:265:GLY:C	1:A:267:LYS:HG3	2.26	0.60
1:B:382:ASP:HA	1:B:461:TYR:OH	2.01	0.60
1:B:959:LEU:HD22	1:B:964:LEU:CB	2.25	0.60
1:B:1005:ILE:O	1:B:1008:ILE:HG22	2.01	0.60
1:B:1139:GLU:H	1:B:1139:GLU:CD	2.09	0.60
1:A:797:VAL:HG21	1:A:1013:GLU:CG	2.26	0.60
1:B:360:GLU:HA	1:B:363:LYS:CE	2.30	0.60
1:B:773:PHE:CD1	1:B:774:GLY:N	2.68	0.60
1:B:1048:VAL:O	1:B:1049:LEU:HD22	2.02	0.60
1:A:318:ILE:HD13	1:A:327:VAL:HG13	1.83	0.60
1:A:365:ILE:HG22	1:A:366:ASP:N	2.15	0.60
1:A:464:GLU:HA	1:A:543:ARG:NH2	2.16	0.60
1:A:482:GLU:O	1:A:483:ASN:C	2.45	0.60
1:B:689:PRO:N	1:B:690:PRO:HD2	2.17	0.60
1:B:711:ILE:HG13	1:B:715:ILE:HD11	1.83	0.60
1:B:855:LEU:O	1:B:858:LEU:HG	2.02	0.60
1:B:894:THR:O	1:B:895:GLU:C	2.45	0.60
1:A:1043:ARG:N	1:A:1044:PRO:HD2	2.17	0.60
1:B:471:GLN:O	1:B:473:PRO:HD3	2.00	0.60
1:B:722:PRO:HA	1:B:979:PHE:CZ	2.36	0.60
1:A:384:ILE:HG22	1:A:385:GLN:N	2.05	0.60
1:A:971:LEU:O	1:A:974:PHE:HB3	2.01	0.60
1:A:1176:GLN:O	1:A:1180:ILE:HG13	2.01	0.60
1:B:238:LYS:C	1:B:238:LYS:HD3	2.27	0.60
1:B:379:HIS:HB2	1:B:456:THR:O	2.01	0.60
1:B:720:LEU:O	1:B:723:ALA:HB3	2.00	0.60
1:B:927:ALA:HA	1:B:930:LYS:CE	2.31	0.60
1:A:374:PHE:CE2	1:A:376:LYS:CB	2.84	0.60
1:A:411:LEU:HD23	1:A:412:LYS:N	2.17	0.60
1:A:711:ILE:HG13	1:A:715:ILE:HD11	1.83	0.60
1:A:727:ILE:HD12	1:A:754:LEU:CA	2.32	0.60
1:A:853:LEU:H	1:A:853:LEU:CD2	1.96	0.60
1:A:858:LEU:HD12	1:A:858:LEU:C	2.26	0.60
1:B:358:ALA:O	1:B:362:PHE:HB2	2.01	0.60
1:B:507:ASP:O	1:B:510:MET:N	2.35	0.60
1:B:762:SER:HA	1:B:765:THR:CG2	2.29	0.60
1:B:827:SER:O	1:B:831:VAL:HG23	2.01	0.60
1:B:1063:ALA:HB3	1:B:1239:ILE:CA	2.24	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1150:ILE:HB	1:B:1179:ARG:HB3	1.83	0.60
1:A:905:SER:O	1:A:907:THR:N	2.35	0.60
1:B:430:SER:O	1:B:434:GLN:HG3	2.02	0.60
1:B:540:ALA:O	1:B:543:ARG:HB3	2.01	0.60
1:A:797:VAL:HG12	1:A:798:SER:N	2.16	0.60
1:A:883:LYS:HA	1:A:886:LEU:CG	2.32	0.60
1:B:1023:LYS:O	1:B:1025:ASN:N	2.35	0.60
1:A:328:LEU:C	1:A:328:LEU:HD12	2.26	0.60
1:B:324:ILE:C	1:B:326:GLN:N	2.56	0.60
1:B:902:THR:O	1:B:904:VAL:N	2.35	0.60
1:B:978:VAL:O	1:B:981:ALA:HB3	2.02	0.60
1:A:136:ALA:HB2	1:A:182:ILE:CB	2.32	0.59
1:A:692:SER:HB2	1:A:695:ARG:HB3	1.84	0.59
1:A:897:ILE:HG13	1:A:898:GLU:N	2.04	0.59
1:A:1178:GLN:O	1:A:1182:ILE:HG12	2.02	0.59
1:B:155:GLU:CB	1:B:156:ILE:HD12	2.30	0.59
1:B:492:THR:HG22	1:B:494:ASP:H	1.66	0.59
1:B:861:VAL:HB	1:B:862:PRO:CD	2.32	0.59
1:A:322:TYR:CZ	1:A:324:ILE:HD12	2.38	0.59
1:A:388:LEU:N	1:A:388:LEU:HD12	2.17	0.59
1:A:713:CYS:O	1:A:716:ILE:HG12	2.02	0.59
1:A:722:PRO:CG	1:A:841:THR:HB	2.31	0.59
1:A:861:VAL:HB	1:A:862:PRO:CD	2.32	0.59
1:A:1150:ILE:HB	1:A:1179:ARG:HB3	1.82	0.59
1:B:39:PHE:HE2	1:B:358:ALA:HB3	1.65	0.59
1:B:175:VAL:HG13	1:B:176:SER:H	1.68	0.59
1:B:321:GLU:HG3	1:B:322:TYR:N	2.17	0.59
1:B:1133:SER:O	1:B:1135:VAL:N	2.35	0.59
1:A:147:PHE:O	1:A:151:ILE:HG13	2.01	0.59
1:A:437:GLN:NE2	1:A:468:VAL:HG21	2.17	0.59
1:A:703:GLU:HB3	1:A:780:LEU:HD23	1.84	0.59
1:A:1062:LEU:HD12	1:A:1224:ILE:HG23	1.85	0.59
1:B:211:THR:O	1:B:214:ILE:HB	2.02	0.59
1:B:554:THR:OG1	1:B:562:GLU:HG3	2.03	0.59
1:A:251:GLU:OE1	1:A:811:THR:HB	2.02	0.59
1:A:267:LYS:HA	1:A:270:LEU:HD21	1.83	0.59
1:A:297:ALA:HB1	1:A:763:PHE:CD2	2.38	0.59
1:A:559:THR:O	1:A:562:GLU:HB3	2.01	0.59
1:A:1048:VAL:O	1:A:1049:LEU:HD22	2.01	0.59
1:A:1059:GLY:HA2	1:A:1221:ARG:C	2.27	0.59
1:A:1113:SER:HA	1:A:1196:ASP:HB3	1.83	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:267:LYS:HB3	1:B:790:LYS:CE	2.30	0.59
1:B:401:LYS:HD2	1:B:401:LYS:N	2.15	0.59
1:B:552:GLU:O	1:B:555:SER:N	2.33	0.59
1:B:850:GLY:O	1:B:852:GLN:N	2.35	0.59
1:B:992:PRO:C	1:B:994:TYR:H	2.11	0.59
1:A:33:VAL:O	1:A:34:SER:C	2.45	0.59
1:A:818:ALA:O	1:A:821:VAL:HG22	2.03	0.59
1:B:858:LEU:HD12	1:B:858:LEU:C	2.27	0.59
1:B:1020:GLN:HB3	1:B:1101:ASN:CB	2.32	0.59
1:B:1058:LYS:O	1:B:1060:GLN:HG3	2.02	0.59
1:A:324:ILE:HG13	1:A:326:GLN:N	2.17	0.59
1:A:324:ILE:C	1:A:326:GLN:N	2.56	0.59
1:A:773:PHE:O	1:A:776:ALA:HB3	2.02	0.59
1:A:784:LEU:HG	1:A:821:VAL:HG21	1.84	0.59
1:A:1189:GLN:N	1:A:1190:PRO:HD3	2.18	0.59
1:B:70:ILE:O	1:B:71:PHE:C	2.46	0.59
1:B:310:PHE:CZ	1:B:331:PHE:HB3	2.38	0.59
1:B:437:GLN:NE2	1:B:468:VAL:HG21	2.17	0.59
1:B:749:ASN:C	1:B:749:ASN:HD22	2.11	0.59
1:B:784:LEU:HG	1:B:821:VAL:HG21	1.84	0.59
1:B:1020:GLN:HB3	1:B:1101:ASN:HB2	1.85	0.59
1:B:1189:GLN:N	1:B:1190:PRO:HD3	2.18	0.59
1:B:1218:ARG:HH22	1:B:1235:ASN:ND2	1.90	0.59
1:A:215:LEU:C	1:A:219:PRO:HD2	2.27	0.59
1:A:324:ILE:HG13	1:A:326:GLN:CA	2.33	0.59
1:B:207:GLY:O	1:B:209:LYS:N	2.33	0.59
1:B:212:LEU:O	1:B:215:LEU:N	2.36	0.59
1:B:238:LYS:HD3	1:B:238:LYS:O	2.03	0.59
1:B:491:VAL:HG21	1:B:496:ILE:HD11	1.85	0.59
1:B:756:LEU:HD12	1:B:757:ILE:HG12	1.85	0.59
1:A:211:THR:O	1:A:214:ILE:HB	2.03	0.59
1:A:611:LEU:O	1:A:614:GLU:HB3	2.03	0.59
1:A:702:THR:C	1:A:704:TRP:H	2.11	0.59
1:B:207:GLY:C	1:B:209:LYS:H	2.11	0.59
1:B:248:ALA:C	1:B:250:ALA:H	2.11	0.59
1:B:317:VAL:O	1:B:317:VAL:HG12	2.03	0.59
1:B:374:PHE:HD1	1:B:375:SER:N	2.01	0.59
1:B:1043:ARG:N	1:B:1044:PRO:HD2	2.17	0.59
1:A:65:PRO:O	1:A:68:MET:N	2.36	0.59
1:A:168:ASN:O	1:A:171:LEU:HB3	2.01	0.59
1:A:297:ALA:HB1	1:A:763:PHE:HA	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:491:VAL:HG21	1:A:496:ILE:HD11	1.85	0.59
1:B:159:PHE:O	1:B:160:ASP:C	2.46	0.59
1:B:328:LEU:C	1:B:328:LEU:HD12	2.28	0.59
1:B:365:ILE:HG22	1:B:366:ASP:N	2.17	0.59
1:B:856:LEU:HD21	1:B:952:CYS:HA	1.85	0.59
1:B:1109:LEU:HD23	1:B:1109:LEU:O	2.03	0.59
1:B:1229:ARG:C	1:B:1231:SER:N	2.59	0.59
1:A:904:VAL:HG13	1:A:905:SER:N	2.17	0.59
1:A:1109:LEU:HD21	1:A:1188:ARG:HH11	1.68	0.59
1:B:313:GLY:O	1:B:317:VAL:HG23	2.03	0.59
1:B:473:PRO:HB3	1:B:533:GLN:HA	1.85	0.59
1:B:603:VAL:HG23	1:B:604:GLU:N	2.14	0.59
1:B:611:LEU:O	1:B:614:GLU:HB3	2.03	0.59
1:B:690:PRO:HG2	1:B:1006:ARG:CZ	2.32	0.59
1:B:853:LEU:O	1:B:854:THR:C	2.45	0.59
1:A:405:ILE:HD12	1:A:427:CYS:HB3	1.85	0.58
1:B:223:LEU:O	1:B:227:ILE:HG13	2.04	0.58
1:B:722:PRO:HG2	1:B:841:THR:OG1	2.03	0.58
1:B:1020:GLN:CG	1:B:1021:GLY:N	2.66	0.58
1:A:358:ALA:O	1:A:362:PHE:HB2	2.02	0.58
1:A:721:GLN:HG3	1:A:979:PHE:HE1	1.67	0.58
1:A:1022:LEU:CD2	1:A:1022:LEU:O	2.51	0.58
1:B:53:GLY:O	1:B:56:ALA:HB3	2.02	0.58
1:B:706:TYR:CD1	1:B:706:TYR:C	2.80	0.58
1:B:749:ASN:O	1:B:750:LEU:C	2.45	0.58
1:B:813:ARG:HA	1:B:817:ASP:OD2	2.02	0.58
1:A:114:TYR:CB	1:A:950:ALA:HB2	2.33	0.58
1:A:209:LYS:O	1:A:212:LEU:HB3	2.04	0.58
1:A:345:SER:HB3	1:A:346:PRO:HD3	1.85	0.58
1:A:686:GLU:H	1:A:686:GLU:CD	2.11	0.58
1:A:756:LEU:CD1	1:A:757:ILE:HG12	2.34	0.58
1:A:960:VAL:CG1	1:A:966:THR:OG1	2.51	0.58
1:B:930:LYS:O	1:B:933:VAL:HB	2.03	0.58
1:A:186:ILE:HG13	1:A:187:GLY:H	1.68	0.58
1:A:214:ILE:HG12	1:A:331:PHE:CD1	2.39	0.58
1:A:693:PHE:C	1:A:695:ARG:H	2.11	0.58
1:B:110:TYR:HA	1:B:113:TYR:CD2	2.35	0.58
1:B:548:LEU:HD22	1:B:550:LEU:HD11	1.85	0.58
1:B:986:GLN:NE2	2:B:6003:2J8:H31	2.17	0.58
1:B:1090:VAL:HG13	1:B:1097:ILE:CB	2.25	0.58
1:B:1195:LEU:N	1:B:1195:LEU:HD12	2.18	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1221:ARG:N	1:B:1221:ARG:HD2	2.19	0.58
1:A:548:LEU:HD22	1:A:550:LEU:HD11	1.85	0.58
1:A:611:LEU:HB3	1:A:618:TYR:HB3	1.86	0.58
1:A:722:PRO:HG2	1:A:841:THR:OG1	2.02	0.58
1:B:65:PRO:O	1:B:68:MET:N	2.36	0.58
1:B:136:ALA:HB2	1:B:182:ILE:CB	2.32	0.58
1:B:958:TYR:O	1:B:966:THR:OG1	2.21	0.58
1:B:1059:GLY:HA2	1:B:1221:ARG:C	2.28	0.58
1:B:1248:LYS:HG2	1:B:1262:ILE:HD12	1.84	0.58
1:A:491:VAL:HG21	1:A:496:ILE:CD1	2.33	0.58
1:B:286:LYS:O	1:B:290:THR:HG23	2.02	0.58
1:B:713:CYS:O	1:B:716:ILE:HG12	2.02	0.58
1:B:787:MET:HE2	1:B:1008:ILE:HD11	1.86	0.58
1:B:806:THR:HG23	1:B:809:ALA:H	1.69	0.58
1:A:72:GLY:HA2	1:A:326:GLN:HE21	1.66	0.58
1:A:103:LEU:HB2	1:A:960:VAL:CG2	2.34	0.58
1:A:207:GLY:HA3	1:A:211:THR:CB	2.34	0.58
1:A:210:LEU:O	1:A:214:ILE:HG13	2.03	0.58
1:A:251:GLU:O	1:A:254:LEU:HD11	2.04	0.58
1:A:286:LYS:NZ	1:A:822:LYS:HZ2	2.02	0.58
1:A:554:THR:OG1	1:A:562:GLU:HG3	2.04	0.58
1:A:749:ASN:C	1:A:749:ASN:HD22	2.10	0.58
1:A:897:ILE:CG1	1:A:898:GLU:H	2.11	0.58
1:B:210:LEU:O	1:B:214:ILE:HG13	2.04	0.58
1:B:818:ALA:O	1:B:821:VAL:HG22	2.04	0.58
1:A:1221:ARG:HD2	1:A:1221:ARG:N	2.19	0.58
1:B:158:TRP:HZ2	1:B:900:PHE:HB2	1.66	0.58
1:B:314:THR:O	1:B:318:ILE:HG22	2.03	0.58
1:B:703:GLU:HB3	1:B:780:LEU:HD23	1.84	0.58
1:B:992:PRO:HB2	1:B:996:LYS:HZ3	1.67	0.58
1:B:1062:LEU:HD12	1:B:1224:ILE:HG23	1.85	0.58
1:B:1081:ARG:NH2	1:B:1098:LYS:O	2.37	0.58
1:B:1176:GLN:O	1:B:1180:ILE:HG13	2.04	0.58
1:A:212:LEU:O	1:A:215:LEU:N	2.37	0.58
1:A:284:GLY:O	1:A:287:LYS:HB3	2.04	0.58
1:A:720:LEU:HD11	1:A:758:LEU:HA	1.85	0.58
1:A:722:PRO:HG2	1:A:841:THR:HB	1.85	0.58
1:A:1012:PRO:O	1:A:1013:GLU:CB	2.51	0.58
1:A:1141:ILE:O	1:A:1144:ALA:HB3	2.04	0.58
1:A:1195:LEU:HD12	1:A:1195:LEU:N	2.18	0.58
1:B:56:ALA:O	1:B:59:ILE:HG13	2.04	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:70:ILE:HG22	1:B:74:MET:HE3	1.86	0.58
1:B:186:ILE:HG13	1:B:187:GLY:H	1.69	0.58
1:B:199:GLY:O	1:B:203:GLY:HA3	2.04	0.58
1:B:290:THR:HG22	1:B:770:GLY:C	2.28	0.58
1:B:374:PHE:HD1	1:B:376:LYS:H	1.50	0.58
1:B:594:ILE:O	1:B:605:GLN:HA	2.04	0.58
1:B:970:VAL:HA	1:B:973:VAL:HG23	1.86	0.58
1:B:1243:GLN:O	1:B:1244:ASN:C	2.47	0.58
1:A:70:ILE:HG22	1:A:74:MET:HE3	1.86	0.58
1:A:603:VAL:HG23	1:A:604:GLU:N	2.15	0.58
1:A:780:LEU:O	1:A:784:LEU:HB2	2.04	0.58
1:B:131:PHE:C	1:B:131:PHE:CD2	2.81	0.58
1:B:491:VAL:HG21	1:B:496:ILE:CD1	2.33	0.58
1:B:1049:LEU:CD1	1:B:1052:LEU:HD22	2.33	0.58
1:A:59:ILE:HG12	1:A:124:VAL:HG11	1.86	0.57
1:A:497:GLU:O	1:A:500:VAL:HG22	2.04	0.57
1:A:856:LEU:HD21	1:A:952:CYS:HA	1.86	0.57
1:A:900:PHE:O	1:A:903:VAL:HG12	2.04	0.57
1:B:37:THR:O	1:B:38:MET:C	2.45	0.57
1:B:59:ILE:HG12	1:B:124:VAL:HG11	1.86	0.57
1:B:279:GLU:O	1:B:282:ARG:HB2	2.04	0.57
1:B:298:ALA:O	1:B:302:ILE:HG13	2.04	0.57
1:B:603:VAL:CG2	1:B:604:GLU:H	2.08	0.57
1:B:827:SER:O	1:B:828:ARG:C	2.47	0.57
1:B:978:VAL:CG2	2:B:6003:2J8:H29	2.34	0.57
1:A:313:GLY:O	1:A:317:VAL:HG23	2.04	0.57
1:A:401:LYS:HD2	1:A:401:LYS:N	2.16	0.57
1:A:432:THR:O	1:A:433:VAL:C	2.48	0.57
1:A:970:VAL:HA	1:A:973:VAL:HG23	1.85	0.57
1:A:1185:ALA:O	1:A:1190:PRO:HD3	2.04	0.57
1:B:158:TRP:HA	1:B:162:HIS:CD2	2.33	0.57
1:B:849:TYR:HD1	1:B:854:THR:CA	2.16	0.57
1:A:749:ASN:O	1:A:750:LEU:C	2.47	0.57
1:A:790:LYS:HB3	1:A:794:ARG:CZ	2.34	0.57
1:A:813:ARG:HA	1:A:817:ASP:OD2	2.03	0.57
1:A:827:SER:HG	1:A:994:TYR:HD2	1.52	0.57
1:B:388:LEU:HD12	1:B:388:LEU:N	2.18	0.57
1:B:611:LEU:HD23	1:B:618:TYR:CB	2.34	0.57
1:B:883:LYS:HA	1:B:886:LEU:CG	2.33	0.57
1:B:921:GLN:HG2	1:B:922:ILE:HD12	1.86	0.57
1:B:1141:ILE:O	1:B:1144:ALA:HB3	2.05	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:210:LEU:HG	1:A:322:TYR:HD2	1.67	0.57
1:A:425:SER:HB3	1:A:599:GLY:HA3	1.86	0.57
1:A:1049:LEU:CD1	1:A:1052:LEU:HD22	2.33	0.57
1:B:251:GLU:O	1:B:254:LEU:HD11	2.03	0.57
1:B:263:PHE:HD1	1:B:1188:ARG:HH22	1.52	0.57
1:B:497:GLU:O	1:B:500:VAL:HG22	2.04	0.57
1:B:1032:GLN:HB2	1:B:1091:PHE:HB2	1.86	0.57
1:B:1043:ARG:NE	1:B:1086:MET:HE3	2.20	0.57
1:B:1109:LEU:HD21	1:B:1188:ARG:HH11	1.68	0.57
1:B:1137:SER:HB3	1:B:1140:GLU:HB2	1.85	0.57
1:A:787:MET:HE2	1:A:1008:ILE:HD11	1.87	0.57
1:A:861:VAL:HB	1:A:862:PRO:HD3	1.86	0.57
1:A:1127:ILE:O	1:A:1129:TYR:N	2.34	0.57
1:B:175:VAL:HA	1:B:178:ILE:HD12	1.87	0.57
1:B:693:PHE:CD2	1:B:693:PHE:N	2.71	0.57
1:B:788:VAL:O	1:B:791:SER:N	2.38	0.57
1:B:826:GLY:O	1:B:829:LEU:HB2	2.05	0.57
1:A:53:GLY:O	1:A:56:ALA:HB3	2.04	0.57
1:A:70:ILE:O	1:A:71:PHE:C	2.44	0.57
1:A:186:ILE:HG13	1:A:187:GLY:N	2.20	0.57
1:A:498:LYS:C	1:A:498:LYS:HD3	2.29	0.57
1:A:611:LEU:HD23	1:A:618:TYR:CB	2.34	0.57
1:A:1072:LYS:HB3	1:A:1226:ILE:HD13	1.87	0.57
1:A:1133:SER:O	1:A:1135:VAL:N	2.37	0.57
1:B:721:GLN:HG3	1:B:979:PHE:HE1	1.67	0.57
1:B:722:PRO:CG	1:B:841:THR:HB	2.34	0.57
1:B:731:VAL:HG22	1:B:750:LEU:CB	2.35	0.57
1:B:797:VAL:HG12	1:B:798:SER:N	2.14	0.57
1:B:921:GLN:HG2	1:B:922:ILE:N	2.20	0.57
1:A:144:ARG:HH12	1:A:175:VAL:HG11	1.70	0.57
1:A:157:GLY:HA2	1:A:160:ASP:CG	2.30	0.57
1:A:175:VAL:HA	1:A:178:ILE:HD12	1.86	0.57
1:A:1208:LYS:HD3	1:A:1208:LYS:C	2.29	0.57
1:B:765:THR:HG23	1:B:766:PHE:N	2.19	0.57
1:B:1149:ASN:OD1	1:B:1209:VAL:HG22	2.05	0.57
1:B:1151:HIS:HA	1:B:1154:ILE:HG13	1.85	0.57
1:A:1043:ARG:NE	1:A:1086:MET:HE3	2.19	0.57
1:A:1092:LEU:HD13	1:A:1100:LEU:CD2	2.34	0.57
1:B:132:TRP:CD2	1:B:183:GLY:HA3	2.40	0.57
1:B:837:ALA:HB1	1:B:982:MET:CE	2.34	0.57
1:B:1014:ILE:HA	1:B:1102:VAL:HG11	1.87	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:56:ALA:O	1:A:59:ILE:HG13	2.04	0.57
1:A:207:GLY:C	1:A:209:LYS:H	2.13	0.57
1:A:238:LYS:HD3	1:A:238:LYS:O	2.03	0.57
1:A:371:ILE:O	1:A:371:ILE:HG22	2.05	0.57
1:A:583:HIS:O	1:A:585:LEU:HD22	2.04	0.57
1:A:612:MET:HA	1:A:619:PHE:HB2	1.86	0.57
1:A:1170:THR:O	1:A:1170:THR:HG22	2.04	0.57
1:B:43:GLY:CA	1:B:46:ASP:HB2	2.35	0.57
1:B:178:ILE:HG12	1:B:358:ALA:HB1	1.85	0.57
1:B:457:ILE:HD11	1:B:462:LEU:HD13	1.87	0.57
1:B:621:LEU:HD22	1:B:621:LEU:H	1.70	0.57
1:B:756:LEU:CD1	1:B:757:ILE:HG12	2.35	0.57
1:A:434:GLN:O	1:A:435:LEU:C	2.46	0.57
1:A:480:ILE:O	1:A:481:ALA:C	2.47	0.57
1:A:765:THR:HG23	1:A:766:PHE:N	2.20	0.57
1:A:1137:SER:HB3	1:A:1140:GLU:HB2	1.85	0.57
1:A:1179:ARG:HH21	1:A:1209:VAL:CG1	2.13	0.57
1:B:118:GLY:O	1:B:121:VAL:N	2.37	0.57
1:B:185:LYS:O	1:B:186:ILE:C	2.46	0.57
1:B:324:ILE:HG13	1:B:326:GLN:CA	2.35	0.57
1:B:470:SER:HA	1:B:551:ASP:HB3	1.85	0.57
1:B:801:ASP:HB3	1:B:1083:TYR:CE2	2.40	0.57
1:B:1142:VAL:HA	1:B:1161:TYR:OH	2.05	0.57
1:A:157:GLY:HA2	1:A:160:ASP:OD2	2.05	0.56
1:A:178:ILE:HG12	1:A:358:ALA:HB1	1.84	0.56
1:A:457:ILE:HD11	1:A:462:LEU:HD13	1.87	0.56
1:A:621:LEU:H	1:A:621:LEU:HD22	1.70	0.56
1:A:806:THR:HG23	1:A:809:ALA:H	1.70	0.56
1:A:1229:ARG:C	1:A:1231:SER:N	2.59	0.56
1:B:186:ILE:HG13	1:B:187:GLY:N	2.20	0.56
1:B:322:TYR:CE2	1:B:324:ILE:CD1	2.88	0.56
1:B:1129:TYR:O	1:B:1131:ASP:N	2.37	0.56
1:A:490:ASP:O	1:A:491:VAL:HB	2.05	0.56
1:A:992:PRO:O	1:A:994:TYR:N	2.37	0.56
1:A:1063:ALA:HB3	1:A:1239:ILE:CA	2.25	0.56
1:B:33:VAL:O	1:B:34:SER:C	2.47	0.56
1:B:57:ALA:O	1:B:60:HIS:N	2.38	0.56
1:B:388:LEU:HB2	1:B:413:VAL:CG1	2.35	0.56
1:B:421:LEU:HD11	1:B:579:ILE:HD11	1.87	0.56
1:B:541:LEU:O	1:B:541:LEU:HD13	2.04	0.56
1:B:612:MET:HA	1:B:619:PHE:HB2	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:752:SER:O	1:B:755:PHE:HB3	2.05	0.56
1:B:777:GLY:CA	1:B:822:LYS:HG3	2.35	0.56
1:A:37:THR:O	1:A:38:MET:C	2.48	0.56
1:A:128:GLN:HG3	1:A:129:VAL:N	2.19	0.56
1:A:278:GLU:HA	1:A:282:ARG:CZ	2.35	0.56
1:A:473:PRO:HB3	1:A:533:GLN:HA	1.87	0.56
1:A:697:LEU:HD12	1:A:697:LEU:C	2.30	0.56
1:A:731:VAL:HG22	1:A:750:LEU:CB	2.34	0.56
1:A:837:ALA:HB1	1:A:982:MET:CE	2.36	0.56
1:A:992:PRO:HB2	1:A:996:LYS:HZ3	1.70	0.56
1:A:1129:TYR:O	1:A:1131:ASP:N	2.39	0.56
1:B:210:LEU:HD13	1:B:210:LEU:C	2.30	0.56
1:B:212:LEU:CD1	1:B:215:LEU:HD12	2.34	0.56
1:B:284:GLY:O	1:B:287:LYS:HB3	2.05	0.56
1:B:358:ALA:O	1:B:362:PHE:CB	2.54	0.56
1:B:379:HIS:HD2	1:B:380:LYS:H	1.53	0.56
1:B:480:ILE:O	1:B:481:ALA:C	2.47	0.56
1:B:790:LYS:HB3	1:B:794:ARG:CZ	2.34	0.56
1:B:825:THR:O	1:B:829:LEU:HG	2.05	0.56
1:B:900:PHE:O	1:B:902:THR:N	2.26	0.56
1:B:1011:THR:N	1:B:1012:PRO:HD2	2.01	0.56
1:B:1092:LEU:HD13	1:B:1100:LEU:CD2	2.34	0.56
1:A:132:TRP:CD2	1:A:183:GLY:HA3	2.41	0.56
1:A:212:LEU:O	1:A:213:VAL:C	2.48	0.56
1:A:270:LEU:HD13	1:A:789:PHE:CZ	2.41	0.56
1:A:279:GLU:HG2	1:A:782:LYS:HZ2	1.69	0.56
1:A:317:VAL:HG12	1:A:317:VAL:O	2.05	0.56
1:A:902:THR:O	1:A:905:SER:N	2.35	0.56
1:B:48:LEU:O	1:B:49:TYR:C	2.46	0.56
1:B:498:LYS:HD3	1:B:498:LYS:C	2.31	0.56
1:B:611:LEU:HB3	1:B:618:TYR:HB3	1.88	0.56
1:A:131:PHE:C	1:A:131:PHE:CD2	2.82	0.56
1:A:199:GLY:O	1:A:203:GLY:HA3	2.05	0.56
1:A:203:GLY:C	1:A:211:THR:OG1	2.49	0.56
1:A:258:ARG:O	1:A:259:THR:C	2.49	0.56
1:A:267:LYS:CA	1:A:270:LEU:HD21	2.36	0.56
1:A:492:THR:C	1:A:494:ASP:N	2.63	0.56
1:A:964:LEU:CD1	1:A:965:MET:H	2.16	0.56
1:A:1101:ASN:O	1:A:1102:VAL:C	2.48	0.56
1:A:1149:ASN:OD1	1:A:1209:VAL:HG22	2.05	0.56
1:A:1214:LEU:HD23	1:A:1218:ARG:HD3	1.87	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1243:GLN:O	1:A:1244:ASN:C	2.48	0.56
1:B:101:ALA:O	1:B:105:GLU:HB2	2.04	0.56
1:B:129:VAL:HB	1:B:935:GLY:HA2	1.88	0.56
1:B:158:TRP:HE1	1:B:900:PHE:HB3	1.69	0.56
1:B:282:ARG:HB3	1:B:778:GLU:OE1	2.06	0.56
1:B:1185:ALA:O	1:B:1190:PRO:HD3	2.04	0.56
1:A:167:LEU:HD23	1:A:167:LEU:C	2.31	0.56
1:A:212:LEU:CD1	1:A:215:LEU:HD12	2.35	0.56
1:B:57:ALA:O	1:B:58:ILE:C	2.49	0.56
1:B:217:ILE:O	1:B:221:LEU:HG	2.05	0.56
1:B:425:SER:HB3	1:B:599:GLY:HA3	1.87	0.56
1:B:779:ILE:HG13	1:B:780:LEU:N	2.20	0.56
1:B:1072:LYS:HB3	1:B:1226:ILE:HD13	1.87	0.56
1:B:1140:GLU:O	1:B:1143:ARG:HB3	2.06	0.56
1:A:449:ILE:O	1:A:450:ASP:C	2.45	0.56
1:A:731:VAL:HA	1:A:750:LEU:HD13	1.87	0.56
1:A:752:SER:O	1:A:755:PHE:HB3	2.06	0.56
1:B:212:LEU:O	1:B:213:VAL:C	2.49	0.56
1:B:278:GLU:HA	1:B:282:ARG:CZ	2.36	0.56
1:B:282:ARG:HB3	1:B:778:GLU:CD	2.31	0.56
1:B:697:LEU:HD12	1:B:697:LEU:C	2.30	0.56
1:B:702:THR:C	1:B:704:TRP:H	2.13	0.56
1:B:847:LEU:C	1:B:849:TYR:N	2.60	0.56
1:B:1120:ASP:HA	1:B:1165:VAL:HG22	1.87	0.56
1:B:1214:LEU:HD23	1:B:1218:ARG:HD3	1.87	0.56
1:A:148:PHE:HB3	1:A:913:GLU:CD	2.31	0.56
1:A:155:GLU:O	1:A:156:ILE:C	2.49	0.56
1:A:777:GLY:CA	1:A:822:LYS:HG3	2.35	0.56
1:B:155:GLU:O	1:B:156:ILE:C	2.48	0.56
1:B:861:VAL:HB	1:B:862:PRO:HD3	1.87	0.56
1:B:962:GLN:O	1:B:963:GLN:HB2	2.06	0.56
1:B:1027:LEU:HD23	1:B:1028:GLU:H	1.71	0.56
1:B:1239:ILE:HD12	1:B:1239:ILE:N	2.20	0.56
1:A:57:ALA:O	1:A:58:ILE:C	2.49	0.56
1:A:153:ASN:HA	1:A:155:GLU:OE2	2.06	0.56
1:A:779:ILE:HG13	1:A:780:LEU:N	2.20	0.56
1:A:1124:ALA:HB2	1:A:1161:TYR:O	2.06	0.56
1:B:306:TYR:CD2	1:B:307:ALA:N	2.74	0.56
1:B:406:LEU:HD23	1:B:431:THR:HG21	1.86	0.56
1:B:490:ASP:O	1:B:491:VAL:HB	2.05	0.56
1:A:101:ALA:O	1:A:105:GLU:HB2	2.06	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:204:PHE:HA	1:A:211:THR:CG2	2.34	0.56
1:A:282:ARG:C	1:A:286:LYS:HD3	2.31	0.56
1:A:358:ALA:O	1:A:362:PHE:CB	2.54	0.56
1:A:857:LEU:CD1	1:A:976:ALA:HB3	2.36	0.56
1:A:1142:VAL:HA	1:A:1161:TYR:OH	2.06	0.56
1:B:214:ILE:HG12	1:B:331:PHE:CZ	2.40	0.56
1:B:311:TRP:HA	1:B:311:TRP:HE3	1.71	0.56
1:B:786:TYR:O	1:B:787:MET:C	2.49	0.56
1:B:1166:GLY:HA3	1:B:1171:GLN:OE1	2.05	0.56
1:B:1172:LEU:HD22	1:B:1176:GLN:HG2	1.88	0.56
1:A:138:ARG:HH22	1:B:515:GLN:HE21	1.53	0.55
1:A:314:THR:O	1:A:315:SER:C	2.48	0.55
1:A:421:LEU:HD11	1:A:579:ILE:HD11	1.88	0.55
1:A:793:LEU:C	1:A:795:GLN:H	2.14	0.55
1:A:862:PRO:O	1:A:866:ILE:HG12	2.06	0.55
1:B:121:VAL:CG2	1:B:122:LEU:N	2.69	0.55
1:B:167:LEU:HD23	1:B:167:LEU:C	2.30	0.55
1:B:959:LEU:HD13	1:B:964:LEU:HG	1.88	0.55
1:A:43:GLY:CA	1:A:46:ASP:HB2	2.37	0.55
1:A:210:LEU:C	1:A:210:LEU:HD13	2.31	0.55
1:A:288:ALA:HA	1:A:291:ALA:CB	2.37	0.55
1:A:288:ALA:CA	1:A:291:ALA:HB3	2.36	0.55
1:A:825:THR:O	1:A:829:LEU:HG	2.06	0.55
1:A:1099:GLN:O	1:A:1099:GLN:HG2	2.06	0.55
1:A:1120:ASP:HA	1:A:1165:VAL:HG22	1.86	0.55
1:A:1207:GLU:O	1:A:1211:GLN:HG2	2.06	0.55
1:B:72:GLY:HA2	1:B:326:GLN:HE21	1.68	0.55
1:B:128:GLN:HG3	1:B:129:VAL:N	2.21	0.55
1:B:207:GLY:CA	1:B:211:THR:H	2.19	0.55
1:B:345:SER:HB3	1:B:346:PRO:HD3	1.86	0.55
1:B:429:LYS:H	1:B:429:LYS:CD	2.07	0.55
1:B:1099:GLN:HG2	1:B:1099:GLN:O	2.05	0.55
1:A:131:PHE:O	1:A:132:TRP:C	2.48	0.55
1:A:322:TYR:CE2	1:A:324:ILE:CD1	2.89	0.55
1:A:788:VAL:O	1:A:791:SER:N	2.40	0.55
1:A:906:LEU:O	1:A:906:LEU:HD23	2.05	0.55
1:A:1145:ALA:HB1	1:A:1154:ILE:HD12	1.88	0.55
1:B:188:MET:HG3	1:B:348:ILE:CD1	2.35	0.55
1:B:201:ILE:HG22	1:B:202:ILE:N	2.21	0.55
1:B:845:ILE:HA	1:B:848:ILE:CG2	2.36	0.55
1:A:470:SER:HA	1:A:551:ASP:HB3	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:899:ASN:OD1	1:A:901:ARG:NH2	2.39	0.55
1:A:1193:LEU:HB2	1:A:1223:CYS:HB2	1.88	0.55
1:A:1199:THR:HG21	1:A:1210:VAL:HG11	1.88	0.55
1:B:459:VAL:O	1:B:462:LEU:HB3	2.06	0.55
1:A:48:LEU:O	1:A:49:TYR:C	2.49	0.55
1:A:133:CYS:O	1:A:135:ALA:N	2.39	0.55
1:A:188:MET:HG3	1:A:348:ILE:CD1	2.35	0.55
1:A:239:GLU:HG3	1:A:288:ALA:HB3	1.89	0.55
1:A:306:TYR:CD2	1:A:307:ALA:N	2.74	0.55
1:A:388:LEU:HB2	1:A:413:VAL:CG1	2.35	0.55
1:A:484:ILE:HG21	1:A:496:ILE:CD1	2.32	0.55
1:A:541:LEU:HD13	1:A:541:LEU:O	2.06	0.55
1:A:817:ASP:OD1	1:A:1000:SER:HB3	2.07	0.55
1:A:921:GLN:HG2	1:A:922:ILE:N	2.21	0.55
1:A:1032:GLN:HB2	1:A:1091:PHE:HB2	1.87	0.55
1:A:1137:SER:O	1:A:1141:ILE:HG23	2.06	0.55
1:B:59:ILE:HG13	1:B:60:HIS:N	2.22	0.55
1:B:106:GLU:HG3	1:B:110:TYR:CE2	2.42	0.55
1:B:144:ARG:HH12	1:B:175:VAL:HG11	1.70	0.55
1:B:1145:ALA:HB2	1:B:1154:ILE:HD12	1.88	0.55
1:A:229:ALA:HA	1:A:295:MET:HE2	1.89	0.55
1:B:131:PHE:C	1:B:131:PHE:HD2	2.15	0.55
1:B:154:GLN:HE21	1:B:157:GLY:HA3	1.71	0.55
1:B:902:THR:O	1:B:905:SER:N	2.36	0.55
1:A:68:MET:HE2	1:A:68:MET:CA	2.37	0.55
1:A:201:ILE:HG22	1:A:202:ILE:N	2.20	0.55
1:A:379:HIS:O	1:A:381:PRO:HD3	2.07	0.55
1:A:461:TYR:O	1:A:465:ILE:HG12	2.06	0.55
1:A:1018:SER:O	1:A:1101:ASN:CB	2.46	0.55
1:B:211:THR:HA	1:B:214:ILE:CD1	2.37	0.55
1:B:311:TRP:HA	1:B:311:TRP:CE3	2.42	0.55
1:B:900:PHE:C	1:B:902:THR:N	2.63	0.55
1:B:1170:THR:O	1:B:1170:THR:HG22	2.06	0.55
1:A:159:PHE:O	1:A:160:ASP:C	2.48	0.55
1:A:214:ILE:CD1	1:A:330:VAL:HB	2.37	0.55
1:A:892:ILE:O	1:A:893:ALA:C	2.49	0.55
1:A:905:SER:C	1:A:907:THR:H	2.14	0.55
1:A:906:LEU:HG	1:A:909:GLU:CD	2.31	0.55
1:B:899:ASN:OD1	1:B:901:ARG:NH2	2.39	0.55
1:B:1056:VAL:CG2	1:B:1062:LEU:HB2	2.37	0.55
1:A:121:VAL:CG2	1:A:122:LEU:N	2.70	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:731:VAL:HA	1:A:750:LEU:CD1	2.36	0.55
1:A:1172:LEU:HD22	1:A:1176:GLN:HG2	1.89	0.55
1:B:131:PHE:O	1:B:132:TRP:C	2.49	0.55
1:B:409:LEU:HD21	1:B:602:ILE:HB	1.88	0.55
1:B:543:ARG:NH2	1:B:905:SER:O	2.40	0.55
1:B:708:VAL:HG13	1:B:709:VAL:N	2.21	0.55
1:B:713:CYS:SG	1:B:768:LEU:HD11	2.47	0.55
1:B:780:LEU:C	1:B:784:LEU:HD23	2.32	0.55
1:B:849:TYR:CB	1:B:854:THR:OG1	2.55	0.55
1:B:902:THR:HG23	1:B:903:VAL:H	1.72	0.55
1:A:311:TRP:CE3	1:A:311:TRP:HA	2.42	0.55
1:A:546:LYS:O	1:A:577:THR:HG23	2.06	0.55
1:A:856:LEU:O	1:A:859:ALA:HB3	2.07	0.55
1:B:328:LEU:O	1:B:332:PHE:HB3	2.07	0.55
1:B:482:GLU:O	1:B:483:ASN:C	2.48	0.55
1:B:566:GLN:HA	1:B:569:LEU:HD12	1.89	0.55
1:B:688:VAL:HG23	1:B:688:VAL:O	2.06	0.55
1:B:722:PRO:HG2	1:B:841:THR:HB	1.87	0.55
1:B:862:PRO:O	1:B:866:ILE:HG12	2.07	0.55
1:B:906:LEU:HG	1:B:909:GLU:CD	2.31	0.55
1:A:35:VAL:HG12	1:A:359:TYR:CZ	2.42	0.54
1:A:245:LYS:HA	1:A:245:LYS:NZ	2.21	0.54
1:A:286:LYS:HE3	1:A:822:LYS:NZ	2.22	0.54
1:A:374:PHE:HE2	1:A:376:LYS:CB	2.20	0.54
1:A:930:LYS:O	1:A:933:VAL:HB	2.07	0.54
1:A:994:TYR:O	1:A:994:TYR:HD1	1.90	0.54
1:B:64:LEU:HD11	1:B:945:MET:CE	2.35	0.54
1:B:171:LEU:HD13	1:B:172:THR:N	2.21	0.54
1:B:727:ILE:HD12	1:B:754:LEU:CA	2.37	0.54
1:A:171:LEU:HD13	1:A:172:THR:N	2.21	0.54
1:A:182:ILE:O	1:A:185:LYS:HB3	2.06	0.54
1:A:548:LEU:HD22	1:A:550:LEU:CD1	2.38	0.54
1:A:801:ASP:HB3	1:A:1083:TYR:CZ	2.42	0.54
1:A:1037:VAL:O	1:A:1037:VAL:HG23	2.08	0.54
1:A:1239:ILE:N	1:A:1239:ILE:HD12	2.22	0.54
1:B:41:TYR:O	1:B:42:ALA:HB3	2.05	0.54
1:B:86:LYS:HE2	1:B:739:GLY:HA2	1.89	0.54
1:B:189:PHE:O	1:B:190:PHE:C	2.51	0.54
1:B:548:LEU:HD22	1:B:550:LEU:CD1	2.37	0.54
1:B:1092:LEU:HD23	1:B:1093:ASP:H	1.72	0.54
1:B:1199:THR:HG21	1:B:1210:VAL:HG11	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:106:GLU:HG3	1:A:110:TYR:CE2	2.42	0.54
1:A:447:VAL:HG13	1:A:454:ILE:HG21	1.90	0.54
1:A:708:VAL:HG13	1:A:709:VAL:N	2.22	0.54
1:A:722:PRO:HA	1:A:979:PHE:HZ	1.72	0.54
1:A:812:THR:HG22	1:A:816:ASN:ND2	2.19	0.54
1:A:961:THR:O	1:A:962:GLN:HB3	2.08	0.54
1:B:129:VAL:CB	1:B:935:GLY:HA2	2.37	0.54
1:B:157:GLY:HA2	1:B:160:ASP:OD2	2.07	0.54
1:B:731:VAL:HA	1:B:750:LEU:HD13	1.89	0.54
1:A:217:ILE:O	1:A:221:LEU:HG	2.08	0.54
1:A:254:LEU:HD23	1:A:811:THR:CG2	2.38	0.54
1:A:282:ARG:N	1:A:282:ARG:HH11	2.04	0.54
1:A:478:THR:HG22	1:A:479:THR:N	2.17	0.54
1:A:778:GLU:O	1:A:779:ILE:C	2.49	0.54
1:A:811:THR:CA	1:A:814:LEU:HD23	2.37	0.54
1:B:905:SER:HB2	1:B:908:ARG:NH1	2.21	0.54
1:B:1204:THR:HG23	1:B:1205:GLU:N	2.21	0.54
1:A:110:TYR:HA	1:A:113:TYR:CD2	2.34	0.54
1:A:118:GLY:O	1:A:121:VAL:N	2.40	0.54
1:A:131:PHE:C	1:A:131:PHE:HD2	2.16	0.54
1:A:211:THR:HA	1:A:214:ILE:CD1	2.37	0.54
1:A:215:LEU:O	1:A:219:PRO:CD	2.56	0.54
1:A:434:GLN:O	1:A:436:MET:N	2.41	0.54
1:B:39:PHE:CD2	1:B:355:ARG:HA	2.42	0.54
1:B:900:PHE:C	1:B:900:PHE:CD1	2.85	0.54
1:B:905:SER:O	1:B:907:THR:N	2.39	0.54
1:B:1064:LEU:HD12	1:B:1226:ILE:HB	1.90	0.54
1:A:45:LEU:HD22	1:A:45:LEU:N	2.22	0.54
1:A:311:TRP:HA	1:A:311:TRP:HE3	1.71	0.54
1:A:328:LEU:O	1:A:332:PHE:HB3	2.08	0.54
1:A:777:GLY:HA2	1:A:822:LYS:HG3	1.90	0.54
1:A:900:PHE:C	1:A:902:THR:N	2.61	0.54
1:A:1052:LEU:HG	1:A:1053:SER:N	2.22	0.54
1:A:1078:LEU:C	1:A:1081:ARG:H	2.15	0.54
1:B:171:LEU:O	1:B:175:VAL:HG12	2.08	0.54
1:B:447:VAL:HG13	1:B:454:ILE:HG21	1.88	0.54
1:B:1246:LYS:HD2	1:B:1246:LYS:H	1.72	0.54
1:A:138:ARG:HH22	1:B:515:GLN:NE2	2.06	0.54
1:A:291:ALA:HA	1:A:294:SER:CB	2.37	0.54
1:A:315:SER:CA	1:A:747:ASN:HD22	2.21	0.54
1:A:507:ASP:O	1:A:510:MET:N	2.39	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:703:GLU:HG2	1:A:784:LEU:HD21	1.90	0.54
1:A:827:SER:O	1:A:831:VAL:HG23	2.08	0.54
1:A:921:GLN:HG2	1:A:922:ILE:CD1	2.37	0.54
1:B:35:VAL:HG12	1:B:359:TYR:CZ	2.42	0.54
1:B:129:VAL:HG11	1:B:935:GLY:N	2.22	0.54
1:B:215:LEU:CA	1:B:219:PRO:HD2	2.38	0.54
1:B:1193:LEU:HB2	1:B:1223:CYS:HB2	1.90	0.54
1:A:39:PHE:CD2	1:A:355:ARG:HA	2.42	0.54
1:A:69:LEU:O	1:A:72:GLY:N	2.40	0.54
1:A:315:SER:CB	1:A:747:ASN:HD22	2.21	0.54
1:B:288:ALA:HA	1:B:291:ALA:CB	2.38	0.54
1:B:730:LYS:HG2	1:B:750:LEU:HD22	1.90	0.54
1:B:731:VAL:HA	1:B:750:LEU:CD1	2.38	0.54
1:B:893:ALA:O	1:B:897:ILE:HG12	2.07	0.54
1:B:921:GLN:HG2	1:B:922:ILE:CD1	2.38	0.54
1:B:1207:GLU:O	1:B:1211:GLN:HG2	2.08	0.54
1:B:1214:LEU:HD23	1:B:1214:LEU:O	2.08	0.54
1:A:171:LEU:HD13	1:A:171:LEU:C	2.33	0.54
1:A:1050:GLN:HG2	1:A:1245:GLY:HA3	1.89	0.54
1:A:1166:GLY:HA3	1:A:1171:GLN:OE1	2.07	0.54
1:B:352:ALA:O	1:B:355:ARG:HB3	2.08	0.54
1:B:492:THR:C	1:B:494:ASP:N	2.64	0.54
1:B:812:THR:HG22	1:B:816:ASN:ND2	2.19	0.54
1:B:835:ASN:O	1:B:836:ILE:C	2.50	0.54
1:B:992:PRO:HB2	1:B:996:LYS:CE	2.38	0.54
1:B:1193:LEU:HD11	1:B:1217:ALA:O	2.08	0.54
1:B:1202:LEU:CG	1:B:1203:ASP:H	2.12	0.54
1:A:936:ILE:HG23	1:A:937:THR:N	2.23	0.54
1:A:962:GLN:O	1:A:963:GLN:HB2	2.06	0.54
1:A:1056:VAL:CG2	1:A:1062:LEU:HB2	2.37	0.54
1:B:65:PRO:O	1:B:66:LEU:C	2.50	0.54
1:B:171:LEU:HD13	1:B:171:LEU:C	2.32	0.54
1:B:182:ILE:O	1:B:185:LYS:HB3	2.07	0.54
1:B:546:LYS:O	1:B:577:THR:HG23	2.08	0.54
1:B:722:PRO:HA	1:B:979:PHE:HZ	1.73	0.54
1:B:741:PRO:O	1:B:742:GLU:HB2	2.07	0.54
1:B:843:ILE:HA	1:B:846:SER:HB2	1.90	0.54
1:B:906:LEU:HD23	1:B:906:LEU:O	2.08	0.54
1:A:713:CYS:SG	1:A:768:LEU:HD11	2.47	0.53
1:A:992:PRO:HB2	1:A:996:LYS:CE	2.38	0.53
1:A:1023:LYS:HG3	1:A:1026:MET:CG	2.38	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:214:ILE:HG12	1:B:331:PHE:CE1	2.43	0.53
1:B:239:GLU:HG3	1:B:288:ALA:HB3	1.88	0.53
1:B:285:ILE:CG2	1:B:286:LYS:HD2	2.38	0.53
1:B:419:VAL:CG2	1:B:593:VAL:HG13	2.38	0.53
1:B:479:THR:HA	1:B:518:THR:O	2.08	0.53
1:B:589:ARG:C	1:B:591:ALA:N	2.65	0.53
1:B:695:ARG:HD3	1:B:699:LEU:HD23	1.90	0.53
1:B:703:GLU:HG2	1:B:784:LEU:HD21	1.90	0.53
1:B:765:THR:O	1:B:768:LEU:HG	2.08	0.53
1:B:817:ASP:OD1	1:B:1000:SER:HB3	2.08	0.53
1:B:827:SER:HG	1:B:994:TYR:HD2	1.56	0.53
1:A:188:MET:HG3	1:A:348:ILE:HD13	1.90	0.53
1:A:248:ALA:C	1:A:250:ALA:H	2.14	0.53
1:A:318:ILE:HG13	1:A:735:PHE:CZ	2.43	0.53
1:A:429:LYS:HB3	1:A:581:ILE:HD13	1.89	0.53
1:A:902:THR:HG23	1:A:903:VAL:H	1.72	0.53
1:B:505:ALA:O	1:B:509:ILE:HG23	2.08	0.53
1:B:561:SER:O	1:B:565:VAL:HG23	2.08	0.53
1:B:729:SER:HA	1:B:971:LEU:HB3	1.90	0.53
1:A:57:ALA:O	1:A:60:HIS:N	2.41	0.53
1:A:171:LEU:O	1:A:175:VAL:HG12	2.09	0.53
1:A:519:LEU:HD11	1:B:925:ARG:HD3	1.88	0.53
1:A:905:SER:HB2	1:A:908:ARG:NH1	2.23	0.53
1:A:921:GLN:OE1	1:B:479:THR:HG21	2.08	0.53
1:A:990:PHE:O	1:A:991:ALA:O	2.26	0.53
1:B:158:TRP:CD1	1:B:158:TRP:C	2.86	0.53
1:B:972:LEU:N	1:B:972:LEU:CD1	2.71	0.53
1:B:1261:GLY:H	1:B:1264:PHE:CB	2.12	0.53
1:A:99:MET:HB3	1:A:960:VAL:O	2.07	0.53
1:A:121:VAL:O	1:A:122:LEU:C	2.51	0.53
1:A:370:SER:O	1:A:371:ILE:HB	2.08	0.53
1:A:422:VAL:HG22	1:A:595:ALA:O	2.08	0.53
1:A:780:LEU:C	1:A:784:LEU:HD23	2.33	0.53
1:A:846:SER:HA	1:A:849:TYR:CG	2.43	0.53
1:B:282:ARG:N	1:B:282:ARG:HH11	2.06	0.53
1:B:484:ILE:HG21	1:B:496:ILE:CD1	2.32	0.53
1:B:885:GLU:HB3	1:B:923:PRO:HG3	1.90	0.53
1:B:905:SER:C	1:B:907:THR:H	2.17	0.53
1:A:38:MET:O	1:A:41:TYR:HB3	2.08	0.53
1:A:154:GLN:HE21	1:A:157:GLY:HA3	1.73	0.53
1:A:376:LYS:HD2	1:A:376:LYS:C	2.33	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:422:VAL:O	1:A:597:PHE:HB2	2.08	0.53
1:A:1032:GLN:HE21	1:A:1055:GLU:HG3	1.71	0.53
1:A:1076:VAL:CG1	1:A:1194:LEU:HD13	2.39	0.53
1:B:188:MET:SD	1:B:188:MET:C	2.92	0.53
1:B:696:ILE:O	1:B:700:ASN:HB2	2.08	0.53
1:B:709:VAL:HG13	1:B:710:GLY:N	2.24	0.53
1:B:934:PHE:O	1:B:935:GLY:C	2.48	0.53
1:B:969:ASN:HD22	1:B:969:ASN:C	2.16	0.53
1:A:184:ASP:O	1:A:187:GLY:N	2.41	0.53
1:A:368:LYS:O	1:A:369:PRO:C	2.51	0.53
1:A:881:LYS:O	1:A:884:LYS:HB2	2.08	0.53
1:A:1014:ILE:HB	1:A:1102:VAL:HG21	1.91	0.53
1:A:1064:LEU:HB3	1:A:1226:ILE:HG22	1.91	0.53
1:B:86:LYS:HE2	1:B:738:GLY:C	2.33	0.53
1:B:215:LEU:HA	1:B:219:PRO:HD2	1.89	0.53
1:B:374:PHE:CD1	1:B:375:SER:N	2.74	0.53
1:B:811:THR:CA	1:B:814:LEU:HD23	2.38	0.53
1:A:51:LEU:O	1:A:52:VAL:C	2.52	0.53
1:A:212:LEU:C	1:A:214:ILE:N	2.65	0.53
1:A:696:ILE:O	1:A:700:ASN:HB2	2.09	0.53
1:A:785:ARG:O	1:A:786:TYR:C	2.52	0.53
1:A:800:PHE:HA	1:A:803:PRO:HB3	1.90	0.53
1:A:1204:THR:OG1	1:A:1205:GLU:N	2.42	0.53
1:B:45:LEU:HD22	1:B:45:LEU:N	2.23	0.53
1:B:133:CYS:O	1:B:135:ALA:N	2.41	0.53
1:B:307:ALA:CB	1:B:754:LEU:HD22	2.39	0.53
1:B:324:ILE:HD11	1:B:327:VAL:HG13	1.90	0.53
1:B:692:SER:HB2	1:B:695:ARG:CB	2.39	0.53
1:B:846:SER:HA	1:B:849:TYR:CG	2.44	0.53
1:B:1052:LEU:HG	1:B:1053:SER:N	2.23	0.53
1:A:68:MET:O	1:A:329:THR:HG23	2.08	0.53
1:A:795:GLN:HE21	1:A:796:ASP:H	1.56	0.53
1:B:144:ARG:O	1:B:145:GLN:C	2.50	0.53
1:B:381:PRO:HD2	1:B:461:TYR:CD2	2.44	0.53
1:B:684:LEU:HD23	1:B:684:LEU:N	2.23	0.53
1:B:881:LYS:HB2	1:B:881:LYS:NZ	2.24	0.53
1:B:906:LEU:C	1:B:908:ARG:HD2	2.34	0.53
1:B:936:ILE:HG23	1:B:937:THR:N	2.24	0.53
1:B:969:ASN:O	1:B:972:LEU:N	2.40	0.53
1:B:1057:LYS:H	1:B:1057:LYS:HD2	1.73	0.53
1:B:1064:LEU:HB3	1:B:1226:ILE:HG22	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:144:ARG:O	1:A:145:GLN:C	2.52	0.53
1:A:721:GLN:O	1:A:722:PRO:C	2.51	0.53
1:A:730:LYS:HG2	1:A:750:LEU:HD22	1.90	0.53
1:A:741:PRO:O	1:A:742:GLU:HB2	2.09	0.53
1:A:861:VAL:O	1:A:862:PRO:C	2.51	0.53
1:A:1076:VAL:HG11	1:A:1111:ILE:HD13	1.90	0.53
1:A:1234:GLN:HG2	1:A:1253:HIS:CD2	2.44	0.53
1:B:69:LEU:O	1:B:72:GLY:N	2.42	0.53
1:B:217:ILE:HD11	1:B:331:PHE:CE2	2.44	0.53
1:B:793:LEU:C	1:B:795:GLN:H	2.17	0.53
1:B:1038:PHE:HB2	1:B:1085:PRO:HA	1.90	0.53
1:B:1179:ARG:HH21	1:B:1209:VAL:CG1	2.14	0.53
1:B:1260:LYS:H	1:B:1260:LYS:CD	2.20	0.53
1:A:158:TRP:C	1:A:158:TRP:CD1	2.87	0.53
1:A:189:PHE:O	1:A:190:PHE:C	2.52	0.53
1:A:203:GLY:O	1:A:215:LEU:HD21	2.08	0.53
1:A:215:LEU:CA	1:A:219:PRO:HD2	2.39	0.53
1:A:215:LEU:HA	1:A:219:PRO:HD2	1.91	0.53
1:A:267:LYS:HB3	1:A:790:LYS:NZ	2.24	0.53
1:A:308:LEU:HA	1:A:751:PHE:CD2	2.44	0.53
1:A:395:PHE:HB3	1:A:406:LEU:HB2	1.91	0.53
1:A:409:LEU:HD21	1:A:602:ILE:HB	1.89	0.53
1:A:702:THR:C	1:A:704:TRP:N	2.66	0.53
1:A:934:PHE:O	1:A:935:GLY:C	2.51	0.53
1:A:978:VAL:O	1:A:981:ALA:HB3	2.08	0.53
1:A:1064:LEU:CD1	1:A:1072:LYS:HG2	2.39	0.53
1:B:38:MET:O	1:B:39:PHE:C	2.52	0.53
1:B:153:ASN:HA	1:B:155:GLU:OE2	2.09	0.53
1:B:246:ALA:CB	1:B:277:LEU:HB3	2.38	0.53
1:B:297:ALA:HB1	1:B:763:PHE:CD2	2.43	0.53
1:B:316:LEU:C	1:B:318:ILE:H	2.17	0.53
1:B:881:LYS:O	1:B:884:LYS:HB2	2.09	0.53
1:A:188:MET:SD	1:A:188:MET:C	2.92	0.52
1:A:223:LEU:O	1:A:227:ILE:HG13	2.09	0.52
1:A:385:GLN:HE21	1:A:386:GLY:N	2.06	0.52
1:A:722:PRO:HG3	1:A:979:PHE:CE1	2.44	0.52
1:A:749:ASN:C	1:A:749:ASN:ND2	2.67	0.52
1:A:765:THR:O	1:A:768:LEU:HG	2.09	0.52
1:A:899:ASN:O	1:A:902:THR:HG22	2.10	0.52
1:A:1193:LEU:HD11	1:A:1217:ALA:O	2.08	0.52
1:A:1199:THR:HG23	1:A:1210:VAL:HG11	1.90	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:722:PRO:HG3	1:B:979:PHE:CE1	2.44	0.52
1:B:992:PRO:O	1:B:994:TYR:N	2.42	0.52
1:B:1032:GLN:HE21	1:B:1055:GLU:HG3	1.72	0.52
1:A:283:LEU:HD12	1:A:284:GLY:N	2.24	0.52
1:A:1064:LEU:HD12	1:A:1226:ILE:HB	1.89	0.52
1:A:1246:LYS:HD2	1:A:1246:LYS:H	1.74	0.52
1:B:215:LEU:O	1:B:219:PRO:CD	2.55	0.52
1:B:288:ALA:CA	1:B:291:ALA:HB3	2.37	0.52
1:B:422:VAL:HG22	1:B:595:ALA:O	2.08	0.52
1:B:532:LYS:O	1:B:533:GLN:C	2.52	0.52
1:A:324:ILE:HG12	1:A:326:GLN:H	1.74	0.52
1:A:566:GLN:HA	1:A:569:LEU:HD12	1.91	0.52
1:A:729:SER:HA	1:A:971:LEU:HB3	1.90	0.52
1:A:773:PHE:CD1	1:A:773:PHE:C	2.87	0.52
1:A:835:ASN:O	1:A:836:ILE:C	2.52	0.52
1:A:972:LEU:N	1:A:972:LEU:CD1	2.72	0.52
1:A:1104:TRP:CD1	1:A:1108:GLN:HE22	2.27	0.52
1:B:231:ILE:HG22	1:B:232:LEU:HD22	1.91	0.52
1:B:297:ALA:HB1	1:B:763:PHE:HA	1.90	0.52
1:B:308:LEU:HD13	1:B:755:PHE:CE1	2.45	0.52
1:B:461:TYR:O	1:B:465:ILE:HG12	2.08	0.52
1:B:478:THR:HG22	1:B:479:THR:N	2.18	0.52
1:B:543:ARG:HH12	1:B:905:SER:HB3	1.73	0.52
1:B:824:ALA:O	1:B:828:ARG:HG2	2.10	0.52
1:B:1118:LEU:O	1:B:1118:LEU:HD12	2.10	0.52
1:B:1270:GLN:HG2	1:B:1271:ALA:N	2.25	0.52
1:A:45:LEU:H	1:A:45:LEU:CD2	2.22	0.52
1:A:124:VAL:HG23	1:A:125:ALA:N	2.25	0.52
1:A:847:LEU:C	1:A:849:TYR:N	2.63	0.52
1:A:1206:SER:O	1:A:1210:VAL:HG23	2.10	0.52
1:B:197:PHE:O	1:B:201:ILE:HG12	2.09	0.52
1:B:397:TYR:HB3	1:B:398:PRO:HD2	1.91	0.52
1:B:449:ILE:HD13	1:B:449:ILE:C	2.34	0.52
1:B:538:ALA:O	1:B:539:ARG:C	2.53	0.52
1:B:795:GLN:HE21	1:B:796:ASP:H	1.57	0.52
1:B:899:ASN:HA	1:B:901:ARG:NH1	2.25	0.52
1:B:990:PHE:O	1:B:991:ALA:O	2.27	0.52
1:B:1124:ALA:HB2	1:B:1161:TYR:O	2.09	0.52
1:B:1144:ALA:CA	1:B:1186:LEU:HD11	2.30	0.52
1:A:430:SER:O	1:A:431:THR:C	2.52	0.52
1:A:709:VAL:HG13	1:A:710:GLY:N	2.24	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:800:PHE:C	1:A:803:PRO:HD3	2.31	0.52
1:A:1031:VAL:HB	1:A:1056:VAL:HG12	1.91	0.52
1:A:1038:PHE:HB2	1:A:1085:PRO:HA	1.91	0.52
1:B:111:ALA:HA	1:B:114:TYR:HE1	1.73	0.52
1:B:282:ARG:C	1:B:286:LYS:HD3	2.35	0.52
1:B:504:ASN:OD1	1:B:568:ALA:HB2	2.09	0.52
1:B:539:ARG:O	1:B:540:ALA:C	2.52	0.52
1:B:780:LEU:O	1:B:784:LEU:HB2	2.09	0.52
1:B:1050:GLN:HG2	1:B:1245:GLY:HA3	1.91	0.52
1:A:504:ASN:OD1	1:A:568:ALA:HB2	2.10	0.52
1:A:523:ARG:CD	1:A:524:GLY:N	2.65	0.52
1:A:1032:GLN:O	1:A:1090:VAL:HA	2.10	0.52
1:B:157:GLY:HA2	1:B:160:ASP:CG	2.34	0.52
1:B:188:MET:HG3	1:B:348:ILE:HD13	1.90	0.52
1:B:191:GLN:O	1:B:192:ALA:C	2.53	0.52
1:B:229:ALA:HA	1:B:295:MET:HE2	1.90	0.52
1:B:258:ARG:O	1:B:259:THR:C	2.52	0.52
1:B:702:THR:C	1:B:704:TRP:N	2.67	0.52
1:B:901:ARG:HD3	1:B:901:ARG:N	2.24	0.52
1:B:1037:VAL:HG23	1:B:1037:VAL:O	2.08	0.52
1:B:1076:VAL:CG1	1:B:1194:LEU:HD13	2.39	0.52
1:B:1234:GLN:HG2	1:B:1253:HIS:CD2	2.44	0.52
1:A:182:ILE:O	1:A:185:LYS:HE3	2.10	0.52
1:A:269:GLU:O	1:A:270:LEU:C	2.52	0.52
1:A:594:ILE:O	1:A:605:GLN:HA	2.09	0.52
1:A:769:GLN:HG3	1:A:773:PHE:CE2	2.43	0.52
1:A:791:SER:CA	1:A:1010:LYS:HE2	2.34	0.52
1:A:1092:LEU:HD23	1:A:1093:ASP:H	1.74	0.52
1:A:1118:LEU:HD12	1:A:1118:LEU:O	2.10	0.52
1:B:121:VAL:O	1:B:122:LEU:C	2.51	0.52
1:B:318:ILE:CG1	1:B:325:GLY:H	2.22	0.52
1:B:712:PHE:O	1:B:715:ILE:N	2.42	0.52
1:B:1067:SER:O	1:B:1068:SER:HB2	2.09	0.52
1:B:1214:LEU:HD23	1:B:1214:LEU:C	2.34	0.52
1:A:59:ILE:HG13	1:A:60:HIS:N	2.24	0.52
1:A:191:GLN:O	1:A:192:ALA:C	2.53	0.52
1:A:231:ILE:HG22	1:A:232:LEU:HD22	1.92	0.52
1:A:288:ALA:C	1:A:291:ALA:HB3	2.35	0.52
1:A:362:PHE:O	1:A:365:ILE:HB	2.10	0.52
1:A:702:THR:HB	1:A:703:GLU:OE1	2.10	0.52
1:A:821:VAL:O	1:A:822:LYS:C	2.52	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:994:TYR:O	1:A:994:TYR:CD1	2.63	0.52
1:A:1202:LEU:HD21	1:A:1206:SER:CB	2.37	0.52
1:A:1267:VAL:HG13	1:A:1270:GLN:OE1	2.10	0.52
1:B:64:LEU:HD22	1:B:64:LEU:N	2.25	0.52
1:B:970:VAL:CG2	1:B:971:LEU:HD22	2.40	0.52
1:B:1023:LYS:C	1:B:1025:ASN:H	2.18	0.52
1:B:1064:LEU:CD1	1:B:1072:LYS:HG2	2.39	0.52
1:A:419:VAL:CG2	1:A:593:VAL:HG13	2.38	0.52
1:A:900:PHE:C	1:A:900:PHE:CD1	2.88	0.52
1:B:50:MET:HG3	1:B:131:PHE:CE2	2.45	0.52
1:B:111:ALA:HA	1:B:114:TYR:CE1	2.45	0.52
1:B:291:ALA:HA	1:B:294:SER:CB	2.38	0.52
1:B:336:ILE:HD12	2:B:6004:2J8:SE3	2.60	0.52
1:B:1057:LYS:HD2	1:B:1057:LYS:N	2.25	0.52
1:B:1076:VAL:HG11	1:B:1111:ILE:HD13	1.90	0.52
1:B:1101:ASN:O	1:B:1102:VAL:C	2.53	0.52
1:A:397:TYR:HB3	1:A:398:PRO:HD2	1.92	0.52
1:A:453:ASP:HB3	1:A:456:THR:CG2	2.40	0.52
1:A:539:ARG:O	1:A:540:ALA:C	2.52	0.52
1:A:784:LEU:O	1:A:785:ARG:C	2.53	0.52
1:A:786:TYR:O	1:A:787:MET:C	2.52	0.52
1:A:1088:GLY:O	1:A:1089:SER:HB2	2.10	0.52
1:A:1140:GLU:O	1:A:1143:ARG:HB3	2.10	0.52
1:B:38:MET:O	1:B:41:TYR:HB3	2.08	0.52
1:B:51:LEU:O	1:B:52:VAL:C	2.52	0.52
1:B:211:THR:HA	1:B:214:ILE:HD12	1.92	0.52
1:B:362:PHE:O	1:B:365:ILE:HB	2.10	0.52
1:B:813:ARG:HD3	1:B:817:ASP:OD2	2.10	0.52
1:A:50:MET:HG3	1:A:131:PHE:CE2	2.45	0.51
1:A:263:PHE:HE1	1:A:1129:TYR:HB3	1.74	0.51
1:A:278:GLU:HA	1:A:282:ARG:NH2	2.24	0.51
1:A:459:VAL:O	1:A:462:LEU:HB3	2.10	0.51
1:A:540:ALA:O	1:A:543:ARG:CB	2.58	0.51
1:A:552:GLU:HB3	1:A:555:SER:OG	2.10	0.51
1:A:686:GLU:CG	1:A:813:ARG:HH22	2.13	0.51
1:A:813:ARG:HD3	1:A:817:ASP:OD2	2.11	0.51
1:A:843:ILE:HA	1:A:846:SER:HB2	1.92	0.51
1:A:957:ALA:O	1:A:960:VAL:HG13	2.10	0.51
1:A:1020:GLN:NE2	1:A:1022:LEU:N	2.58	0.51
1:A:1132:ASN:OD1	1:A:1134:ARG:HG2	2.10	0.51
1:B:321:GLU:O	1:B:322:TYR:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:336:ILE:CD1	2:B:6004:2J8:SE3	3.09	0.51
1:B:353:ASN:O	1:B:354:ALA:C	2.53	0.51
1:B:395:PHE:HB3	1:B:406:LEU:HB2	1.91	0.51
1:B:463:ARG:HH11	1:B:463:ARG:HG3	1.76	0.51
1:B:861:VAL:O	1:B:862:PRO:C	2.50	0.51
1:B:1267:VAL:HG13	1:B:1270:GLN:OE1	2.10	0.51
1:B:53:GLY:HA2	1:B:127:ILE:HG22	1.92	0.51
1:B:68:MET:O	1:B:329:THR:HG23	2.11	0.51
1:B:184:ASP:O	1:B:187:GLY:N	2.43	0.51
1:B:185:LYS:HZ2	1:B:186:ILE:CA	2.23	0.51
1:B:278:GLU:O	1:B:279:GLU:C	2.53	0.51
1:B:360:GLU:O	1:B:363:LYS:HB2	2.10	0.51
1:B:469:VAL:HG12	1:B:553:ALA:HB2	1.91	0.51
1:B:892:ILE:O	1:B:893:ALA:C	2.53	0.51
1:B:976:ALA:HA	1:B:979:PHE:HD2	1.75	0.51
1:B:1023:LYS:HB3	1:B:1026:MET:CG	2.38	0.51
1:A:156:ILE:HG23	1:A:439:LEU:HD12	1.91	0.51
1:A:695:ARG:HD3	1:A:699:LEU:HD23	1.91	0.51
1:A:976:ALA:HA	1:A:979:PHE:HD2	1.74	0.51
1:A:1019:THR:HB	1:A:1099:GLN:O	2.09	0.51
1:A:1079:LEU:C	1:A:1081:ARG:H	2.17	0.51
1:A:1249:GLU:CD	1:A:1262:ILE:HB	2.35	0.51
1:B:55:LEU:HD23	1:B:55:LEU:C	2.35	0.51
1:B:106:GLU:HG3	1:B:110:TYR:CZ	2.45	0.51
1:B:125:ALA:O	1:B:128:GLN:HG2	2.11	0.51
1:B:384:ILE:CG2	1:B:385:GLN:N	2.72	0.51
1:B:551:ASP:HA	1:B:581:ILE:CG2	2.40	0.51
1:B:702:THR:O	1:B:704:TRP:N	2.43	0.51
1:B:730:LYS:HG2	1:B:750:LEU:CD2	2.40	0.51
1:B:773:PHE:CD1	1:B:773:PHE:C	2.88	0.51
1:B:800:PHE:C	1:B:803:PRO:HD3	2.35	0.51
1:B:899:ASN:O	1:B:902:THR:HG22	2.11	0.51
1:B:905:SER:OG	1:B:908:ARG:NH2	2.43	0.51
1:B:1104:TRP:CD1	1:B:1108:GLN:HE22	2.28	0.51
1:B:1154:ILE:CD1	1:B:1161:TYR:CE2	2.93	0.51
1:B:1173:SER:HB3	1:B:1176:GLN:NE2	2.25	0.51
1:A:62:VAL:C	1:A:65:PRO:HD2	2.35	0.51
1:A:70:ILE:O	1:A:74:MET:HG2	2.11	0.51
1:A:285:ILE:CG2	1:A:286:LYS:HD2	2.40	0.51
1:A:845:ILE:HA	1:A:848:ILE:CG2	2.40	0.51
1:A:853:LEU:CG	1:A:973:VAL:HG22	2.38	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:885:GLU:HB3	1:A:923:PRO:HG3	1.92	0.51
1:A:916:TYR:O	1:A:920:LEU:HD23	2.11	0.51
1:A:970:VAL:O	1:A:973:VAL:CB	2.58	0.51
1:A:1122:SER:O	1:A:1125:GLU:HB2	2.11	0.51
1:B:45:LEU:H	1:B:45:LEU:CD2	2.23	0.51
1:B:81:VAL:HG22	1:B:102:LYS:HG3	1.93	0.51
1:B:232:LEU:HD22	1:B:232:LEU:N	2.26	0.51
1:B:260:VAL:O	1:B:263:PHE:HB3	2.09	0.51
1:B:1127:ILE:C	1:B:1129:TYR:H	2.17	0.51
1:A:41:TYR:O	1:A:42:ALA:HB3	2.10	0.51
1:A:106:GLU:HG3	1:A:110:TYR:CZ	2.46	0.51
1:A:131:PHE:CZ	1:A:185:LYS:NZ	2.75	0.51
1:A:133:CYS:SG	1:A:931:ALA:HA	2.51	0.51
1:A:135:ALA:O	1:A:136:ALA:C	2.53	0.51
1:A:460:ARG:O	1:A:461:TYR:C	2.53	0.51
1:A:730:LYS:HG2	1:A:750:LEU:CD2	2.41	0.51
1:A:907:THR:C	1:A:908:ARG:NE	2.60	0.51
1:A:992:PRO:C	1:A:994:TYR:N	2.68	0.51
1:A:1067:SER:O	1:A:1068:SER:HB2	2.10	0.51
1:A:1173:SER:HB3	1:A:1176:GLN:NE2	2.25	0.51
1:B:51:LEU:O	1:B:54:THR:HB	2.10	0.51
1:B:278:GLU:HA	1:B:282:ARG:NH2	2.26	0.51
1:B:342:GLY:O	1:B:345:SER:N	2.43	0.51
1:B:348:ILE:O	1:B:349:GLU:C	2.52	0.51
1:B:534:ARG:O	1:B:537:ILE:HB	2.10	0.51
1:B:721:GLN:O	1:B:722:PRO:C	2.51	0.51
1:A:59:ILE:C	1:A:59:ILE:HD12	2.36	0.51
1:A:65:PRO:O	1:A:66:LEU:C	2.53	0.51
1:A:136:ALA:CB	1:A:182:ILE:HB	2.38	0.51
1:A:210:LEU:C	1:A:212:LEU:N	2.65	0.51
1:A:425:SER:HB3	1:A:599:GLY:CA	2.40	0.51
1:A:711:ILE:CD1	1:A:832:ILE:HD13	2.40	0.51
1:A:824:ALA:O	1:A:828:ARG:HG2	2.09	0.51
1:A:905:SER:OG	1:A:908:ARG:NH2	2.44	0.51
1:A:1038:PHE:CG	1:A:1039:ASN:N	2.78	0.51
1:A:1078:LEU:HD23	1:A:1083:TYR:O	2.11	0.51
1:A:1214:LEU:HD23	1:A:1214:LEU:C	2.36	0.51
1:B:62:VAL:C	1:B:65:PRO:HD2	2.36	0.51
1:B:147:PHE:CE2	1:B:365:ILE:HG12	2.46	0.51
1:B:371:ILE:O	1:B:373:SER:N	2.43	0.51
1:B:536:ALA:O	1:B:537:ILE:C	2.54	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:742:GLU:HA	1:B:742:GLU:OE2	2.11	0.51
1:B:799:TRP:O	1:B:803:PRO:HB3	2.10	0.51
1:B:1031:VAL:HB	1:B:1056:VAL:HG12	1.91	0.51
1:A:111:ALA:HA	1:A:114:TYR:HE1	1.76	0.51
1:A:348:ILE:O	1:A:349:GLU:C	2.52	0.51
1:A:352:ALA:O	1:A:355:ARG:HB3	2.10	0.51
1:A:374:PHE:HE2	1:A:376:LYS:HB2	1.76	0.51
1:A:551:ASP:HA	1:A:581:ILE:CG2	2.41	0.51
1:A:881:LYS:HB2	1:A:881:LYS:NZ	2.26	0.51
1:A:1080:GLU:CD	1:A:1109:LEU:HD12	2.36	0.51
1:A:1242:ILE:HG12	1:A:1246:LYS:O	2.11	0.51
1:B:137:GLY:O	1:B:138:ARG:C	2.54	0.51
1:B:218:SER:O	1:B:219:PRO:C	2.52	0.51
1:A:38:MET:O	1:A:39:PHE:C	2.54	0.51
1:A:51:LEU:O	1:A:54:THR:HB	2.10	0.51
1:A:64:LEU:HD22	1:A:64:LEU:N	2.26	0.51
1:A:137:GLY:O	1:A:138:ARG:C	2.53	0.51
1:A:286:LYS:NZ	1:A:822:LYS:NZ	2.59	0.51
1:A:353:ASN:O	1:A:354:ALA:C	2.53	0.51
1:A:532:LYS:O	1:A:533:GLN:C	2.53	0.51
1:A:1013:GLU:O	1:A:1014:ILE:CG2	2.52	0.51
1:A:1057:LYS:H	1:A:1057:LYS:HD2	1.74	0.51
1:B:214:ILE:O	1:B:215:LEU:C	2.54	0.51
1:B:958:TYR:O	1:B:966:THR:HG21	2.10	0.51
1:B:1014:ILE:O	1:B:1015:ASP:CG	2.53	0.51
1:B:1038:PHE:CG	1:B:1039:ASN:N	2.78	0.51
1:B:1132:ASN:OD1	1:B:1134:ARG:HG2	2.11	0.51
1:B:1144:ALA:HB2	1:B:1187:VAL:HG23	1.93	0.51
1:B:1148:ALA:HB1	1:B:1179:ARG:O	2.11	0.51
1:A:72:GLY:O	1:A:75:THR:N	2.43	0.51
1:A:225:ALA:HB2	1:A:302:ILE:HG21	1.92	0.51
1:A:324:ILE:HD11	1:A:327:VAL:HG13	1.92	0.51
1:A:398:PRO:HD3	1:A:440:TYR:CE2	2.46	0.51
1:A:588:VAL:O	1:A:591:ALA:CB	2.57	0.51
1:A:686:GLU:HG2	1:A:813:ARG:NH2	2.13	0.51
1:A:901:ARG:HD3	1:A:901:ARG:N	2.23	0.51
1:A:1001:ALA:O	1:A:1004:ILE:HG22	2.11	0.51
1:A:1093:ASP:C	1:A:1093:ASP:OD2	2.53	0.51
1:B:225:ALA:HB2	1:B:302:ILE:HG21	1.91	0.51
1:B:245:LYS:HA	1:B:245:LYS:NZ	2.23	0.51
1:B:261:ILE:C	1:B:263:PHE:N	2.62	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:282:ARG:HB3	1:B:778:GLU:HG2	1.93	0.51
1:B:288:ALA:C	1:B:291:ALA:HB3	2.35	0.51
1:B:356:GLY:O	1:B:357:ALA:C	2.54	0.51
1:B:769:GLN:HG3	1:B:773:PHE:CE2	2.43	0.51
1:B:856:LEU:O	1:B:859:ALA:HB3	2.10	0.51
1:B:949:TYR:CE2	1:B:977:ILE:HG21	2.46	0.51
1:B:955:PHE:O	1:B:958:TYR:HB3	2.11	0.51
1:B:1199:THR:HG23	1:B:1210:VAL:HG11	1.92	0.51
1:A:113:TYR:CG	1:A:114:TYR:N	2.79	0.51
1:A:573:ARG:O	1:A:575:GLY:N	2.43	0.51
1:A:1050:GLN:H	1:A:1245:GLY:HA2	1.76	0.51
1:A:1057:LYS:HD2	1:A:1057:LYS:N	2.26	0.51
1:A:1114:GLN:HE22	1:A:1200:SER:CB	2.23	0.51
1:B:65:PRO:C	1:B:67:MET:N	2.65	0.51
1:B:121:VAL:HG23	1:B:122:LEU:H	1.74	0.51
1:B:462:LEU:HD12	1:B:466:ILE:CD1	2.40	0.51
1:B:806:THR:OG1	1:B:807:THR:N	2.44	0.51
1:B:1123:ILE:HG12	1:B:1124:ALA:N	2.26	0.51
1:A:74:MET:HG3	1:A:75:THR:N	2.26	0.50
1:A:81:VAL:HG22	1:A:102:LYS:HG3	1.93	0.50
1:A:702:THR:O	1:A:704:TRP:N	2.44	0.50
1:A:703:GLU:HA	1:A:783:ARG:HH12	1.75	0.50
1:B:1037:VAL:HG12	1:B:1051:GLY:N	2.24	0.50
1:A:68:MET:SD	1:A:332:PHE:CE1	3.02	0.50
1:A:72:GLY:O	1:A:73:ASP:C	2.54	0.50
1:A:118:GLY:HA3	1:A:946:TYR:CE2	2.46	0.50
1:A:183:GLY:O	1:A:184:ASP:C	2.54	0.50
1:A:185:LYS:HZ2	1:A:186:ILE:CA	2.23	0.50
1:A:260:VAL:O	1:A:263:PHE:HB3	2.11	0.50
1:A:279:GLU:O	1:A:282:ARG:HB2	2.11	0.50
1:A:566:GLN:NE2	1:A:569:LEU:HD12	2.26	0.50
1:B:552:GLU:HB3	1:B:555:SER:HB2	1.93	0.50
1:B:748:SER:O	1:B:751:PHE:HD1	1.94	0.50
1:B:762:SER:O	1:B:763:PHE:C	2.53	0.50
1:B:910:GLN:O	1:B:913:GLU:N	2.44	0.50
1:B:970:VAL:O	1:B:973:VAL:CB	2.58	0.50
1:B:1079:LEU:C	1:B:1081:ARG:N	2.67	0.50
1:B:1149:ASN:OD1	1:B:1213:ALA:HB2	2.11	0.50
1:A:55:LEU:O	1:A:56:ALA:C	2.53	0.50
1:A:449:ILE:HD13	1:A:449:ILE:C	2.35	0.50
1:A:775:LYS:O	1:A:776:ALA:C	2.54	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:922:ILE:CB	1:A:923:PRO:HD3	2.38	0.50
1:A:1023:LYS:HB3	1:A:1023:LYS:HZ3	1.77	0.50
1:A:1214:LEU:HD23	1:A:1214:LEU:O	2.11	0.50
1:B:248:ALA:C	1:B:250:ALA:N	2.68	0.50
1:B:411:LEU:HD23	1:B:411:LEU:C	2.37	0.50
1:B:583:HIS:O	1:B:585:LEU:HD22	2.10	0.50
1:B:1080:GLU:CD	1:B:1109:LEU:HD12	2.36	0.50
1:B:1093:ASP:C	1:B:1093:ASP:OD2	2.55	0.50
1:A:53:GLY:HA2	1:A:127:ILE:HG22	1.93	0.50
1:A:113:TYR:CD1	1:A:114:TYR:N	2.80	0.50
1:A:114:TYR:HB3	1:A:950:ALA:HB2	1.94	0.50
1:A:207:GLY:CA	1:A:211:THR:H	2.22	0.50
1:A:218:SER:CB	1:A:219:PRO:CD	2.90	0.50
1:A:286:LYS:HE3	1:A:822:LYS:HZ1	1.75	0.50
1:A:1067:SER:OG	1:A:1244:ASN:ND2	2.45	0.50
1:A:1149:ASN:OD1	1:A:1213:ALA:HB2	2.10	0.50
1:B:59:ILE:C	1:B:59:ILE:HD12	2.36	0.50
1:B:74:MET:HG3	1:B:75:THR:N	2.27	0.50
1:B:604:GLU:OE2	1:B:616:GLY:HA3	2.12	0.50
1:B:702:THR:HB	1:B:703:GLU:OE1	2.11	0.50
1:B:777:GLY:HA2	1:B:822:LYS:HG3	1.93	0.50
1:B:1032:GLN:O	1:B:1090:VAL:HA	2.11	0.50
1:A:267:LYS:HB3	1:A:790:LYS:CE	2.41	0.50
1:A:326:GLN:HE21	1:A:329:THR:HG1	1.57	0.50
1:A:384:ILE:CG2	1:A:385:GLN:H	2.03	0.50
1:A:433:VAL:CG1	1:A:549:LEU:HD23	2.41	0.50
1:A:932:HIS:O	1:A:933:VAL:C	2.55	0.50
1:A:1027:LEU:HD12	1:A:1027:LEU:N	2.26	0.50
1:A:1037:VAL:HG12	1:A:1051:GLY:N	2.24	0.50
1:A:1144:ALA:HB2	1:A:1187:VAL:HG23	1.92	0.50
1:B:433:VAL:O	1:B:434:GLN:C	2.54	0.50
1:B:573:ARG:O	1:B:575:GLY:N	2.45	0.50
1:B:1079:LEU:C	1:B:1081:ARG:H	2.18	0.50
1:A:91:MET:HB3	1:A:93:GLU:OE2	2.12	0.50
1:A:362:PHE:HA	1:A:365:ILE:CD1	2.41	0.50
1:A:462:LEU:HD12	1:A:466:ILE:CD1	2.40	0.50
1:A:463:ARG:HH11	1:A:463:ARG:HG3	1.76	0.50
1:A:469:VAL:HG12	1:A:553:ALA:HB2	1.94	0.50
1:A:505:ALA:O	1:A:509:ILE:HG23	2.10	0.50
1:A:561:SER:O	1:A:565:VAL:HG23	2.10	0.50
1:A:1028:GLU:HB2	1:A:1093:ASP:OD1	2.12	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1081:ARG:NH1	1:A:1098:LYS:O	2.44	0.50
1:B:72:GLY:O	1:B:73:ASP:C	2.55	0.50
1:B:113:TYR:CG	1:B:114:TYR:N	2.79	0.50
1:B:139:GLN:O	1:B:140:ILE:C	2.54	0.50
1:B:283:LEU:HD12	1:B:284:GLY:N	2.25	0.50
1:B:454:ILE:HG23	1:B:455:ARG:N	2.27	0.50
1:B:695:ARG:HD3	1:B:699:LEU:CD2	2.42	0.50
1:B:1078:LEU:C	1:B:1081:ARG:H	2.20	0.50
1:A:342:GLY:O	1:A:346:PRO:CD	2.60	0.50
1:A:544:ASN:HB2	1:A:576:ARG:HH21	1.77	0.50
1:A:710:GLY:O	1:A:711:ILE:C	2.55	0.50
1:A:899:ASN:HA	1:A:901:ARG:NH1	2.25	0.50
1:B:113:TYR:CD1	1:B:114:TYR:N	2.79	0.50
1:B:186:ILE:CG1	1:B:187:GLY:N	2.75	0.50
1:B:566:GLN:NE2	1:B:569:LEU:HD12	2.26	0.50
1:B:603:VAL:HG21	1:B:617:ILE:HG13	1.94	0.50
1:B:785:ARG:O	1:B:786:TYR:C	2.54	0.50
1:B:957:ALA:O	1:B:960:VAL:HG13	2.12	0.50
1:B:1001:ALA:O	1:B:1004:ILE:HG22	2.12	0.50
1:B:1206:SER:O	1:B:1207:GLU:C	2.55	0.50
1:A:374:PHE:CD2	1:A:376:LYS:HB3	2.47	0.50
1:A:384:ILE:O	1:A:385:GLN:O	2.30	0.50
1:A:603:VAL:HG21	1:A:617:ILE:HG13	1.94	0.50
1:A:945:MET:O	1:A:949:TYR:HD1	1.95	0.50
1:A:955:PHE:O	1:A:958:TYR:HB3	2.12	0.50
1:A:1127:ILE:C	1:A:1129:TYR:H	2.17	0.50
1:B:68:MET:HE2	1:B:68:MET:CA	2.38	0.50
1:B:124:VAL:HG23	1:B:125:ALA:N	2.26	0.50
1:B:453:ASP:HB3	1:B:456:THR:CG2	2.41	0.50
1:B:853:LEU:H	1:B:853:LEU:CD2	2.16	0.50
1:B:993:ASP:C	1:B:995:ALA:H	2.19	0.50
1:B:1023:LYS:CB	1:B:1026:MET:HG2	2.41	0.50
1:A:118:GLY:HA3	1:A:946:TYR:CD2	2.46	0.50
1:A:528:SER:O	1:A:529:GLY:C	2.53	0.50
1:A:534:ARG:O	1:A:537:ILE:HB	2.12	0.50
1:A:697:LEU:HB3	1:A:828:ARG:CZ	2.41	0.50
1:A:762:SER:O	1:A:763:PHE:C	2.53	0.50
1:A:846:SER:C	1:A:849:TYR:HB2	2.37	0.50
1:A:906:LEU:C	1:A:908:ARG:HD2	2.37	0.50
1:A:1196:ASP:OD2	1:A:1226:ILE:HD11	2.12	0.50
1:B:114:TYR:CB	1:B:950:ALA:HB2	2.42	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:182:ILE:O	1:B:185:LYS:HE3	2.11	0.50
1:B:218:SER:CB	1:B:219:PRO:CD	2.90	0.50
1:B:269:GLU:O	1:B:270:LEU:C	2.54	0.50
1:B:820:GLN:HG3	1:B:1000:SER:HB3	1.92	0.50
1:B:1178:GLN:O	1:B:1182:ILE:HG12	2.11	0.50
1:B:1196:ASP:OD2	1:B:1226:ILE:HD11	2.12	0.50
1:A:200:PHE:O	1:A:201:ILE:C	2.54	0.49
1:A:689:PRO:HB2	1:A:690:PRO:CD	2.37	0.49
1:A:799:TRP:O	1:A:803:PRO:HB3	2.12	0.49
1:A:848:ILE:O	1:A:848:ILE:HG12	2.12	0.49
1:A:972:LEU:O	1:A:975:SER:CB	2.60	0.49
1:B:91:MET:HB3	1:B:93:GLU:OE2	2.12	0.49
1:B:140:ILE:O	1:B:141:HIS:C	2.55	0.49
1:B:212:LEU:C	1:B:214:ILE:N	2.66	0.49
1:B:528:SER:O	1:B:529:GLY:C	2.55	0.49
1:B:897:ILE:CG1	1:B:898:GLU:H	2.10	0.49
1:B:1035:GLY:C	1:B:1052:LEU:O	2.55	0.49
1:B:1067:SER:OG	1:B:1244:ASN:ND2	2.45	0.49
1:B:1154:ILE:HD13	1:B:1161:TYR:CE2	2.47	0.49
1:A:55:LEU:C	1:A:55:LEU:HD23	2.36	0.49
1:A:232:LEU:HD22	1:A:232:LEU:N	2.27	0.49
1:A:238:LYS:HZ3	1:A:242:ALA:HB2	1.77	0.49
1:A:304:ALA:HB2	1:A:758:LEU:HD23	1.94	0.49
1:A:393:ILE:HG13	1:A:409:LEU:HB3	1.94	0.49
1:A:507:ASP:OD1	1:A:508:PHE:N	2.35	0.49
1:B:70:ILE:O	1:B:74:MET:HG2	2.12	0.49
1:B:366:ASP:O	1:B:367:ASN:C	2.55	0.49
1:B:406:LEU:HD12	1:B:409:LEU:HB2	1.93	0.49
1:B:531:GLN:O	1:B:532:LYS:C	2.55	0.49
1:B:536:ALA:O	1:B:537:ILE:O	2.30	0.49
1:B:937:THR:OG1	1:B:938:PHE:N	2.45	0.49
1:B:1050:GLN:H	1:B:1245:GLY:HA2	1.77	0.49
1:B:1175:GLY:O	1:B:1179:ARG:HG3	2.12	0.49
1:B:1249:GLU:OE1	1:B:1262:ILE:HB	2.12	0.49
1:A:150:ALA:O	1:A:151:ILE:C	2.55	0.49
1:A:265:GLY:O	1:A:267:LYS:HG3	2.12	0.49
1:A:361:VAL:O	1:A:365:ILE:CD1	2.59	0.49
1:A:812:THR:O	1:A:813:ARG:C	2.54	0.49
1:A:937:THR:OG1	1:A:938:PHE:N	2.44	0.49
1:A:969:ASN:O	1:A:972:LEU:N	2.44	0.49
1:A:1255:GLN:HG2	1:A:1259:GLN:HE22	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:265:GLY:O	1:B:267:LYS:HG3	2.11	0.49
1:B:342:GLY:O	1:B:346:PRO:CD	2.60	0.49
1:B:544:ASN:HB2	1:B:576:ARG:HH21	1.77	0.49
1:B:969:ASN:HD22	1:B:970:VAL:H	1.57	0.49
1:B:1229:ARG:O	1:B:1231:SER:N	2.45	0.49
1:A:44:TRP:CD1	1:A:45:LEU:HD22	2.47	0.49
1:A:214:ILE:O	1:A:215:LEU:C	2.56	0.49
1:A:406:LEU:HD12	1:A:409:LEU:HB2	1.93	0.49
1:A:454:ILE:HG23	1:A:455:ARG:N	2.27	0.49
1:A:520:VAL:HG12	1:A:523:ARG:O	2.11	0.49
1:A:695:ARG:HD3	1:A:699:LEU:CD2	2.42	0.49
1:A:730:LYS:O	1:A:733:GLY:N	2.46	0.49
1:A:748:SER:O	1:A:751:PHE:HD1	1.94	0.49
1:A:795:GLN:NE2	1:A:796:ASP:H	2.10	0.49
1:A:810:LEU:O	1:A:811:THR:C	2.55	0.49
1:A:893:ALA:O	1:A:897:ILE:HG12	2.13	0.49
1:A:1076:VAL:HG22	1:A:1194:LEU:HD22	1.95	0.49
1:A:1216:LYS:HA	1:A:1216:LYS:CE	2.36	0.49
1:B:326:GLN:O	1:B:327:VAL:C	2.55	0.49
1:B:535:ILE:O	1:B:536:ALA:C	2.54	0.49
1:B:697:LEU:HB3	1:B:828:ARG:CZ	2.43	0.49
1:B:907:THR:C	1:B:908:ARG:NE	2.59	0.49
1:B:1022:LEU:O	1:B:1023:LYS:O	2.31	0.49
1:B:1046:ILE:HD12	1:B:1046:ILE:N	2.28	0.49
1:B:1062:LEU:HB3	1:B:1224:ILE:HA	1.94	0.49
1:A:52:VAL:O	1:A:53:GLY:C	2.53	0.49
1:A:111:ALA:HA	1:A:114:TYR:CE1	2.47	0.49
1:A:214:ILE:HG12	1:A:331:PHE:CE2	2.48	0.49
1:A:246:ALA:CB	1:A:277:LEU:HB3	2.39	0.49
1:A:585:LEU:HD12	1:A:618:TYR:CE1	2.43	0.49
1:A:585:LEU:H	1:A:585:LEU:CD2	2.25	0.49
1:A:712:PHE:O	1:A:715:ILE:N	2.45	0.49
1:A:806:THR:OG1	1:A:807:THR:N	2.45	0.49
1:A:883:LYS:CA	1:A:886:LEU:HG	2.43	0.49
1:A:962:GLN:O	1:A:962:GLN:HG2	2.13	0.49
1:A:1041:PRO:O	1:A:1042:THR:HB	2.13	0.49
1:B:44:TRP:CD1	1:B:45:LEU:HD22	2.47	0.49
1:B:50:MET:O	1:B:51:LEU:C	2.55	0.49
1:B:68:MET:HA	1:B:68:MET:CE	2.39	0.49
1:B:118:GLY:HA3	1:B:946:TYR:CD2	2.48	0.49
1:B:588:VAL:O	1:B:591:ALA:CB	2.59	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:974:PHE:O	1:B:978:VAL:HG12	2.13	0.49
1:B:1032:GLN:NE2	1:B:1055:GLU:HG3	2.28	0.49
1:A:121:VAL:CG2	1:A:122:LEU:H	2.25	0.49
1:A:128:GLN:O	1:A:129:VAL:C	2.51	0.49
1:A:186:ILE:CG1	1:A:187:GLY:N	2.75	0.49
1:A:788:VAL:O	1:A:789:PHE:C	2.54	0.49
1:A:807:THR:O	1:A:811:THR:HG23	2.13	0.49
1:A:1249:GLU:OE1	1:A:1262:ILE:HB	2.13	0.49
1:A:1270:GLN:O	1:A:1271:ALA:C	2.53	0.49
1:B:68:MET:SD	1:B:332:PHE:CE1	3.02	0.49
1:B:174:ASP:O	1:B:175:VAL:C	2.54	0.49
1:B:425:SER:HB3	1:B:599:GLY:CA	2.43	0.49
1:B:703:GLU:HA	1:B:783:ARG:HH12	1.76	0.49
1:B:711:ILE:CD1	1:B:832:ILE:HD13	2.42	0.49
1:B:1041:PRO:O	1:B:1042:THR:HB	2.13	0.49
1:B:1076:VAL:HG22	1:B:1194:LEU:HD22	1.95	0.49
1:B:1137:SER:O	1:B:1141:ILE:HG23	2.12	0.49
1:A:99:MET:N	1:A:99:MET:SD	2.85	0.49
1:A:286:LYS:CE	1:A:822:LYS:NZ	2.76	0.49
1:A:742:GLU:HA	1:A:742:GLU:OE2	2.12	0.49
1:A:969:ASN:HD22	1:A:970:VAL:H	1.56	0.49
1:B:749:ASN:C	1:B:749:ASN:ND2	2.68	0.49
1:B:836:ILE:O	1:B:837:ALA:C	2.55	0.49
1:B:846:SER:C	1:B:849:TYR:HB2	2.37	0.49
1:A:207:GLY:O	1:A:209:LYS:N	2.46	0.49
1:A:418:THR:HG22	1:A:578:THR:CG2	2.43	0.49
1:A:1011:THR:O	1:A:1012:PRO:C	2.55	0.49
1:A:1186:LEU:HD12	1:A:1187:VAL:N	2.28	0.49
1:A:1260:LYS:H	1:A:1260:LYS:CD	2.23	0.49
1:B:286:LYS:HG2	1:B:778:GLU:CG	2.43	0.49
1:B:398:PRO:HD3	1:B:440:TYR:CE2	2.47	0.49
1:B:422:VAL:O	1:B:597:PHE:HB2	2.12	0.49
1:B:1114:GLN:HE22	1:B:1200:SER:CB	2.25	0.49
1:A:120:GLY:O	1:A:121:VAL:C	2.56	0.49
1:A:158:TRP:NE1	1:A:900:PHE:HB3	2.12	0.49
1:A:248:ALA:C	1:A:250:ALA:N	2.71	0.49
1:A:342:GLY:O	1:A:346:PRO:HD2	2.12	0.49
1:A:411:LEU:HD23	1:A:411:LEU:C	2.38	0.49
1:A:922:ILE:HB	1:A:923:PRO:CD	2.41	0.49
1:B:324:ILE:HG13	1:B:326:GLN:N	2.28	0.49
1:B:409:LEU:HD13	1:B:409:LEU:C	2.38	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:431:THR:O	1:B:432:THR:C	2.55	0.49
1:B:962:GLN:O	1:B:962:GLN:HG2	2.13	0.49
1:B:1147:GLU:HB3	1:B:1186:LEU:CD2	2.40	0.49
1:A:174:ASP:O	1:A:175:VAL:C	2.54	0.49
1:A:316:LEU:C	1:A:318:ILE:H	2.20	0.49
1:A:345:SER:O	1:A:346:PRO:C	2.53	0.49
1:A:433:VAL:HG13	1:A:549:LEU:HD23	1.95	0.49
1:A:849:TYR:OH	1:A:976:ALA:CB	2.61	0.49
1:A:1057:LYS:N	1:A:1060:GLN:NE2	2.61	0.49
1:B:55:LEU:O	1:B:56:ALA:C	2.55	0.49
1:B:113:TYR:CD1	1:B:113:TYR:C	2.90	0.49
1:B:121:VAL:CG2	1:B:122:LEU:H	2.25	0.49
1:B:321:GLU:HG3	1:B:322:TYR:H	1.76	0.49
1:B:385:GLN:HE21	1:B:386:GLY:N	2.08	0.49
1:B:432:THR:O	1:B:433:VAL:C	2.55	0.49
1:B:848:ILE:O	1:B:848:ILE:HG12	2.11	0.49
1:B:932:HIS:O	1:B:933:VAL:C	2.54	0.49
1:B:957:ALA:O	1:B:958:TYR:C	2.56	0.49
1:B:1249:GLU:CD	1:B:1262:ILE:HB	2.37	0.49
1:A:77:SER:O	1:A:81:VAL:HG23	2.13	0.48
1:A:520:VAL:CG1	1:A:524:GLY:HA2	2.43	0.48
1:A:589:ARG:C	1:A:591:ALA:N	2.62	0.48
1:A:1032:GLN:NE2	1:A:1055:GLU:HG3	2.27	0.48
1:A:1037:VAL:CG2	1:A:1037:VAL:O	2.61	0.48
1:A:1046:ILE:HD12	1:A:1046:ILE:N	2.28	0.48
1:A:1079:LEU:C	1:A:1081:ARG:N	2.66	0.48
1:B:52:VAL:O	1:B:53:GLY:C	2.55	0.48
1:B:71:PHE:C	1:B:71:PHE:CD2	2.91	0.48
1:B:99:MET:N	1:B:99:MET:SD	2.86	0.48
1:B:158:TRP:HE1	1:B:900:PHE:CB	2.26	0.48
1:B:202:ILE:O	1:B:204:PHE:N	2.45	0.48
1:B:303:TYR:O	1:B:306:TYR:CB	2.60	0.48
1:B:418:THR:HG22	1:B:578:THR:CG2	2.42	0.48
1:B:460:ARG:O	1:B:461:TYR:C	2.54	0.48
1:B:1088:GLY:O	1:B:1089:SER:HB2	2.12	0.48
1:A:154:GLN:O	1:A:154:GLN:HG2	2.13	0.48
1:A:342:GLY:O	1:A:345:SER:N	2.47	0.48
1:A:360:GLU:O	1:A:363:LYS:HB2	2.13	0.48
1:B:210:LEU:C	1:B:212:LEU:N	2.66	0.48
1:B:280:ALA:C	1:B:282:ARG:H	2.21	0.48
1:B:916:TYR:O	1:B:920:LEU:HD23	2.13	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1186:LEU:HD12	1:B:1187:VAL:N	2.28	0.48
1:A:199:GLY:HA2	1:A:334:VAL:HG23	1.95	0.48
1:A:211:THR:HA	1:A:214:ILE:HD12	1.95	0.48
1:A:218:SER:O	1:A:219:PRO:C	2.56	0.48
1:A:479:THR:O	1:A:482:GLU:HB2	2.13	0.48
1:A:781:THR:HG23	1:A:818:ALA:HB1	1.95	0.48
1:B:291:ALA:CA	1:B:294:SER:HB2	2.40	0.48
1:B:484:ILE:CG2	1:B:496:ILE:CD1	2.91	0.48
1:B:1145:ALA:CB	1:B:1154:ILE:HD12	2.44	0.48
1:A:113:TYR:CD1	1:A:113:TYR:C	2.91	0.48
1:A:121:VAL:HG23	1:A:122:LEU:H	1.76	0.48
1:A:170:ARG:HB2	1:A:174:ASP:CG	2.39	0.48
1:A:301:LEU:O	1:A:304:ALA:HB3	2.13	0.48
1:A:327:VAL:HG23	1:A:328:LEU:N	2.28	0.48
1:A:374:PHE:CE2	1:A:376:LYS:HB2	2.48	0.48
1:A:464:GLU:C	1:A:466:ILE:H	2.20	0.48
1:A:550:LEU:HD12	1:A:550:LEU:N	2.29	0.48
1:A:728:PHE:O	1:A:732:VAL:HG22	2.13	0.48
1:A:783:ARG:HG2	1:A:783:ARG:HH11	1.78	0.48
1:A:978:VAL:HG21	2:A:6001:2J8:H29	1.95	0.48
1:B:71:PHE:C	1:B:71:PHE:HD2	2.22	0.48
1:B:154:GLN:O	1:B:154:GLN:HG2	2.13	0.48
1:B:207:GLY:HA2	1:B:210:LEU:HD12	1.94	0.48
1:B:324:ILE:HG13	1:B:326:GLN:H	1.76	0.48
1:B:753:LEU:O	1:B:754:LEU:C	2.56	0.48
1:B:781:THR:HG23	1:B:818:ALA:HB1	1.94	0.48
1:B:894:THR:HA	1:B:897:ILE:HD11	1.96	0.48
1:B:922:ILE:CB	1:B:923:PRO:HD3	2.41	0.48
1:B:945:MET:O	1:B:949:TYR:HD1	1.96	0.48
1:B:1037:VAL:CG2	1:B:1037:VAL:O	2.61	0.48
1:B:1064:LEU:C	1:B:1064:LEU:HD13	2.38	0.48
1:A:204:PHE:O	1:A:211:THR:HG21	2.14	0.48
1:A:420:ALA:O	1:A:421:LEU:HD12	2.14	0.48
1:A:479:THR:HA	1:A:518:THR:O	2.14	0.48
1:A:728:PHE:CE1	2:A:6002:2J8:SE2	3.16	0.48
1:A:797:VAL:O	1:A:801:ASP:HB2	2.14	0.48
1:A:908:ARG:CD	1:A:908:ARG:N	2.76	0.48
1:A:1075:VAL:O	1:A:1076:VAL:C	2.55	0.48
1:B:35:VAL:HA	1:B:359:TYR:CD2	2.49	0.48
1:B:77:SER:O	1:B:81:VAL:HG23	2.14	0.48
1:B:238:LYS:HZ2	1:B:242:ALA:HB2	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:243:TYR:C	1:B:243:TYR:CD2	2.91	0.48
1:B:306:TYR:CE1	1:B:335:LEU:HD22	2.49	0.48
1:B:318:ILE:HD13	1:B:327:VAL:HG22	1.95	0.48
1:B:324:ILE:HD11	1:B:327:VAL:CG1	2.43	0.48
1:B:464:GLU:HA	1:B:543:ARG:CZ	2.43	0.48
1:B:509:ILE:HD12	1:B:509:ILE:C	2.39	0.48
1:B:711:ILE:HD11	1:B:832:ILE:CG2	2.27	0.48
1:B:711:ILE:O	1:B:714:ALA:HB3	2.14	0.48
1:B:907:THR:N	1:B:908:ARG:NE	2.60	0.48
1:B:1057:LYS:N	1:B:1060:GLN:NE2	2.62	0.48
1:A:214:ILE:CG2	1:A:334:VAL:HG11	2.43	0.48
1:A:348:ILE:O	1:A:351:PHE:N	2.47	0.48
1:A:465:ILE:O	1:A:465:ILE:HG22	2.13	0.48
1:A:538:ALA:O	1:A:539:ARG:C	2.56	0.48
1:A:755:PHE:O	1:A:756:LEU:C	2.56	0.48
1:A:912:PHE:O	1:A:913:GLU:C	2.57	0.48
1:A:970:VAL:CG2	1:A:971:LEU:HD22	2.40	0.48
1:A:1147:GLU:HB3	1:A:1186:LEU:CD2	2.42	0.48
1:B:181:GLY:HA3	1:B:354:ALA:CB	2.44	0.48
1:B:332:PHE:O	1:B:335:LEU:HB3	2.13	0.48
1:B:471:GLN:OE1	1:B:472:GLU:N	2.45	0.48
1:B:614:GLU:O	1:B:615:LYS:C	2.56	0.48
1:B:883:LYS:CA	1:B:886:LEU:HG	2.43	0.48
1:B:1255:GLN:O	1:B:1258:ALA:HB3	2.13	0.48
1:A:128:GLN:O	1:A:131:PHE:N	2.47	0.48
1:A:148:PHE:CD2	1:A:913:GLU:OE2	2.64	0.48
1:A:183:GLY:O	1:A:186:ILE:CG1	2.58	0.48
1:A:361:VAL:C	1:A:365:ILE:HD12	2.38	0.48
1:A:993:ASP:C	1:A:995:ALA:H	2.21	0.48
1:A:1137:SER:HB3	1:A:1140:GLU:HB3	1.94	0.48
1:B:106:GLU:OE2	1:B:109:THR:HB	2.14	0.48
1:B:293:ILE:HG21	1:B:770:GLY:HA3	1.96	0.48
1:B:529:GLY:HA2	1:B:532:LYS:HD3	1.96	0.48
1:B:540:ALA:O	1:B:543:ARG:CB	2.61	0.48
1:B:1001:ALA:O	1:B:1005:ILE:CG1	2.62	0.48
1:B:1078:LEU:HD23	1:B:1083:TYR:O	2.13	0.48
1:B:1242:ILE:HG12	1:B:1246:LYS:O	2.14	0.48
1:A:209:LYS:C	1:A:212:LEU:HB3	2.38	0.48
1:A:479:THR:OG1	1:A:482:GLU:HG2	2.13	0.48
1:A:886:LEU:HD12	1:A:887:GLU:N	2.28	0.48
1:A:1032:GLN:HE21	1:A:1055:GLU:HB2	1.79	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:218:SER:CB	1:B:219:PRO:HD3	2.44	0.48
1:B:342:GLY:O	1:B:346:PRO:HD2	2.12	0.48
1:B:520:VAL:HG12	1:B:523:ARG:O	2.13	0.48
1:B:523:ARG:CD	1:B:524:GLY:N	2.63	0.48
1:B:690:PRO:O	1:B:691:ALA:C	2.54	0.48
1:B:710:GLY:O	1:B:711:ILE:C	2.55	0.48
1:B:849:TYR:OH	1:B:976:ALA:CB	2.61	0.48
1:B:1204:THR:OG1	1:B:1205:GLU:N	2.42	0.48
1:A:65:PRO:C	1:A:67:MET:N	2.67	0.48
1:A:217:ILE:HG13	1:A:218:SER:H	1.78	0.48
1:A:271:GLU:C	1:A:271:GLU:OE2	2.56	0.48
1:A:318:ILE:HD13	1:A:327:VAL:CG1	2.44	0.48
1:A:366:ASP:O	1:A:367:ASN:C	2.56	0.48
1:A:531:GLN:O	1:A:535:ILE:HG12	2.14	0.48
1:B:128:GLN:O	1:B:131:PHE:N	2.47	0.48
1:B:393:ILE:HG13	1:B:409:LEU:HB3	1.95	0.48
1:B:449:ILE:O	1:B:450:ASP:C	2.56	0.48
1:B:783:ARG:HG2	1:B:783:ARG:HH11	1.77	0.48
1:A:116:GLY:O	1:A:117:ILE:C	2.56	0.48
1:A:140:ILE:HG13	1:A:179:ASN:HB2	1.95	0.48
1:A:197:PHE:O	1:A:201:ILE:HG12	2.13	0.48
1:A:257:ILE:O	1:A:257:ILE:HD13	2.12	0.48
1:A:480:ILE:C	1:A:482:GLU:N	2.71	0.48
1:A:506:TYR:O	1:A:510:MET:HG2	2.14	0.48
1:A:538:ALA:O	1:A:541:LEU:HB3	2.13	0.48
1:A:711:ILE:CD1	1:A:832:ILE:HG21	2.28	0.48
1:A:727:ILE:HD11	1:A:753:LEU:CG	2.44	0.48
1:A:923:PRO:HA	1:A:926:ASN:HB3	1.96	0.48
1:A:1029:GLY:O	1:A:1031:VAL:N	2.47	0.48
1:A:1217:ALA:O	1:A:1221:ARG:HD3	2.14	0.48
1:B:484:ILE:O	1:B:487:GLY:N	2.46	0.48
1:B:533:GLN:O	1:B:536:ALA:HB3	2.14	0.48
1:B:573:ARG:C	1:B:575:GLY:H	2.22	0.48
1:B:730:LYS:O	1:B:733:GLY:N	2.46	0.48
1:B:902:THR:OG1	1:B:908:ARG:HD3	2.14	0.48
1:B:908:ARG:CD	1:B:908:ARG:N	2.77	0.48
1:B:1032:GLN:HE21	1:B:1055:GLU:HB2	1.78	0.48
1:B:1255:GLN:HG2	1:B:1259:GLN:HE22	1.78	0.48
1:A:175:VAL:CG1	1:A:176:SER:H	2.27	0.47
1:A:369:PRO:O	1:A:370:SER:C	2.57	0.47
1:A:386:GLY:HA3	1:A:450:ASP:CA	2.39	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:959:LEU:O	1:A:964:LEU:HB3	2.13	0.47
1:A:1020:GLN:NE2	1:A:1104:TRP:CE3	2.77	0.47
1:A:1025:ASN:O	1:A:1025:ASN:CG	2.57	0.47
1:A:1092:LEU:O	1:A:1093:ASP:HB3	2.14	0.47
1:B:136:ALA:O	1:B:139:GLN:HB2	2.14	0.47
1:B:282:ARG:HG3	1:B:782:LYS:HD3	1.96	0.47
1:B:311:TRP:CD1	1:B:754:LEU:HD13	2.49	0.47
1:B:327:VAL:HG23	1:B:328:LEU:N	2.27	0.47
1:B:550:LEU:N	1:B:550:LEU:HD12	2.28	0.47
1:B:1032:GLN:NE2	1:B:1055:GLU:HB2	2.29	0.47
1:A:71:PHE:C	1:A:71:PHE:CD2	2.92	0.47
1:A:202:ILE:C	1:A:204:PHE:H	2.22	0.47
1:A:530:GLY:O	1:A:531:GLN:C	2.56	0.47
1:A:625:GLN:O	1:A:626:THR:HB	2.14	0.47
1:A:706:TYR:O	1:A:707:PHE:CG	2.67	0.47
1:A:734:VAL:HG11	1:A:746:GLN:HB3	1.96	0.47
1:A:861:VAL:O	1:A:864:ILE:HG13	2.14	0.47
1:A:908:ARG:HD2	1:A:908:ARG:N	2.29	0.47
1:A:910:GLN:O	1:A:913:GLU:N	2.46	0.47
1:A:948:SER:O	1:A:952:CYS:HB2	2.13	0.47
1:A:1009:GLU:O	1:A:1010:LYS:HG3	2.13	0.47
1:A:1057:LYS:H	1:A:1060:GLN:NE2	2.12	0.47
1:B:308:LEU:HD12	1:B:751:PHE:CE2	2.48	0.47
1:B:479:THR:OG1	1:B:482:GLU:HG2	2.15	0.47
1:B:625:GLN:O	1:B:626:THR:HB	2.14	0.47
1:B:821:VAL:O	1:B:822:LYS:C	2.58	0.47
1:B:1019:THR:O	1:B:1101:ASN:N	2.43	0.47
1:B:1117:ILE:HG13	1:B:1118:LEU:N	2.30	0.47
1:A:207:GLY:CA	1:A:211:THR:HB	2.39	0.47
1:A:270:LEU:HD23	1:A:270:LEU:N	2.17	0.47
1:A:324:ILE:HD11	1:A:327:VAL:CG1	2.45	0.47
1:A:324:ILE:O	1:A:325:GLY:C	2.58	0.47
1:A:326:GLN:O	1:A:327:VAL:C	2.57	0.47
1:A:356:GLY:O	1:A:357:ALA:C	2.56	0.47
1:A:398:PRO:O	1:A:400:ARG:N	2.46	0.47
1:A:464:GLU:HA	1:A:543:ARG:CZ	2.43	0.47
1:A:896:ALA:O	1:A:897:ILE:C	2.56	0.47
1:A:1117:ILE:HG13	1:A:1118:LEU:N	2.30	0.47
1:B:128:GLN:O	1:B:129:VAL:C	2.56	0.47
1:B:135:ALA:O	1:B:136:ALA:C	2.57	0.47
1:B:204:PHE:N	1:B:211:THR:OG1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:285:ILE:HG22	1:B:286:LYS:HD2	1.96	0.47
1:B:397:TYR:CB	1:B:398:PRO:HD2	2.44	0.47
1:B:784:LEU:O	1:B:785:ARG:C	2.56	0.47
1:B:1154:ILE:CD1	1:B:1161:TYR:HE2	2.27	0.47
1:A:464:GLU:C	1:A:466:ILE:N	2.72	0.47
1:A:533:GLN:HE21	1:A:553:ALA:HB1	1.79	0.47
1:A:722:PRO:HG2	1:A:841:THR:HG1	1.78	0.47
1:A:732:VAL:HG21	1:A:971:LEU:HG	1.97	0.47
1:A:853:LEU:HG	1:A:973:VAL:CG2	2.40	0.47
1:A:1062:LEU:HB3	1:A:1224:ILE:HA	1.95	0.47
1:B:200:PHE:O	1:B:201:ILE:C	2.57	0.47
1:B:212:LEU:HD12	1:B:215:LEU:HD12	1.95	0.47
1:B:282:ARG:HB3	1:B:778:GLU:CG	2.44	0.47
1:B:348:ILE:O	1:B:351:PHE:N	2.48	0.47
1:B:566:GLN:HA	1:B:569:LEU:CD1	2.44	0.47
1:B:785:ARG:NH2	1:B:815:ALA:HA	2.29	0.47
1:B:795:GLN:NE2	1:B:796:ASP:H	2.11	0.47
1:B:820:GLN:CB	1:B:1000:SER:HB2	2.44	0.47
1:B:886:LEU:HD12	1:B:887:GLU:N	2.30	0.47
1:B:904:VAL:CG1	1:B:905:SER:N	2.77	0.47
1:B:959:LEU:O	1:B:964:LEU:HB3	2.14	0.47
1:A:125:ALA:O	1:A:128:GLN:HG2	2.15	0.47
1:A:188:MET:HB2	1:A:347:ASN:HB3	1.96	0.47
1:A:202:ILE:O	1:A:204:PHE:N	2.45	0.47
1:A:243:TYR:C	1:A:243:TYR:CD2	2.92	0.47
1:A:376:LYS:NZ	1:A:377:SER:HB2	2.30	0.47
1:A:469:VAL:HG12	1:A:553:ALA:CB	2.45	0.47
1:A:536:ALA:O	1:A:537:ILE:C	2.58	0.47
1:A:573:ARG:C	1:A:575:GLY:H	2.22	0.47
1:A:928:MET:O	1:A:931:ALA:HB3	2.14	0.47
1:A:943:ALA:HA	1:A:946:TYR:HE1	1.79	0.47
1:A:1064:LEU:HD13	1:A:1064:LEU:C	2.39	0.47
1:B:286:LYS:CA	1:B:289:ILE:HB	2.39	0.47
1:B:362:PHE:CA	1:B:365:ILE:HD12	2.41	0.47
1:B:432:THR:O	1:B:435:LEU:HB2	2.15	0.47
1:B:465:ILE:O	1:B:465:ILE:HG22	2.14	0.47
1:B:492:THR:C	1:B:494:ASP:H	2.23	0.47
1:B:727:ILE:HD12	1:B:754:LEU:HB2	1.97	0.47
1:B:861:VAL:O	1:B:864:ILE:HG13	2.15	0.47
1:B:915:MET:O	1:B:918:GLN:HB2	2.14	0.47
1:B:923:PRO:HA	1:B:926:ASN:HB3	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:943:ALA:HA	1:B:946:TYR:CE1	2.50	0.47
1:B:1077:GLN:O	1:B:1080:GLU:HB2	2.15	0.47
1:A:212:LEU:HD12	1:A:215:LEU:HD12	1.96	0.47
1:A:535:ILE:O	1:A:536:ALA:C	2.58	0.47
1:A:796:ASP:O	1:A:797:VAL:HB	2.14	0.47
1:A:867:ALA:O	1:A:870:VAL:HG12	2.14	0.47
1:A:1032:GLN:NE2	1:A:1055:GLU:HB2	2.29	0.47
1:A:1077:GLN:O	1:A:1080:GLU:HB2	2.15	0.47
1:B:90:ASN:CB	1:B:91:MET:HE3	2.43	0.47
1:B:120:GLY:O	1:B:121:VAL:C	2.56	0.47
1:B:159:PHE:HD2	1:B:440:TYR:HH	1.62	0.47
1:B:267:LYS:CA	1:B:270:LEU:HD21	2.45	0.47
1:B:290:THR:HG22	1:B:771:PHE:N	2.30	0.47
1:B:346:PRO:O	1:B:347:ASN:C	2.57	0.47
1:B:382:ASP:HA	1:B:461:TYR:HH	1.80	0.47
1:B:384:ILE:CG2	1:B:385:GLN:H	2.12	0.47
1:B:886:LEU:HD12	1:B:886:LEU:C	2.39	0.47
1:B:912:PHE:O	1:B:913:GLU:C	2.58	0.47
1:A:50:MET:O	1:A:51:LEU:C	2.56	0.47
1:A:106:GLU:OE2	1:A:109:THR:HB	2.15	0.47
1:A:278:GLU:O	1:A:279:GLU:C	2.57	0.47
1:A:308:LEU:HD13	1:A:755:PHE:CE1	2.50	0.47
1:A:409:LEU:HD13	1:A:409:LEU:C	2.39	0.47
1:A:519:LEU:HD11	1:B:925:ARG:CD	2.45	0.47
1:A:533:GLN:O	1:A:536:ALA:HB3	2.14	0.47
1:A:708:VAL:O	1:A:709:VAL:C	2.58	0.47
1:A:753:LEU:O	1:A:754:LEU:C	2.58	0.47
1:A:897:ILE:O	1:A:898:GLU:C	2.57	0.47
1:A:902:THR:OG1	1:A:908:ARG:HD3	2.15	0.47
1:A:1035:GLY:C	1:A:1052:LEU:O	2.57	0.47
1:A:1225:VAL:HG13	1:A:1225:VAL:O	2.15	0.47
1:A:1229:ARG:O	1:A:1231:SER:N	2.47	0.47
1:B:140:ILE:HG13	1:B:179:ASN:HB2	1.95	0.47
1:B:212:LEU:HD13	1:B:215:LEU:HD12	1.96	0.47
1:B:249:VAL:O	1:B:249:VAL:HG12	2.15	0.47
1:B:290:THR:HG21	1:B:771:PHE:HA	1.97	0.47
1:B:315:SER:HB3	1:B:747:ASN:HD22	1.77	0.47
1:B:394:HIS:HB2	1:B:444:ASP:HB3	1.97	0.47
1:B:429:LYS:N	1:B:429:LYS:CD	2.74	0.47
1:B:782:LYS:O	1:B:783:ARG:C	2.57	0.47
1:B:786:TYR:HE2	1:B:790:LYS:HZ3	1.62	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:807:THR:O	1:B:811:THR:HG23	2.14	0.47
1:B:943:ALA:HA	1:B:946:TYR:HE1	1.79	0.47
1:B:976:ALA:O	1:B:979:PHE:HB2	2.14	0.47
1:B:992:PRO:HB2	1:B:996:LYS:HE2	1.96	0.47
1:A:90:ASN:CB	1:A:91:MET:HE3	2.43	0.47
1:A:114:TYR:O	1:A:115:THR:C	2.55	0.47
1:A:140:ILE:O	1:A:141:HIS:C	2.57	0.47
1:A:144:ARG:NH1	1:A:175:VAL:HG21	2.30	0.47
1:A:332:PHE:O	1:A:335:LEU:HB3	2.14	0.47
1:A:519:LEU:CD1	1:B:925:ARG:HD3	2.45	0.47
1:A:535:ILE:O	1:A:538:ALA:HB3	2.15	0.47
1:B:47:ARG:O	1:B:48:LEU:C	2.57	0.47
1:B:140:ILE:O	1:B:143:ILE:N	2.48	0.47
1:B:236:THR:O	1:B:239:GLU:HB2	2.15	0.47
1:B:257:ILE:HG23	1:B:258:ARG:N	2.30	0.47
1:B:320:LYS:O	1:B:323:SER:OG	2.32	0.47
1:B:464:GLU:C	1:B:466:ILE:H	2.22	0.47
1:B:479:THR:O	1:B:482:GLU:HB2	2.15	0.47
1:B:506:TYR:O	1:B:510:MET:HG2	2.14	0.47
1:B:779:ILE:HG13	1:B:780:LEU:H	1.79	0.47
1:A:136:ALA:O	1:A:139:GLN:HB2	2.15	0.47
1:A:584:ARG:O	1:A:585:LEU:C	2.57	0.47
1:A:943:ALA:HA	1:A:946:TYR:CE1	2.49	0.47
1:A:1141:ILE:HG13	1:A:1142:VAL:N	2.30	0.47
1:B:183:GLY:O	1:B:186:ILE:CG1	2.57	0.47
1:B:295:MET:HA	1:B:295:MET:CE	2.45	0.47
1:B:530:GLY:O	1:B:531:GLN:C	2.57	0.47
1:B:552:GLU:HB3	1:B:555:SER:CB	2.45	0.47
1:B:732:VAL:HG21	1:B:971:LEU:HG	1.97	0.47
1:B:792:MET:O	1:B:793:LEU:C	2.58	0.47
1:B:841:THR:O	1:B:845:ILE:HG13	2.14	0.47
1:B:875:LEU:HD23	1:B:875:LEU:C	2.40	0.47
1:B:986:GLN:C	1:B:988:SER:H	2.23	0.47
1:B:1141:ILE:HG13	1:B:1142:VAL:N	2.30	0.47
1:B:1252:THR:HG23	1:B:1255:GLN:CB	2.44	0.47
1:A:100:PHE:HB2	1:A:961:THR:HG23	1.97	0.47
1:A:139:GLN:O	1:A:140:ILE:C	2.55	0.47
1:A:686:GLU:CD	1:A:686:GLU:N	2.73	0.47
1:A:836:ILE:O	1:A:837:ALA:C	2.55	0.47
1:A:903:VAL:HG23	1:A:906:LEU:HD12	1.97	0.47
1:B:72:GLY:O	1:B:75:THR:N	2.48	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:114:TYR:O	1:B:115:THR:C	2.58	0.47
1:B:144:ARG:NH1	1:B:175:VAL:HG21	2.30	0.47
1:B:183:GLY:O	1:B:184:ASP:C	2.55	0.47
1:B:362:PHE:HA	1:B:365:ILE:CD1	2.40	0.47
1:B:554:THR:HG23	1:B:555:SER:N	2.29	0.47
1:B:706:TYR:O	1:B:707:PHE:CG	2.67	0.47
1:B:726:VAL:HA	1:B:729:SER:OG	2.15	0.47
1:B:810:LEU:O	1:B:811:THR:C	2.58	0.47
1:B:1056:VAL:HG13	1:B:1056:VAL:O	2.15	0.47
1:B:1122:SER:O	1:B:1125:GLU:HB2	2.15	0.47
1:A:71:PHE:C	1:A:71:PHE:HD2	2.22	0.46
1:A:181:GLY:HA3	1:A:354:ALA:CB	2.44	0.46
1:A:212:LEU:HD13	1:A:215:LEU:HD12	1.95	0.46
1:A:249:VAL:O	1:A:249:VAL:HG12	2.15	0.46
1:A:484:ILE:CG2	1:A:496:ILE:CD1	2.91	0.46
1:A:554:THR:HG23	1:A:555:SER:N	2.31	0.46
1:A:566:GLN:CD	1:A:569:LEU:HD12	2.40	0.46
1:A:849:TYR:OH	1:A:976:ALA:HB2	2.15	0.46
1:A:1043:ARG:N	1:A:1044:PRO:CD	2.78	0.46
1:B:202:ILE:CD1	1:B:203:GLY:H	2.19	0.46
1:B:263:PHE:HD1	1:B:1188:ARG:NH2	2.14	0.46
1:B:271:GLU:OE2	1:B:271:GLU:C	2.57	0.46
1:B:314:THR:HG22	1:B:315:SER:N	2.30	0.46
1:B:538:ALA:O	1:B:541:LEU:HB3	2.15	0.46
1:B:812:THR:O	1:B:813:ARG:C	2.58	0.46
1:B:882:ASP:O	1:B:886:LEU:HG	2.16	0.46
1:B:885:GLU:CB	1:B:923:PRO:HG3	2.45	0.46
1:B:1127:ILE:O	1:B:1129:TYR:N	2.36	0.46
1:A:165:GLY:O	1:A:168:ASN:OD1	2.34	0.46
1:A:218:SER:CB	1:A:219:PRO:HD3	2.43	0.46
1:A:382:ASP:OD2	1:A:382:ASP:N	2.47	0.46
1:A:397:TYR:CB	1:A:398:PRO:HD2	2.46	0.46
1:A:711:ILE:CD1	1:A:832:ILE:CD1	2.94	0.46
1:A:718:GLY:HA3	1:A:837:ALA:HB2	1.97	0.46
1:A:894:THR:O	1:A:896:ALA:N	2.48	0.46
1:A:1023:LYS:C	1:A:1025:ASN:H	2.23	0.46
1:A:1056:VAL:O	1:A:1056:VAL:HG13	2.14	0.46
1:A:1255:GLN:O	1:A:1258:ALA:HB3	2.16	0.46
1:B:255:ALA:C	1:B:257:ILE:N	2.71	0.46
1:B:324:ILE:O	1:B:325:GLY:C	2.58	0.46
1:B:734:VAL:CG1	1:B:735:PHE:N	2.79	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:788:VAL:O	1:B:789:PHE:C	2.58	0.46
1:B:791:SER:O	1:B:795:GLN:CB	2.60	0.46
1:B:1216:LYS:HA	1:B:1216:LYS:CE	2.34	0.46
1:A:210:LEU:HD23	1:A:317:VAL:CG1	2.41	0.46
1:A:236:THR:O	1:A:239:GLU:HB2	2.14	0.46
1:A:282:ARG:O	1:A:283:LEU:C	2.58	0.46
1:A:303:TYR:CD1	1:A:303:TYR:C	2.93	0.46
1:A:318:ILE:O	1:A:735:PHE:HZ	1.99	0.46
1:A:716:ILE:HG13	1:A:717:ASN:N	2.30	0.46
1:A:994:TYR:N	1:A:996:LYS:HZ1	2.13	0.46
1:A:1026:MET:C	1:A:1028:GLU:H	2.23	0.46
1:B:464:GLU:C	1:B:466:ILE:N	2.74	0.46
1:B:604:GLU:OE1	1:B:617:ILE:HB	2.15	0.46
1:B:908:ARG:HD2	1:B:908:ARG:N	2.30	0.46
1:B:1137:SER:HB3	1:B:1140:GLU:HB3	1.96	0.46
1:A:604:GLU:OE2	1:A:616:GLY:HA3	2.15	0.46
1:A:796:ASP:O	1:A:797:VAL:CB	2.62	0.46
1:A:908:ARG:O	1:A:911:LYS:N	2.49	0.46
1:A:962:GLN:O	1:A:963:GLN:CB	2.63	0.46
1:A:1026:MET:HE3	1:A:1095:LYS:CD	2.43	0.46
1:A:1092:LEU:HD23	1:A:1093:ASP:N	2.30	0.46
1:B:35:VAL:HG21	1:B:355:ARG:NH2	2.29	0.46
1:B:116:GLY:O	1:B:117:ILE:C	2.58	0.46
1:B:281:LYS:O	1:B:285:ILE:HB	2.15	0.46
1:B:528:SER:OG	1:B:531:GLN:HG3	2.15	0.46
1:B:566:GLN:CD	1:B:569:LEU:HD12	2.40	0.46
1:B:994:TYR:N	1:B:996:LYS:HZ1	2.13	0.46
1:B:1225:VAL:HG13	1:B:1225:VAL:O	2.14	0.46
1:A:35:VAL:HA	1:A:359:TYR:CD2	2.50	0.46
1:A:71:PHE:CZ	1:A:328:LEU:HD11	2.51	0.46
1:A:308:LEU:HD12	1:A:751:PHE:CE2	2.51	0.46
1:A:428:GLY:O	1:A:432:THR:HG23	2.16	0.46
1:A:492:THR:C	1:A:494:ASP:H	2.24	0.46
1:A:604:GLU:OE1	1:A:617:ILE:HB	2.14	0.46
1:A:730:LYS:O	1:A:731:VAL:C	2.58	0.46
1:A:770:GLY:HA2	1:A:773:PHE:CE2	2.50	0.46
1:A:882:ASP:O	1:A:886:LEU:HG	2.15	0.46
1:A:902:THR:C	1:A:904:VAL:HG12	2.41	0.46
1:A:902:THR:CA	1:A:904:VAL:HG12	2.46	0.46
1:A:1019:THR:O	1:A:1020:GLN:HB3	2.14	0.46
1:B:150:ALA:O	1:B:151:ILE:C	2.58	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:311:TRP:CZ2	1:B:728:PHE:CE2	3.04	0.46
1:B:386:GLY:HA3	1:B:450:ASP:CA	2.37	0.46
1:B:480:ILE:C	1:B:482:GLU:N	2.70	0.46
1:B:775:LYS:O	1:B:776:ALA:C	2.58	0.46
1:B:921:GLN:CG	1:B:922:ILE:HD12	2.44	0.46
1:B:969:ASN:O	1:B:972:LEU:HB2	2.15	0.46
1:B:1022:LEU:O	1:B:1026:MET:HG2	2.16	0.46
1:A:257:ILE:HG23	1:A:258:ARG:N	2.30	0.46
1:A:762:SER:C	1:A:765:THR:HG22	2.41	0.46
1:A:841:THR:O	1:A:845:ILE:HG13	2.15	0.46
1:A:1062:LEU:C	1:A:1062:LEU:HD13	2.40	0.46
1:A:1218:ARG:C	1:A:1220:GLY:H	2.23	0.46
1:B:266:GLN:HB2	1:B:270:LEU:CD2	2.46	0.46
1:B:270:LEU:H	1:B:270:LEU:CD2	2.16	0.46
1:B:286:LYS:HE2	1:B:778:GLU:HG3	1.97	0.46
1:B:303:TYR:C	1:B:303:TYR:CD1	2.94	0.46
1:B:800:PHE:HA	1:B:803:PRO:HB3	1.97	0.46
1:B:897:ILE:O	1:B:898:GLU:C	2.58	0.46
1:B:962:GLN:O	1:B:963:GLN:CB	2.63	0.46
1:B:1043:ARG:N	1:B:1044:PRO:CD	2.79	0.46
1:B:1092:LEU:HD23	1:B:1093:ASP:N	2.30	0.46
1:B:1092:LEU:O	1:B:1093:ASP:HB3	2.16	0.46
1:A:346:PRO:O	1:A:347:ASN:C	2.54	0.46
1:A:1078:LEU:O	1:A:1081:ARG:N	2.48	0.46
1:B:131:PHE:CZ	1:B:185:LYS:NZ	2.75	0.46
1:B:170:ARG:HB2	1:B:174:ASP:CG	2.40	0.46
1:B:286:LYS:HE3	1:B:822:LYS:HZ1	1.80	0.46
1:B:727:ILE:HD11	1:B:753:LEU:CG	2.46	0.46
1:B:1142:VAL:HG22	1:B:1161:TYR:HE1	1.80	0.46
1:A:327:VAL:O	1:A:328:LEU:C	2.59	0.46
1:A:354:ALA:O	1:A:355:ARG:C	2.57	0.46
1:A:528:SER:OG	1:A:531:GLN:HG3	2.16	0.46
1:A:543:ARG:NH1	1:A:905:SER:HB3	2.31	0.46
1:A:1056:VAL:HG23	1:A:1060:GLN:HE22	1.81	0.46
1:A:1154:ILE:CD1	1:A:1161:TYR:CE2	2.96	0.46
1:B:207:GLY:HA3	1:B:211:THR:CA	2.44	0.46
1:B:267:LYS:HA	1:B:270:LEU:HD21	1.98	0.46
1:B:318:ILE:HD12	1:B:324:ILE:H	1.79	0.46
1:B:327:VAL:O	1:B:328:LEU:C	2.59	0.46
1:B:466:ILE:HD12	1:B:466:ILE:N	2.31	0.46
1:B:585:LEU:HD12	1:B:618:TYR:CE1	2.43	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:896:ALA:O	1:B:897:ILE:C	2.59	0.46
1:B:902:THR:CA	1:B:904:VAL:HG12	2.46	0.46
1:B:1033:PHE:CD1	1:B:1036:VAL:HG22	2.51	0.46
1:A:324:ILE:C	1:A:326:GLN:H	2.22	0.46
1:A:475:LEU:HD12	1:A:532:LYS:HG2	1.98	0.46
1:A:498:LYS:HZ3	1:A:502:GLU:CD	2.23	0.46
1:A:712:PHE:O	1:A:713:CYS:C	2.58	0.46
1:A:729:SER:CB	1:A:971:LEU:HB3	2.46	0.46
1:A:885:GLU:CB	1:A:923:PRO:HG3	2.46	0.46
1:A:973:VAL:O	1:A:974:PHE:C	2.59	0.46
1:A:1203:ASP:C	1:A:1204:THR:HG22	2.40	0.46
1:A:1252:THR:HG23	1:A:1255:GLN:CB	2.45	0.46
1:B:113:TYR:OH	1:B:950:ALA:HA	2.15	0.46
1:B:118:GLY:HA3	1:B:946:TYR:CZ	2.50	0.46
1:B:199:GLY:HA2	1:B:334:VAL:HG23	1.97	0.46
1:B:295:MET:HE3	1:B:298:ALA:CB	2.46	0.46
1:B:817:ASP:O	1:B:821:VAL:HG13	2.16	0.46
1:B:849:TYR:OH	1:B:976:ALA:HB2	2.16	0.46
1:B:1131:ASP:OD1	1:B:1134:ARG:HG3	2.15	0.46
1:A:531:GLN:O	1:A:532:LYS:C	2.57	0.46
1:A:549:LEU:N	1:A:549:LEU:CD1	2.79	0.46
1:A:817:ASP:O	1:A:821:VAL:HG13	2.15	0.46
1:A:875:LEU:C	1:A:875:LEU:HD23	2.41	0.46
1:A:1131:ASP:OD1	1:A:1134:ARG:HG3	2.15	0.46
1:B:165:GLY:O	1:B:168:ASN:OD1	2.34	0.46
1:B:203:GLY:O	1:B:215:LEU:HD21	2.16	0.46
1:B:475:LEU:HD12	1:B:532:LYS:HG2	1.98	0.46
1:B:1057:LYS:H	1:B:1060:GLN:NE2	2.13	0.46
1:A:118:GLY:C	1:A:121:VAL:HG22	2.41	0.45
1:A:227:ILE:HG22	1:A:228:TRP:N	2.31	0.45
1:A:472:GLU:OE1	1:A:472:GLU:HA	2.15	0.45
1:A:614:GLU:O	1:A:615:LYS:C	2.58	0.45
1:A:782:LYS:O	1:A:783:ARG:C	2.58	0.45
1:A:904:VAL:CG1	1:A:905:SER:N	2.78	0.45
1:A:974:PHE:O	1:A:978:VAL:HG12	2.15	0.45
1:A:986:GLN:C	1:A:988:SER:H	2.24	0.45
1:A:1095:LYS:H	1:A:1095:LYS:CD	2.29	0.45
1:A:1148:ALA:HB1	1:A:1179:ARG:O	2.14	0.45
1:A:1193:LEU:HB2	1:A:1223:CYS:CB	2.45	0.45
1:B:268:LYS:C	1:B:268:LYS:HD3	2.41	0.45
1:B:585:LEU:H	1:B:585:LEU:CD2	2.26	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:705:PRO:O	1:B:706:TYR:HB3	2.16	0.45
1:B:778:GLU:O	1:B:779:ILE:C	2.58	0.45
1:B:790:LYS:O	1:B:793:LEU:N	2.49	0.45
1:B:796:ASP:O	1:B:797:VAL:HB	2.15	0.45
1:B:851:TRP:CA	1:B:854:THR:HB	2.26	0.45
1:A:458:ASN:HD22	1:A:459:VAL:N	2.11	0.45
1:A:489:GLU:O	1:A:491:VAL:HG12	2.16	0.45
1:A:728:PHE:CD1	1:A:728:PHE:C	2.95	0.45
1:A:886:LEU:HD12	1:A:886:LEU:C	2.41	0.45
1:A:921:GLN:HG2	1:A:922:ILE:HD13	1.98	0.45
1:A:969:ASN:HD22	1:A:969:ASN:C	2.15	0.45
1:A:976:ALA:O	1:A:979:PHE:HB2	2.16	0.45
1:A:1196:ASP:HA	1:A:1226:ILE:CG1	2.47	0.45
1:B:188:MET:HB2	1:B:347:ASN:HB3	1.97	0.45
1:B:235:PHE:O	1:B:239:GLU:HG2	2.16	0.45
1:B:326:GLN:HE21	1:B:329:THR:HG1	1.60	0.45
1:B:394:HIS:O	1:B:443:LEU:HB3	2.17	0.45
1:B:734:VAL:HG11	1:B:746:GLN:HB3	1.98	0.45
1:B:770:GLY:HA2	1:B:773:PHE:CE2	2.50	0.45
1:B:821:VAL:C	1:B:823:GLY:N	2.71	0.45
1:B:850:GLY:C	1:B:852:GLN:N	2.65	0.45
1:B:890:GLY:O	1:B:893:ALA:HB3	2.16	0.45
1:B:908:ARG:O	1:B:911:LYS:N	2.49	0.45
1:A:401:LYS:O	1:A:402:GLU:C	2.59	0.45
1:A:463:ARG:HG3	1:A:463:ARG:NH1	2.32	0.45
1:A:504:ASN:HB3	1:A:571:LYS:NZ	2.32	0.45
1:A:509:ILE:HD12	1:A:509:ILE:C	2.40	0.45
1:A:541:LEU:HD13	1:A:541:LEU:C	2.41	0.45
1:B:133:CYS:HB2	1:B:931:ALA:HB1	1.98	0.45
1:B:257:ILE:O	1:B:257:ILE:HD13	2.16	0.45
1:B:295:MET:C	1:B:297:ALA:N	2.73	0.45
1:B:381:PRO:HD2	1:B:461:TYR:CE2	2.51	0.45
1:B:478:THR:HG22	1:B:482:GLU:HG3	1.99	0.45
1:B:484:ILE:O	1:B:485:ARG:C	2.60	0.45
1:B:527:LEU:N	1:B:527:LEU:CD2	2.77	0.45
1:B:717:ASN:ND2	1:B:765:THR:CG2	2.79	0.45
1:B:821:VAL:CG2	1:B:822:LYS:N	2.80	0.45
1:B:948:SER:O	1:B:952:CYS:HB2	2.15	0.45
1:B:964:LEU:CD1	1:B:965:MET:H	2.18	0.45
1:B:1150:ILE:HD13	1:B:1176:GLN:HA	1.98	0.45
1:A:57:ALA:O	1:A:60:HIS:HB3	2.17	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:235:PHE:O	1:A:239:GLU:HG2	2.16	0.45
1:A:693:PHE:O	1:A:694:TRP:HB2	2.15	0.45
1:A:789:PHE:O	1:A:792:MET:HB2	2.16	0.45
1:A:804:LYS:N	1:A:804:LYS:HE3	2.32	0.45
1:A:820:GLN:CB	1:A:1000:SER:HB2	2.46	0.45
1:A:992:PRO:HB2	1:A:996:LYS:HE2	1.98	0.45
1:A:1020:GLN:OE1	1:A:1020:GLN:C	2.59	0.45
1:A:1063:ALA:CB	1:A:1239:ILE:HG13	2.46	0.45
1:A:1142:VAL:HG22	1:A:1161:TYR:HE1	1.80	0.45
1:B:359:TYR:O	1:B:362:PHE:HB3	2.16	0.45
1:B:580:VAL:HG22	1:B:581:ILE:N	2.31	0.45
1:B:949:TYR:HE2	1:B:977:ILE:HG21	1.82	0.45
1:B:1036:VAL:CG1	1:B:1052:LEU:HB3	2.45	0.45
1:A:261:ILE:C	1:A:263:PHE:N	2.64	0.45
1:A:286:LYS:CA	1:A:289:ILE:HB	2.40	0.45
1:A:413:VAL:HG21	1:A:419:VAL:CG1	2.47	0.45
1:A:533:GLN:HA	1:A:533:GLN:OE1	2.17	0.45
1:A:578:THR:OG1	1:A:579:ILE:N	2.47	0.45
1:A:717:ASN:ND2	1:A:765:THR:CG2	2.79	0.45
1:A:907:THR:N	1:A:908:ARG:NE	2.64	0.45
1:A:1020:GLN:HB3	1:A:1100:LEU:HD12	1.97	0.45
1:A:1032:GLN:HE21	1:A:1055:GLU:CB	2.29	0.45
1:A:1101:ASN:OD1	1:A:1103:GLN:HB3	2.17	0.45
1:B:71:PHE:HD2	1:B:71:PHE:O	1.98	0.45
1:B:114:TYR:CB	1:B:950:ALA:CB	2.95	0.45
1:B:114:TYR:HB3	1:B:950:ALA:CB	2.46	0.45
1:B:390:PHE:HZ	1:B:436:MET:HG2	1.82	0.45
1:B:428:GLY:O	1:B:431:THR:HB	2.16	0.45
1:B:504:ASN:HB3	1:B:571:LYS:NZ	2.31	0.45
1:B:578:THR:OG1	1:B:579:ILE:N	2.48	0.45
1:B:922:ILE:HB	1:B:923:PRO:CD	2.45	0.45
1:B:972:LEU:O	1:B:975:SER:CB	2.63	0.45
1:A:359:TYR:O	1:A:362:PHE:HB3	2.17	0.45
1:A:519:LEU:H	1:A:519:LEU:HD22	1.80	0.45
1:A:779:ILE:HG13	1:A:780:LEU:H	1.82	0.45
1:A:1033:PHE:CD1	1:A:1036:VAL:HG22	2.52	0.45
1:A:1036:VAL:CG1	1:A:1052:LEU:HB3	2.45	0.45
1:A:1119:PHE:O	1:A:1165:VAL:HG11	2.17	0.45
1:A:1157:LEU:O	1:A:1158:PRO:C	2.60	0.45
1:B:71:PHE:CZ	1:B:328:LEU:HD11	2.52	0.45
1:B:114:TYR:HB3	1:B:950:ALA:HB2	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:188:MET:O	1:B:189:PHE:C	2.58	0.45
1:B:202:ILE:C	1:B:204:PHE:H	2.24	0.45
1:B:318:ILE:CD1	1:B:324:ILE:H	2.29	0.45
1:B:346:PRO:O	1:B:349:GLU:HB3	2.16	0.45
1:B:712:PHE:O	1:B:713:CYS:C	2.59	0.45
1:A:47:ARG:O	1:A:48:LEU:C	2.58	0.45
1:A:136:ALA:HB2	1:A:182:ILE:CG2	2.47	0.45
1:A:152:MET:HG3	1:A:909:GLU:HG3	1.98	0.45
1:A:208:TRP:O	1:A:209:LYS:HE3	2.17	0.45
1:A:426:GLY:O	1:A:427:CYS:HB2	2.17	0.45
1:B:257:ILE:C	1:B:257:ILE:CD1	2.90	0.45
1:B:265:GLY:O	1:B:267:LYS:NZ	2.43	0.45
1:B:322:TYR:CE2	1:B:327:VAL:HG12	2.52	0.45
1:B:324:ILE:C	1:B:326:GLN:H	2.23	0.45
1:B:472:GLU:OE1	1:B:472:GLU:HA	2.16	0.45
1:B:559:THR:O	1:B:562:GLU:N	2.49	0.45
1:B:711:ILE:HG23	1:B:712:PHE:N	2.32	0.45
1:B:729:SER:CB	1:B:971:LEU:HB3	2.47	0.45
1:B:852:GLN:O	1:B:856:LEU:HB3	2.16	0.45
1:B:1056:VAL:HG23	1:B:1060:GLN:HE22	1.81	0.45
1:B:1195:LEU:N	1:B:1195:LEU:CD1	2.80	0.45
1:A:270:LEU:HB3	1:A:789:PHE:CE1	2.52	0.45
1:A:376:LYS:HZ1	1:A:377:SER:HB2	1.82	0.45
1:A:529:GLY:HA2	1:A:532:LYS:HD3	1.97	0.45
1:A:566:GLN:HA	1:A:569:LEU:CD1	2.47	0.45
1:A:603:VAL:CG2	1:A:604:GLU:H	2.09	0.45
1:A:718:GLY:CA	1:A:837:ALA:CB	2.94	0.45
1:A:788:VAL:HG21	1:A:1004:ILE:HD11	1.98	0.45
1:A:821:VAL:C	1:A:823:GLY:N	2.69	0.45
1:A:930:LYS:O	1:A:931:ALA:C	2.58	0.45
1:A:954:ARG:CD	1:A:954:ARG:C	2.90	0.45
1:A:1022:LEU:O	1:A:1022:LEU:HD22	2.17	0.45
1:A:1029:GLY:O	1:A:1031:VAL:HG23	2.16	0.45
1:B:301:LEU:O	1:B:304:ALA:HB3	2.17	0.45
1:B:431:THR:O	1:B:435:LEU:HD23	2.17	0.45
1:B:607:ASN:O	1:B:608:HIS:C	2.59	0.45
1:B:762:SER:C	1:B:765:THR:HG22	2.40	0.45
1:B:792:MET:HA	1:B:795:GLN:HB2	1.98	0.45
1:B:834:GLN:O	1:B:835:ASN:O	2.35	0.45
1:B:1075:VAL:O	1:B:1076:VAL:C	2.58	0.45
1:B:1095:LYS:H	1:B:1095:LYS:CD	2.30	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:295:MET:O	1:A:298:ALA:N	2.50	0.45
1:A:466:ILE:HD12	1:A:466:ILE:N	2.32	0.45
1:A:559:THR:O	1:A:560:GLU:C	2.60	0.45
1:A:792:MET:O	1:A:793:LEU:C	2.58	0.45
1:A:792:MET:HA	1:A:795:GLN:HB2	1.98	0.45
1:A:957:ALA:O	1:A:958:TYR:C	2.59	0.45
1:B:175:VAL:CG1	1:B:176:SER:N	2.79	0.45
1:B:282:ARG:O	1:B:283:LEU:C	2.60	0.45
1:B:711:ILE:CD1	1:B:832:ILE:CD1	2.94	0.45
1:B:820:GLN:HG3	1:B:1000:SER:HB2	1.98	0.45
1:B:857:LEU:C	1:B:857:LEU:HD23	2.41	0.45
1:B:902:THR:C	1:B:904:VAL:HG12	2.42	0.45
1:B:1037:VAL:HA	1:B:1049:LEU:O	2.16	0.45
1:A:110:TYR:O	1:A:111:ALA:C	2.60	0.45
1:A:314:THR:HG22	1:A:315:SER:N	2.31	0.45
1:A:322:TYR:CE2	1:A:327:VAL:HG12	2.52	0.45
1:A:374:PHE:CD2	1:A:374:PHE:C	2.95	0.45
1:A:389:GLU:OE1	1:A:412:LYS:HB2	2.16	0.45
1:A:734:VAL:CG1	1:A:735:PHE:N	2.79	0.45
1:A:1094:GLY:O	1:A:1095:LYS:O	2.35	0.45
1:B:549:LEU:N	1:B:549:LEU:CD1	2.79	0.45
1:B:716:ILE:HG13	1:B:717:ASN:N	2.30	0.45
1:B:728:PHE:O	1:B:732:VAL:HG22	2.17	0.45
1:B:903:VAL:HG23	1:B:906:LEU:HD12	1.98	0.45
1:B:1062:LEU:C	1:B:1062:LEU:HD13	2.41	0.45
1:B:1248:LYS:CG	1:B:1262:ILE:HD12	2.46	0.45
1:A:35:VAL:HG21	1:A:355:ARG:NH2	2.29	0.44
1:A:132:TRP:HB2	1:A:186:ILE:HG12	1.99	0.44
1:A:140:ILE:O	1:A:143:ILE:N	2.50	0.44
1:A:278:GLU:O	1:A:282:ARG:NH1	2.49	0.44
1:A:280:ALA:C	1:A:282:ARG:H	2.25	0.44
1:A:295:MET:HE3	1:A:298:ALA:CB	2.47	0.44
1:A:370:SER:OG	1:A:374:PHE:CD1	2.65	0.44
1:A:388:LEU:N	1:A:388:LEU:CD1	2.80	0.44
1:A:436:MET:O	1:A:436:MET:HE3	2.17	0.44
1:A:693:PHE:O	1:A:693:PHE:CD1	2.70	0.44
1:A:827:SER:C	1:A:829:LEU:N	2.72	0.44
1:A:918:GLN:O	1:A:919:SER:C	2.60	0.44
1:B:270:LEU:HD23	1:B:270:LEU:N	2.17	0.44
1:B:354:ALA:O	1:B:355:ARG:C	2.57	0.44
1:B:371:ILE:C	1:B:373:SER:N	2.74	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:537:ILE:O	1:B:540:ALA:N	2.51	0.44
1:B:795:GLN:CD	1:B:1012:PRO:HD3	2.42	0.44
1:B:899:ASN:HA	1:B:901:ARG:CZ	2.47	0.44
1:B:913:GLU:OE2	1:B:913:GLU:CA	2.64	0.44
1:B:954:ARG:C	1:B:954:ARG:CD	2.90	0.44
1:B:972:LEU:HA	1:B:975:SER:OG	2.18	0.44
1:B:1064:LEU:HB3	1:B:1226:ILE:HA	1.98	0.44
1:A:49:TYR:O	1:A:50:MET:C	2.60	0.44
1:A:303:TYR:O	1:A:306:TYR:N	2.50	0.44
1:A:404:GLN:HG2	1:A:404:GLN:O	2.18	0.44
1:A:721:GLN:HG3	1:A:979:PHE:CE1	2.51	0.44
1:A:1035:GLY:O	1:A:1036:VAL:C	2.59	0.44
1:A:1037:VAL:HG22	1:A:1087:ALA:HB3	1.99	0.44
1:A:1156:SER:O	1:A:1157:LEU:O	2.35	0.44
1:A:1178:GLN:OE1	1:A:1178:GLN:HA	2.17	0.44
1:B:136:ALA:HB2	1:B:182:ILE:CG2	2.47	0.44
1:B:314:THR:HG23	1:B:327:VAL:CG2	2.42	0.44
1:B:463:ARG:HG3	1:B:463:ARG:NH1	2.32	0.44
1:B:974:PHE:CB	2:B:6004:2J8:SE2	3.09	0.44
1:B:1179:ARG:O	1:B:1182:ILE:HB	2.18	0.44
1:A:89:THR:O	1:A:90:ASN:CG	2.60	0.44
1:A:109:THR:O	1:A:113:TYR:HB3	2.17	0.44
1:A:131:PHE:CZ	1:A:186:ILE:HG22	2.53	0.44
1:A:147:PHE:CG	1:A:365:ILE:HG12	2.52	0.44
1:A:175:VAL:CG1	1:A:176:SER:N	2.76	0.44
1:A:184:ASP:O	1:A:185:LYS:C	2.61	0.44
1:A:257:ILE:HG13	1:A:800:PHE:CD2	2.52	0.44
1:A:308:LEU:HA	1:A:751:PHE:HE2	1.81	0.44
1:A:471:GLN:OE1	1:A:472:GLU:N	2.46	0.44
1:A:732:VAL:O	1:A:736:THR:HG23	2.18	0.44
1:A:764:ILE:HG22	1:A:768:LEU:HD23	2.00	0.44
1:A:894:THR:HA	1:A:897:ILE:HD11	1.97	0.44
1:A:1027:LEU:N	1:A:1027:LEU:CD1	2.81	0.44
1:A:1150:ILE:HD13	1:A:1176:GLN:HA	1.99	0.44
1:B:506:TYR:O	1:B:509:ILE:HG13	2.17	0.44
1:B:509:ILE:HD13	1:B:516:PHE:CE1	2.52	0.44
1:B:519:LEU:H	1:B:519:LEU:HD22	1.82	0.44
1:B:537:ILE:O	1:B:539:ARG:N	2.51	0.44
1:B:539:ARG:O	1:B:542:VAL:N	2.50	0.44
1:B:559:THR:O	1:B:560:GLU:C	2.59	0.44
1:B:849:TYR:CD1	1:B:854:THR:HA	2.44	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1005:ILE:O	1:B:1006:ARG:C	2.60	0.44
1:B:1063:ALA:CB	1:B:1239:ILE:HG13	2.46	0.44
1:B:1119:PHE:O	1:B:1165:VAL:HG11	2.16	0.44
1:B:1192:ILE:HD13	1:B:1192:ILE:C	2.42	0.44
1:B:1217:ALA:O	1:B:1221:ARG:HD3	2.16	0.44
1:A:509:ILE:HD13	1:A:516:PHE:CE1	2.52	0.44
1:A:510:MET:SD	1:A:515:GLN:OE1	2.76	0.44
1:A:609:ASP:O	1:A:613:ARG:HB2	2.18	0.44
1:A:899:ASN:HA	1:A:901:ARG:CZ	2.47	0.44
1:A:996:LYS:HD3	1:A:996:LYS:N	2.12	0.44
1:A:1005:ILE:O	1:A:1006:ARG:C	2.60	0.44
1:A:1023:LYS:HD2	1:A:1095:LYS:NZ	2.32	0.44
1:A:1128:ALA:HB2	1:A:1141:ILE:CG2	2.38	0.44
1:B:132:TRP:HB2	1:B:186:ILE:HG12	1.99	0.44
1:B:345:SER:O	1:B:346:PRO:C	2.56	0.44
1:B:541:LEU:HD13	1:B:541:LEU:C	2.42	0.44
1:B:543:ARG:NH1	1:B:905:SER:CB	2.76	0.44
1:B:718:GLY:HA3	1:B:837:ALA:HB2	1.99	0.44
1:B:797:VAL:O	1:B:798:SER:C	2.60	0.44
1:B:1038:PHE:CD1	1:B:1039:ASN:N	2.85	0.44
1:B:1101:ASN:OD1	1:B:1103:GLN:HB3	2.18	0.44
1:A:266:GLN:HB2	1:A:270:LEU:CD2	2.47	0.44
1:A:286:LYS:CE	1:A:822:LYS:HZ2	2.30	0.44
1:A:406:LEU:HD11	1:A:432:THR:HG22	1.97	0.44
1:A:429:LYS:O	1:A:430:SER:C	2.61	0.44
1:A:468:VAL:CG2	1:A:549:LEU:HD13	2.47	0.44
1:A:536:ALA:O	1:A:537:ILE:O	2.36	0.44
1:A:791:SER:O	1:A:795:GLN:CB	2.62	0.44
1:A:821:VAL:CG2	1:A:822:LYS:N	2.80	0.44
1:A:921:GLN:HG2	1:A:922:ILE:HD12	1.99	0.44
1:A:972:LEU:HA	1:A:975:SER:OG	2.18	0.44
1:A:1033:PHE:O	1:A:1053:SER:HA	2.17	0.44
1:A:1195:LEU:O	1:A:1226:ILE:HG13	2.18	0.44
1:B:39:PHE:CZ	1:B:178:ILE:HG23	2.53	0.44
1:B:239:GLU:O	1:B:243:TYR:HB2	2.17	0.44
1:B:764:ILE:HG22	1:B:768:LEU:HD23	2.00	0.44
1:B:788:VAL:O	1:B:791:SER:HB2	2.18	0.44
1:B:802:ASP:CG	1:B:1041:PRO:HB2	2.43	0.44
1:B:938:PHE:O	1:B:941:THR:N	2.50	0.44
1:B:974:PHE:CE2	1:B:978:VAL:HB	2.53	0.44
1:B:1156:SER:O	1:B:1157:LEU:O	2.36	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:279:GLU:HG2	1:A:782:LYS:CD	2.47	0.44
1:A:369:PRO:C	1:A:370:SER:O	2.59	0.44
1:A:431:THR:O	1:A:434:GLN:HB3	2.18	0.44
1:A:559:THR:O	1:A:562:GLU:N	2.51	0.44
1:A:585:LEU:HD22	1:A:585:LEU:N	2.31	0.44
1:A:766:PHE:O	1:A:767:PHE:C	2.60	0.44
1:A:915:MET:O	1:A:918:GLN:HB2	2.17	0.44
1:A:1038:PHE:CD1	1:A:1039:ASN:N	2.86	0.44
1:A:1114:GLN:OE1	1:A:1197:GLU:HB2	2.17	0.44
1:A:1204:THR:HG23	1:A:1205:GLU:N	2.33	0.44
1:B:78:PHE:HZ	1:B:967:PHE:O	2.01	0.44
1:B:142:LYS:O	1:B:143:ILE:C	2.61	0.44
1:B:398:PRO:O	1:B:400:ARG:N	2.47	0.44
1:B:718:GLY:CA	1:B:837:ALA:CB	2.95	0.44
1:B:727:ILE:HG22	1:B:728:PHE:N	2.33	0.44
1:B:977:ILE:O	1:B:980:GLY:N	2.50	0.44
1:B:1032:GLN:HE21	1:B:1055:GLU:CB	2.28	0.44
1:A:112:TYR:CD2	1:A:112:TYR:N	2.85	0.44
1:A:147:PHE:O	1:A:148:PHE:C	2.61	0.44
1:A:247:GLY:O	1:A:250:ALA:HB3	2.17	0.44
1:A:438:ARG:CZ	1:A:455:ARG:HA	2.48	0.44
1:A:833:PHE:CG	1:A:834:GLN:N	2.86	0.44
1:A:967:PHE:N	1:A:967:PHE:CD2	2.86	0.44
1:A:1014:ILE:CD1	1:A:1106:ARG:HH12	2.27	0.44
1:A:1027:LEU:CD1	1:A:1027:LEU:H	2.30	0.44
1:A:1030:ASN:HA	1:A:1056:VAL:O	2.17	0.44
1:B:81:VAL:HG13	1:B:99:MET:HG3	2.00	0.44
1:B:89:THR:O	1:B:90:ASN:CG	2.60	0.44
1:B:150:ALA:O	1:B:153:ASN:N	2.41	0.44
1:B:282:ARG:HD3	1:B:282:ARG:HA	1.81	0.44
1:B:361:VAL:O	1:B:365:ILE:CD1	2.63	0.44
1:B:468:VAL:CG2	1:B:549:LEU:HD13	2.47	0.44
1:B:498:LYS:HZ3	1:B:502:GLU:CD	2.26	0.44
1:B:507:ASP:O	1:B:508:PHE:C	2.58	0.44
1:B:688:VAL:HB	1:B:1006:ARG:HH22	1.82	0.44
1:B:754:LEU:C	1:B:754:LEU:HD23	2.42	0.44
1:B:885:GLU:HB3	1:B:923:PRO:CG	2.48	0.44
1:B:1196:ASP:HA	1:B:1226:ILE:CG1	2.48	0.44
1:B:1202:LEU:HG	1:B:1203:ASP:N	2.21	0.44
1:A:258:ARG:O	1:A:261:ILE:N	2.51	0.44
1:A:267:LYS:HB3	1:A:790:LYS:HE3	1.99	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:268:LYS:C	1:A:268:LYS:HD3	2.41	0.44
1:A:282:ARG:HD3	1:A:282:ARG:HA	1.82	0.44
1:A:303:TYR:O	1:A:306:TYR:CB	2.60	0.44
1:A:449:ILE:HG21	1:A:457:ILE:HD13	2.00	0.44
1:A:476:PHE:O	1:A:520:VAL:HB	2.18	0.44
1:A:580:VAL:HG22	1:A:581:ILE:N	2.32	0.44
1:A:711:ILE:O	1:A:714:ALA:HB3	2.17	0.44
1:A:726:VAL:HA	1:A:729:SER:OG	2.18	0.44
1:A:925:ARG:HG2	1:B:514:HIS:ND1	2.33	0.44
1:A:974:PHE:CE2	1:A:978:VAL:HB	2.52	0.44
1:A:1023:LYS:HD2	1:A:1095:LYS:CE	2.48	0.44
1:A:1195:LEU:N	1:A:1195:LEU:CD1	2.81	0.44
1:B:118:GLY:C	1:B:121:VAL:HG22	2.40	0.44
1:B:227:ILE:HG22	1:B:228:TRP:N	2.32	0.44
1:B:431:THR:HG22	1:B:435:LEU:HD23	1.99	0.44
1:B:449:ILE:HG21	1:B:457:ILE:HD13	2.00	0.44
1:B:510:MET:SD	1:B:515:GLN:OE1	2.76	0.44
1:B:584:ARG:O	1:B:585:LEU:C	2.61	0.44
1:B:689:PRO:N	1:B:690:PRO:CD	2.81	0.44
1:B:766:PHE:O	1:B:767:PHE:C	2.61	0.44
1:B:788:VAL:HG21	1:B:1004:ILE:HD11	1.99	0.44
1:B:1252:THR:CG2	1:B:1255:GLN:HB2	2.47	0.44
1:A:39:PHE:CZ	1:A:178:ILE:HG23	2.53	0.44
1:A:147:PHE:CE2	1:A:365:ILE:HG12	2.53	0.44
1:A:214:ILE:HA	1:A:331:PHE:CE2	2.53	0.44
1:A:584:ARG:C	1:A:586:SER:N	2.75	0.44
1:A:927:ALA:HA	1:A:930:LYS:HG2	1.99	0.44
1:A:969:ASN:O	1:A:972:LEU:HB2	2.18	0.44
1:A:1049:LEU:HD11	1:A:1052:LEU:HD22	2.00	0.44
1:B:112:TYR:N	1:B:112:TYR:CD2	2.86	0.44
1:B:208:TRP:O	1:B:209:LYS:HG2	2.18	0.44
1:B:476:PHE:O	1:B:520:VAL:HB	2.18	0.44
1:A:72:GLY:HA2	1:A:326:GLN:CD	2.41	0.43
1:A:255:ALA:C	1:A:257:ILE:N	2.73	0.43
1:A:394:HIS:HB2	1:A:444:ASP:HB3	1.99	0.43
1:A:711:ILE:HG23	1:A:712:PHE:N	2.33	0.43
1:A:1059:GLY:HA2	1:A:1222:THR:N	2.33	0.43
1:A:1167:ASP:O	1:A:1167:ASP:CG	2.61	0.43
1:B:60:HIS:O	1:B:63:ALA:CB	2.65	0.43
1:B:119:ALA:O	1:B:120:GLY:C	2.60	0.43
1:B:210:LEU:HD23	1:B:317:VAL:CG1	2.41	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:459:VAL:O	1:B:460:ARG:C	2.60	0.43
1:B:514:HIS:HB2	1:B:518:THR:OG1	2.18	0.43
1:B:699:LEU:O	1:B:703:GLU:CD	2.61	0.43
1:B:755:PHE:O	1:B:756:LEU:C	2.60	0.43
1:B:777:GLY:HA3	1:B:822:LYS:HG3	2.00	0.43
1:A:156:ILE:HG23	1:A:439:LEU:CD1	2.48	0.43
1:A:185:LYS:NZ	1:A:186:ILE:HG22	2.33	0.43
1:A:281:LYS:O	1:A:285:ILE:HB	2.18	0.43
1:A:285:ILE:HG22	1:A:286:LYS:HD2	1.99	0.43
1:A:527:LEU:N	1:A:527:LEU:CD2	2.77	0.43
1:A:936:ILE:HG23	1:A:937:THR:H	1.83	0.43
1:A:1037:VAL:HA	1:A:1049:LEU:O	2.18	0.43
1:B:57:ALA:O	1:B:60:HIS:HB3	2.17	0.43
1:B:109:THR:O	1:B:113:TYR:HB3	2.17	0.43
1:B:148:PHE:HD2	1:B:913:GLU:OE2	2.01	0.43
1:B:151:ILE:C	1:B:153:ASN:N	2.75	0.43
1:B:175:VAL:CG1	1:B:176:SER:H	2.31	0.43
1:B:388:LEU:HD22	1:B:413:VAL:HG11	2.00	0.43
1:B:1154:ILE:HD12	1:B:1161:TYR:CE2	2.53	0.43
1:A:377:SER:O	1:A:458:ASN:ND2	2.51	0.43
1:A:751:PHE:CD1	1:A:752:SER:N	2.86	0.43
1:A:905:SER:C	1:A:907:THR:N	2.76	0.43
1:B:159:PHE:HD2	1:B:440:TYR:OH	2.00	0.43
1:B:339:PHE:CZ	2:B:6003:2J8:C21	3.01	0.43
1:B:533:GLN:HA	1:B:533:GLN:OE1	2.18	0.43
1:B:535:ILE:H	1:B:535:ILE:HG12	1.48	0.43
1:B:784:LEU:O	1:B:788:VAL:HG23	2.18	0.43
1:B:823:GLY:O	1:B:824:ALA:C	2.60	0.43
1:B:936:ILE:O	1:B:937:THR:C	2.60	0.43
1:B:1049:LEU:HD11	1:B:1052:LEU:HD22	2.00	0.43
1:B:1056:VAL:HG21	1:B:1062:LEU:HB2	2.00	0.43
1:B:1167:ASP:O	1:B:1167:ASP:CG	2.60	0.43
1:A:291:ALA:CA	1:A:294:SER:HB2	2.39	0.43
1:A:482:GLU:O	1:A:484:ILE:N	2.51	0.43
1:A:717:ASN:O	1:A:720:LEU:HB3	2.18	0.43
1:A:727:ILE:HD11	1:A:753:LEU:HD23	2.00	0.43
1:B:428:GLY:O	1:B:432:THR:HG23	2.19	0.43
1:B:592:ASP:O	1:B:593:VAL:HB	2.19	0.43
1:B:821:VAL:HG23	1:B:822:LYS:N	2.34	0.43
1:B:833:PHE:O	1:B:834:GLN:C	2.61	0.43
1:B:860:ILE:CG2	1:B:948:SER:HB3	2.48	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:891:LYS:O	1:B:892:ILE:C	2.60	0.43
1:B:1114:GLN:OE1	1:B:1197:GLU:HB2	2.18	0.43
1:B:1193:LEU:HB2	1:B:1223:CYS:CB	2.48	0.43
1:B:1260:LYS:HA	1:B:1264:PHE:HB2	2.00	0.43
1:A:95:ASP:O	1:A:99:MET:HB2	2.18	0.43
1:A:172:THR:O	1:A:175:VAL:CG1	2.66	0.43
1:A:239:GLU:O	1:A:243:TYR:HB2	2.17	0.43
1:A:287:LYS:HA	1:A:290:THR:OG1	2.19	0.43
1:A:347:ASN:O	1:A:348:ILE:C	2.61	0.43
1:A:388:LEU:HD22	1:A:413:VAL:HG11	2.01	0.43
1:A:492:THR:HB	1:A:495:GLU:OE2	2.18	0.43
1:A:497:GLU:O	1:A:498:LYS:C	2.61	0.43
1:A:534:ARG:O	1:A:535:ILE:C	2.61	0.43
1:A:607:ASN:O	1:A:608:HIS:C	2.61	0.43
1:A:718:GLY:HA3	1:A:837:ALA:CB	2.48	0.43
1:A:757:ILE:HG23	1:A:761:ILE:HD12	2.01	0.43
1:A:790:LYS:O	1:A:791:SER:C	2.61	0.43
1:A:820:GLN:HG3	1:A:1000:SER:HB3	1.95	0.43
1:A:1019:THR:OG1	1:A:1101:ASN:CA	2.63	0.43
1:A:1042:THR:O	1:A:1042:THR:HG23	2.18	0.43
1:A:1151:HIS:HA	1:A:1154:ILE:HB	2.01	0.43
1:A:1175:GLY:O	1:A:1179:ARG:HG3	2.17	0.43
1:B:131:PHE:CZ	1:B:186:ILE:HG22	2.52	0.43
1:B:132:TRP:CG	1:B:183:GLY:HA3	2.53	0.43
1:B:307:ALA:HB1	1:B:754:LEU:HD22	1.99	0.43
1:B:387:ASN:N	1:B:450:ASP:HA	2.33	0.43
1:B:1010:LYS:HB3	1:B:1012:PRO:HD2	2.00	0.43
1:A:71:PHE:HD2	1:A:71:PHE:O	2.02	0.43
1:A:140:ILE:HG13	1:A:179:ASN:ND2	2.23	0.43
1:A:295:MET:C	1:A:297:ALA:N	2.74	0.43
1:A:857:LEU:O	1:A:860:ILE:N	2.51	0.43
1:A:971:LEU:HD22	1:A:971:LEU:N	2.34	0.43
1:A:1150:ILE:O	1:A:1150:ILE:HG13	2.19	0.43
1:B:158:TRP:O	1:B:158:TRP:HD1	2.01	0.43
1:B:404:GLN:O	1:B:404:GLN:HG2	2.17	0.43
1:B:405:ILE:HD12	1:B:427:CYS:CB	2.48	0.43
1:B:721:GLN:HG3	1:B:979:PHE:CE1	2.51	0.43
1:B:722:PRO:HG3	1:B:979:PHE:CZ	2.54	0.43
1:B:786:TYR:HE2	1:B:790:LYS:NZ	2.17	0.43
1:B:802:ASP:CB	1:B:1041:PRO:HB2	2.48	0.43
1:B:927:ALA:HA	1:B:930:LYS:HG2	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1035:GLY:O	1:B:1036:VAL:C	2.60	0.43
1:A:150:ALA:O	1:A:153:ASN:N	2.43	0.43
1:A:552:GLU:C	1:A:554:THR:H	2.27	0.43
1:A:692:SER:OG	1:A:692:SER:O	2.37	0.43
1:A:754:LEU:C	1:A:754:LEU:HD23	2.44	0.43
1:A:764:ILE:O	1:A:768:LEU:HD23	2.19	0.43
1:A:785:ARG:NH2	1:A:815:ALA:HA	2.30	0.43
1:A:793:LEU:C	1:A:795:GLN:N	2.77	0.43
1:A:838:ASN:OD1	1:A:838:ASN:C	2.62	0.43
1:A:857:LEU:HD23	1:A:857:LEU:C	2.43	0.43
1:A:1252:THR:CG2	1:A:1255:GLN:HB2	2.48	0.43
1:B:283:LEU:HA	1:B:778:GLU:OE2	2.18	0.43
1:B:438:ARG:CZ	1:B:455:ARG:HA	2.48	0.43
1:B:727:ILE:HD11	1:B:753:LEU:HD23	2.00	0.43
1:B:834:GLN:O	1:B:835:ASN:C	2.62	0.43
1:B:934:PHE:H	1:B:934:PHE:HD1	1.66	0.43
1:B:1031:VAL:HB	1:B:1056:VAL:CG1	2.49	0.43
1:B:1123:ILE:HG12	1:B:1124:ALA:H	1.82	0.43
1:B:1150:ILE:O	1:B:1150:ILE:HG13	2.18	0.43
1:B:1196:ASP:HA	1:B:1226:ILE:HG13	2.00	0.43
1:A:114:TYR:CG	1:A:950:ALA:CB	3.01	0.43
1:A:279:GLU:CG	1:A:782:LYS:HD2	2.48	0.43
1:A:308:LEU:CA	1:A:751:PHE:HE2	2.32	0.43
1:A:393:ILE:CG1	1:A:409:LEU:HB3	2.48	0.43
1:A:757:ILE:O	1:A:758:LEU:C	2.62	0.43
1:A:1123:ILE:HG12	1:A:1124:ALA:N	2.33	0.43
1:A:1250:HIS:N	1:A:1256:LEU:HD21	2.34	0.43
1:B:136:ALA:CB	1:B:182:ILE:HB	2.40	0.43
1:B:320:LYS:O	1:B:321:GLU:O	2.36	0.43
1:B:389:GLU:OE1	1:B:412:LYS:HB2	2.18	0.43
1:B:751:PHE:CG	1:B:752:SER:N	2.86	0.43
1:B:930:LYS:O	1:B:931:ALA:C	2.62	0.43
1:B:1138:TYR:O	1:B:1141:ILE:HG12	2.18	0.43
1:B:1143:ARG:O	1:B:1146:LYS:HB2	2.18	0.43
1:A:67:MET:HE2	1:A:117:ILE:CG2	2.33	0.43
1:A:119:ALA:O	1:A:120:GLY:C	2.61	0.43
1:A:286:LYS:HZ2	1:A:822:LYS:NZ	2.16	0.43
1:A:351:PHE:CD1	1:A:351:PHE:C	2.96	0.43
1:A:387:ASN:N	1:A:450:ASP:HA	2.33	0.43
1:A:707:PHE:O	1:A:710:GLY:N	2.51	0.43
1:A:751:PHE:CG	1:A:752:SER:N	2.85	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:936:ILE:O	1:A:937:THR:C	2.62	0.43
1:B:72:GLY:HA2	1:B:326:GLN:CD	2.44	0.43
1:B:247:GLY:O	1:B:250:ALA:HB3	2.18	0.43
1:B:266:GLN:C	1:B:267:LYS:HG3	2.44	0.43
1:B:303:TYR:O	1:B:304:ALA:C	2.59	0.43
1:B:303:TYR:O	1:B:306:TYR:N	2.51	0.43
1:B:351:PHE:CD1	1:B:351:PHE:C	2.96	0.43
1:B:389:GLU:O	1:B:447:VAL:HA	2.19	0.43
1:B:435:LEU:HD13	1:B:435:LEU:HA	1.82	0.43
1:B:492:THR:H	1:B:495:GLU:CD	2.27	0.43
1:B:497:GLU:O	1:B:498:LYS:C	2.60	0.43
1:B:551:ASP:C	1:B:553:ALA:H	2.26	0.43
1:B:730:LYS:O	1:B:731:VAL:C	2.62	0.43
1:B:751:PHE:CD1	1:B:752:SER:N	2.87	0.43
1:B:1126:ASN:O	1:B:1129:TYR:CG	2.72	0.43
1:A:81:VAL:HG13	1:A:99:MET:HG3	2.01	0.43
1:A:151:ILE:C	1:A:153:ASN:N	2.76	0.43
1:A:217:ILE:HD11	1:A:331:PHE:HE2	1.84	0.43
1:A:495:GLU:O	1:A:496:ILE:C	2.61	0.43
1:A:601:VAL:HG13	1:A:601:VAL:O	2.19	0.43
1:A:727:ILE:HG22	1:A:728:PHE:N	2.34	0.43
1:A:1114:GLN:O	1:A:1116:PRO:HD3	2.19	0.43
1:A:1127:ILE:C	1:A:1129:TYR:N	2.77	0.43
1:B:413:VAL:HG21	1:B:419:VAL:CG1	2.48	0.43
1:B:492:THR:O	1:B:494:ASP:N	2.52	0.43
1:B:520:VAL:CG1	1:B:524:GLY:HA2	2.49	0.43
1:B:756:LEU:O	1:B:760:ILE:HB	2.17	0.43
1:B:814:LEU:HD22	1:B:814:LEU:N	2.34	0.43
1:B:1092:LEU:HB3	1:B:1097:ILE:CD1	2.44	0.43
1:B:1109:LEU:HD21	1:B:1188:ARG:NH1	2.33	0.43
1:A:102:LYS:HE3	1:A:102:LYS:CA	2.44	0.42
1:A:282:ARG:HB3	1:A:778:GLU:CG	2.45	0.42
1:A:318:ILE:HD11	1:A:324:ILE:H	1.84	0.42
1:A:421:LEU:HD12	1:A:421:LEU:N	2.34	0.42
1:A:492:THR:O	1:A:494:ASP:N	2.52	0.42
1:A:507:ASP:O	1:A:508:PHE:C	2.62	0.42
1:A:790:LYS:O	1:A:793:LEU:N	2.52	0.42
1:A:792:MET:CE	1:A:810:LEU:HD22	2.49	0.42
1:A:857:LEU:HD12	1:A:973:VAL:HG13	1.99	0.42
1:A:1022:LEU:O	1:A:1022:LEU:HD23	2.18	0.42
1:A:1026:MET:SD	1:A:1104:TRP:CH2	3.12	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:1197:GLU:O	1:A:1198:ALA:C	2.62	0.42
1:A:1204:THR:HG23	1:A:1206:SER:H	1.84	0.42
1:A:1229:ARG:HA	1:A:1229:ARG:HD2	1.81	0.42
1:B:54:THR:O	1:B:57:ALA:HB3	2.18	0.42
1:B:184:ASP:O	1:B:185:LYS:C	2.62	0.42
1:B:266:GLN:HB2	1:B:270:LEU:HD21	2.01	0.42
1:B:278:GLU:O	1:B:282:ARG:NH1	2.52	0.42
1:B:393:ILE:CG1	1:B:409:LEU:HB3	2.49	0.42
1:B:484:ILE:CG2	1:B:542:VAL:HG21	2.46	0.42
1:B:492:THR:HB	1:B:495:GLU:OE2	2.18	0.42
1:B:728:PHE:O	1:B:729:SER:C	2.61	0.42
1:B:857:LEU:O	1:B:860:ILE:N	2.52	0.42
1:B:936:ILE:HG23	1:B:937:THR:H	1.83	0.42
1:B:967:PHE:CD2	1:B:967:PHE:N	2.86	0.42
1:B:1143:ARG:HG2	1:B:1143:ARG:HH11	1.83	0.42
1:B:1178:GLN:OE1	1:B:1178:GLN:HA	2.19	0.42
1:A:38:MET:HE2	1:A:38:MET:HA	2.02	0.42
1:A:346:PRO:O	1:A:349:GLU:HB3	2.18	0.42
1:A:389:GLU:O	1:A:447:VAL:HA	2.19	0.42
1:A:402:GLU:CA	1:A:402:GLU:OE2	2.67	0.42
1:A:484:ILE:O	1:A:485:ARG:C	2.61	0.42
1:A:686:GLU:HB2	1:A:687:ASP:H	1.61	0.42
1:A:705:PRO:O	1:A:706:TYR:HB3	2.19	0.42
1:A:722:PRO:HG3	1:A:979:PHE:CZ	2.54	0.42
1:A:722:PRO:CB	1:A:841:THR:HB	2.50	0.42
1:A:810:LEU:O	1:A:813:ARG:N	2.52	0.42
1:A:827:SER:OG	1:A:994:TYR:HD2	2.02	0.42
1:A:993:ASP:O	1:A:994:TYR:HB3	2.18	0.42
1:A:1117:ILE:O	1:A:1184:ARG:NH2	2.53	0.42
1:A:1126:ASN:O	1:A:1127:ILE:C	2.61	0.42
1:A:1143:ARG:HG2	1:A:1143:ARG:HH11	1.84	0.42
1:A:1202:LEU:HG	1:A:1203:ASP:N	2.22	0.42
1:B:118:GLY:C	1:B:120:GLY:N	2.77	0.42
1:B:140:ILE:HG13	1:B:179:ASN:ND2	2.23	0.42
1:B:185:LYS:NZ	1:B:186:ILE:HG22	2.34	0.42
1:B:304:ALA:CA	1:B:758:LEU:HD23	2.49	0.42
1:B:304:ALA:O	1:B:307:ALA:HB3	2.19	0.42
1:B:473:PRO:HB3	1:B:533:GLN:CA	2.48	0.42
1:B:482:GLU:O	1:B:484:ILE:N	2.52	0.42
1:B:717:ASN:O	1:B:720:LEU:HB3	2.18	0.42
1:B:728:PHE:CD1	1:B:728:PHE:C	2.96	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:783:ARG:O	1:B:784:LEU:C	2.62	0.42
1:B:827:SER:OG	1:B:994:TYR:HD2	2.02	0.42
1:B:1218:ARG:C	1:B:1220:GLY:H	2.26	0.42
1:A:365:ILE:O	1:A:366:ASP:C	2.62	0.42
1:A:381:PRO:O	1:A:461:TYR:OH	2.33	0.42
1:A:449:ILE:HD13	1:A:450:ASP:HB2	2.01	0.42
1:A:549:LEU:C	1:A:550:LEU:HD12	2.44	0.42
1:A:693:PHE:C	1:A:695:ARG:N	2.77	0.42
1:A:699:LEU:O	1:A:703:GLU:CD	2.62	0.42
1:A:708:VAL:CG1	1:A:709:VAL:N	2.83	0.42
1:A:722:PRO:HB2	1:A:841:THR:HG21	2.01	0.42
1:A:857:LEU:O	1:A:858:LEU:C	2.62	0.42
1:A:892:ILE:CG1	1:A:916:TYR:HE1	2.32	0.42
1:A:1153:PHE:O	1:A:1157:LEU:HD23	2.19	0.42
1:A:1182:ILE:C	1:A:1184:ARG:N	2.76	0.42
1:A:1196:ASP:HA	1:A:1226:ILE:HG13	1.99	0.42
1:B:83:ASN:HD22	1:B:83:ASN:HA	1.53	0.42
1:B:375:SER:HB2	1:B:376:LYS:NZ	2.33	0.42
1:B:718:GLY:HA3	1:B:837:ALA:CB	2.49	0.42
1:B:732:VAL:O	1:B:736:THR:HG23	2.19	0.42
1:B:860:ILE:HG21	1:B:948:SER:HB3	2.01	0.42
1:B:931:ALA:O	1:B:932:HIS:C	2.60	0.42
1:B:964:LEU:CD1	1:B:965:MET:N	2.72	0.42
1:B:971:LEU:HD22	1:B:971:LEU:N	2.34	0.42
1:B:972:LEU:CD1	1:B:972:LEU:H	2.31	0.42
1:B:1081:ARG:HG2	1:B:1081:ARG:O	2.19	0.42
1:A:34:SER:O	1:A:35:VAL:C	2.63	0.42
1:A:214:ILE:HG12	1:A:331:PHE:CG	2.53	0.42
1:A:217:ILE:HD11	1:A:331:PHE:CE2	2.55	0.42
1:A:293:ILE:HG22	1:A:766:PHE:HB3	2.01	0.42
1:A:457:ILE:CD1	1:A:462:LEU:HD13	2.50	0.42
1:A:539:ARG:O	1:A:542:VAL:N	2.52	0.42
1:A:718:GLY:CA	1:A:837:ALA:HB2	2.50	0.42
1:A:758:LEU:O	1:A:759:GLY:C	2.62	0.42
1:A:885:GLU:HB3	1:A:923:PRO:CG	2.49	0.42
1:A:987:VAL:HG22	1:A:987:VAL:O	2.19	0.42
1:A:1023:LYS:HD2	1:A:1095:LYS:HE2	2.01	0.42
1:A:1039:ASN:CG	1:A:1047:PRO:HA	2.44	0.42
1:B:56:ALA:O	1:B:57:ALA:C	2.63	0.42
1:B:74:MET:SD	1:B:953:PHE:CE1	3.13	0.42
1:B:132:TRP:CD2	1:B:183:GLY:CA	3.03	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:433:VAL:O	1:B:436:MET:N	2.41	0.42
1:B:711:ILE:CD1	1:B:832:ILE:HG21	2.27	0.42
1:B:714:ALA:O	1:B:715:ILE:C	2.61	0.42
1:B:764:ILE:O	1:B:768:LEU:HD23	2.19	0.42
1:B:789:PHE:HD2	1:B:789:PHE:O	2.01	0.42
1:B:993:ASP:O	1:B:994:TYR:HB3	2.20	0.42
1:B:1050:GLN:HG2	1:B:1245:GLY:CA	2.49	0.42
1:A:54:THR:O	1:A:55:LEU:C	2.61	0.42
1:A:208:TRP:O	1:A:209:LYS:CE	2.68	0.42
1:A:369:PRO:O	1:A:370:SER:O	2.38	0.42
1:A:506:TYR:O	1:A:509:ILE:HG13	2.19	0.42
1:A:790:LYS:CB	1:A:794:ARG:NH2	2.82	0.42
1:A:1081:ARG:NH1	1:A:1098:LYS:C	2.77	0.42
1:B:38:MET:HE2	1:B:38:MET:HA	2.00	0.42
1:B:155:GLU:C	1:B:157:GLY:N	2.75	0.42
1:B:212:LEU:O	1:B:214:ILE:N	2.52	0.42
1:B:280:ALA:C	1:B:282:ARG:N	2.76	0.42
1:B:357:ALA:O	1:B:361:VAL:HG13	2.19	0.42
1:B:388:LEU:N	1:B:388:LEU:CD1	2.81	0.42
1:B:401:LYS:O	1:B:402:GLU:C	2.62	0.42
1:B:535:ILE:O	1:B:538:ALA:HB3	2.20	0.42
1:B:747:ASN:O	1:B:748:SER:C	2.63	0.42
1:B:757:ILE:HG23	1:B:761:ILE:HD12	2.02	0.42
1:B:792:MET:CE	1:B:810:LEU:HD22	2.49	0.42
1:B:859:ALA:O	1:B:863:ILE:CG1	2.60	0.42
1:B:1015:ASP:O	1:B:1016:SER:C	2.62	0.42
1:A:83:ASN:HD22	1:A:83:ASN:HA	1.50	0.42
1:A:132:TRP:CG	1:A:183:GLY:HA3	2.54	0.42
1:A:206:ARG:C	1:A:211:THR:HB	2.45	0.42
1:A:492:THR:H	1:A:495:GLU:CD	2.27	0.42
1:A:724:PHE:O	1:A:725:SER:C	2.60	0.42
1:A:848:ILE:O	1:A:849:TYR:O	2.38	0.42
1:A:972:LEU:CD1	1:A:972:LEU:H	2.33	0.42
1:A:1263:TYR:O	1:A:1266:MET:HB2	2.20	0.42
1:B:225:ALA:O	1:B:226:GLY:C	2.63	0.42
1:B:270:LEU:O	1:B:274:ASN:CG	2.62	0.42
1:B:315:SER:C	1:B:318:ILE:HG22	2.44	0.42
1:B:604:GLU:CD	1:B:617:ILE:H	2.27	0.42
1:B:838:ASN:OD1	1:B:838:ASN:C	2.62	0.42
1:B:1126:ASN:O	1:B:1127:ILE:C	2.62	0.42
1:B:1153:PHE:HA	1:B:1157:LEU:HD23	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:266:GLN:C	1:A:267:LYS:HG3	2.45	0.42
1:A:357:ALA:O	1:A:361:VAL:HG13	2.19	0.42
1:A:707:PHE:O	1:A:708:VAL:C	2.60	0.42
1:A:727:ILE:HD12	1:A:754:LEU:HA	2.01	0.42
1:A:732:VAL:CG2	1:A:971:LEU:HG	2.50	0.42
1:A:821:VAL:HG23	1:A:822:LYS:N	2.34	0.42
1:A:860:ILE:CG2	1:A:948:SER:HB3	2.50	0.42
1:B:75:THR:HB	1:B:326:GLN:HE22	1.84	0.42
1:B:207:GLY:C	1:B:209:LYS:N	2.78	0.42
1:B:318:ILE:HG23	1:B:735:PHE:CZ	2.54	0.42
1:B:379:HIS:CD2	1:B:380:LYS:N	2.84	0.42
1:B:429:LYS:O	1:B:430:SER:C	2.62	0.42
1:B:439:LEU:HB3	1:B:440:TYR:H	1.71	0.42
1:B:454:ILE:O	1:B:457:ILE:HG12	2.20	0.42
1:B:531:GLN:O	1:B:535:ILE:HG12	2.20	0.42
1:B:585:LEU:HD22	1:B:585:LEU:N	2.33	0.42
1:B:754:LEU:HD23	1:B:754:LEU:O	2.19	0.42
1:B:1153:PHE:O	1:B:1157:LEU:HD23	2.20	0.42
1:A:270:LEU:CB	1:A:789:PHE:CE1	3.02	0.42
1:A:394:HIS:O	1:A:443:LEU:HB3	2.19	0.42
1:A:483:ASN:O	1:A:486:TYR:HB2	2.20	0.42
1:A:509:ILE:HD11	1:A:510:MET:HG2	2.01	0.42
1:A:535:ILE:HG12	1:A:535:ILE:H	1.46	0.42
1:A:711:ILE:CG1	1:A:715:ILE:HD11	2.49	0.42
1:A:831:VAL:O	1:A:832:ILE:C	2.61	0.42
1:A:902:THR:O	1:A:903:VAL:C	2.63	0.42
1:A:934:PHE:HD1	1:A:934:PHE:H	1.66	0.42
1:A:935:GLY:O	1:A:936:ILE:C	2.62	0.42
1:A:968:GLU:O	1:A:971:LEU:HD23	2.20	0.42
1:A:1064:LEU:HB3	1:A:1226:ILE:HA	2.00	0.42
1:A:1143:ARG:O	1:A:1146:LYS:HB2	2.20	0.42
1:A:1241:VAL:HB	1:A:1249:GLU:HB2	2.00	0.42
1:B:147:PHE:O	1:B:148:PHE:C	2.61	0.42
1:B:349:GLU:O	1:B:352:ALA:HB3	2.20	0.42
1:B:365:ILE:O	1:B:366:ASP:C	2.63	0.42
1:B:376:LYS:HD2	1:B:376:LYS:N	2.35	0.42
1:B:727:ILE:HD12	1:B:754:LEU:CB	2.50	0.42
1:B:796:ASP:O	1:B:797:VAL:CB	2.67	0.42
1:B:1057:LYS:H	1:B:1057:LYS:CD	2.33	0.42
1:A:163:ASP:O	1:A:165:GLY:N	2.50	0.42
1:A:333:SER:O	1:A:336:ILE:HB	2.19	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:817:ASP:OD1	1:A:1000:SER:CB	2.68	0.42
1:A:827:SER:O	1:A:830:ALA:N	2.52	0.42
1:A:1022:LEU:HG	1:A:1104:TRP:HE1	1.74	0.42
1:B:49:TYR:OH	1:B:130:SER:CB	2.60	0.42
1:B:509:ILE:HD11	1:B:510:MET:HG2	2.01	0.42
1:B:549:LEU:C	1:B:550:LEU:HD12	2.45	0.42
1:B:724:PHE:O	1:B:725:SER:C	2.63	0.42
1:B:765:THR:CG2	1:B:766:PHE:N	2.83	0.42
1:B:1043:ARG:CZ	1:B:1086:MET:HE3	2.50	0.42
1:A:74:MET:SD	1:A:953:PHE:HE1	2.38	0.42
1:A:173:ASP:O	1:A:177:LYS:HG3	2.19	0.42
1:A:263:PHE:CE1	1:A:1129:TYR:HB3	2.54	0.42
1:A:303:TYR:O	1:A:304:ALA:C	2.60	0.42
1:A:307:ALA:HB1	1:A:754:LEU:HD22	1.98	0.42
1:A:373:SER:O	1:A:374:PHE:CB	2.44	0.42
1:A:388:LEU:HD12	1:A:388:LEU:H	1.84	0.42
1:A:421:LEU:O	1:A:581:ILE:HD12	2.20	0.42
1:A:710:GLY:O	1:A:713:CYS:SG	2.76	0.42
1:A:823:GLY:O	1:A:824:ALA:C	2.63	0.42
1:A:827:SER:O	1:A:829:LEU:N	2.52	0.42
1:A:833:PHE:O	1:A:834:GLN:C	2.61	0.42
1:A:1001:ALA:O	1:A:1005:ILE:CG1	2.63	0.42
1:A:1052:LEU:HG	1:A:1054:LEU:CD2	2.50	0.42
1:A:1063:ALA:HA	1:A:1225:VAL:CG1	2.49	0.42
1:A:1131:ASP:OD2	1:A:1188:ARG:NE	2.53	0.42
1:B:91:MET:H	1:B:91:MET:HG3	1.49	0.42
1:B:347:ASN:O	1:B:348:ILE:C	2.63	0.42
1:B:388:LEU:HD12	1:B:388:LEU:H	1.85	0.42
1:B:490:ASP:O	1:B:491:VAL:CB	2.68	0.42
1:B:552:GLU:HB3	1:B:555:SER:OG	2.19	0.42
1:B:609:ASP:O	1:B:613:ARG:HB2	2.20	0.42
1:B:749:ASN:O	1:B:752:SER:N	2.53	0.42
1:B:921:GLN:CG	1:B:922:ILE:N	2.81	0.42
1:B:1042:THR:O	1:B:1042:THR:HG23	2.20	0.42
1:B:1058:LYS:HB2	1:B:1058:LYS:HE3	1.86	0.42
1:B:1127:ILE:C	1:B:1129:TYR:N	2.77	0.42
1:B:1239:ILE:HD12	1:B:1239:ILE:H	1.84	0.42
1:A:75:THR:HB	1:A:326:GLN:HE22	1.84	0.41
1:A:318:ILE:CG1	1:A:735:PHE:CZ	3.03	0.41
1:A:534:ARG:HH21	1:A:564:VAL:CG1	2.29	0.41
1:A:714:ALA:O	1:A:715:ILE:C	2.63	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:789:PHE:O	1:A:789:PHE:HD2	2.03	0.41
1:A:891:LYS:O	1:A:892:ILE:C	2.59	0.41
1:A:1011:THR:O	1:A:1011:THR:HG23	2.20	0.41
1:B:844:ILE:O	1:B:847:LEU:HB2	2.20	0.41
1:B:867:ALA:O	1:B:870:VAL:HG12	2.20	0.41
1:B:1039:ASN:CG	1:B:1047:PRO:HA	2.44	0.41
1:B:1076:VAL:HG13	1:B:1194:LEU:CD1	2.45	0.41
1:B:1128:ALA:HB2	1:B:1141:ILE:CG2	2.38	0.41
1:B:1147:GLU:CB	1:B:1186:LEU:HD22	2.46	0.41
1:B:1241:VAL:HB	1:B:1249:GLU:HB2	2.01	0.41
1:B:1248:LYS:HG2	1:B:1262:ILE:CD1	2.48	0.41
1:B:1250:HIS:N	1:B:1256:LEU:HD21	2.35	0.41
1:A:462:LEU:O	1:A:463:ARG:C	2.63	0.41
1:A:764:ILE:O	1:A:765:THR:C	2.62	0.41
1:A:814:LEU:HD22	1:A:814:LEU:N	2.34	0.41
1:A:890:GLY:O	1:A:893:ALA:HB3	2.20	0.41
1:A:1052:LEU:HD11	1:A:1054:LEU:HD21	2.02	0.41
1:B:95:ASP:O	1:B:99:MET:HB2	2.20	0.41
1:B:229:ALA:HB1	1:B:299:PHE:CE2	2.54	0.41
1:B:239:GLU:HG3	1:B:288:ALA:HB2	1.98	0.41
1:B:462:LEU:O	1:B:463:ARG:C	2.61	0.41
1:B:489:GLU:O	1:B:491:VAL:HG12	2.19	0.41
1:B:611:LEU:HA	1:B:614:GLU:HB3	2.02	0.41
1:B:708:VAL:O	1:B:709:VAL:C	2.63	0.41
1:B:790:LYS:CB	1:B:794:ARG:NH2	2.82	0.41
1:B:843:ILE:O	1:B:846:SER:HB2	2.20	0.41
1:B:1113:SER:OG	1:B:1114:GLN:N	2.53	0.41
1:B:1114:GLN:O	1:B:1116:PRO:HD3	2.19	0.41
1:A:128:GLN:CG	1:A:129:VAL:N	2.82	0.41
1:A:155:GLU:HB3	1:A:156:ILE:CD1	2.45	0.41
1:A:239:GLU:HB3	1:A:285:ILE:HG13	1.99	0.41
1:A:266:GLN:HB2	1:A:270:LEU:HD21	2.01	0.41
1:A:318:ILE:CD1	1:A:324:ILE:H	2.32	0.41
1:A:466:ILE:HG22	1:A:468:VAL:HG23	2.02	0.41
1:A:490:ASP:O	1:A:491:VAL:CB	2.67	0.41
1:A:604:GLU:H	1:A:604:GLU:HG3	1.52	0.41
1:A:905:SER:O	1:A:907:THR:HG23	2.20	0.41
1:A:938:PHE:O	1:A:941:THR:N	2.53	0.41
1:A:1081:ARG:O	1:A:1081:ARG:HG2	2.20	0.41
1:A:1113:SER:OG	1:A:1114:GLN:N	2.52	0.41
1:A:1179:ARG:O	1:A:1182:ILE:HB	2.20	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:49:TYR:O	1:B:50:MET:C	2.62	0.41
1:B:100:PHE:O	1:B:103:LEU:HB3	2.21	0.41
1:B:147:PHE:CG	1:B:365:ILE:HG12	2.56	0.41
1:B:354:ALA:O	1:B:358:ALA:HB2	2.20	0.41
1:B:503:ALA:O	1:B:504:ASN:C	2.62	0.41
1:B:543:ARG:NH1	1:B:543:ARG:HG2	2.35	0.41
1:B:715:ILE:O	1:B:718:GLY:N	2.53	0.41
1:B:1028:GLU:O	1:B:1093:ASP:OD1	2.39	0.41
1:B:1076:VAL:HG13	1:B:1194:LEU:CD2	2.46	0.41
1:B:1151:HIS:HA	1:B:1154:ILE:HB	2.02	0.41
1:B:1157:LEU:O	1:B:1158:PRO:C	2.63	0.41
1:A:74:MET:SD	1:A:953:PHE:CD1	3.13	0.41
1:A:362:PHE:CA	1:A:365:ILE:HD12	2.47	0.41
1:A:467:GLY:H	1:A:545:PRO:HG3	1.82	0.41
1:A:478:THR:HG22	1:A:482:GLU:HG3	1.99	0.41
1:A:492:THR:O	1:A:493:MET:C	2.64	0.41
1:A:1000:SER:O	1:A:1004:ILE:HG22	2.20	0.41
1:A:1031:VAL:HB	1:A:1056:VAL:CG1	2.49	0.41
1:A:1050:GLN:HG2	1:A:1245:GLY:CA	2.49	0.41
1:A:1052:LEU:HG	1:A:1053:SER:H	1.84	0.41
1:A:1058:LYS:HB2	1:A:1058:LYS:HE3	1.87	0.41
1:A:1144:ALA:CA	1:A:1186:LEU:HD11	2.30	0.41
1:B:36:LEU:HD12	1:B:36:LEU:C	2.46	0.41
1:B:155:GLU:HB3	1:B:156:ILE:CD1	2.46	0.41
1:B:186:ILE:C	1:B:186:ILE:HD12	2.45	0.41
1:B:290:THR:CG2	1:B:771:PHE:HA	2.51	0.41
1:B:415:SER:HA	1:B:577:THR:HB	2.01	0.41
1:B:420:ALA:O	1:B:421:LEU:HD12	2.19	0.41
1:B:421:LEU:HD12	1:B:421:LEU:N	2.35	0.41
1:B:722:PRO:HB2	1:B:841:THR:HG21	2.03	0.41
1:B:787:MET:O	1:B:790:LYS:HB2	2.21	0.41
1:B:892:ILE:CG1	1:B:916:TYR:HE1	2.33	0.41
1:B:987:VAL:O	1:B:987:VAL:HG22	2.21	0.41
1:B:1131:ASP:OD2	1:B:1188:ARG:NE	2.53	0.41
1:B:1261:GLY:N	1:B:1264:PHE:HB3	2.20	0.41
1:A:270:LEU:O	1:A:274:ASN:CG	2.63	0.41
1:A:383:ASN:O	1:A:384:ILE:HB	2.20	0.41
1:A:592:ASP:O	1:A:593:VAL:HB	2.20	0.41
1:A:756:LEU:O	1:A:760:ILE:HB	2.20	0.41
1:A:834:GLN:O	1:A:835:ASN:C	2.64	0.41
1:A:961:THR:O	1:A:962:GLN:CB	2.69	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:967:PHE:CD1	1:A:968:GLU:N	2.88	0.41
1:A:1076:VAL:HG13	1:A:1194:LEU:CD1	2.45	0.41
1:A:1138:TYR:HA	1:A:1141:ILE:HG12	2.03	0.41
1:A:1147:GLU:CB	1:A:1186:LEU:HD22	2.48	0.41
1:A:1177:LYS:O	1:A:1180:ILE:N	2.53	0.41
1:A:1202:LEU:CG	1:A:1203:ASP:N	2.81	0.41
1:B:34:SER:O	1:B:35:VAL:C	2.63	0.41
1:B:133:CYS:HB3	1:B:931:ALA:CB	2.50	0.41
1:B:309:ALA:O	1:B:310:PHE:O	2.39	0.41
1:B:817:ASP:OD1	1:B:1000:SER:CB	2.68	0.41
1:B:928:MET:O	1:B:931:ALA:HB3	2.20	0.41
1:B:1102:VAL:CG1	1:B:1103:GLN:N	2.83	0.41
1:A:92:SER:O	1:A:96:LYS:HG3	2.20	0.41
1:A:103:LEU:HB2	1:A:960:VAL:HG23	2.02	0.41
1:A:186:ILE:C	1:A:186:ILE:HD12	2.46	0.41
1:A:747:ASN:O	1:A:748:SER:C	2.64	0.41
1:A:913:GLU:OE2	1:A:913:GLU:CA	2.63	0.41
1:A:1109:LEU:HD23	1:A:1109:LEU:N	2.35	0.41
1:A:1166:GLY:O	1:A:1167:ASP:CB	2.64	0.41
1:A:1182:ILE:O	1:A:1183:ALA:C	2.63	0.41
1:A:1192:ILE:HD13	1:A:1192:ILE:C	2.45	0.41
1:B:173:ASP:O	1:B:177:LYS:HG3	2.21	0.41
1:B:197:PHE:O	1:B:201:ILE:N	2.54	0.41
1:B:215:LEU:HA	1:B:219:PRO:CD	2.49	0.41
1:B:314:THR:O	1:B:316:LEU:N	2.54	0.41
1:B:727:ILE:HD11	1:B:753:LEU:HB3	2.01	0.41
1:B:764:ILE:O	1:B:765:THR:C	2.62	0.41
1:B:1078:LEU:O	1:B:1081:ARG:N	2.53	0.41
1:B:1150:ILE:O	1:B:1154:ILE:CG1	2.68	0.41
1:A:56:ALA:O	1:A:57:ALA:C	2.64	0.41
1:A:689:PRO:O	1:A:690:PRO:C	2.64	0.41
1:A:921:GLN:CG	1:A:922:ILE:N	2.84	0.41
1:A:954:ARG:HE	1:A:955:PHE:HA	1.85	0.41
1:A:978:VAL:HG22	2:A:6001:2J8:H29	2.01	0.41
1:A:993:ASP:N	1:A:996:LYS:HZ1	2.19	0.41
1:A:1043:ARG:CZ	1:A:1086:MET:HE3	2.50	0.41
1:A:1192:ILE:HA	1:A:1222:THR:O	2.21	0.41
1:A:1260:LYS:HA	1:A:1264:PHE:HB2	2.01	0.41
1:B:133:CYS:CB	1:B:931:ALA:HB1	2.50	0.41
1:B:295:MET:O	1:B:298:ALA:N	2.53	0.41
1:B:358:ALA:O	1:B:362:PHE:N	2.52	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:387:ASN:O	1:B:450:ASP:O	2.39	0.41
1:B:449:ILE:HD13	1:B:450:ASP:HB2	2.03	0.41
1:B:717:ASN:HB3	1:B:833:PHE:CE1	2.56	0.41
1:B:718:GLY:CA	1:B:837:ALA:HB2	2.51	0.41
1:B:776:ALA:O	1:B:780:LEU:HG	2.21	0.41
1:B:833:PHE:CG	1:B:834:GLN:N	2.88	0.41
1:B:968:GLU:O	1:B:971:LEU:HD23	2.21	0.41
1:B:1000:SER:O	1:B:1004:ILE:HG22	2.21	0.41
1:B:1052:LEU:HD11	1:B:1054:LEU:HD21	2.02	0.41
1:B:1109:LEU:HD23	1:B:1109:LEU:N	2.36	0.41
1:A:148:PHE:HB3	1:A:913:GLU:OE1	2.21	0.41
1:A:168:ASN:O	1:A:169:THR:C	2.64	0.41
1:A:229:ALA:HB1	1:A:299:PHE:CE2	2.55	0.41
1:A:354:ALA:O	1:A:358:ALA:HB2	2.19	0.41
1:A:480:ILE:O	1:A:482:GLU:N	2.54	0.41
1:A:727:ILE:HD11	1:A:753:LEU:HB3	2.02	0.41
1:A:730:LYS:NZ	1:A:750:LEU:HD21	2.36	0.41
1:A:788:VAL:O	1:A:791:SER:HB2	2.21	0.41
1:A:797:VAL:CG1	1:A:798:SER:H	2.20	0.41
1:A:814:LEU:H	1:A:814:LEU:CD2	2.34	0.41
1:A:1017:TYR:HB3	1:A:1018:SER:H	1.42	0.41
1:A:1056:VAL:HG21	1:A:1062:LEU:HB2	2.01	0.41
1:A:1065:VAL:HG13	1:A:1241:VAL:HG22	2.02	0.41
1:B:255:ALA:C	1:B:257:ILE:H	2.27	0.41
1:B:402:GLU:CA	1:B:402:GLU:OE2	2.68	0.41
1:B:491:VAL:HG23	1:B:495:GLU:OE1	2.21	0.41
1:B:507:ASP:OD1	1:B:508:PHE:N	2.37	0.41
1:B:604:GLU:H	1:B:604:GLU:HG3	1.51	0.41
1:B:762:SER:O	1:B:764:ILE:N	2.54	0.41
1:B:843:ILE:HA	1:B:846:SER:CB	2.50	0.41
1:B:946:TYR:CG	1:B:947:PHE:N	2.89	0.41
1:B:1059:GLY:HA2	1:B:1222:THR:N	2.35	0.41
1:B:1197:GLU:O	1:B:1198:ALA:C	2.63	0.41
1:A:36:LEU:HD12	1:A:36:LEU:C	2.46	0.41
1:A:39:PHE:CE2	1:A:358:ALA:HB3	2.52	0.41
1:A:132:TRP:C	1:A:132:TRP:CD1	2.99	0.41
1:A:214:ILE:HG21	1:A:334:VAL:HG11	2.01	0.41
1:A:251:GLU:O	1:A:252:GLU:HB2	2.21	0.41
1:A:267:LYS:O	1:A:790:LYS:NZ	2.52	0.41
1:A:282:ARG:HD3	1:A:286:LYS:NZ	2.36	0.41
1:A:311:TRP:CE3	1:A:311:TRP:CA	3.04	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:315:SER:C	1:A:318:ILE:HG22	2.45	0.41
1:A:358:ALA:O	1:A:362:PHE:N	2.54	0.41
1:A:362:PHE:CD1	1:A:362:PHE:C	2.98	0.41
1:A:415:SER:HA	1:A:577:THR:HB	2.03	0.41
1:A:438:ARG:O	1:A:439:LEU:O	2.39	0.41
1:A:711:ILE:HD11	1:A:832:ILE:CG2	2.29	0.41
1:A:713:CYS:SG	1:A:769:GLN:HB3	2.61	0.41
1:A:722:PRO:O	1:A:725:SER:OG	2.32	0.41
1:A:1022:LEU:O	1:A:1023:LYS:C	2.63	0.41
1:A:1109:LEU:HD23	1:A:1109:LEU:H	1.86	0.41
1:A:1153:PHE:HA	1:A:1157:LEU:HD23	2.02	0.41
1:B:58:ILE:H	1:B:58:ILE:CD1	2.33	0.41
1:B:110:TYR:O	1:B:111:ALA:C	2.62	0.41
1:B:178:ILE:HG13	1:B:178:ILE:H	1.73	0.41
1:B:185:LYS:HB3	1:B:185:LYS:HE3	1.90	0.41
1:B:268:LYS:NZ	1:B:272:ARG:HD3	2.36	0.41
1:B:276:ASN:HD22	1:B:276:ASN:HA	1.70	0.41
1:B:308:LEU:HD13	1:B:755:PHE:CD1	2.55	0.41
1:B:356:GLY:O	1:B:358:ALA:N	2.54	0.41
1:B:432:THR:OG1	1:B:433:VAL:N	2.53	0.41
1:B:434:GLN:C	1:B:436:MET:N	2.78	0.41
1:B:457:ILE:CD1	1:B:462:LEU:HD13	2.49	0.41
1:B:713:CYS:SG	1:B:769:GLN:HB3	2.61	0.41
1:B:730:LYS:NZ	1:B:750:LEU:HD21	2.36	0.41
1:B:733:GLY:O	1:B:734:VAL:C	2.64	0.41
1:B:757:ILE:O	1:B:758:LEU:C	2.63	0.41
1:B:757:ILE:HG22	1:B:758:LEU:N	2.35	0.41
1:B:774:GLY:O	1:B:775:LYS:C	2.64	0.41
1:B:789:PHE:O	1:B:792:MET:HB2	2.20	0.41
1:B:1007:ILE:C	1:B:1009:GLU:N	2.76	0.41
1:B:1037:VAL:HG22	1:B:1087:ALA:HB3	1.99	0.41
1:B:1052:LEU:HG	1:B:1054:LEU:CD2	2.50	0.41
1:B:1108:GLN:HE21	1:B:1108:GLN:H	1.68	0.41
1:B:1203:ASP:C	1:B:1204:THR:HG22	2.45	0.41
1:B:1233:ILE:O	1:B:1233:ILE:HG13	2.21	0.41
1:A:103:LEU:HD13	1:A:960:VAL:HG22	2.02	0.41
1:A:291:ALA:C	1:A:294:SER:H	2.29	0.41
1:A:318:ILE:HD12	1:A:322:TYR:O	2.21	0.41
1:A:349:GLU:O	1:A:352:ALA:HB3	2.21	0.41
1:A:364:ILE:HG22	1:A:364:ILE:O	2.20	0.41
1:A:604:GLU:CD	1:A:617:ILE:H	2.28	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:611:LEU:HA	1:A:614:GLU:HB3	2.03	0.41
1:A:783:ARG:O	1:A:784:LEU:C	2.62	0.41
1:A:1108:GLN:HE21	1:A:1108:GLN:H	1.68	0.41
1:A:1126:ASN:O	1:A:1129:TYR:CG	2.74	0.41
1:A:1233:ILE:O	1:A:1233:ILE:HG13	2.20	0.41
1:B:132:TRP:C	1:B:132:TRP:CD1	2.99	0.41
1:B:142:LYS:C	1:B:144:ARG:N	2.77	0.41
1:B:167:LEU:O	1:B:170:ARG:HG2	2.20	0.41
1:B:430:SER:O	1:B:433:VAL:HB	2.21	0.41
1:B:433:VAL:O	1:B:436:MET:HB2	2.21	0.41
1:B:466:ILE:HG22	1:B:468:VAL:HG23	2.03	0.41
1:B:722:PRO:HA	1:B:979:PHE:CE1	2.55	0.41
1:B:802:ASP:CG	1:B:1041:PRO:O	2.63	0.41
1:B:804:LYS:HE3	1:B:804:LYS:N	2.35	0.41
1:B:992:PRO:C	1:B:994:TYR:N	2.74	0.41
1:B:1027:LEU:HD23	1:B:1028:GLU:N	2.34	0.41
1:A:52:VAL:O	1:A:55:LEU:HB3	2.22	0.40
1:A:54:THR:O	1:A:57:ALA:HB3	2.22	0.40
1:A:167:LEU:O	1:A:170:ARG:HG2	2.21	0.40
1:A:207:GLY:C	1:A:209:LYS:N	2.78	0.40
1:A:214:ILE:HG12	1:A:331:PHE:CD2	2.56	0.40
1:A:279:GLU:CG	1:A:782:LYS:CD	2.99	0.40
1:A:295:MET:O	1:A:296:GLY:C	2.64	0.40
1:A:484:ILE:O	1:A:487:GLY:N	2.55	0.40
1:A:706:TYR:O	1:A:707:PHE:CD2	2.74	0.40
1:A:729:SER:HA	1:A:971:LEU:CB	2.50	0.40
1:A:1138:TYR:O	1:A:1141:ILE:HG12	2.21	0.40
1:A:1234:GLN:O	1:A:1236:ALA:N	2.51	0.40
1:A:1267:VAL:O	1:A:1270:GLN:HB3	2.21	0.40
1:B:298:ALA:O	1:B:302:ILE:CG1	2.68	0.40
1:B:298:ALA:C	1:B:302:ILE:HG13	2.46	0.40
1:B:310:PHE:HB3	1:B:311:TRP:H	1.61	0.40
1:B:362:PHE:CD1	1:B:362:PHE:C	2.99	0.40
1:B:433:VAL:CG1	1:B:549:LEU:HD23	2.48	0.40
1:B:855:LEU:O	1:B:856:LEU:C	2.63	0.40
1:B:914:THR:O	1:B:915:MET:C	2.64	0.40
1:B:1033:PHE:O	1:B:1053:SER:HA	2.21	0.40
1:B:1065:VAL:HG13	1:B:1241:VAL:HG22	2.03	0.40
1:A:132:TRP:CD2	1:A:183:GLY:CA	3.04	0.40
1:A:151:ILE:C	1:A:153:ASN:H	2.29	0.40
1:A:188:MET:O	1:A:189:PHE:C	2.60	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:212:LEU:O	1:A:214:ILE:N	2.55	0.40
1:A:318:ILE:HD11	1:A:324:ILE:HG12	2.02	0.40
1:A:436:MET:HE3	1:A:454:ILE:HD12	2.03	0.40
1:A:491:VAL:HG23	1:A:495:GLU:OE1	2.21	0.40
1:A:611:LEU:HB2	1:A:618:TYR:HD2	1.86	0.40
1:A:861:VAL:CB	1:A:862:PRO:CD	2.99	0.40
1:A:931:ALA:O	1:A:932:HIS:C	2.64	0.40
1:A:990:PHE:HB3	1:A:991:ALA:H	1.72	0.40
1:A:1109:LEU:HD21	1:A:1188:ARG:NH1	2.33	0.40
1:A:1218:ARG:O	1:A:1219:GLU:HB3	2.21	0.40
1:B:128:GLN:CG	1:B:129:VAL:N	2.83	0.40
1:B:151:ILE:C	1:B:153:ASN:H	2.29	0.40
1:B:258:ARG:O	1:B:261:ILE:N	2.54	0.40
1:B:404:GLN:HE21	1:B:404:GLN:HB3	1.64	0.40
1:B:473:PRO:O	1:B:532:LYS:HE2	2.22	0.40
1:B:601:VAL:O	1:B:601:VAL:HG13	2.20	0.40
1:B:726:VAL:O	1:B:727:ILE:C	2.65	0.40
1:B:967:PHE:CD1	1:B:968:GLU:N	2.87	0.40
1:B:993:ASP:N	1:B:996:LYS:HZ1	2.18	0.40
1:B:1071:GLY:O	1:B:1075:VAL:HG23	2.21	0.40
1:B:1173:SER:HB3	1:B:1176:GLN:HE22	1.85	0.40
1:B:1182:ILE:O	1:B:1183:ALA:C	2.62	0.40
1:B:1186:LEU:HD12	1:B:1186:LEU:C	2.46	0.40
1:B:1263:TYR:O	1:B:1266:MET:HB2	2.20	0.40
1:A:53:GLY:O	1:A:54:THR:C	2.63	0.40
1:A:158:TRP:O	1:A:158:TRP:HD1	2.03	0.40
1:A:258:ARG:C	1:A:260:VAL:N	2.78	0.40
1:A:298:ALA:C	1:A:302:ILE:HG13	2.45	0.40
1:A:977:ILE:O	1:A:980:GLY:N	2.53	0.40
1:A:1057:LYS:H	1:A:1057:LYS:CD	2.34	0.40
1:A:1261:GLY:N	1:A:1264:PHE:HB3	2.20	0.40
1:B:39:PHE:CE2	1:B:358:ALA:HB3	2.52	0.40
1:B:191:GLN:O	1:B:194:ALA:N	2.54	0.40
1:B:437:GLN:HE21	1:B:468:VAL:HG21	1.86	0.40
1:B:548:LEU:HD23	1:B:549:LEU:H	1.86	0.40
1:B:608:HIS:O	1:B:609:ASP:C	2.64	0.40
1:B:689:PRO:HG2	1:B:690:PRO:HD3	2.02	0.40
1:B:732:VAL:CG2	1:B:971:LEU:HG	2.51	0.40
1:B:765:THR:HG23	1:B:766:PHE:H	1.84	0.40
1:B:864:ILE:HD12	1:B:864:ILE:C	2.46	0.40
1:B:913:GLU:CA	1:B:916:TYR:HD2	2.31	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:B:1036:VAL:HB	1:B:1052:LEU:C	2.47	0.40
1:B:1165:VAL:O	1:B:1171:GLN:HG2	2.21	0.40
1:A:195:THR:HB	1:A:337:GLY:O	2.22	0.40
1:A:268:LYS:NZ	1:A:272:ARG:HD3	2.36	0.40
1:A:721:GLN:HB3	1:A:722:PRO:HD3	2.04	0.40
1:A:791:SER:CB	1:A:1010:LYS:HE2	2.52	0.40
1:A:799:TRP:O	1:A:803:PRO:CA	2.70	0.40
1:A:947:PHE:HD2	1:A:947:PHE:HA	1.77	0.40
1:A:969:ASN:CA	1:A:972:LEU:HD13	2.43	0.40
1:A:1083:TYR:CD1	1:A:1083:TYR:N	2.89	0.40
1:B:146:LYS:O	1:B:150:ALA:HB2	2.21	0.40
1:B:282:ARG:HD3	1:B:286:LYS:NZ	2.37	0.40
1:B:361:VAL:C	1:B:365:ILE:HD12	2.45	0.40
1:B:495:GLU:O	1:B:496:ILE:C	2.63	0.40
1:B:534:ARG:HH21	1:B:564:VAL:CG1	2.29	0.40
1:B:778:GLU:HB3	1:B:782:LYS:HE2	2.03	0.40
1:B:990:PHE:HB3	1:B:991:ALA:H	1.72	0.40
1:A:395:PHE:HA	1:A:443:LEU:CB	2.52	0.40
1:A:404:GLN:HE21	1:A:404:GLN:HB3	1.63	0.40
1:A:472:GLU:OE1	1:A:473:PRO:HD2	2.22	0.40
1:A:476:PHE:CD2	1:A:486:TYR:HE1	2.39	0.40
1:A:727:ILE:HD12	1:A:754:LEU:CB	2.52	0.40
1:A:784:LEU:O	1:A:788:VAL:HG23	2.21	0.40
1:A:789:PHE:C	1:A:789:PHE:CD2	3.00	0.40
1:A:834:GLN:O	1:A:835:ASN:O	2.39	0.40
1:A:860:ILE:HG21	1:A:948:SER:HB3	2.02	0.40
1:A:946:TYR:CG	1:A:947:PHE:N	2.90	0.40
1:A:1036:VAL:HB	1:A:1052:LEU:C	2.47	0.40
1:A:1056:VAL:HG23	1:A:1062:LEU:HB2	2.04	0.40
1:B:311:TRP:CE3	1:B:311:TRP:CA	3.04	0.40
1:B:429:LYS:NZ	1:B:581:ILE:HD11	2.37	0.40
1:B:480:ILE:O	1:B:482:GLU:N	2.54	0.40
1:B:708:VAL:CG1	1:B:709:VAL:N	2.83	0.40
1:B:721:GLN:HG2	1:B:982:MET:SD	2.62	0.40
1:B:814:LEU:CD2	1:B:814:LEU:H	2.35	0.40
1:B:852:GLN:OE1	1:B:955:PHE:O	2.39	0.40
1:B:1083:TYR:CD1	1:B:1083:TYR:N	2.89	0.40
1:B:1234:GLN:O	1:B:1236:ALA:N	2.52	0.40

There are no symmetry-related clashes.

5.3 Torsion angles

5.3.1 Protein backbone

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	1178/1284 (92%)	685 (58%)	305 (26%)	188 (16%)	0	2
1	B	1178/1284 (92%)	678 (58%)	318 (27%)	182 (15%)	0	2
All	All	2356/2568 (92%)	1363 (58%)	623 (26%)	370 (16%)	0	2

All (370) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	A	35	VAL
1	A	52	VAL
1	A	88	SER
1	A	131	PHE
1	A	133	CYS
1	A	134	LEU
1	A	135	ALA
1	A	155	GLU
1	A	156	ILE
1	A	164	VAL
1	A	201	ILE
1	A	208	TRP
1	A	209	LYS
1	A	267	LYS
1	A	276	ASN
1	A	310	PHE
1	A	371	ILE
1	A	374	PHE
1	A	384	ILE
1	A	385	GLN
1	A	400	ARG
1	A	439	LEU
1	A	489	GLU
1	A	491	VAL
1	A	537	ILE

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Mol	Chain	Res	Type
1	A	553	ALA
1	A	574	GLU
1	A	590	ASN
1	A	593	VAL
1	A	731	VAL
1	A	755	PHE
1	A	757	ILE
1	A	788	VAL
1	A	797	VAL
1	A	799	TRP
1	A	835	ASN
1	A	849	TYR
1	A	901	ARG
1	A	906	LEU
1	A	909	GLU
1	A	933	VAL
1	A	963	GLN
1	A	990	PHE
1	A	993	ASP
1	A	1012	PRO
1	A	1014	ILE
1	A	1020	GLN
1	A	1042	THR
1	A	1057	LYS
1	A	1093	ASP
1	A	1098	LYS
1	A	1134	ARG
1	A	1158	PRO
1	A	1244	ASN
1	B	35	VAL
1	B	52	VAL
1	B	88	SER
1	B	131	PHE
1	B	133	CYS
1	B	134	LEU
1	B	135	ALA
1	B	155	GLU
1	B	156	ILE
1	B	164	VAL
1	B	201	ILE
1	B	274	ASN
1	B	276	ASN

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Mol	Chain	Res	Type
1	B	310	PHE
1	B	321	GLU
1	B	322	TYR
1	B	370	SER
1	B	372	ASP
1	B	400	ARG
1	B	439	LEU
1	B	489	GLU
1	B	491	VAL
1	B	537	ILE
1	B	553	ALA
1	B	574	GLU
1	B	590	ASN
1	B	593	VAL
1	B	731	VAL
1	B	755	PHE
1	B	757	ILE
1	B	797	VAL
1	B	798	SER
1	B	835	ASN
1	B	849	TYR
1	B	901	ARG
1	B	906	LEU
1	B	909	GLU
1	B	933	VAL
1	B	963	GLN
1	B	990	PHE
1	B	993	ASP
1	B	1011	THR
1	B	1012	PRO
1	B	1014	ILE
1	B	1023	LYS
1	B	1042	THR
1	B	1057	LYS
1	B	1093	ASP
1	B	1134	ARG
1	B	1158	PRO
1	B	1244	ASN
1	A	34	SER
1	A	44	TRP
1	A	72	GLY
1	A	90	ASN

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Mol	Chain	Res	Type
1	A	132	TRP
1	A	137	GLY
1	A	140	ILE
1	A	144	ARG
1	A	160	ASP
1	A	203	GLY
1	A	216	ALA
1	A	274	ASN
1	A	308	LEU
1	A	356	GLY
1	A	373	SER
1	A	404	GLN
1	A	407	LYS
1	A	408	GLY
1	A	424	ASN
1	A	521	GLY
1	A	539	ARG
1	A	620	LYS
1	A	687	ASP
1	A	712	PHE
1	A	796	ASP
1	A	815	ALA
1	A	837	ALA
1	A	947	PHE
1	A	959	LEU
1	A	991	ALA
1	A	1028	GLU
1	A	1030	ASN
1	A	1095	LYS
1	A	1114	GLN
1	A	1128	ALA
1	A	1129	TYR
1	A	1130	GLY
1	A	1155	ASP
1	A	1157	LEU
1	A	1160	LYS
1	A	1198	ALA
1	A	1262	ILE
1	B	34	SER
1	B	44	TRP
1	B	72	GLY
1	B	132	TRP

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Mol	Chain	Res	Type
1	B	140	ILE
1	B	160	ASP
1	B	190	PHE
1	B	203	GLY
1	B	216	ALA
1	B	267	LYS
1	B	308	LEU
1	B	320	LYS
1	B	356	GLY
1	B	404	GLN
1	B	408	GLY
1	B	424	ASN
1	B	521	GLY
1	B	522	GLU
1	B	539	ARG
1	B	620	LYS
1	B	712	PHE
1	B	788	VAL
1	B	796	ASP
1	B	799	TRP
1	B	814	LEU
1	B	815	ALA
1	B	837	ALA
1	B	851	TRP
1	B	947	PHE
1	B	959	LEU
1	B	991	ALA
1	B	1016	SER
1	B	1024	PRO
1	B	1095	LYS
1	B	1098	LYS
1	B	1114	GLN
1	B	1128	ALA
1	B	1129	TYR
1	B	1130	GLY
1	B	1155	ASP
1	B	1198	ALA
1	B	1262	ILE
1	A	73	ASP
1	A	118	GLY
1	A	190	PHE
1	A	317	VAL

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Mol	Chain	Res	Type
1	A	320	LYS
1	A	355	ARG
1	A	369	PRO
1	A	370	SER
1	A	434	GLN
1	A	435	LEU
1	A	522	GLU
1	A	552	GLU
1	A	703	GLU
1	A	707	PHE
1	A	758	LEU
1	A	778	GLU
1	A	794	ARG
1	A	814	LEU
1	A	833	PHE
1	A	839	LEU
1	A	908	ARG
1	A	935	GLY
1	A	945	MET
1	A	965	MET
1	A	969	ASN
1	A	975	SER
1	A	995	ALA
1	A	1013	GLU
1	A	1017	TYR
1	A	1018	SER
1	A	1027	LEU
1	A	1041	PRO
1	A	1230	LEU
1	A	1235	ASN
1	B	73	ASP
1	B	90	ASN
1	B	118	GLY
1	B	137	GLY
1	B	144	ARG
1	B	208	TRP
1	B	355	ARG
1	B	373	SER
1	B	385	GLN
1	B	407	LYS
1	B	703	GLU
1	B	707	PHE

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Mol	Chain	Res	Type
1	B	758	LEU
1	B	772	THR
1	B	778	GLU
1	B	833	PHE
1	B	839	LEU
1	B	854	THR
1	B	908	ARG
1	B	935	GLY
1	B	945	MET
1	B	965	MET
1	B	969	ASN
1	B	975	SER
1	B	1010	LYS
1	B	1015	ASP
1	B	1041	PRO
1	B	1157	LEU
1	B	1159	ASP
1	B	1160	LYS
1	B	1230	LEU
1	A	152	MET
1	A	402	GLU
1	A	523	ARG
1	A	538	ALA
1	A	558	ASP
1	A	608	HIS
1	A	766	PHE
1	A	772	THR
1	A	786	TYR
1	A	806	THR
1	A	854	THR
1	A	894	THR
1	A	895	GLU
1	A	912	PHE
1	A	958	TYR
1	A	1046	ILE
1	A	1102	VAL
1	A	1156	SER
1	A	1159	ASP
1	A	1204	THR
1	B	317	VAL
1	B	369	PRO
1	B	377	SER

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Mol	Chain	Res	Type
1	B	384	ILE
1	B	433	VAL
1	B	538	ALA
1	B	608	HIS
1	B	691	ALA
1	B	766	PHE
1	B	786	TYR
1	B	794	ARG
1	B	912	PHE
1	B	958	TYR
1	B	1013	GLU
1	B	1020	GLN
1	B	1046	ILE
1	B	1102	VAL
1	B	1156	SER
1	B	1235	ASN
1	A	218	SER
1	A	258	ARG
1	A	269	GLU
1	A	352	ALA
1	A	429	LYS
1	A	559	THR
1	A	690	PRO
1	A	705	PRO
1	A	748	SER
1	A	753	LEU
1	A	793	LEU
1	A	1024	PRO
1	A	1036	VAL
1	A	1101	ASN
1	B	209	LYS
1	B	218	SER
1	B	258	ARG
1	B	352	ALA
1	B	381	PRO
1	B	402	GLU
1	B	507	ASP
1	B	558	ASP
1	B	559	THR
1	B	692	SER
1	B	705	PRO
1	B	753	LEU

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Mol	Chain	Res	Type
1	B	894	THR
1	B	1036	VAL
1	B	1206	SER
1	A	161	VAL
1	A	280	ALA
1	A	322	TYR
1	A	507	ASP
1	A	759	GLY
1	A	897	ILE
1	A	1085	PRO
1	B	161	VAL
1	B	315	SER
1	B	523	ARG
1	B	598	ASP
1	B	759	GLY
1	B	806	THR
1	B	1019	THR
1	B	1136	VAL
1	B	1168	LYS
1	A	214	ILE
1	A	545	PRO
1	A	603	VAL
1	A	689	PRO
1	A	1069	GLY
1	A	1136	VAL
1	A	1166	GLY
1	B	603	VAL
1	B	1085	PRO
1	A	381	PRO
1	B	214	ILE
1	B	897	ILE
1	B	1166	GLY
1	A	227	ILE
1	A	1047	PRO
1	A	1094	GLY
1	B	545	PRO
1	B	999	VAL
1	B	1069	GLY
1	B	1094	GLY
1	A	121	VAL
1	A	601	VAL
1	A	999	VAL

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Mol	Chain	Res	Type
1	A	1127	ILE
1	B	116	GLY
1	B	121	VAL
1	B	227	ILE
1	B	601	VAL
1	B	1047	PRO
1	B	1127	ILE
1	A	116	GLY
1	A	831	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	976/1065 (92%)	831 (85%)	145 (15%)	3	14
1	B	976/1065 (92%)	840 (86%)	136 (14%)	3	15
All	All	1952/2130 (92%)	1671 (86%)	281 (14%)	3	15

All (281) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
1	A	45	LEU
1	A	59	ILE
1	A	70	ILE
1	A	71	PHE
1	A	76	ASP
1	A	83	ASN
1	A	91	MET
1	A	102	LYS
1	A	113	TYR
1	A	123	ILE
1	A	131	PHE
1	A	156	ILE
1	A	158	TRP
1	A	163	ASP

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Mol	Chain	Res	Type
1	A	171	LEU
1	A	186	ILE
1	A	189	PHE
1	A	202	ILE
1	A	209	LYS
1	A	210	LEU
1	A	219	PRO
1	A	227	ILE
1	A	228	TRP
1	A	231	ILE
1	A	238	LYS
1	A	245	LYS
1	A	252	GLU
1	A	254	LEU
1	A	257	ILE
1	A	261	ILE
1	A	267	LYS
1	A	270	LEU
1	A	282	ARG
1	A	285	ILE
1	A	289	ILE
1	A	295	MET
1	A	302	ILE
1	A	306	TYR
1	A	308	LEU
1	A	314	THR
1	A	324	ILE
1	A	328	LEU
1	A	330	VAL
1	A	336	ILE
1	A	366	ASP
1	A	382	ASP
1	A	388	LEU
1	A	397	TYR
1	A	401	LYS
1	A	402	GLU
1	A	404	GLN
1	A	405	ILE
1	A	429	LYS
1	A	438	ARG
1	A	439	LEU
1	A	447	VAL

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Mol	Chain	Res	Type
1	A	449	ILE
1	A	471	GLN
1	A	484	ILE
1	A	493	MET
1	A	495	GLU
1	A	496	ILE
1	A	519	LEU
1	A	527	LEU
1	A	535	ILE
1	A	549	LEU
1	A	577	THR
1	A	578	THR
1	A	602	ILE
1	A	604	GLU
1	A	613	ARG
1	A	686	GLU
1	A	694	TRP
1	A	697	LEU
1	A	703	GLU
1	A	711	ILE
1	A	721	GLN
1	A	722	PRO
1	A	727	ILE
1	A	734	VAL
1	A	743	THR
1	A	751	PHE
1	A	795	GLN
1	A	799	TRP
1	A	804	LYS
1	A	816	ASN
1	A	836	ILE
1	A	841	THR
1	A	843	ILE
1	A	853	LEU
1	A	862	PRO
1	A	863	ILE
1	A	872	MET
1	A	881	LYS
1	A	892	ILE
1	A	902	THR
1	A	905	SER
1	A	909	GLU

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Mol	Chain	Res	Type
1	A	912	PHE
1	A	922	ILE
1	A	936	ILE
1	A	945	MET
1	A	947	PHE
1	A	953	PHE
1	A	964	LEU
1	A	968	GLU
1	A	969	ASN
1	A	982	MET
1	A	993	ASP
1	A	996	LYS
1	A	1005	ILE
1	A	1007	ILE
1	A	1008	ILE
1	A	1010	LYS
1	A	1011	THR
1	A	1012	PRO
1	A	1013	GLU
1	A	1014	ILE
1	A	1020	GLN
1	A	1023	LYS
1	A	1025	ASN
1	A	1041	PRO
1	A	1047	PRO
1	A	1049	LEU
1	A	1060	GLN
1	A	1083	TYR
1	A	1108	GLN
1	A	1118	LEU
1	A	1123	ILE
1	A	1131	ASP
1	A	1139	GLU
1	A	1140	GLU
1	A	1154	ILE
1	A	1158	PRO
1	A	1161	TYR
1	A	1182	ILE
1	A	1187	VAL
1	A	1192	ILE
1	A	1229	ARG
1	A	1233	ILE

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Mol	Chain	Res	Type
1	A	1242	ILE
1	A	1246	LYS
1	A	1254	GLN
1	A	1259	GLN
1	A	1262	ILE
1	B	45	LEU
1	B	59	ILE
1	B	70	ILE
1	B	71	PHE
1	B	76	ASP
1	B	83	ASN
1	B	91	MET
1	B	102	LYS
1	B	113	TYR
1	B	123	ILE
1	B	131	PHE
1	B	156	ILE
1	B	158	TRP
1	B	163	ASP
1	B	171	LEU
1	B	186	ILE
1	B	189	PHE
1	B	202	ILE
1	B	210	LEU
1	B	219	PRO
1	B	227	ILE
1	B	228	TRP
1	B	231	ILE
1	B	238	LYS
1	B	245	LYS
1	B	252	GLU
1	B	254	LEU
1	B	257	ILE
1	B	261	ILE
1	B	267	LYS
1	B	270	LEU
1	B	282	ARG
1	B	285	ILE
1	B	295	MET
1	B	302	ILE
1	B	306	TYR
1	B	308	LEU

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Mol	Chain	Res	Type
1	B	314	THR
1	B	324	ILE
1	B	328	LEU
1	B	330	VAL
1	B	336	ILE
1	B	366	ASP
1	B	388	LEU
1	B	397	TYR
1	B	401	LYS
1	B	402	GLU
1	B	404	GLN
1	B	405	ILE
1	B	429	LYS
1	B	436	MET
1	B	438	ARG
1	B	439	LEU
1	B	447	VAL
1	B	449	ILE
1	B	471	GLN
1	B	484	ILE
1	B	493	MET
1	B	495	GLU
1	B	496	ILE
1	B	519	LEU
1	B	527	LEU
1	B	535	ILE
1	B	549	LEU
1	B	577	THR
1	B	578	THR
1	B	602	ILE
1	B	604	GLU
1	B	613	ARG
1	B	684	LEU
1	B	693	PHE
1	B	694	TRP
1	B	697	LEU
1	B	703	GLU
1	B	711	ILE
1	B	721	GLN
1	B	722	PRO
1	B	727	ILE
1	B	734	VAL

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Mol	Chain	Res	Type
1	B	743	THR
1	B	751	PHE
1	B	795	GLN
1	B	799	TRP
1	B	804	LYS
1	B	816	ASN
1	B	836	ILE
1	B	841	THR
1	B	853	LEU
1	B	862	PRO
1	B	863	ILE
1	B	872	MET
1	B	881	LYS
1	B	892	ILE
1	B	902	THR
1	B	905	SER
1	B	909	GLU
1	B	912	PHE
1	B	936	ILE
1	B	945	MET
1	B	947	PHE
1	B	953	PHE
1	B	964	LEU
1	B	968	GLU
1	B	969	ASN
1	B	982	MET
1	B	993	ASP
1	B	996	LYS
1	B	1005	ILE
1	B	1007	ILE
1	B	1008	ILE
1	B	1011	THR
1	B	1013	GLU
1	B	1022	LEU
1	B	1041	PRO
1	B	1047	PRO
1	B	1049	LEU
1	B	1060	GLN
1	B	1083	TYR
1	B	1108	GLN
1	B	1118	LEU
1	B	1123	ILE

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Mol	Chain	Res	Type
1	B	1131	ASP
1	B	1140	GLU
1	B	1154	ILE
1	B	1158	PRO
1	B	1161	TYR
1	B	1182	ILE
1	B	1187	VAL
1	B	1192	ILE
1	B	1229	ARG
1	B	1233	ILE
1	B	1242	ILE
1	B	1246	LYS
1	B	1254	GLN
1	B	1259	GLN
1	B	1262	ILE

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (92) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	60	HIS
1	A	83	ASN
1	A	87	ASN
1	A	153	ASN
1	A	154	GLN
1	A	168	ASN
1	A	179	ASN
1	A	191	GLN
1	A	266	GLN
1	A	274	ASN
1	A	275	ASN
1	A	276	ASN
1	A	292	ASN
1	A	385	GLN
1	A	387	ASN
1	A	394	HIS
1	A	404	GLN
1	A	437	GLN
1	A	458	ASN
1	A	515	GLN
1	A	605	GLN
1	A	625	GLN
1	A	717	ASN

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Mol	Chain	Res	Type
1	A	721	GLN
1	A	747	ASN
1	A	749	ASN
1	A	769	GLN
1	A	795	GLN
1	A	816	ASN
1	A	820	GLN
1	A	834	GLN
1	A	878	GLN
1	A	962	GLN
1	A	969	ASN
1	A	1003	HIS
1	A	1025	ASN
1	A	1032	GLN
1	A	1039	ASN
1	A	1099	GLN
1	A	1108	GLN
1	A	1114	GLN
1	A	1152	GLN
1	A	1191	HIS
1	A	1235	ASN
1	A	1244	ASN
1	A	1253	HIS
1	B	60	HIS
1	B	83	ASN
1	B	87	ASN
1	B	128	GLN
1	B	153	ASN
1	B	154	GLN
1	B	179	ASN
1	B	191	GLN
1	B	266	GLN
1	B	274	ASN
1	B	276	ASN
1	B	292	ASN
1	B	379	HIS
1	B	385	GLN
1	B	387	ASN
1	B	394	HIS
1	B	404	GLN
1	B	434	GLN
1	B	437	GLN

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Mol	Chain	Res	Type
1	B	458	ASN
1	B	515	GLN
1	B	605	GLN
1	B	625	GLN
1	B	717	ASN
1	B	721	GLN
1	B	747	ASN
1	B	749	ASN
1	B	769	GLN
1	B	795	GLN
1	B	820	GLN
1	B	834	GLN
1	B	852	GLN
1	B	878	GLN
1	B	910	GLN
1	B	963	GLN
1	B	969	ASN
1	B	1003	HIS
1	B	1032	GLN
1	B	1039	ASN
1	B	1099	GLN
1	B	1114	GLN
1	B	1152	GLN
1	B	1191	HIS
1	B	1235	ASN
1	B	1244	ASN
1	B	1253	HIS

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no oligosaccharides in this entry.

5.6 Ligand geometry

4 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
2	2J8	A	6001	-	33,39,39	1.37	3 (9%)	51,57,57	1.26	6 (11%)
2	2J8	B	6004	-	16,18,39	3.36	4 (25%)	20,24,57	2.88	6 (30%)
2	2J8	A	6002	-	16,18,39	3.22	4 (25%)	20,24,57	2.82	6 (30%)
2	2J8	B	6003	-	33,39,39	1.48	4 (12%)	51,57,57	1.41	8 (15%)

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

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
2	2J8	A	6001	-	-	0/42/48/48	0/4/4/4
2	2J8	B	6004	-	-	0/14/16/48	0/2/2/4
2	2J8	A	6002	-	-	0/14/16/48	0/2/2/4
2	2J8	B	6003	-	-	0/42/48/48	0/4/4/4

All (15) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6004	2J8	C12-N23	11.44	1.38	1.28
2	A	6002	2J8	C12-N23	11.23	1.38	1.28
2	B	6004	2J8	C16-N17	4.94	1.44	1.34
2	A	6002	2J8	C16-N17	4.64	1.43	1.34
2	B	6003	2J8	C16-N17	4.56	1.43	1.34
2	A	6001	2J8	C16-N17	4.07	1.42	1.34
2	A	6001	2J8	C02-N03	3.97	1.42	1.34
2	A	6001	2J8	C09-N10	3.96	1.42	1.34
2	B	6003	2J8	C09-N10	3.78	1.42	1.34
2	B	6004	2J8	SE2-C14	3.50	1.91	1.86
2	B	6003	2J8	C02-N03	3.29	1.41	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
2	B	6003	2J8	C21-C01	-2.97	1.30	1.35
2	A	6002	2J8	SE2-C14	2.68	1.90	1.86
2	A	6002	2J8	SE2-C12	2.52	1.93	1.86
2	B	6004	2J8	SE2-C12	2.29	1.92	1.86

All (26) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	B	6004	2J8	C01-N22-C19	8.58	112.77	104.86
2	A	6002	2J8	C01-N22-C19	8.52	112.71	104.86
2	A	6002	2J8	C12-N23-C15	5.88	114.64	109.51
2	B	6004	2J8	C12-N23-C15	5.80	114.57	109.51
2	B	6004	2J8	SE2-C14-C15	5.58	116.06	111.61
2	A	6002	2J8	SE2-C14-C15	5.12	115.69	111.61
2	B	6003	2J8	SE3-C21-C01	4.95	118.18	111.07
2	A	6001	2J8	SE3-C21-C01	3.57	116.20	111.07
2	B	6003	2J8	SE2-C14-C15	3.25	115.74	111.07
2	A	6001	2J8	SE2-C14-C15	3.14	115.58	111.07
2	A	6001	2J8	SE1-C07-C08	3.02	115.41	111.07
2	B	6004	2J8	C18-N17-C16	2.81	127.28	121.57
2	A	6001	2J8	C11-N10-C09	2.80	127.26	121.57
2	B	6003	2J8	SE1-C07-C08	2.80	115.08	111.07
2	B	6003	2J8	C21-SE3-C19	-2.76	81.01	84.61
2	B	6004	2J8	C14-C15-N23	-2.65	113.67	116.53
2	A	6001	2J8	C04-N03-C02	2.59	126.84	121.57
2	B	6003	2J8	C11-N10-C09	2.58	126.82	121.57
2	B	6003	2J8	C18-N17-C16	2.53	126.72	121.57
2	A	6001	2J8	C18-N17-C16	2.50	126.66	121.57
2	A	6002	2J8	C18-N17-C16	2.36	126.37	121.57
2	B	6003	2J8	C15-C16-N17	2.26	118.44	115.22
2	A	6002	2J8	C14-C15-N23	-2.19	114.17	116.53
2	B	6003	2J8	C01-C02-N03	2.16	118.30	115.22
2	B	6004	2J8	C14-SE2-C12	-2.08	81.33	85.29
2	A	6002	2J8	C19-C18-N17	2.04	111.20	108.05

There are no chirality outliers.

There are no torsion outliers.

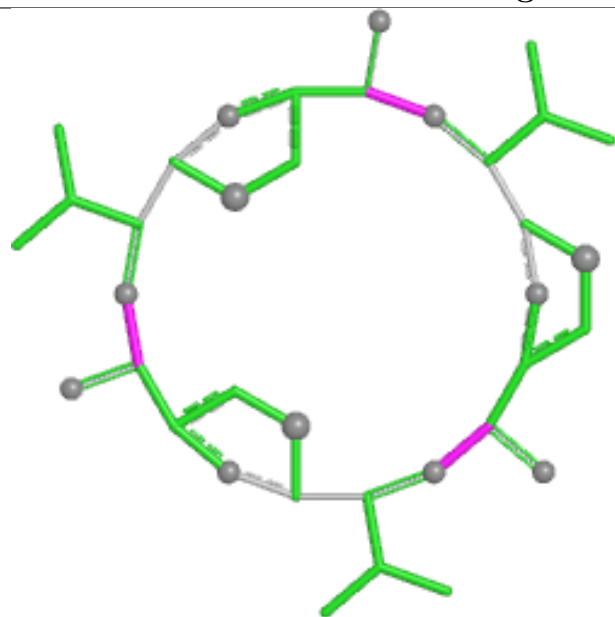
There are no ring outliers.

4 monomers are involved in 25 short contacts:

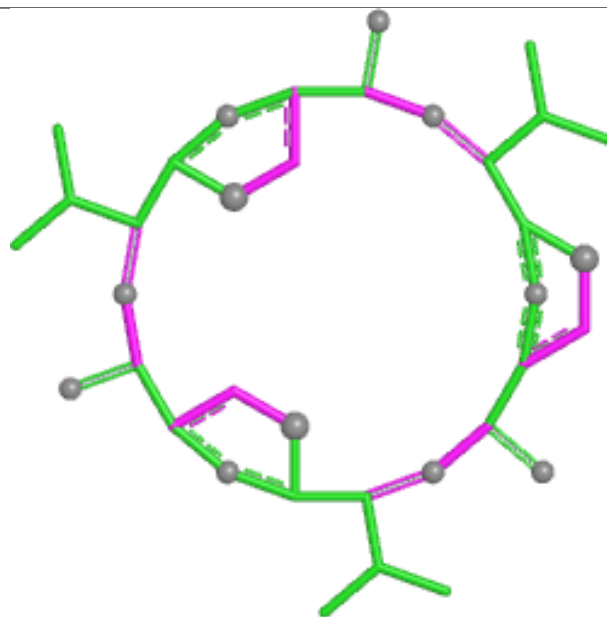
Mol	Chain	Res	Type	Clashes	Symm-Clashes
2	A	6001	2J8	4	0
2	B	6004	2J8	4	0
2	A	6002	2J8	1	0
2	B	6003	2J8	16	0

The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. For torsion angles, if less than 5% of the Mogul distribution of torsion angles is within 10 degrees of the torsion angle in question, then that torsion angle is considered an outlier. Any bond that is central to one or more torsion angles identified as an outlier by Mogul will be highlighted in the graph. For rings, the root-mean-square deviation (RMSD) between the ring in question and similar rings identified by Mogul is calculated over all ring torsion angles. If the average RMSD is greater than 60 degrees and the minimal RMSD between the ring in question and any Mogul-identified rings is also greater than 60 degrees, then that ring is considered an outlier. The outliers are highlighted in purple. The color gray indicates Mogul did not find sufficient equivalents in the CSD to analyse the geometry.

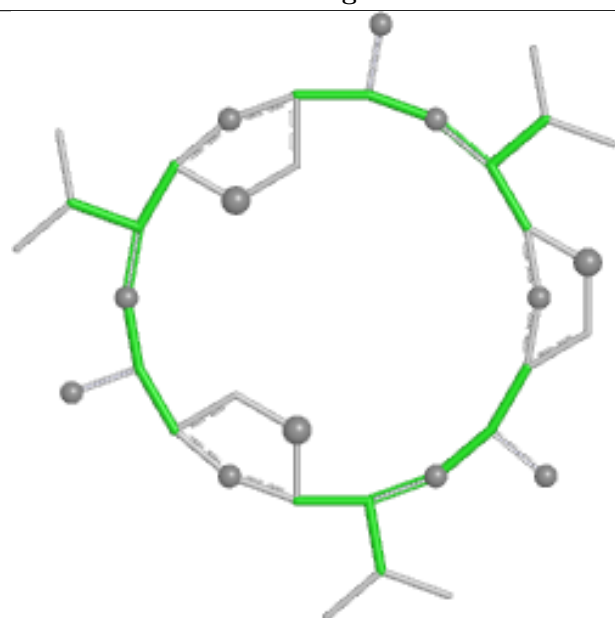
Ligand 2J8 A 6001



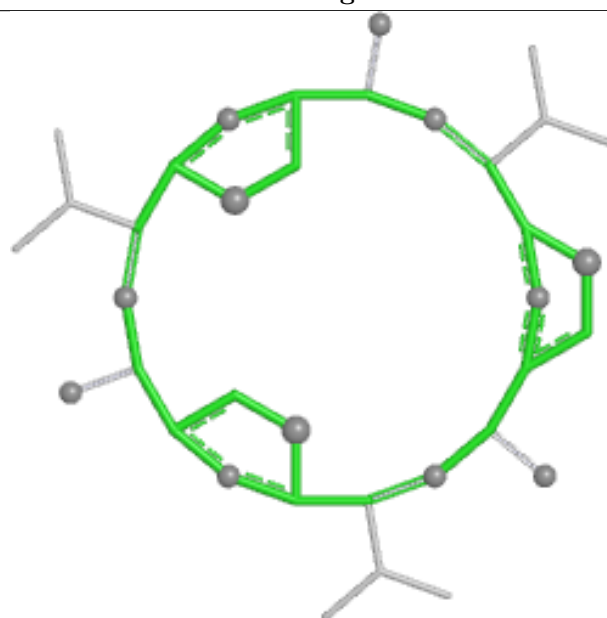
Bond lengths



Bond angles

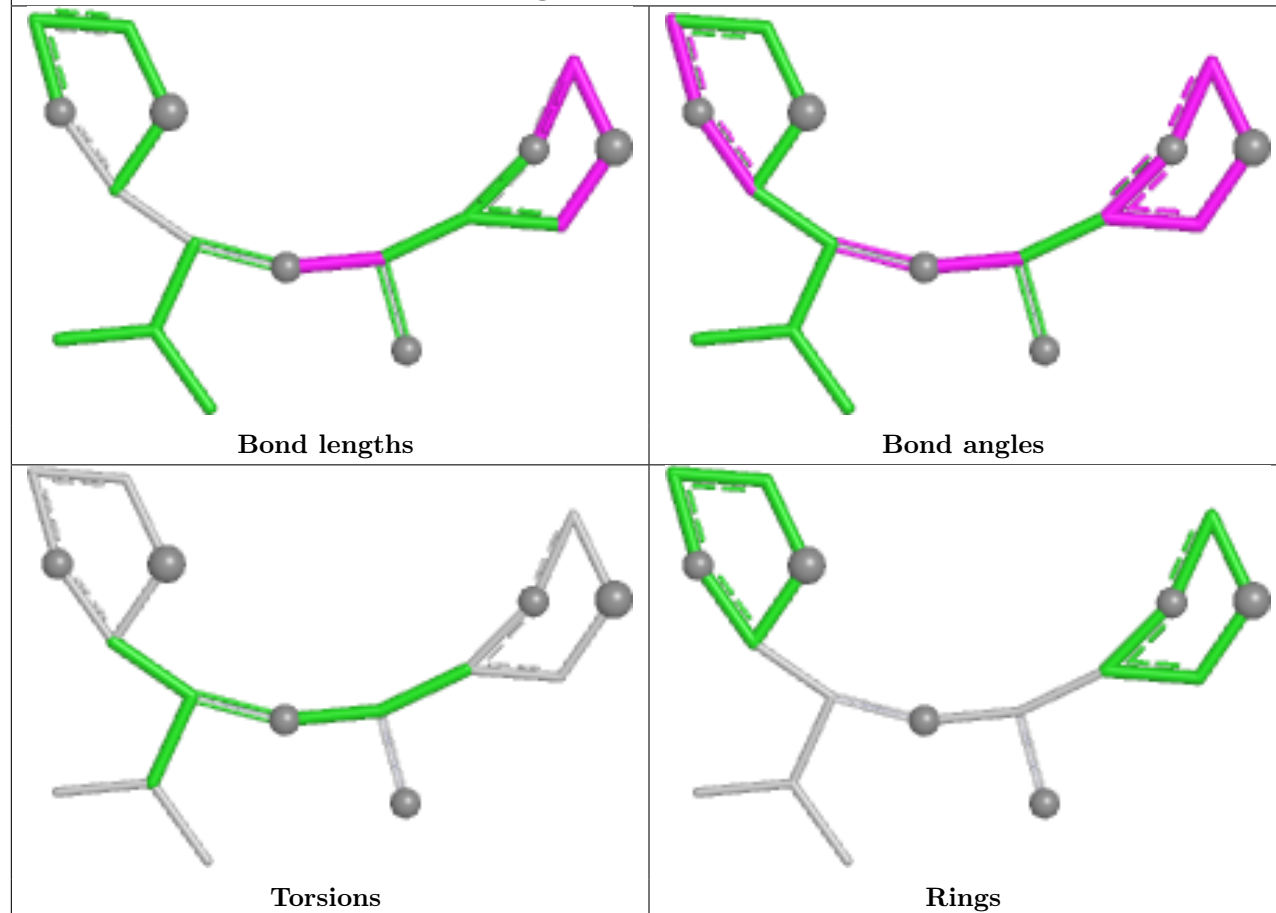


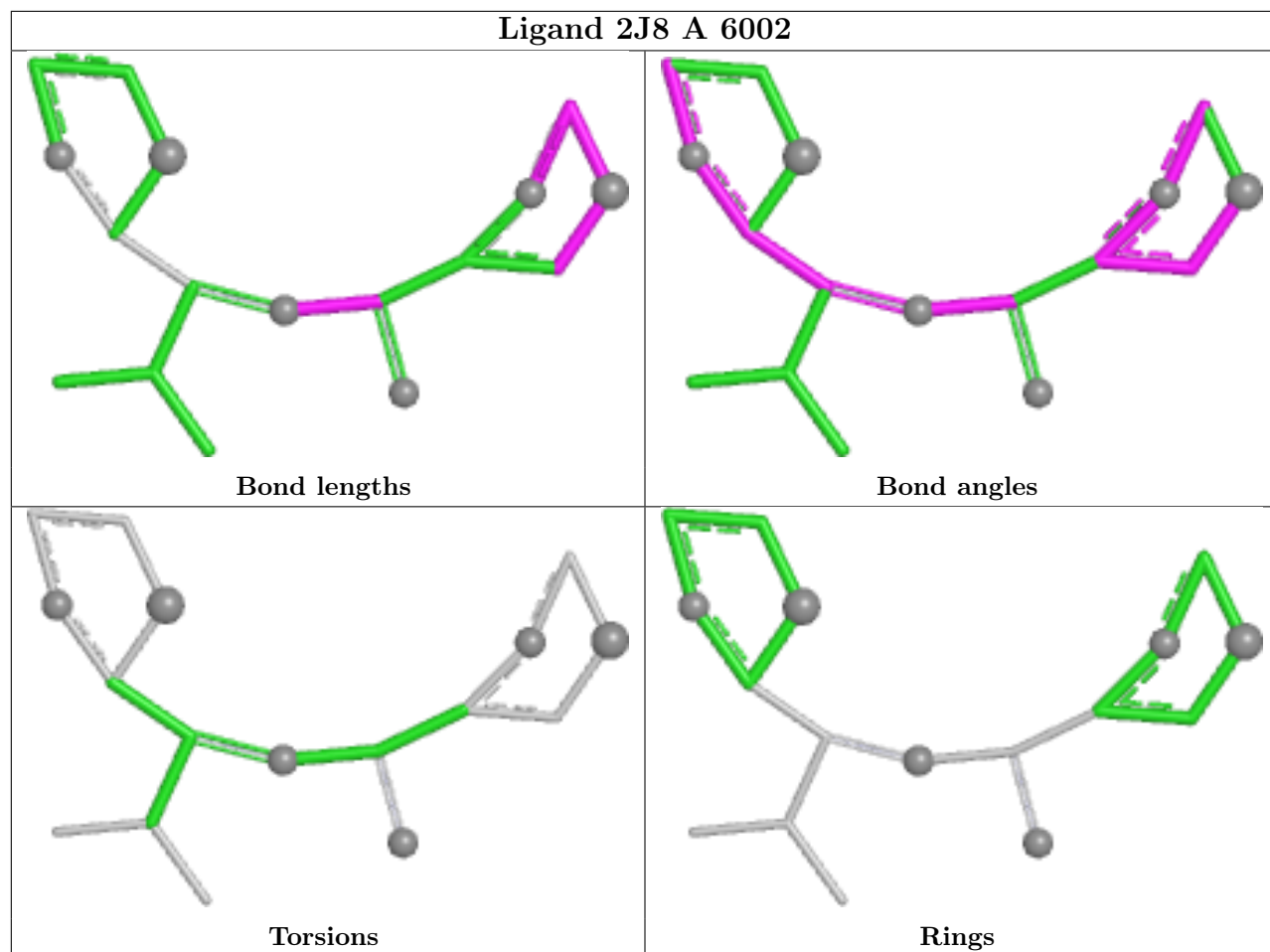
Torsions

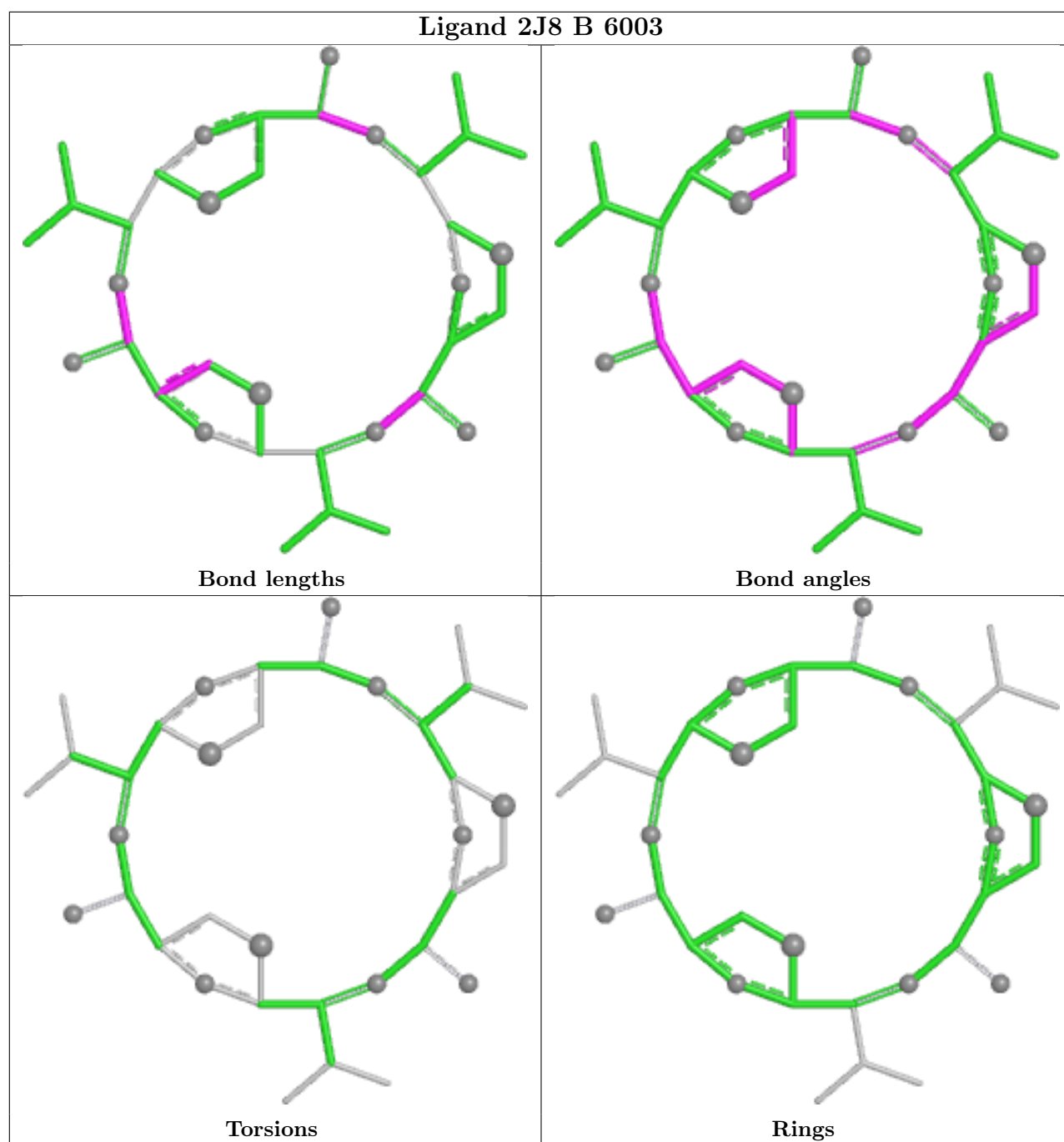


Rings

Ligand 2J8 B 6004







5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

6 Fit of model and data

6.1 Protein, DNA and RNA chains

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

Mol	Chain	Analysed	<RSRZ>	#RSRZ>2		OWAB(Å ²)	Q<0.9
1	A	1182/1284 (92%)	0.06	28 (2%)	59 47	115, 180, 210, 247	0
1	B	1182/1284 (92%)	0.03	29 (2%)	58 45	97, 183, 214, 303	0
All	All	2364/2568 (92%)	0.05	57 (2%)	59 47	97, 182, 212, 303	0

All (57) RSRZ outliers are listed below:

Mol	Chain	Res	Type	RSRZ
1	A	66	LEU	5.6
1	A	948	SER	4.7
1	A	69	LEU	4.3
1	A	952	CYS	4.3
1	B	1161	TYR	4.2
1	B	299	PHE	4.1
1	A	949	TYR	4.0
1	A	191	GLN	3.7
1	A	275	ASN	3.7
1	A	274	ASN	3.6
1	A	207	GLY	3.6
1	A	317	VAL	3.5
1	B	415	SER	3.3
1	A	340	SER	3.3
1	A	1025	ASN	3.2
1	B	1198	ALA	3.2
1	B	184	ASP	3.2
1	B	407	LYS	3.1
1	A	827	SER	3.1
1	B	1244	ASN	3.0
1	B	800	PHE	2.9
1	A	624	THR	2.9
1	B	1008	ILE	2.6
1	B	313	GLY	2.6

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Mol	Chain	Res	Type	RSRZ
1	B	306	TYR	2.6
1	B	331	PHE	2.6
1	A	375	SER	2.5
1	B	1220	GLY	2.5
1	B	63	ALA	2.5
1	A	1229	ARG	2.5
1	A	38	MET	2.5
1	B	228	TRP	2.5
1	B	971	LEU	2.5
1	B	1024	PRO	2.4
1	B	311	TRP	2.4
1	A	299	PHE	2.4
1	B	278	GLU	2.4
1	B	802	ASP	2.4
1	B	373	SER	2.4
1	A	801	ASP	2.4
1	A	845	ILE	2.4
1	A	164	VAL	2.3
1	A	329	THR	2.3
1	B	292	ASN	2.2
1	B	303	TYR	2.2
1	A	1017	TYR	2.2
1	A	158	TRP	2.2
1	B	185	LYS	2.2
1	B	274	ASN	2.1
1	A	623	MET	2.1
1	A	838	ASN	2.1
1	B	205	THR	2.1
1	B	370	SER	2.1
1	A	1083	TYR	2.1
1	A	852	GLN	2.1
1	B	785	ARG	2.1
1	B	66	LEU	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](#)

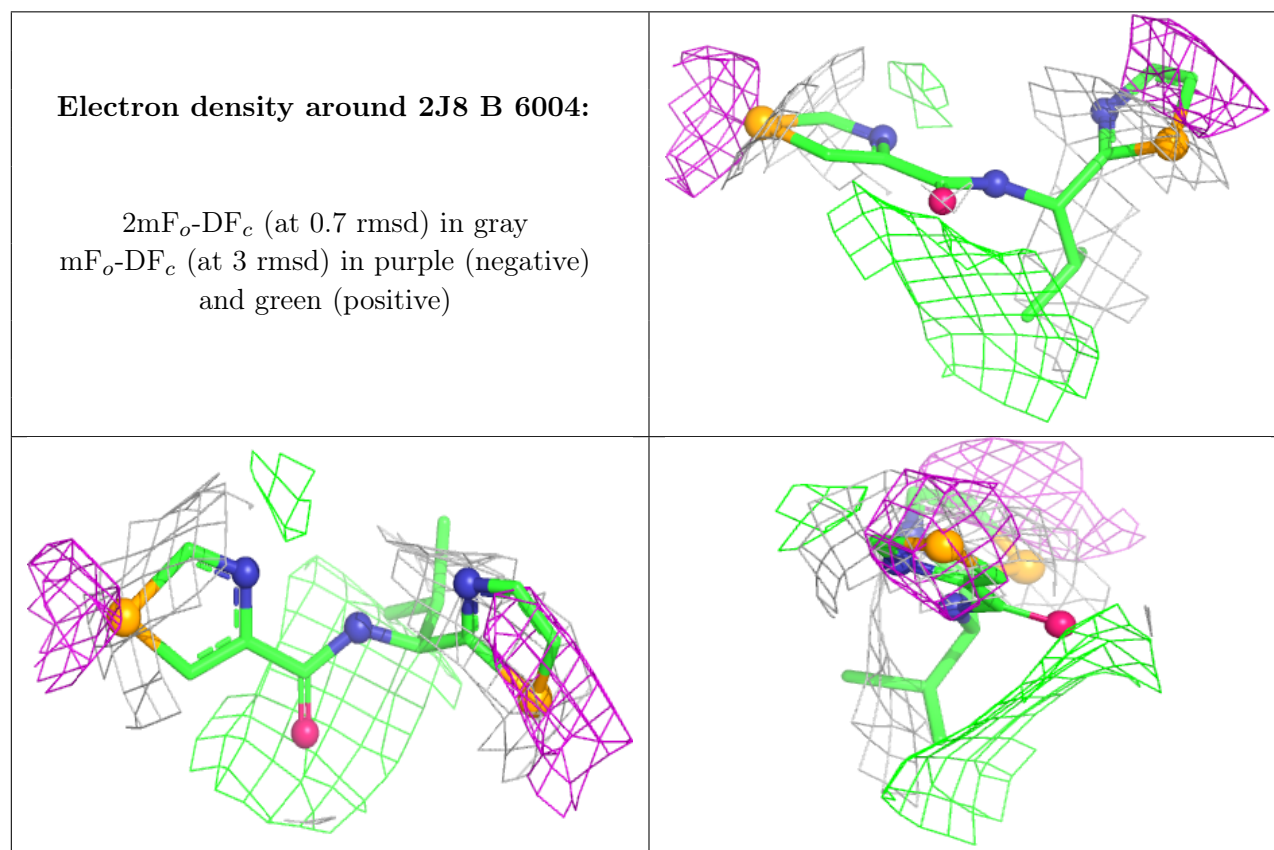
There are no oligosaccharides in this entry.

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, 95th 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.

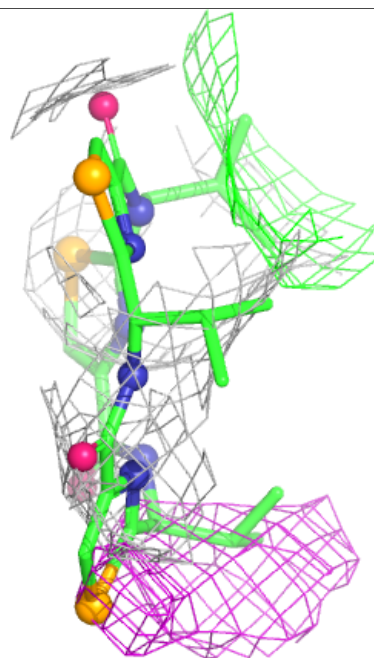
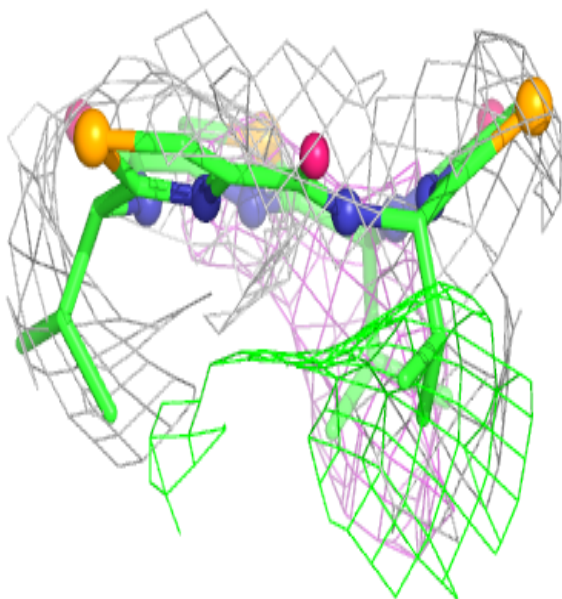
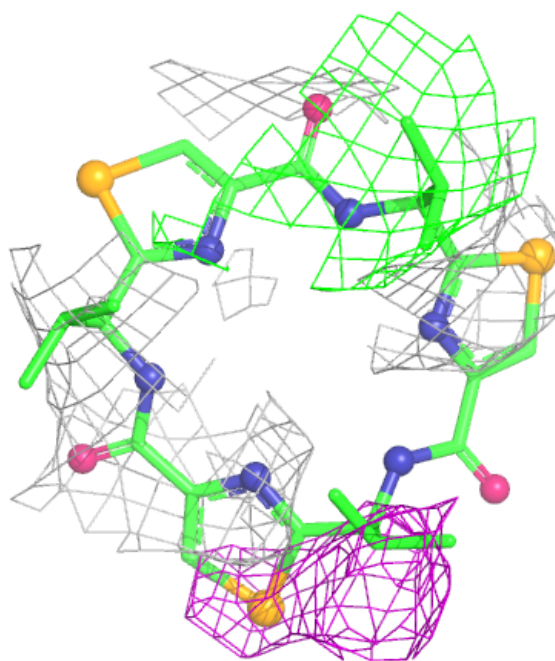
Mol	Type	Chain	Res	Atoms	RSCC	RSR	B-factors($\text{\AA}^2$)	Q<0.9
2	2J8	B	6004	17/36	0.41	0.21	185,185,185,185	0
2	2J8	B	6003	36/36	0.61	0.19	185,185,185,185	0
2	2J8	A	6002	17/36	0.66	0.13	185,185,185,185	0
2	2J8	A	6001	36/36	0.71	0.16	185,185,185,185	0

The following is a graphical depiction of the model fit to experimental electron density of all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the geometry validation Tables will also be included. Each fit is shown from different orientation to approximate a three-dimensional view.



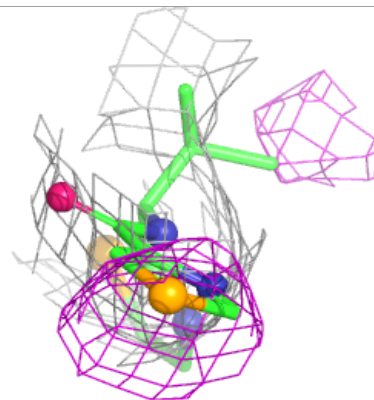
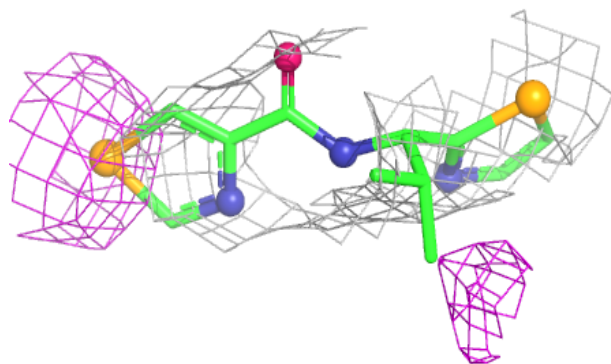
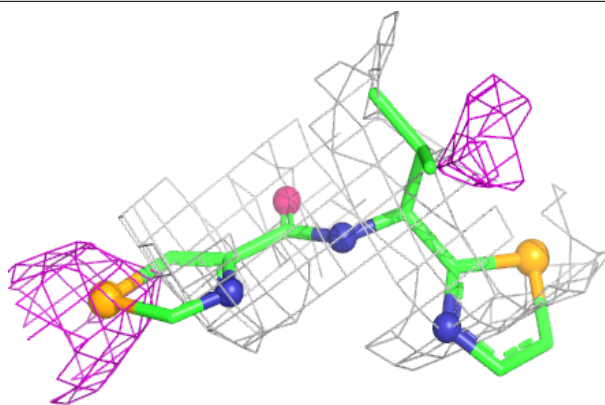
Electron density around 2J8 B 6003:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



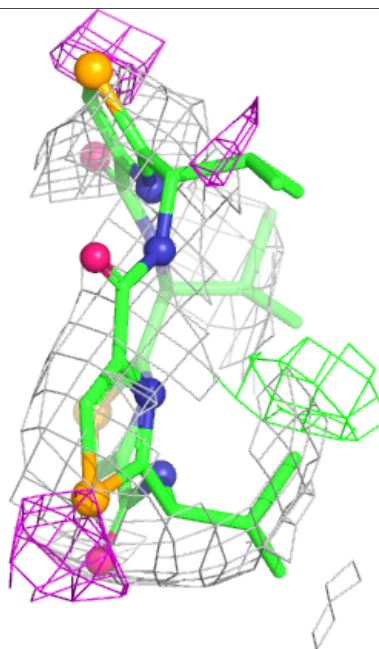
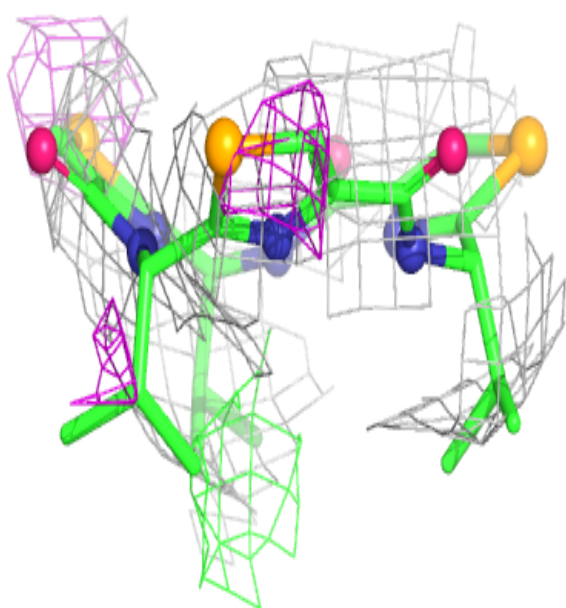
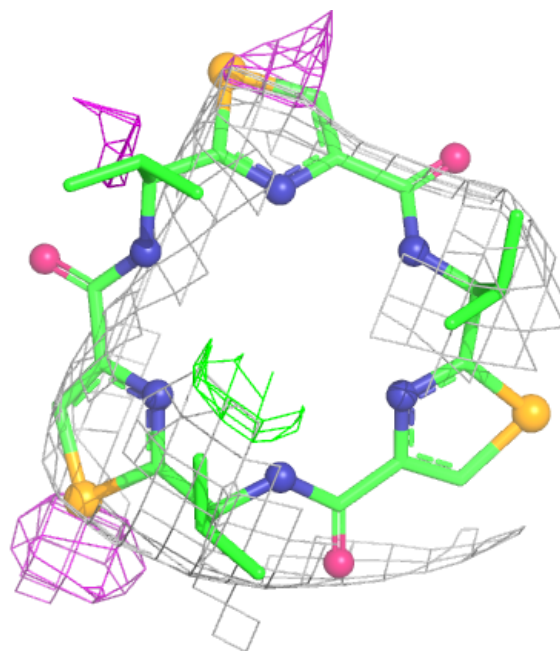
Electron density around 2J8 A 6002:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



Electron density around 2J8 A 6001:

$2mF_o-DF_c$ (at 0.7 rmsd) in gray
 mF_o-DF_c (at 3 rmsd) in purple (negative)
and green (positive)



6.5 Other polymers ⓘ

There are no such residues in this entry.